Multiscale analysis of non-convex discrete systems via Γ-convergence

Dissertationsschrift zur Erlangung des
naturwissenschaftlichen Doktorgrades
der Julius-Maximilians-Universität Würzburg

vorgelegt von

Mathias Schäffner

aus

Leipzig

Würzburg 2015

Contents

Notation

$\mathbb{R}$, $\mathbb{N}$, $\mathbb{Z}$	real numbers, positive integers, integers
$\mathbb{R}_+$, $\mathbb{N}_0$	positive real numbers, non-negative integers
$a \wedge b$, $a \vee b$	for real numbers a, b, $a \wedge b := \min\{a, b\}$ and $a \vee b := \max\{a, b\}$
χ_A	the indicator function of a set A, i.e. $\chi_A(x) = 1$ if $x \in A$, and $\chi_A(x) = 0$ if $x \notin A$
$\bar{\chi}_A$	the characteristic function of a set A, i.e. $\bar{\chi}_A = 0$ if $x \in A$, and $\bar{\chi}_A(x) = +\infty$ if $x \notin A$
$⨍_\Omega u(x)dx$	$:= \frac{1}{\|\Omega\|} \int_\Omega u(x)dx$
$\mathcal{M}(\Omega)$	the space of finite Radon measures on Ω
$(S)BV(\Omega)$	space of (special) functions of bounded variation, cf. Section 2.1
$(S)BV^\ell(0,1)$	$(S)BV$-functions with boundary values, cf. Section 2.1.1
Du	distributional derivative of $u \in BV$
$D^a u$	absolutely continuous part of derivative
$D^s u$	singular part of derivative
$D^j u$, $D^c u$	jump part and Cantor part of the derivative
K	interaction range
J_j	interaction potential of Lennard-Jones type
$J_{0,j}, \psi_j$	effective potentials, cf. (3.8) and (3.14)
J_{CB}	Cauchy-Born energy density, cf. (3.17)
$B(\theta, \ell)$, $\widetilde{B}(\theta, \ell)$	elastic boundary layer energies, cf. (3.50) and (3.64)
$B(\gamma)$, $\widetilde{B}(\gamma)$	boundary layer energies at free surfaces, cf. (3.71) and (3.112)
$B_b(\theta)$, $\widetilde{B}_b(\theta)$	boundary layer energies, cf. (3.70) and (3.111)
B_{BJ}, B_{IJ}	jump energies, cf. (3.74) and (3.75)
$\mathcal{T}_n$	set of representative atoms, cf. Section 4.1
$\hat{r}_n^{\mathcal{T}}, \hat{l}_n^{\mathcal{T}}, \hat{r}^{\mathcal{T}}, \hat{l}^{\mathcal{T}}$	representative atoms at the atomistic/continuum interface, cf. (4.26) and (4.28)
$B_{IF}^{(1)}$, $B_{IF}^{(2)}$, $B_{IF}^{(3)}$	boundary layer energies due to jumps at the atomistic/continuum interface, cf. (4.35), (4.38) and (4.39)

Chapter 1

Introduction

A number of phenomena in continuum mechanics can be modelled in terms of minimisation problems. A prominent example is the variational theory of nonlinear elasticity. Consider a homogeneous solid body with a given reference configuration $\Omega \subset \mathbb{R}^d$, $d \in \{1, 2, 3\}$. The stored elastic energy of a deformation $u : \Omega \to u(\Omega) \subset \mathbb{R}^d$ is given by

$$I_{el}(u) = \int_\Omega W(\nabla u(x))dx, \tag{1.1}$$

where W denotes the *stored elastic energy density*. In practice, W is mostly chosen phenomenologically but it is desirable to obtain it from microscopic models; or as it is asked in John Ball's open problems [4]: *Is it possible to derive elasticity theory from atomistic models?* Motivated by this, the analysis of microscopic models, in particular of discrete lattice systems, and their relation to continuum mechanics is a growing subject within the applied analysis, see e.g. [7] for an overview. A common approach is to apply Γ-convergence to discrete energy functionals which are parametrised by the number of atoms (see e.g. [2, 12, 13, 14]). This ensures that minimisers and minima of the discrete energy converge to minimisers and minima of the limiting continuum energy.

In the first part of this thesis, we analyse a one-dimensional atomistic model with finite range Lennard-Jones type interactions. In particular, we refine a result by Braides and Gelli [14] and give an explicit expression for the Γ-limit of the discrete functionals in this case. Moreover, we provide an asymptotic expansion by Γ-convergence, see [1, 20]. In this way, we recover boundary layer energies due to lattice asymmetries at the boundary and at cracks of the specimen. We derive a macroscopic model which allows for fracture and inherits the atomic length scale. This generalises results of Braides and Cicalese [11] and Scardia, Schlömerkemper and Zanini [50, 51] for Lennard-Jones systems with nearest and next-to-nearest neighbour interactions to the case of general finite range interactions which is a step towards the physical case of long range interactions.

In the second part, we study the validity of the so-called quasicontinuum method [59]. This is a computational multiscale method which couples atomistic and continuum descriptions of crystalline solids and became very popular in the last two decades for studying phenomena, such as the behaviour of grain boundaries, dislocation nucleation and crack growth etc., in which there exist isolated regions of interest where a very detailed model is desirable (e.g. the crack tip) and regions where a continuum model is sufficient. We construct a quasicontinuum approximation of the one-dimensional Lennard-Jones system discussed before and compare this approximation and the original model in terms of their Γ-limits.

Before we discuss the results of this thesis, let us briefly review some related contributions in the literature. Consider $\varepsilon\mathbb{Z}^d \cap \Omega$ with $\Omega \subset \mathbb{R}^d$ and $\varepsilon > 0$ as the reference lattice and let $u : \varepsilon\mathbb{Z}^d \cap \Omega \to \mathbb{R}^d$ be a deformation of the reference lattice. Then a typical discrete energy is given by

$$E_\varepsilon(u) = \sum_{\substack{i,j \in \varepsilon\mathbb{Z}^d \cap \Omega \\ i \neq j}} \varepsilon^d J\left(\frac{|u(i) - u(j)|}{\varepsilon}\right). \tag{1.2}$$

The prototypical example for the interaction potential J is given by the Lennard-Jones potential [37], i.e.

$$J(z) = \frac{k_1}{z^{12}} - \frac{k_2}{z^6}, \quad z > 0, \tag{1.3}$$

with $k_1, k_2 > 0$.

Blanc, Le Bris and Lions [6] derive the pointwise limit $\lim_{\varepsilon\to 0} E_\varepsilon(u)$ for sufficiently smooth deformations u. They recover the structure of (1.1) and give an explicit expression for W. By further expansions with respect to the lattice parameter ε, they derive additional surface terms. In the core of this derivation lies the assumption that the microscopic deformation of the atoms follows the macroscopic deformation. This kind of assumptions are often called Cauchy-Born hypotheses, cf. i.e. [28]. The validity of the Cauchy-Born hypotheses is a delicate issue. Friesecke and Theil [32] proved for a square lattice spring model that the global minimiser in a certain parameter regime satisfies the Cauchy-Born hypotheses and showed that there exists a parameter regime where this is not the case, see also [23]. In [27, 47], it is shown that there exist local minimisers of atomistic models which satisfy the Cauchy-Born hypotheses in more general situations.

As mentioned previously, we consider the passage from discrete systems to continuum models via Γ-convergence. This is at present an active field of research. Alicandro and Cicalese [2] proved a general integral representation result for the Γ-limit of a class discrete energies with pair interactions. The limiting functional has the form (1.1). In contrast to the result given in [6], the energy density W of the Γ-limit is given rather implicitly and it is assumed that the interaction potentials satisfies certain growth conditions from below. This rules out interatomic potentials such as Lennard-Jones potentials. Further results in this direction are given in [16, 19, 21, 35, 52].

Here, we are interested in models which allow for fracture. A first contribution in the discrete-to-continuum derivation of fracture mechanics is due to Truskinovsky [60]. Truskinovsky considers a chain of atoms which interact through Lennard-Jones potentials.

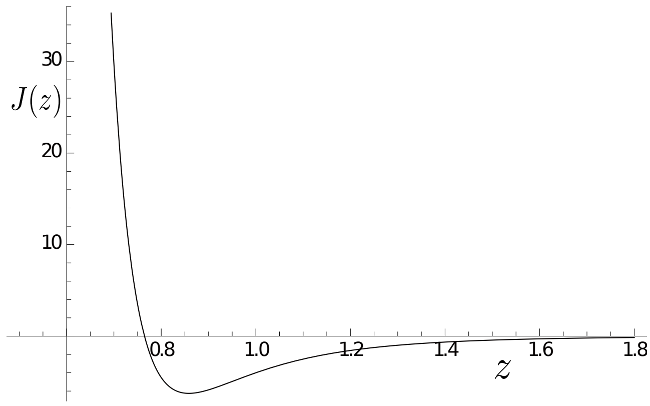

FIGURE 1.1: A typical example of a Lennard-Jones potential.

From this, he derives, by minimising the discrete energy, a continuum model for fracture which inherits the atomistic length scale. More precisely, he proposes an energy consisting of a bulk term and a contribution which accounts for cracks and is scaled with the lattice parameter.

To the best of our knowledge, Braides, Dal Maso and Garroni [12] provide the first derivation of fracture mechanics from a discrete system using Γ-convergence. They start from a chain of atoms (or material points) linked by nearest neighbour interactions and obtain a continuum limit which allows for fracture. Braides and Gelli [13, 14] give a description of the Γ-limit for discrete systems in one dimension with general interatomic pair potentials, including Lennard-Jones interactions with finite range. It is shown that the limiting functional involves, at least if one allows for interactions beyond next-to-nearest neighbour interactions, a homogenisation process similar to the vector-valued case [2], see (1.7).

In order to derive a discrete-to-continuum limit which captures a small scale variable, Braides and Cicalese [11] and Scardia, Schlömerkemper and Zanini [50] used the notion of a development by Γ-convergence in the sense of Anzelotti and Baldo, see [1]. In both articles the authors start with a chain of atoms with nearest and next-to-nearest neighbour interactions of Lennard-Jones type and compute the Γ-limit and the Γ-limit of first order. The Γ-limit yields an integral functional which allows for positive jumps, i.e. of fracture, which do not contribute to the energy. In the first-order Γ-limit boundary layer energies are recovered which penalise fracture. Later on Scardia, Schlömerkemper and Zanini in [51] used the concept of equivalence by Γ-convergence, due to Braides and Truskinovsky [20], to step further towards a mathematical understanding of Truskinovsky's original idea. Especially the works [50, 51], serve as a starting point for the analysis presented in Chapter 3 of this thesis.

Let us now give some details of the obtained results. Let $\lambda_n\mathbb{Z} \cap [0,1]$ with $\lambda_n := \frac{1}{n}$ be the reference lattice. The deformation of the ith lattice point is denoted by u^i and we identify the deformation $u : \lambda_n\mathbb{Z} \cap [0,1] \to \mathbb{R}$ with its piecewise affine interpolation. The nearest K neighbours in the reference lattice $\lambda_n\mathbb{Z} \cap [0,1]$ interact via a potential J_j, $j \in \{1,\dots,K\}$ with $K \in \mathbb{N}$ be fixed. The energy of the system under consideration is the sum of all pair interactions up to range K with the canonical bulk scaling. It reads

$$H_n(u) = \sum_{j=1}^{K} \sum_{i=0}^{n-j} \lambda_n J_j\left(\frac{u^{i+j} - u^i}{j\lambda_n}\right). \tag{1.4}$$

The mathematical assumptions on the potentials J_j, $j = 1,\dots,K$, are phrased in Section 3.1. As mentioned above, the main example that we have in mind are the Lennard-Jones potentials, that is $J_j(z) = J(jz)$ if $z > 0$, and $+\infty$ if $z \le 0$, where J is given in (1.3). Therefore, we call the potentials which satisfy our assumptions potentials of Lennard-Jones type. Furthermore, we impose boundary conditions on the deformation of the first K and last K atoms. For given $\ell > 0$ and $u_0^{(1)}, u_1^{(1)} \in \mathbb{R}_+^{K-1}$, we set

$$u^0 = 0, \quad u^n = \ell, \quad u^s - u^{s-1} = \lambda_n u_{0,s}^{(1)}, \quad u^{n+1-s} - u^{n-s} = \lambda_n u_{1,s}^{(1)} \tag{1.5}$$

for $s \in \{1,\dots,K-1\}$, see (3.3). Note that for the piecewise affine interpolation u the above conditions imply Dirichlet boundary conditions $u(0) = 0$ and $u(1) = \ell$ respectively, and prescribe the derivative u' in $(0,(K-1)\lambda_n)$ and $(1-(K-1)\lambda_n, 1)$ respectively. In the case of nearest and next-to-nearest neighbour interactions ($K = 2$), the boundary conditions considered here coincide with the boundary conditions studied in [50, 51]. We denote by H_n^ℓ the functional given by $H_n^\ell(u) = H_n(u)$ if u satisfies the boundary conditions (1.5), and $+\infty$ else.

On Lennard-Jones type systems and their asymptotic analysis

Next, we outline the results on the asymptotic analysis of the sequence $(H_n^\ell)_n$ via Γ-convergence which is the subject of Chapter 3.

1. Zero-order Γ-limit. The Γ-limit of discrete functionals of the form H_n was derived under very general assumptions on the interatomic potentials in [14]. The Γ-limit result of [14, Theorem 3.2] phrased for Lennard-Jones type potentials asserts that the sequence (H_n) Γ-converges to an integral functional H, which is defined on the space of functions of bounded variations and has the form

$$H(u) := \Gamma\text{-}\lim_{n\to\infty} H_n(u) = \begin{cases} \int_0^1 \phi(u')dx & \text{if } D^s u \ge 0 \text{ in } (0,1), \\ +\infty & \text{otherwise,} \end{cases} \tag{1.6}$$

where $D^s u$ denotes the singular part with respect to the Lebesgue measure of the distributional derivative $Du = u'\mathcal{L}^1 + D^s u$. The energy density ϕ is given via an asymptotic homogenisation formula, see Theorem 3.4 below. For Lennard-Jones potentials this homogenisation formula reduces to

$$\phi(z) = \lim_{N\to\infty} \min\Bigg\{ \frac{1}{N} \sum_{j=1}^{K} \sum_{i=0}^{N-j} J_j\left(\frac{u^{i+j}-u^i}{j}\right) :\ u:\mathbb{N}_0 \to \mathbb{R},$$
$$u^i = zi \text{ if } i \in \{0,\dots,K\} \cup \{N-K,\dots,N\} \Bigg\}, \tag{1.7}$$

see [15, Theorem 2.21]. It is desirable to have a more explicit expression for ϕ. For Lennard-Jones type potentials, we prove that

$$\phi \equiv J_{CB}^{**}, \quad \text{where} \quad J_{CB}(z) := \sum_{j=1}^{K} J_j(z)$$

and J_{CB}^{**} is the lower semicontinuous and convex envelope of J_{CB}, see Theorem 3.5. This was previously known in the cases $K \in \{1, 2\}$ only, see e.g. [11, 13].

Let us give some ideas of the proof, since they are crucial also for other parts of the thesis: in the case of nearest and next-to-nearest neighbour interactions, there exists a more explicit formula for ϕ given by $\phi \equiv J_0^{**}$, where J_0 is an effective potential given by the following infimal convolution-type formula, which takes possible oscillations on the lattice-level into account

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

see e.g. [14, Remark 3.3]. For Lennard-Jones potentials and z such that $J_0(z) = J_0^{**}(z)$, it is not difficult to show that the infimum in the definition of J_0 is attained if and only if $z_1 = z_2 = z$ and that $\phi(z) = (J_1 + J_2)^{**}(z) = J_{CB}^{**}(z)$, see [50, Remark 4.1]. From this it follows that, roughly speaking, no oscillations on the lattice-level occur in Lennard-Jones systems with nearest and next-to-nearest neighbour interactions. In order to show this also for Lennard-Jones systems beyond next-to-nearest neighbour interactions, it would be beneficial to have a description of ϕ similar to in the case of nearest and next-to-nearest neighbour interactions via a minimisation problem on a fixed 'cell' (as in the definition of J_0). However, up to our knowledge, there has not been a result in the literature which asserts whether or how the formula for the effective potential J_0 extends to a larger interaction range.

To show $\phi \equiv J_{CB}^{**}$, we use suitable generalisations of the function J_0. These are explicitly tailored for potentials of Lennard-Jones type and make use of their convex-concave shape, see Figure 1.1. To motivate the definition of the generalisations, we note that the terms in the minimisation problem in (1.7) can be rewritten as

$$\frac{1}{N} \sum_{j=2}^{K} \sum_{i=0}^{N-j} \left\{ J_j\left(\frac{u^{i+j}-u^i}{j}\right) + \frac{c_j}{j} \sum_{s=i}^{i+j-1} J_1\left(u^{s+1}-u^s\right) \right\} + \mathcal{O}\left(\frac{1}{N}\right) \tag{1.8}$$

for any set of constants $c_2, \dots, c_K > 0$ that satisfy $\sum_{j=2}^K c_j = 1$. Thus, in order to find a lower bound on the terms in the curly brackets, it is useful to define

$$J_{0,j}(z) := J_j(z) + \frac{c_j}{j} \inf \left\{ \sum_{s=1}^j J_1(z_s),\ \sum_{s=1}^j z_s = jz \right\}, \quad j = 2, \dots, K,$$

cf. (3.8). These serve as extensions of the effective potential J_0. The crucial observation is now that in the case of Lennard-Jones potentials it is possible to choose $c_2, \dots, c_K$, see Proposition 3.2, such that

$$J_{CB}^{**}(z) = \sum_{j=2}^K J_{0,j}^{**}(z) = \begin{cases} J_{CB}(z) & \text{if } z \le \gamma, \\ J_{CB}(\gamma) & \text{if } z \ge \gamma, \end{cases}$$

where $\gamma > 0$ is the (unique) minimiser of J_{CB} and $J_{0,j}(z)$ for $j \in \{2, \dots, K\}$, see Proposition 3.2 and Remark 3.1. Jensen's inequality, the constraints in the minimisation problem in (1.7), and the definition of the potentials $J_{0,j}$ yield $\phi(z) \ge J_{CB}^{**}(z)$. We make this precise and show the reverse inequality in Theorem 3.5 for the Lennard-Jones type potentials. Furthermore, we provide in Theorem 3.7 a Γ-limit result for the sequence (H_n^ℓ) without using the homogenisation formula ϕ. For this, we use a similar decomposition as in (1.8) of the energy H_n^ℓ:

$$H_n^\ell(u) = \sum_{j=2}^K \sum_{i=0}^{n-j} \lambda_n \left\{ J_j\left(\frac{u^{i+j} - u^i}{j\lambda_n}\right) + \frac{c_j}{j} \sum_{s=i}^{i+j-1} J_1\left(\frac{u^{s+1} - u^s}{\lambda_n}\right) \right\} + \mathcal{O}(\lambda_n), \tag{1.9}$$

see (3.7). The Γ-limit H^ℓ of the sequence (H_n^ℓ) is given by the restriction of H to a suitable set $BV^\ell(0,1)$, see Section 2.1.1, which inherits the boundary conditions $u(0) = 0$ and $u(1) = \ell$ in H_n^ℓ. We present this alternative proof because its arguments can be easily adapted to the quasicontinuum model that we consider in Chapter 4.

From the modelling point of view the functional H is not rich enough. For example it allows for (positive) jumps which do not cost any energy. Hence, a refined analysis is needed, see e.g. [20]. For this, we follow the approach of Scardia, Schlömerkemper and Zanini [50, 51]: we derive the first-order Γ-limit of the sequence (H_n^ℓ) and consider suitable rescaled functionals for which the contribution of elastic deformations and surface contributions due to jumps are on the same order of magnitude. Using a decomposition of the energy as in (1.9), we can apply similar arguments as are used in [50, 51], which are based on the more explicit characterisation of the Γ-limit in the case $K = 2$ via the effective potential J_0. We extend several results from [50, 51] to the case of finite range interactions:

2. First-order Γ-limit. In Section 3.3, we derive in analogy to [11, 50] the first-order Γ-limit of the sequence (H_n^ℓ). That is we compute the Γ-limit of the sequence $(H_{1,n}^\ell)$ given by

$$H^{\ell}_{1,n}(u) = \frac{H^{\ell}_n(u) - \min_u H^{\ell}(u)}{\lambda_n}.$$

It turns out that the limiting functional is similar to in the case of nearest and next-to-nearest neighbour interactions: we have to distinguish between the cases when $0 < \ell \le \gamma$ and $\ell > \gamma$ where ℓ denotes the deformation of the last atom in the chain (see (1.5)) and γ the (unique) minimiser of J_{CB}. In the case $0 < \ell \le \gamma$ the limiting functional is finite only for the elastic deformation $u(x) = \ell x$. As in [11, 50], the first-order Γ-limit recovers boundary layer energies at both ends of the specimen. This elastic boundary layer energies depend on the additional boundary conditions which are described by $u_0^{(1)}$ and $u_1^{(1)}$, cf. Theorem 3.12 and Proposition 3.15.

In the case $\ell > \gamma$ fracture occurs. Each crack yields additional boundary layer energies due to the new surfaces created by the crack. The limiting functional distinguishes between fracture at the boundary and in the interior of the specimen. For $\ell > \gamma$ and $u_0^{(1)}, u_1^{(1)} \in \mathbb{R}^{K-1}_+$, we show that $(H^{\ell}_{1,n})$ Γ-converges with respect to the $L^1(0,1)$-topology to the functional H^{ℓ}_1, where

$$\begin{aligned} H^{\ell}_1(u) =& \widetilde{B}(u_0^{(1)}, \gamma) + \widetilde{B}(u_1^{(1)}, \gamma) - \sum_{j=2}^{K} (j-1) J_j(\gamma) \\ &+ \beta_{BJ}(u_0^{(1)}) \#(S_u \cap \{0\}) + \beta_{IJ} \#(S_u \cap (0,1)) + \beta_{BJ}(u_1^{(1)}) \#(S_u \cap \{1\}) \end{aligned}$$

if $u \in SBV^{\ell}(0,1)$, $0 < \#S_u < +\infty$, $[u] \ge 0$ in $[0,1]$, and $u' = \gamma$ a.e. in $(0,1)$, and $+\infty$ otherwise, where the jump energies $\beta_{BJ}(\theta)$, for $\theta \in \mathbb{R}^{K-1}_+$, and β_{IJ} are given by

$$\beta_{BJ}(\theta) = \widetilde{B}_b(\theta) + \widetilde{B}(\gamma) - \sum_{j=1}^{K} j J_j(\gamma) - \widetilde{B}(\theta, \gamma), \quad \beta_{IJ} = 2\widetilde{B}(\gamma) - \sum_{j=1}^{K} j J_j(\gamma),$$

cf. Theorem 3.19 and Proposition 3.21. The $\widetilde{B}$ terms denote certain boundary layer energies, which are defined via asymptotic cell formulas, for instance $\widetilde{B}(\gamma)$ is given by

$$\begin{aligned} \widetilde{B}(\gamma) := \inf_{N \in \mathbb{N}_0} \min \Bigg\{ & \sum_{i \ge 0} \Bigg\{ \sum_{j=1}^{K} J_j \left(\frac{u^{i+j} - u^i}{j} \right) - J_{CB}(\gamma) \Bigg\} : \\ & u : \mathbb{N}_0 \to \mathbb{R},\ u^0 = 0,\ u^{i+1} - u^i = \gamma \text{ if } i \ge N \Bigg\}, \end{aligned}$$

see (3.112). In Section 3.4, we study the minimisation problem given by H^{ℓ}_1 for $\ell > \gamma$. In particular, we show that there exists no boundary condition which would imply that fracture in the interior of the specimen is more favourable than fracture at the boundary. Moreover, we give examples for the choices of $u_0^{(1)}$ and $u_1^{(1)}$ which ensure that either fracture appears at the boundary of the specimen or fracture appears indifferently everywhere in the specimen, see Proposition 3.24. This extends the result [50, Theorem 5.1] to the case $K > 2$.

In Section 3.4.3, we study the minimal configurations of an asymptotic cell formula, which is equivalent to $\widetilde{B}(\gamma)$, in the case of nearest an next-to-nearest neighbour interactions only ($K = 2$). We derive a relaxed minimisation problem which is defined on a suitable sequence space and show exponential decay for minimisers of this relaxed minimisation problem, cf. Proposition 3.30. For this, we build on a related result by Hudson [35] for discrete systems with convex nearest and concave next-to-nearest neighbour interactions, which mimic Lennard-Jones interactions.

3. Rescaled energies and Γ*-equivalence.* As it was already pointed out in [20, 51], in the formal development by Γ-convergence fracture happens at zero tension and the minimal energies are not continuous in the boundary condition ℓ with the discontinuity at $\ell = \gamma$. This is not physical and does not reflect the behaviour of minimisers for finite n. Therefore, we perform a refined analysis of $H^{\ell}_{1,n}$ with ℓ close to γ. We follow [51] and consider a sequence $(\ell_n) \subset \mathbb{R}$ and replace ℓ in the boundary conditions (1.5) by ℓ_n. We assume that $\ell_n \geq \gamma$ and $\ell_n \to \gamma$ such that $\delta_n := \frac{\ell_n - \gamma}{\sqrt{\lambda_n}} \to \delta \geq 0$ as $n \to \infty$. This defines a new sequence of functionals $(H^{\ell_n}_n)$. By introducing the change of variables, we have $H^{\ell_n}_{1,n}(u) = E^{\delta_n}_n(v)$, where v is the piecewise affine interpolation of $v^i = \frac{u^i - \gamma i \lambda_n}{\sqrt{\lambda_n}}$ for $i = 0, \ldots, n$, and

$$E^{\delta_n}_n(v) = \sum_{j=1}^{K} \sum_{i=0}^{n-j} J_j \left(\gamma + \frac{v^{i+j} - v^i}{j\sqrt{\lambda_n}} \right) - nJ_{CB}(\gamma).$$

The scaling in the energy $E^{\delta_n}_n$, was investigated previously in one dimension (see [17, 18, 51]) and recently by Friedrich and Schmidt [30, 31] in higher dimensions. In Theorem 3.34, we show that $(E^{\delta_n}_n)$ Γ-converges with respect to the $L^1(0,1)$-topology to the functional E^{δ} given by

$$\begin{aligned} E^{\delta}(v) =& \alpha \int_0^1 |v'|^2 dx + \widetilde{B}(u_0^{(1)}, \gamma) + \widetilde{B}(u_1^{(1)}, \gamma) - \sum_{j=2}^{K} (j-1) J_j(\gamma) \\ &+ \beta_{BJ}(u_0^{(1)}) \#(S_v \cap \{0\}) + \beta_{IJ} \#(S_v \cap (0,1)) + \beta_{BJ}(u_1^{(1)}) \#(S_v \cap \{1\}) \end{aligned}$$

if $v \in SBV^{\delta}(0,1)$, $\#S_v < +\infty$, and $[v] \geq 0$ in $[0,1]$, and $+\infty$ otherwise, where $\alpha = \frac{1}{2} J''_{CB}(\gamma)$ and the β terms are as above, cf. Theorem 3.34 and Corollary 3.35. We notice that E^{δ} is a one-dimensional version of Griffith energy for fracture. This result is proven in [51, Theorem 6.1] in the case of nearest and next-to-nearest neighbour interactions; and we can follow arguments of [17, 51] to show Theorem 3.34 which is valid for general finite range interactions of Lennard-Jones type. Note that in [17, Theorem 4] a similar result for K interacting neighbours and periodic boundary conditions is shown. However, that result is proven under assumptions on the interaction potentials which are not always applicable to pair potentials, e.g. Lennard-Jones potentials, if $K > 2$, see Remark 3.36, and also [17, Remark 3], [18, Section 4].

In Section 3.6, we combine the formal development by Γ-convergence, which is a good approximation of the discrete model for $\ell \neq \gamma$, and the result for the rescaled sequence $(E_n^{\delta_n})$ which yields an approximation to H_n^ℓ in the vicinity of $\ell = \gamma$. We define the functional G_n^ℓ for functions $u \in SBV^\ell(0,1)$ with positive jumps by

$$G_n^\ell(u) = \int_0^1 W(u')dx + \lambda_n \beta_{IJ} \#(S_u \cap [0,1]) - \lambda_n \sum_{j=2}^K (j-1) J_j(\min\{\ell, \gamma\}),$$

where $W(z) = J_{CB}(z)$ for $z \leq \gamma$ and $W(z) = \frac{1}{2} J''_{CB}(\gamma)(z-\gamma)^2$ for $z \geq \gamma$ and β_{IJ} is given as above. We show that for $\ell > 0$ that the sequence (G_n^ℓ) has the same Γ-limit and first-order Γ-limit as the discrete energy H_n^ℓ for a particular choice of $u_0^{(1)}$ and $u_1^{(1)}$, see Proposition 3.39. This implies that (H_n^ℓ) and (G_n^ℓ) are Γ-equivalent, in the sense of Braides and Truskinovsky [20]. Notice that minima of G_n^ℓ are continuous in ℓ and fracture occurs for finite tension, see Remark 3.41.

Γ-convergence analysis of a quasicontinuum method in one dimension

The quasicontinuum (QC) method was introduced by Tadmor, Ortiz and Phillips [59] as a computational tool for atomistic simulations of crystalline solids at zero temperature. The key idea is to split the computational domain into regions where a very detailed (atomistic, nonlocal) description is needed and regions where a coarser (continuum, local) description is sufficient. This allows for simulations of relatively large systems with a full atomistic resolution at regions of interest. This idea has been successfully used to study crystal defects such as dislocations, nanoindentations or cracks and their impact on the overall behaviour of the material, see e.g. [42] for an overview of the method and the references therein for several applications.

There are various types of QC-methods: some are formulated in an energy based framework, some in a force based framework; further, different couplings between the atomistic and continuum parts and different models in the continuum region are considered. A first contribution to the mathematical analysis of those methods is given by Lin [40], where a QC-approximation of a Lennard-Jones system without boundary conditions and external forces is considered. By deriving explicit estimates for the minimisers of the full atomistic system and the QC-model Lin obtains an error estimate for the difference of the two minimisers. In the last decade, many articles related to the systematic error analysis of such coupling methods were published, e.g. [38, 43, 45, 46, 48] for one-dimensional problems and [26, 57] for higher dimensional problems. In particular, we refer to [41] for a recent overview.

In Chapter 4, we consider a variant of the so-called quasinonlocal quasicontinuum (QNL) method, first proposed by Shimokawa et al. [58]. QNL-methods are energy-based QC-methods which are constructed to overcome asymmetries (so-called ghost-forces) at the atomistic/continuum interface which arise in the classical energy based QC-method. Here, we focus on a generalization of the QNL-method given by Li and Luskin [38] which allows for a treatment of general finite range interactions; see also [26, 57] for further generalisations of QNL idea.

We are interested in an analytical approach to verify the QNL-method as an appropriate mechanical model by means of a discrete-to-continuum limit via Γ-convergence. To our knowledge Γ-convergence was used by Español et al. [29] to study a QC-approximation for the first time. In [29], the authors consider an atomistic model different from ours, namely a harmonic and defect-free crystal in arbitrary dimensions. Under general conditions it is shown that a quasicontinuum approximation based on summation rules has the same continuum limit as the fully atomistic system.

We aim for a Γ-convergence analysis of a QC-method in the presence of defects (i.e fracture). To this end, we consider the discrete energy H_n^ℓ as the fully atomistic model problem and construct an approximation based on the QNL-method. In particular, we keep all interactions in the atomistic (nonlocal) region and approximate the interactions beyond nearest neighbours in the continuum (local) region by appropriate nearest neighbour interactions:

$$J_j\left(\frac{u^{i+j}-u^i}{j\lambda_n}\right) \approx \frac{1}{j}\sum_{s=i}^{i+j-1} J_j\left(\frac{u^{s+1}-u^s}{\lambda_n}\right).$$

Furthermore, we reduce the degrees of freedom of the energy by fixing certain representative atoms and let the deformation of all atoms depend only on the deformation of these representative atoms. This yields a new sequence of functionals of which we derive a development by Γ-convergence similarly as for the fully atomistic model.

In Theorem 4.1, we show that the fully atomistic model and the quasicontinuum model have the same zero-order Γ-limit. If the boundary conditions are such that the specimen behaves elastically (i.e. $\ell \leq \gamma$), we prove that the first-order Γ-limits of both models coincide, see Theorem 4.5.

If the boundary conditions are such that fracture occurs (i.e. $\ell > \gamma$), the quasicontinuum approximation leads to a first-order Γ-limit (Theorem 4.11) that is in general different from the one obtained for the fully atomistic model (Theorem 3.19). To compare the fully atomistic and the quasicontinuum models also in this regime, we further analyse the first-order Γ-limits in Section 4.4. For this, we focus on the case of nearest and next-to-nearest neighbour interactions. It turns out that the choice of the representative atoms has a considerable impact on the validity of the QC-method. In Theorem 4.19, we provide sufficient conditions for the validity of the QC-method, in the sense that the minimal energies of the first-order Γ-limit coincide with the one for the fully atomistic model. We show that the QC-method is valid if the representative atoms are chosen in such a way that there is at least one non-representative atom between two neighbouring representative atoms in the continuum region. With this choice, fracture occurs always in the atomistic region, as desired. In Proposition 4.22, we provide examples in which the mentioned sufficient conditions on the choice of the representative atoms are not satisfied and the minima of the first-order Γ-limits of the fully atomistic model and the QC-model do not coincide. In this case, the QC-method should not be considered an appropriate approximation. This implies by means of analytical tools that in quasicontinuum simulations of fracture one has to make sure to pick a sufficiently large mesh in the continuum region and at the interface. In fact we show that in our particular model problem, with nearest and next-to-nearest neighbour interactions, it is sufficient that the mesh size in the continuum region is at least twice the size of the atomistic lattice distance.

Similar models as the one we consider here, were investigated previously in terms of numerical analysis. We refer the reader especially to [25, 38, 43, 45, 48] where the QNL-method is studied in one dimension. By proving notions of consistency and stability, those authors perform an error analysis in terms of the lattice spacing. To our knowledge, most of the results do not hold for “fractured” deformations. However, in [46] a Galerkin approximation of a discrete system is considered and error bounds are proven also for states with a single crack of which the position is prescribed. Recently, a different approach based on bifurcation theory is used in [39] to study the QC-approximation in the context of crack growth.

In [5], a different one-dimensional atomistic-continuum coupling method is investigated. Similar as in the QC-method the domain is splitted in a discrete and a continuum region. In the discrete part the energy is given by nearest neighbour Lennard-Jones interaction and in the continuum part by an integral functional with Lennard-Jones energy density. It is shown that fracture is more favourable in the continuum than in the discrete region. To overcome this, the energy density of the continuum model is modified by introducing an additional term which depends on the lattice distance in the discrete region. Furthermore, in [7, p. 420] it is remarked that if the continuum model is replaced by a typical discretized version, the fracture is favourable in the discrete region. As mentioned above, we here treat a similar issue in the QNL-method, see in particular Theorem 4.19, Proposition 4.22.

Several results of this thesis are based on the works [55, 56] obtained by the author jointly with Anja Schlömerkemper. In [56], a 1D Lennard-Jones type model with finite range interactions and periodic boundary conditions is considered. In that setting Theorem 3.5 and an analogous result to Theorem 3.34 for rescaled energies are proven (see Theorem 3.37). Here, we consider different boundary conditions and give a more detailed analysis for the discrete system including the first-order Γ-limit which we study in more detail. In [55], the analysis of the QC-method in the spirit of Chapter 4 is presented for the case of nearest and next-to-nearest neighbour interactions (see also [53, 54] for abridged versions). Here, we generalise those results to the case of finite range interactions.

Chapter 2

Mathematical background

2.1 Functions of bounded variations

In this section, we briefly recall some definitions and basic properties of (special) functions of bounded variations. For further details and proofs, we refer to [3, 8].

Let $\Omega = (a, b) \subset \mathbb{R}$ be a bounded interval. We denote by $C_0(\Omega)$ the space of continuous functions $\Omega \to \mathbb{R}$ vanishing at the boundary. Following [3, Definition 1.40], we denote by $\mathcal{M}(\Omega)$ the space of finite Radon measures on Ω. For $\mu \in \mathcal{M}(\Omega)$, we define for every Borel set $B \in \mathcal{B}(\Omega)$ the total variation $|\mu|(B)$ as

$$|\mu|(B) := \sup \left\{ \sum_{i \in \mathbb{N}} |\mu(E_i)| : \ E_i \in \mathcal{B}(\Omega) \text{ pairwise disjoint, } B = \bigcup_{i \in \mathbb{N}} E_i \right\}.$$

Recall that by the Riesz representation Theorem the space $\mathcal{M}(\Omega)$ is isometrically isomorphic to the dual space of $C_0(\Omega)$. This motivates the following definition

Definition 2.1. Let $\mu, \mu_n \in \mathcal{M}(\Omega)$. We say that μ_n weakly* converges to μ in the sense of measures (and write $\mu_n \overset{*}{\rightharpoonup} \mu$) if

$$\lim_{n \to \infty} \int_\Omega \phi d\mu_n = \int_\Omega \phi d\mu \quad \forall \phi \in C_0(\Omega).$$

Proposition 2.2. *Let $(\mu_n) \subset \mathcal{M}(\Omega)$ be such that $\sup_n |\mu_n|(\Omega) < +\infty$. Then there exists a subsequence converging weakly* to some $\mu \in \mathcal{M}(\Omega)$ in the sense of measures.*

Next, we define the functions of bounded variations.

Definition 2.3. Let $u \in L^1(\Omega)$; we say that u is a *function of bounded variation* in Ω if its distributional derivative is a finite Radon measure in Ω; i.e. there exists $\mu \in \mathcal{M}(\Omega)$ such that

$$\int_\Omega u\phi' dx = -\int_\Omega \phi d\mu \quad \forall \phi \in C_c^1(\Omega).$$

The measure μ will be denoted by Du. The space of all functions of bounded variation in Ω is denoted by $BV(\Omega)$.

The space $BV(\Omega)$ endowed with the norm

$$\|u\|_{BV(\Omega)} := \|u\|_{L^1(\Omega)} + |Du|(\Omega)$$

is a Banach space. However, the norm topology is too strong and we will mostly use the following weaker notion of convergence

Definition 2.4. We say that $(u_n) \subset BV(\Omega)$ weakly* converges in $BV(\Omega)$ to some $u \in BV(\Omega)$, if $u_n \to u$ in $L^1(\Omega)$ and $Du_n \overset{*}{\rightharpoonup} Du$ in $\mathcal{M}(\Omega)$.

The following proposition gives a useful criterion for weak* convergence, cf. i.e. [3, Proposition 3.13].

Proposition 2.5. *Let $(u_n) \subset BV(\Omega)$. Then (u_n) weakly* converges to u in $BV(\Omega)$ if and only if (u_n) is bounded in $BV(\Omega)$ and $u_n \to u$ in $L^1(\Omega)$.*

Let us now state a compactness theorem for functions in BV, cf. i.e. [3, Proposition 3.23].

Theorem 2.6. *Let $(u_n) \subset BV(\Omega)$ be such that $\sup_n \|u_n\|_{BV(\Omega)} < \infty$ then there exists a subsequence (u_{n_k}) weakly* converging to some $u \in BV(\Omega)$.*

We notice that a direct consequence of Theorem 2.6 is that equibounded sequences in $W^{1,1}$ converge, up to subsequences, in $L^1(\Omega)$ to some $u \in BV(\Omega)$.

Let $u \in BV(\Omega)$ be given. By the Radon-Nikodyn Theorem, we can split Du into an *absolutely continuous part* $D^a u$ with respect to the Lebesgue measure $\mathcal{L}^1$, and a *singular part* $D^s u$. Moreover, we can decompose the singular part $D^s u$ into a *jump part* $D^j u$ and a *Cantor part* $D^c u$. To this end, we denote $A = \{x \in \Omega : \; Du(\{x\}) \neq 0\}$ the set of atoms of Du. Since Du is a finite Radon measure the set A is at most countable. Finally, we set $D^j u = D^s u \llcorner A$ and $D^c u = D^s u \llcorner (\Omega \setminus A)$. In this way we obtain

$$Du = D^a u + D^s u = D^a u + D^j u + D^c u. \tag{2.1}$$

Notice that all the previous definitions and statements including the decomposition of the derivative Du can be extended in a suitable sense to the case $\Omega \subset \mathbb{R}^n$ and $u : \Omega \to \mathbb{R}^m$ with $n, m \in \mathbb{N}$.

Next, we use the fact that u depends only on one variable. We say that $u \in BV(\Omega)$ is a jump function if $Du = D^j u$, and we say that u is a Cantor function if $Du = D^c u$. For given $u \in BV(\Omega)$, there exist $u^a \in W^{1,1}$, a jump function u^j, and a Cantor function u^c such that $u = u^a + u^j + u^c$.

For a function $u \in BV(\Omega)$, the right-hand side and left-hand side limits

$$u(x+) = \lim_{h \to 0+} \int_x^{x+h} u(s)ds, \quad u(x-) = \lim_{h \to 0+} \int_{x-h}^{x} u(s)ds$$

exist at all $x \in [a, b)$, and $x \in (a, b]$, respectively. We can define the *jump set* $S_u := \{x \in \Omega : \; u(x+) \neq u(x-)\}$. We notice that S_u coincides with the set of atoms of the measure Du and thus is at most countable.

For a given $u \in BV(\Omega)$, we denote by $u' \in L^1(\Omega)$ the density of $D^a u$ and we set $[u](x) := u(x+) - u(x-)$ for all $x \in \Omega$. Then the jump part $D^j u$ is given by $\sum_{x \in S_u} [u](x)\delta_x$ and the decomposition in (2.1) reads

$$Du = u'\mathcal{L}^1 + \sum_{x \in S_u} [u](x)\delta_x + D^c u.$$

An important subspace of $BV(\Omega)$ is given by the special functions of bounded variations

Definition 2.7. We say that a function $u \in BV(\Omega)$ is a *special function of bounded variation* if $D^c u \equiv 0$. We denote the space of special functions of bounded variations by $SBV(\Omega)$.

For a given $u \in SBV(\Omega)$, we can use the previous decomposition and find $u^a \in W^{1,1}(\Omega)$ and a jump function $u^j \in SBV(\Omega)$ such that $u = u^a + u^j$. The space $SBV(\Omega)$ enjoys the following useful closure and compactness properties, cf. i.e. [3, Theorem 4.7, Theorem 4.8].

Theorem 2.8. *Let $\varphi : [0, +\infty) \to [0, +\infty]$ be a lower semicontinuous increasing function and assume that*

$$\lim_{t \to \infty} \frac{\varphi(t)}{t} = +\infty.$$

Let $(u_n) \subset SBV(\Omega)$ be such that

$$\sup_n \left(\int_\Omega \varphi(|u_n'|)dx + \#S_u \right) < +\infty. \tag{2.2}$$

If (u_n) weakly converges in $BV(\Omega)$ to u, then $u \in SBV(\Omega)$, $u_n' \rightharpoonup u'$ in $L^1(\Omega)$, $D^j u_n \overset{*}{\rightharpoonup} D^j u$ in $\mathcal{M}(\Omega)$ and $\#S_u \leq \liminf_{n \to \infty} \#S_{u_n}$.*

Theorem 2.9. *Let φ be as in Theorem 2.8. Let $(u_n) \subset SBV(\Omega)$ be satisfying* (2.2) *and assume that $\sup_n \|u_n\|_{L^\infty(\Omega)} < +\infty$. Then there exists a subsequence (u_{n_k}) weakly* converging in $BV(\Omega)$ to $u \in SBV(\Omega)$.*

2.1.1 Boundary values in BV

As mentioned in the introduction, we consider discrete minimisation problems for functions defined on $[0, 1]$ with fixed Dirichlet boundary data and derive a limiting minimisation problem which is defined on the space of bounded variations. For this we have to introduce appropriate function spaces which take jumps at the boundary into account. To this end, we follow [11, 12, 50]: for given $\ell > 0$, we say that $u \in BV^\ell(0, 1)$ if u is a function of bounded variation on $(0, 1)$ and we set $u(0-) = 0$ and $u(1+) = \ell$. Then we define $[u](x) := u(x+) - u(x-)$ for every $x \in [0, 1]$ and the set $S_u^\ell = \{x \in [0, 1] : [u](x) \neq 0\}$. Moreover, we extend the measures Du and $D^s u$ to $[0, 1]$ by

$$Du = u'\mathcal{L}^1 + \sum_{x \in S_u^\ell} [u](x)\delta_x + D^c u, \quad D^s u = \sum_{x \in S_u^\ell} [u](x)\delta_x + D^c u.$$

We notice that, if $v \in BV_{\text{loc}}(\mathbb{R})$ is the extension of u defined by $v(x) = 0$ for $x \leq 0$ and $v(x) = \ell$ for $x \geq 1$, then Du and $D^s u$ are the restrictions to $[0,1]$ of the distributional derivative Dv and of its singular part $D^s v$. Note also that for every $u \in BV^\ell(0,1)$, we have

$$Du([0,1]) = \int_0^1 u' dx + \sum_{x \in S_u^\ell} [u](x)\delta_x + D^c u(0,1) = \ell$$

and that u is uniquely determined by the measure Du on $[0,1]$. We define the set $SBV^\ell(0,1)$ correspondingly.

In the remainder of this thesis, we will omit the superscript ℓ in S_u^ℓ and set $S_u = S_u^\ell$ for $u \in BV^\ell(0,1)$ (or $u \in SBV^\ell(0,1)$).

2.2 Γ–convergence

In this section, we give a brief introduction to the notion of Γ-convergence. For a comprehensive introduction to Γ-convergence we refer to [9, 24]. We follow here the overview given in [8, Section 3.1].

Definition 2.10. Let (X, d) be a metric space. For any $n \in \mathbb{N}$, let $F_n : X \to [-\infty, +\infty]$. The sequence (F_n) Γ-converges to $F : X \to [-\infty, +\infty]$ if for all $u \in X$ the following hold true

(i) (*liminf inequality*) for every sequence (u_n) converging to u

$$\liminf_{n\to\infty} F_n(u_n) \geq F(u);$$

(ii) (*limsup inequality*) there exists a sequence (u_n) converging to u such that

$$\limsup_{n\to\infty} F_n(u_n) \leq F(u),$$

or equivalently (by (i))

$$\lim_{n\to\infty} F_n(u_n) = F(u).$$

The function F is called the Γ-limit of (F_n) (with respect to d), and we write $F = \Gamma\text{-}\lim_{n\to\infty} F_n$ or $F = \Gamma(d)\text{-}\lim_{n\to\infty}$ to emphasize the metric d if this is needed.

The following result is one of the main reasons for introducing Γ-convergence.

Theorem 2.11. *Let (X, d) be a metric space, let $F_n, F : X \to [-\infty, +\infty]$ be such $F = \Gamma\text{-}\lim_n F_n$. If there exists a compact set $K \subset X$ such that $\inf_X F_n = \inf_K F_n$ for all n, then*

$$\exists \min_X F = \lim_{n\to\infty} \inf_X F_n.$$

Moreover, if (u_n) is a converging sequence such that $\lim_{n\to\infty} F_n(u_n) = \lim_{n\to\infty} \inf_X F_n$ then its limit is a minimum point for F.

It is often useful to use the following pointwise definition of Γ-convergence.

Definition 2.12. Let (X, d) be a metric space. For any $n \in \mathbb{N}$, let $F_n : X \to [-\infty, +\infty]$ and let $u \in X$. The Γ-lower and Γ-upper limits of (F_n) at u, denoted by $\Gamma\text{-}\liminf F_n(u)$ and $\Gamma\text{-}\limsup F_n(u)$, are defined by

$$\Gamma\text{-}\liminf_{n\to\infty} F_n(u) = \inf\left\{\liminf_{n\to\infty} F_n(u_n) : \; u_n \to u\right\},$$
$$\Gamma\text{-}\limsup_{n\to\infty} F_n(u) = \inf\left\{\limsup_{n\to\infty} F_n(u_n) : \; u_n \to u\right\}.$$

If $\Gamma\text{-}\liminf_n F_n(u) = \Gamma\text{-}\limsup_n F_n(u)$ then the common value is called the Γ-limit of (F_n) at u, and is denoted by $\Gamma\text{-}\lim_n F_n(u)$. Note that this definition is in accord with Definition 2.10, and that (F_n) Γ-converges to F if and only if $F(u) = \Gamma\text{-}\lim_n F_n(u)$ at all $u \in X$.

Remark 2.13. Let $F_n : X \to [-\infty, +\infty]$ be a sequence of functionals on X.
(a) Let $G : X \to [-\infty, +\infty]$ be continuous with respect to d and (F_n) Γ-converges to F. Then $\Gamma\text{-}\lim_n(F_n + G) = F + G$.
(b) Let $F_n = F_1$ for all $n \in \mathbb{N}$. Then (F_n) Γ-converges to the lower semicontinuous envelope $\overline{F}_1$ of F_1, i.e.

$$\overline{F}_1(u) = \sup\{G(u) : \; G \text{ is lower semicontinuous and } G \le F_1\}.$$

(c) The Γ-lower and Γ-upper limits are lower semicontinuous.

In this thesis, we consider Γ-limit of higher (first) order. This is motivated by the following result.

Theorem 2.14. *Let $F_n : X \to (-\infty, +\infty]$ be a sequence of d-equi-coercive functions and let $F = \Gamma(d)\text{-}\lim_{n\to\infty} F_n$. Let $m_n = \inf_X F_n$, $m^0 = \min F$ and denote $\lambda_n = \frac{1}{n}$. Suppose that for $\alpha > 0$ there exists the Γ-limit*

$$F^\alpha = \Gamma(d')\text{-}\lim_{n\to\infty} \frac{F_n - m^0}{\lambda_n^\alpha},$$

and that the sequence $F_n^\alpha = (F_n - m^0)/\lambda_n^\alpha$ is d'-equi-coercive for a metric d' which is not weaker than d. Define $m^\alpha = \min F^\alpha$ and suppose that $m^\alpha \neq +\infty$; then we have that

$$m_n = m^0 + \lambda_n^\alpha m^\alpha + o(\lambda_n^\alpha)$$

and from all sequences (u_n) such that $F_n(u_n) - m_n = o(\lambda_n)$ there exists a subsequence converging in (X, d') to a point u which minimises both F and F^α.

2.3 Lower semicontinuity and relaxation

In this section, we give a relaxation result for integral functionals defined on $W^{1,1}(\Omega)$ which is used at several occasions in the remainder of the thesis.

Proposition 2.15. *Let $f : \mathbb{R} \to \mathbb{R} \cup \{+\infty\}$ be convex, lower semicontinuous, monotone decreasing with*

$$\lim_{z \to -\infty} \frac{f(z)}{|z|} = +\infty \quad \text{and} \quad \lim_{z \to +\infty} f(z) = c \in \mathbb{R}. \tag{2.3}$$

Let $F : BV(a,b) \to \mathbb{R} \cup \{+\infty\}$ be defined as

$$F(u) := \begin{cases} \displaystyle\int_a^b f(u')dx & \text{if } u \in W^{1,1}(0,1), \\ +\infty & \text{else.} \end{cases}$$

Let the functional $\mathcal{F} : BV(a,b) \to \mathbb{R} \cup \{+\infty\}$ be defined as

$$\mathcal{F}(u) := \begin{cases} \displaystyle\int_a^b f(u')dx & \text{if } u \in BV(a,b),\ D^s u \geq 0, \\ +\infty & \text{else.} \end{cases}$$

Let $\overline{F}$ denote the lower semicontinuous envelope of F with respect to the weak* convergence in $BV(a,b)$. Then it holds $\mathcal{F} \equiv \overline{F}$.

The above Proposition can be deduced from [34, Theorem 1.62]. For the convenience of the reader, we present a self contained proof here. We follow the arguments of [33, Theorem 2.4], where a similar result is proven for functions $f : (0,+\infty) \to \mathbb{R}$.

Proof. Let us first show $\mathcal{F} \leq \overline{F}$. By definition of $\mathcal{F}$ it holds $\mathcal{F} \leq F$ and it is left to show that the functional $\mathcal{F}$ is lower semicontinuous with respect to the weak* convergence in $BV(a,b)$. Indeed, from (2.3), we deduce for the recession function f_∞ of f that

$$f_\infty(p) := \lim_{t \to +\infty} \frac{f(p_0 + tp) - f(p_0)}{t} = \begin{cases} +\infty & \text{if } p < 0, \\ 0 & \text{if } p \geq 0, \end{cases}$$

with $p_0 \in \operatorname{dom} f$ arbitrary, see [3, Definition 2.32]. For given $u \in BV(a,b)$, we have that

$$\mathcal{F}(u) = \mathcal{H}(Du) := \int_a^b f(D^a u)dx + \sum_{x \in S_u} f_\infty(D^j u(\{x\})) + \int_a^b f_\infty\left(\frac{D^c u}{|D^c u|}\right) d|D^c u|.$$

Since $u_n \overset{*}{\rightharpoonup} u$ in $BV(a,b)$ implies $Du_n \overset{*}{\rightharpoonup} Du$ in $\mathcal{M}(a,b)$, we have that lower semicontinuity of $\mathcal{H}$ (with respect to weak* convergence in $\mathcal{M}(a,b)$) implies lower semicontinuity of $\mathcal{F}$ (with respect to weak* convergence in $BV(a,b)$). Since f is decreasing, we have that $f : \mathbb{R} \to [c,+\infty]$. In the case $c \geq 0$ the lower semicontinuity of $\mathcal{H}$ follows by [3, Proposition 5.1, Theorem 5.2]. If $c < 0$ we apply the above cited lower semicontinuity results on the functional $\tilde{\mathcal{H}}$ which is defined as $\mathcal{H}$ but f is replaced by $\tilde{f} : \mathbb{R} \to [0, +\infty]$ with $\tilde{f}(z) = f(z) - c$. Since $\tilde{\mathcal{H}}$ and $\mathcal{H}$ share the same lower semicontinuity properties the assertion follows.

Let us show that $\overline{F} \leq \mathcal{F}$. To this end, we provide for every $u \in BV(0,1)$ a sequence (u_N) such that $u_N \overset{*}{\rightharpoonup} u$ weakly* in $BV(a,b)$ and

$$\limsup_{N\to\infty} F(u_N) \leq \mathcal{F}(u). \tag{2.4}$$

Without loss of generality, we can assume that $D^s u \geq 0$ on (a,b), otherwise the above inequality is trivial. Let $(g_N) \subset L^1(a,b)$ be such that $g_N \geq 0$ on (a,b) and $g_N \mathcal{L}^1 \overset{*}{\rightharpoonup} D^s u$ weakly* in measure on (a,b). Let $x_0 \in (a,b)$ be a Lebesgue point of u. We define the sequence $(u_N) \subset W^{1,1}(a,b)$ by

$$u_N(x) := u(x_0) + \int_{x_0}^{x} u'(s) + g_N(s) ds.$$

Since g_N is equibounded in $L^1(a,b)$, we have that $\|u_N\|_{W^{1,1}(a,b)}$ is equibounded and thus there exists a subsequence, not relabelled, (u_N) which weakly* converges in $BV(a,b)$ to some $v \in BV(a,b)$. From $u_N(x_0) = u(x_0)$ for all $N \in \mathbb{N}$ and $Du_N = (u' + g_N)\mathcal{L}^1$ converges weakly* to Du in measure we deduce that $v \equiv u$. Since $u'_N = u' + g_N$ and $g_N \geq 0$ by construction, we deduce from the monotonicity of f that

$$F(u_N) = \int_a^b f(u'_N) dx \leq \int_a^b f(u') dx = \mathcal{F}(u)$$

for every $N \in \mathbb{N}$. This yields inequality (2.4). □

Chapter 3

On Lennard-Jones type systems and their asymptotic analysis

3.1 Setting of the problem

We consider a one-dimensional lattice given by $\lambda_n\mathbb{Z}\cap[0,1]$ with $\lambda_n = \frac{1}{n}$ and interpret this as a chain of $n+1$ atoms. We denote by $u : \lambda_n\mathbb{Z}\cap[0,1]\to\mathbb{R}$ the deformation of the atoms from the reference configuration and write $u(i\lambda_n) = u^i$ as shorthand. We identify such functions with their piecewise affine interpolations and define

$$\mathcal{A}_n(0,1) := \{u \in C([0,1]) : \ u \text{ is affine on } (i,i+1)\lambda_n,\ i \in \{0,\dots,n-1\}\}\,. \tag{3.1}$$

For a given $K\in\mathbb{N}$, $K\geq 2$ the energy of a deformation $u\in\mathcal{A}_n(0,1)$ is defined by

$$H_n(u) = \sum_{j=1}^{K}\sum_{i=0}^{n-j}\lambda_n J_j\left(\frac{u^{i+j}-u^i}{j\lambda_n}\right), \tag{3.2}$$

where $J_1,\dots,J_K$ are potentials of Lennard-Jones type which will be specified below. In analogy to [50], we impose the following boundary conditions: for given $\ell>0$ and $u_0^{(1)} = (u_{0,s}^{(1)})_{s=1}^{K-1}$, $u_1^{(1)} = (u_{1,s}^{(1)})_{s=1}^{K-1}\in\mathbb{R}_+^{K-1}$ we set

$$\begin{aligned} &u^0 = 0,\ u^n = \ell,\\ &u^s - u^{s-1} = \lambda_n u_{0,s}^{(1)},\ u^{n+1-s} - u^{n-s} = \lambda_n u_{1,s}^{(1)} \quad \text{for } s\in\{1,\dots,K-1\}. \end{aligned} \tag{3.3}$$

Note that (3.3) yields $2K$ boundary conditions. This compensates the fact that the first (last) K atoms in the chain have more interactions with atoms on the right-hand side (left-hand side) than on the left-hand side (right-hand side); cf. e.g. [22] for a further discussion of boundary conditions in discrete systems beyond nearest neighbour interactions. In [11] the energy H_n is studied in the case of nearest and next-to-nearest neighbour interactions ($K=2$). The authors consider two different boundary conditions: (i) Dirichlet boundary conditions on the first and the last atom only, and (ii) periodic boundary conditions. In

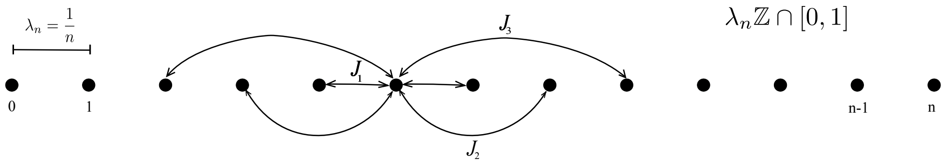

FIGURE 3.1: A chain of $n+1$ atoms.

the case of fracture, it is shown that either the crack appears at the boundary (case (i)), or fracture appears indifferently everywhere (case (ii)). On the contrary, the extra degree of freedom in the boundary conditions (3.3) allow for both behaviours, see [50, Theorem 5.1] for the case $K = 2$ and Theorem 3.118 for the general case $K \geq 2$.

For given $\ell > 0$ and $u_0^{(1)}, u_1^{(1)} \in \mathbb{R}_+^{K-1}$, we consider the functional $H_n^\ell : L^1(0,1) \to (-\infty, +\infty]$ defined by

$$H_n^\ell(u) = \begin{cases} H_n(u) & \text{if } u \in \mathcal{A}_n(0,1) \text{ satisfies (3.3)}, \\ +\infty & \text{else.} \end{cases} \tag{3.4}$$

Before we state the assumptions on the interaction potentials J_j let us rewrite the energy H_n in a suitable way. For given $j \in \{2, \dots, K\}$ and $u \in \mathcal{A}_n(0,1)$, we can rewrite the nearest neighbour interactions in (3.2) by

$$\begin{aligned} \sum_{i=0}^{n-1} \lambda_n J_1\left(\frac{u^{i+1}-u^i}{\lambda_n}\right) =& \sum_{s=1}^{j-1} \frac{j-s}{j} \lambda_n J_1\left(\frac{u^s - u^{s-1}}{\lambda_n}\right) + \sum_{i=0}^{n-j} \frac{1}{j} \sum_{s=i}^{i+j-1} \lambda_n J_1\left(\frac{u^{s+1}-u^s}{\lambda_n}\right) \\ &+ \sum_{s=1}^{j-1} \frac{j-s}{j} \lambda_n J_1\left(\frac{u^{n-s+1}-u^{n-s}}{\lambda_n}\right). \end{aligned} \tag{3.5}$$

Indeed, this follows from the following calculation with $a_i = \lambda_n J_1(\frac{u^{i+1}-u^i}{\lambda_n})$

$$\begin{aligned} \frac{1}{j} \sum_{i=0}^{n-j} \sum_{s=i}^{i+j-1} a_s =& \frac{1}{j} \sum_{i=0}^{n-j} \sum_{s=0}^{j-1} a_{i+s} = \frac{1}{j} \sum_{s=0}^{j-1} \sum_{i=s}^{n+s-j} a_i \\ =& \frac{1}{j} \sum_{s=0}^{j-1} \sum_{i=0}^{n-1} a_i - \frac{1}{j} \sum_{s=0}^{j-1} \left\{ \sum_{i=0}^{s-1} a_i + \sum_{i=n+s-j+1}^{n-1} a_i \right\} \\ =& \sum_{i=0}^{n-1} a_i - \sum_{i=1}^{j-1} \frac{j-i}{j} \left\{ a_{i-1} + a_{n-i} \right\}. \end{aligned} \tag{3.6}$$

Let $c = (c_j)_{j=2}^K \in \mathbb{R}_+^{K-1}$ be such that $\sum_{j=2}^K c_j = 1$. Using (3.5), we can rewrite the energy (3.2) as

$$H_n(u) = \sum_{j=2}^{K}\sum_{i=0}^{n-j} \lambda_n \left\{ J_j\left(\frac{u^{i+j}-u^i}{j\lambda_n}\right) + \frac{c_j}{j}\sum_{s=i}^{i+j-1} \lambda_n J_1\left(\frac{u^{s+1}-u^s}{\lambda_n}\right)\right\}$$
$$+ \sum_{j=2}^{K} c_j \sum_{s=1}^{j-1} \frac{j-s}{j}\lambda_n \left\{ J_1\left(\frac{u^s-u^{s-1}}{\lambda_n}\right) + J_1\left(\frac{u^{n-s+1}-u^{n-s}}{\lambda_n}\right)\right\}. \tag{3.7}$$

For given $j \in \{2, \dots, K\}$, we define the following functions

$$J_{0,j}(z) := J_j(z) + \frac{c_j}{j}\inf\left\{\sum_{s=1}^{j} J_1(z_s),\ \sum_{s=1}^{j} z_s = jz\right\}. \tag{3.8}$$

Note that the definition of $J_{0,j}$ yields a lower bound for the terms in the sum from $i = 0$ to $i = n - j$ in (3.7). In the case of nearest and next-to-nearest neighbour interactions, i.e. $K = 2$, we have $c_2 = c_K = 1$ and

$$J_0(z) := J_{0,2}(z) = J_2(z) + \frac{1}{2}\inf\left\{J_1(z_1) + J_1(z_2),\ z_1 + z_2 = 2z\right\},$$

which is exactly the effective energy density J_0 which show up in [11, 50].

Let us now state assumptions on the potentials J_j for $j \in \{1, \dots, K\}$:

(LJ1) The function $J_j : \mathbb{R} \to (-\infty, +\infty]$, $j = 1, \dots, K$ be lower semicontinuous and in $C^{1,\alpha}$, $0 < \alpha \leq 1$ on their domains, i.e. on $\operatorname{dom} J_j = \{z \in \mathbb{R} : J_j(z) < +\infty\}$. It holds $\operatorname{dom} J_1 = \operatorname{dom} J_j$ for $j = 2, \dots, K$ and $(0, +\infty) \subset \operatorname{dom} J_1$. Moreover, we assume that

$$\lim_{z\to+\infty} J_j(z) = 0,\ j = 1, \dots, K \tag{3.9}$$

(LJ2) The potentials J_j, $j = 1, \dots, K$ are such that there exists a convex function $\Psi : \mathbb{R} \to [0, +\infty]$ and constants d_1, d_2 such that

$$\lim_{z\to-\infty} \frac{\Psi(z)}{|z|} = +\infty \tag{3.10}$$

and

$$d_1(\Psi(z) - 1) \leq J_j(z) \leq d_2 \max\{\Psi(z), |z|\} \quad \text{for all } z \in \mathbb{R} \quad j = 1, \dots, K. \tag{3.11}$$

Further, J_j has a unique minimum point δ_j and it is strictly convex in $(-\infty, \delta_j)$ on its domain for $j = 1, \dots, K$.

(LJ3) There exists $c = (c_j)_{j=2}^K \in \mathbb{R}_+^{K-1}$ such that $\sum_{j=2}^K c_j = 1$, and $J_{0,j}$ defined in (3.8) satisfies the assumptions (LJ4) and (LJ5) for $j \in \{2, \dots, K\}$.

(LJ4) There exists a unique $\gamma > 0$, independent of j, such that

$$\{\gamma\} = \arg\min_{z\in\mathbb{R}} J_{0,j}(z). \tag{3.12}$$

Furthermore, there exists $\gamma^c > \gamma$ such that for $z \in (-\infty, \gamma^c] \cap \operatorname{dom} J_1$ it holds:

$$\{(z, \dots, z)\} = \arg\min_{(z_1,\dots,z_j)\in\mathbb{R}^j} \left\{ \sum_{s=1}^{j} J_1(z_s) : \ \sum_{s=1}^{j} z_s = jz \right\}. \tag{3.13}$$

This implies $J_{0,j}(z) = \psi_j(z)$ for $z \le \gamma^c$, where $\psi_j : \mathbb{R} \to (-\infty, +\infty]$ is defined by

$$\psi_j(z) := J_j(z) + c_j J_1(z). \tag{3.14}$$

(LJ5) The convex and lower semicontinuous envelopes $J_{0,j}^{**}$ and ψ_j^{**} of $J_{0,j}$ and ψ_j satisfy

$$J_{0,j}^{**}(z) = \psi_j^{**}(z) = \begin{cases} \psi_j(z) & \text{if } z \le \gamma, \\ \psi_j(\gamma) & \text{if } z > \gamma. \end{cases} \tag{3.15}$$

Furthermore, ψ_j is strictly convex in $(-\infty, \gamma)$ on its domain and it holds

$$\liminf_{z\to+\infty} J_{0,j}(z) > J_{0,j}(\gamma). \tag{3.16}$$

Remark 3.1. Let $J_1, \dots, J_K$ satisfy the assumptions (LJ1)–(LJ5).

(a) We have that $\{\gamma\} = \arg\min_z J_{CB}(z)$, where γ is given in (3.12) and $J_{CB} : \mathbb{R} \to (-\infty, +\infty]$ is defined by

$$J_{CB}(z) := \sum_{j=1}^{K} J_j(z), \tag{3.17}$$

and is called Cauchy-Born energy density, see e.g. [59]. Indeed assume for contradiction that there exists $\hat{\gamma} \in \arg\min J_{CB}$ such that $\hat{\gamma} \neq \gamma$. Using $\sum_{j=2}^{K} c_j = 1$ and (3.12), we obtain

$$J_{CB}(\gamma) \ge J_{CB}(\hat{\gamma}) = \sum_{j=2}^{K} (J_j(\hat{\gamma}) + c_j J_1(\hat{\gamma})) \ge \sum_{j=2}^{K} J_{0,j}(\hat{\gamma}) > \sum_{j=2}^{K} J_{0,j}(\gamma) = J_{CB}(\gamma),$$

which is a contradiction. Moreover, it holds

$$J_{CB}^{**}(z) = \sum_{j=2}^{K} \psi_j^{**}(z) = \begin{cases} J_{CB}(z) & \text{if } z \le \gamma \\ J_{CB}(\gamma) & \text{if } z \ge \gamma. \end{cases} \tag{3.18}$$

From (3.9), $J_{0,j} \le \psi_j$ and (3.16), we deduce that

$$\psi_j(\gamma) = J_{0,j}(\gamma) < 0. \tag{3.19}$$

(b) From (LJ4), we deduce that $\{\gamma\} = \arg\min_z \psi_j(z)$ for all $j \in \{2, \dots, K\}$ and thus, by (LJ1), that

$$0 = \psi_j'(\gamma) = J_j'(\gamma) + c_j J_1'(\gamma) \quad \forall j \in \{2, \dots, K\}. \tag{3.20}$$

From equation (3.20) and $c_j > 0$, we deduce that $J_1'(\gamma) \neq 0$ implies $J_j'(\gamma) \neq 0$ for all $j \in \{2, \dots, K\}$. In this case $c = (c_j)_{j=2}^K$ is uniquely determined by

$$c_j = -\frac{J_j'(\gamma)}{J_1'(\gamma)}. \tag{3.21}$$

Note that $\{\gamma\} = \arg\min_z J_{CB}(z)$ implies $\sum_{j=2}^K J_j'(\gamma) = -J_1'(\gamma)$ and thus $\sum_{j=2}^K c_j = 1$ for c_j as in (3.21).

(c) The assumptions (LJ1) and (LJ2) imply that either $\operatorname{dom} J_j = \mathbb{R}$ or there exists $r_* \leq 0$ such that $\operatorname{dom} J_j = (r_*, +\infty)$ or $\operatorname{dom} J_j = [r_*, +\infty)$ for all $j \in \{1, \dots, K\}$.

Next, we show that the assumptions (LJ1)–(LJ5) are reasonable in the sense that they are satisfied by the classical Lennard-Jones potentials.

Proposition 3.2. *For $j \in \{1, \dots, K\}$ let $J_j : \mathbb{R} \to \mathbb{R} \cup \{+\infty\}$ be defined as*

$$J_j(z) = J(jz) \text{ with } J(z) = \frac{k_1}{z^{12}} - \frac{k_2}{z^6}, \text{ for } z > 0 \text{ and } J(z) = +\infty \text{ for } z \leq 0 \tag{3.22}$$

and $k_1, k_2 > 0$. Then the there exists a unique $\gamma > 0$ such that the assumptions (LJ1)–(LJ5) are satisfied with $c = (c_j)_{j=2}^K$ given as in (3.21)*. Moreover, it holds $\gamma < \delta_1$, where δ_1 is the unique minimiser of J, and $\psi_j''(\gamma) > 0$ for all $j \in \{2, \dots, K\}$, see* (3.14)*.*

Proof. By the definition of J_j, $j \in \{1, \dots, K\}$ it is clear that they satisfy (LJ1) and (LJ2). Note that the unique minimiser δ_j of J_j is given by

$$\delta_j = \frac{1}{j}\left(\frac{2k_1}{k_2}\right)^{\frac{1}{6}} = \frac{1}{j}\delta_1,$$

and J is strictly convex on $(0, z_c)$ with $z_c = (\frac{13}{7})^{\frac{1}{6}}\delta_1 > \delta_1$. Let us show (LJ3)–(LJ5). The function J_{CB} is given by

$$J_{CB}(z) = \sum_{j=1}^K J(jz) = \frac{k_1}{z^{12}} \sum_{j=1}^K \frac{1}{j^{12}} - \frac{k_2}{z^6} \sum_{j=1}^K \frac{1}{j^6}.$$

Hence, J_{CB} is also a Lennard-Jones potential with the constants $\tilde{k}_1 = k_1 \sum_{j=1}^K j^{-12}$ and $\tilde{k}_2 = k_2 \sum_{j=1}^K j^{-6}$. The unique minimiser γ of J_{CB} is given by

$$\gamma = \left(\frac{2\tilde{k}_1}{\tilde{k}_2}\right)^{\frac{1}{6}} = \left(\frac{2k_1}{k_2}\right)^{\frac{1}{6}} \left(\frac{\sum_{j=1}^K \frac{1}{j^{12}}}{\sum_{j=1}^K \frac{1}{j^6}}\right)^{\frac{1}{6}} < \delta_1. \tag{3.23}$$

Since $\gamma < \delta_1$ it holds $J'(\gamma) < 0$. For given $j \in \{2, \dots, K\}$, we have that

$$\delta_j \le \delta_2 = \frac{1}{2}\delta_1 < \left(\frac{1}{\zeta(6)}\right)^{\frac{1}{6}} \delta_1 < \left(\frac{\sum_{j=1}^K j^{-12}}{\sum_{j=1}^K j^{-6}}\right)^{\frac{1}{6}} \delta_1 = \gamma,$$

where we denote by $\zeta(s) = \sum_{n\ge1} n^{-s}$ the Riemann zeta function and we used $\zeta(6) = \frac{\pi^6}{945} \approx 1.017$. Since J_j is strictly increasing on $\{z \in \mathbb{R} : z > \delta_j\}$ this implies that $J_j'(\gamma) = jJ'(j\gamma) > 0$ for $j \in \{2, \dots, K\}$. Hence, we have $c_j := -\frac{J_j(\gamma)}{J_1(\gamma)} > 0$ for $j \in \{2, \dots, K\}$ and it holds $\sum_{j=2}^K c_j = 1$ (see Remark 3.1 (b)).

Let $z \le \delta_1$, where δ_1 denotes the unique minimum of J. We show (3.13) for $j = 2, \dots, K$. Firstly, we note that the existence of a minimiser is clear since $z_s > 0$ for $s \in \{1, \dots, j\}$. Let $z < \delta_1$ and $(z_1, \dots, z_j) \in \arg\min\{\sum_{s=1}^j J_1(z_s) : \sum_{s=1}^j z_s = jz\}$ (see (3.13)). By the optimality conditions, there exists $\lambda \in \mathbb{R}$ such that $J'(z_s) = \lambda$ for $s \in \{1, \dots, j\}$. From $\sum_{s=1}^j z_s = jz < j\delta_1$, we deduce that there exists $\bar{j} \in \{1, \dots, j\}$ such that $z_{\bar{j}} < \delta_1$. Since $J' > 0$ on $(\delta_1, +\infty)$ and J' strictly increasing and ≤ 0 on $(0, \delta_1)$, we deduce that $z_s = z_{\bar{j}}$ for all $s = 1, \dots, j$. Hence, $z_s = z$ for $s = 1, \dots, j$. The case $z = \delta_1$ is trivial.

Let us show that γ is the unique minimiser of $J_{0,j}$ for $j = 2, \dots, K$. From the definition of $J_{0,j}$ and since J is increasing on $(\delta_1, +\infty)$, we deduce $J_{0,j}(z) \ge J(jz) + c_j J(\delta_1) \ge J_{0,j}(\delta_1)$ for $z \ge \delta_1$. Thus it is enough to consider $z \le \delta_1$ in order to find the minimum. Since $J_{0,j}(z) = J_j(z) + c_j J_1(z) = \psi_j(z)$ for $z \le \delta_1$ it holds

$$J_{0,j}(z) = \psi_j(z) = \frac{k_1}{z^{12}}\left(\frac{1}{j^{12}} + c_j\right) - \frac{k_2}{z^6}\left(\frac{1}{j^6} + c_j\right)$$

for $z \le \delta_1$. This is again a Lennard-Jones potential, thus it has only one critical point which is a minimum. Since c_j is defined such that $J_j'(\gamma) + c_j J_1'(\gamma) = 0$, we deduce that γ is the unique minimiser of $J_{0,j}$ and ψ_j for $j \in \{2, \dots, K\}$. Hence, we have shown (LJ4), where we set $\gamma^c = \delta_1 > \gamma$. Since ψ_j is a Lennard-Jones potential with minimiser γ, we obtain that $\psi_j'' > 0$ on $(0, (\frac{13}{7})^{\frac{1}{6}}\gamma)$. Hence, $\psi_j''(\gamma) > 0$ for all $j \in \{2, \dots, K\}$.

Let us show (LJ5). Since $\psi_j = J_j + c_j J_1$ is a Lennard-Jones potential with minimiser γ, we have that $\psi_j^{**}(z) = \psi_j(z)$ if $z \le \gamma$ and $\psi_j^{**}(z) = \psi_j(\gamma)$ for $z > \gamma$. Combining $J_{0,j}(z) \le \psi_j(z)$ and $\psi_j^{**}(z) \le J_{0,j}(z)$ for all $z > 0$ yields that $J_{0,j}^{**} \equiv \psi_j^{**}$. It is left to show that $\liminf_{z\to+\infty} J_{0,j}(z) > J_{0,j}(\gamma)$ for $j \in \{2, \dots, K\}$. Let (z_n) be such that $\lim_{n\to\infty} z_n = +\infty$ and

$$\liminf_{z\to+\infty} J_{0,j}(z) = \lim_{n\to\infty} J_{0,j}(z_n).$$

By the definition of $J_{0,j}$ there exists for every $\eta > 0$ and $n \in \mathbb{N}$ a tupel z_n^s with $s \in \{1, \dots, j\}$ such that

$$J_{0,j}(z_n) \ge J_j(z_n) + \frac{c_j}{j}\sum_{s=1}^j J_1(z_n^s) - \eta \quad \text{with} \quad \sum_{s=1}^j z_n^s = jz_n.$$

From $z_n \to \infty$, we deduce that, up to subsequences, there exists $s \in \{1, \dots, j\}$ such that $z_n^s \to +\infty$ as $n \to \infty$. Without loss of generality we assume that $s = 1$ and from $\lim_{z\to\infty} J(z) = 0$, we deduce

$$\liminf_{n\to\infty} J_{0,j}(z_n) \geq \frac{c_j}{j} \liminf_{n\to\infty} \sum_{s=2}^{j} J_1(z_n^s) - \eta \geq c_j \frac{j-1}{j} J_1(\delta_1) - \eta.$$

Since $J_j(\delta_1) < 0$ for $j = 1, \dots, K$ the assertion follows by choosing $\eta = -\frac{1}{2} J_j(\delta_1)$ and

$$\begin{aligned} c_j \frac{j-1}{j} J_1(\delta_1) - \eta >& c_j \frac{j-1}{j} J_1(\delta_1) - \eta + \frac{1}{2} J_j(\delta_1) + \frac{c_j}{j} J_1(\delta_1) \\ =& J_j(\delta_1) + c_j J_1(\delta_1) > \psi_j(\gamma), \end{aligned}$$

and since $\psi_j(\gamma) = J_{0,j}(\gamma)$, the assertion is proven. □

Remark 3.3. A further example of an interatomic interaction potential is the so-called Morse potential[44], given by

$$J_j(z) = J(jz) \quad \text{with} \quad J(z) = k_1 \left(1 - e^{-k_2(z-\delta_1)}\right)^2 - k_1 \quad \text{for } z \in \mathbb{R} \tag{3.24}$$

and $k_1, k_2, \delta_1 > 0$. The definition of J implies $\min_{\mathbb{R}} J = -k_1$, $\arg\min_z J(z) = \{\delta_1\}$ and the potential J has the same convex/concave shape as the Lennard-Jones potential. It is straightforward to check that $J_1, \dots, J_K$ given in (3.24) satisfy (LJ1) and (LJ2). Using the convex/concave shape of J and similar arguments as in the proof of Proposition 3.2, we can show that the crucial assumption (3.13) holds true for all $z \leq \delta_1$. Moreover, in the case $K = 2$ the potentials J_1 and J_2 satisfy all assumptions (LJ1)–(LJ5).

Contrary to the Lennard-Jones potential the Morse potential does not satisfy the assumptions (LJ3)–(LJ5) for all choices of parameters $k_1, k_2, \delta_1 > 0$ in the case $K > 2$. To illustrate this, we set δ_1 such that $1 \in \arg\min_z J_{CB}(z)$, where $J_{CB}(z) = \sum_{j=1}^{K} J(jz)$. This implies

$$0 = J_{CB}'(1) = 2k_1k_2 \sum_{j=1}^{K} j \left(e^{-jk_2} - e^{-2jk_2} e^{k_2\delta_1}\right) \Leftrightarrow \delta_1 = \frac{1}{k_2} \ln\left(\frac{\sum_{j=1}^{K} je^{-jk_2}}{\sum_{j=1}^{K} je^{-2jk_2}}\right).$$

Next, we derive a necessary condition for (LJ3)–(LJ5) to hold. Assume that $J_1, \dots, J_K$ given in (3.24) with δ_1 as above satisfy (LJ1)–(LJ5). Then it holds $\gamma = 1 < \delta_1$ and thus $J'(1) < 0$ (otherwise $J_{CB}'(1) > 0$). Hence, $c = (c_j)_{j=2}^{K}$ is given by (3.21) and $c_2 > 0$ implies $J_2'(\gamma) = 2J'(2) > 0$, i.e. $\delta_1 < 2$. This yields a nontrivial condition on k_2. Indeed, we have in the case $K = 3$:

$$\delta_1 = \frac{1}{k_2} \ln\left(\frac{e^{-k_2} + 2e^{-2k_2} + 3e^{-3k_2}}{e^{-2k_2} + 2e^{-4k_2} + 3e^{-6k_2}}\right) = 2 + \frac{1}{k_2} \ln\left(\frac{e^{-k_2} + 2e^{-2k_2} + 3e^{-3k_2}}{1 + 2e^{-2k_2} + 3e^{-4k_2}}\right).$$

Hence, $\delta_1 < 2$ is equivalent to

$$e^{-k_2} + 3e^{-3k_2} < 1 + 3e^{-4k_2} \;\Leftrightarrow\; 0 < e^{4k_2} - e^{3k_2} + 3 - 3e^{k_2} \;\Leftrightarrow\; 0 < (e^{3k_2} - 3)(e^{k_2} - 1)$$

which yields $k_2 > \frac{\ln 3}{3}$ as a necessary condition for (LJ3)–(LJ5) to hold in the case $K = 3$. Note that the condition $\delta_1 < 2$ is ensured by $k_2 > \ln(\frac{2}{3-\sqrt{5}})$ for all $K \geq 2$. Indeed,

$$\begin{aligned}\delta_1 =& \frac{1}{k_2} \ln\left(\frac{\sum_{j=1}^K je^{-jk_2}}{\sum_{j=1}^K je^{-2jk_2}}\right) \leq \frac{1}{k_2} \ln\left(\frac{\sum_{j=1}^\infty je^{-jk_2}}{e^{-2k_2}}\right) = 2 + \frac{1}{k_2}\ln\sum_{j=1}^\infty j\left(e^{-k_2}\right)^j \\ <& 2 + \frac{1}{k_2}\ln\sum_{j=1}^\infty j\left(\frac{3-\sqrt{5}}{2}\right)^j = 2.\end{aligned}$$

For the last equality, we used $\sum_{j=1}^\infty jq^j = \frac{q}{(1-q)^2}$ if $|q| < 1$ (variant of geometric series) and that $q = \frac{3-\sqrt{5}}{2}$ satisfies $\frac{q}{(1-q)^2} = 1$.

3.2 Γ-limit of zeroth order

In this section, we give a description of the (zero-order) Γ-limits of the sequences (H_n) and (H_n^ℓ), see (3.2) and (3.4). In [14], Braides and Gelli provide a Γ-limit result for functionals of the form (3.2) under very general assumptions on the interaction potentials J_j. In Theorem 3.5, we refine their statement in the particular case of Lennard-Jones type potentials, that is (LJ1)–(LJ5) holds true. In the spirit of [50, Theorem 3.1], the result by Braides and Gelli can be extended to the sequence (H_n^ℓ). However, we give in Theorem 3.7 a self contained proof of this result which makes use of the specific structure of the interaction potentials.

3.2.1 Γ-limit of H_n

The following result is a direct consequence of [14, Theorem 3.2].

Theorem 3.4. *Let $J_j : \mathbb{R} \to (-\infty, +\infty]$ be Borel functions bounded from below and satisfy* (3.9)*. Assume there exist a convex function $\Psi : \mathbb{R} \to [0, +\infty]$ and constants $d^1, d^2 > 0$ such that* (3.10) *and* (3.11) *hold true. Then the Γ-limit of the sequence (H_n) with respect to the $L^1_{\mathrm{loc}}(0,1)$-topology is given by the functional H defined by*

$$H(u) = \begin{cases} \displaystyle\int_0^1 \overline{\phi}(u'(x))dx & \text{if } u \in BV_{\mathrm{loc}}(0,1),\ D^s u \geq 0 \text{ in } (0,1), \\ +\infty & \text{else on } L^1(0,1), \end{cases}$$

where $D^s u$ denotes the singular part of the measure Du with respect to the Lebesgue measure and the function $\overline{\phi}$ is defined as $\overline{\phi}(z) = \inf\{\phi(z_1) + g(z_2) : z_1 + z_2 = z\}$, where

$g(z) = 0$ *for* $z \geq 0$ *and* $g(z) = +\infty$ *for* $z < 0$*, and* $\phi = \Gamma\text{-}\lim_{N\to\infty} \phi_N^{**}$ *with*

$$\phi_N(z) = \min \left\{ \frac{1}{N} \sum_{j=1}^{K} \sum_{i=0}^{N-j} J_j \left(\frac{u^{i+j} - u^i}{j} \right) : \ u : \mathbb{N}_0 \to \mathbb{R}, \right.$$
$$\left. u^i = zi \ \text{if}\ i \in \{0, \dots, K\} \cup \{N-K, \dots, N\} \right\}. \tag{3.25}$$

Next, we show that $\overline{\phi}$ can be solved explicitly for potentials J_j which satisfy the assumptions (LJ1)–(LJ5), which includes in particular the Lennard-Jones potentials, cf. Proposition 3.2.

Theorem 3.5. *Let* J_j*,* $j = 1, \dots, K$ *satisfy the assumptions (LJ1)–(LJ5). Then it holds*

$$\overline{\phi} \equiv \phi \equiv J_{CB}^{**}$$

with $\overline{\phi}$ *and* ϕ *as in Theorem 3.4 and* J_{CB} *as in* (3.17)*.*

Proof. Let us first show that $\phi \equiv J_{CB}^{**}$. We begin with proving the lower bound of the Γ-limit, i.e., we show that for every sequence $(z_N) \subset \mathbb{R}$ such that $z_N \to z$ it holds $\liminf_{N\to\infty} \phi_N^{**}(z_N) \geq J_{CB}^{**}(z)$. By a similar calculation as in (3.7), combined with the definition of $J_{0,j}$, (3.15) and setting $C = J_1(\delta_1) \sum_{j=2}^{K} c_j(j-1)$, we obtain

$$\begin{aligned}
&\frac{1}{N} \sum_{j=1}^{K} \sum_{i=0}^{N-j} J_j \left(\frac{u^{i+j} - u^i}{j} \right) \\
&\geq \frac{1}{N} \sum_{j=2}^{K} \sum_{i=0}^{N-j} \left\{ J_j \left(\frac{u^{i+j} - u^i}{j} \right) + \frac{c_j}{j} \sum_{s=i}^{i+j-1} J_1(u^{s+1} - u^s) \right\} + \frac{C}{N} \\
&\geq \frac{1}{N} \sum_{j=2}^{K} \sum_{i=0}^{N-j} J_{0,j}^{**} \left(\frac{u^{i+j} - u^i}{j} \right) + \frac{C}{N} \\
&\geq \sum_{j=2}^{K} \frac{N-j+1}{N} \sum_{i=0}^{N-j} \frac{1}{N-j+1} \psi_j^{**} \left(\frac{u^{i+j} - u^i}{j} \right) + \frac{C}{N} \\
&\geq \sum_{j=2}^{K} \frac{N-j+1}{N} \psi_j^{**} \left(\sum_{i=0}^{N-j} \frac{u^{i+j} - u^i}{j(N-j+1)} \right) + \frac{C}{N} \\
&\geq \sum_{j=2}^{K} \left(1 - \frac{j-1}{N} \right) \psi_j^{**}(z) + \frac{C}{N}.
\end{aligned}$$

In the last inequality, we have used $u^i = iz$ for $i \in \{0, \dots, K\} \cup \{N-K, \dots, N\}$ and

$$\begin{aligned}\sum_{i=0}^{N-j}(u^{i+j}-u^i) &= \sum_{i=0}^{N-j}\sum_{s=0}^{j-1}(u^{i+1+s}-u^{i+s}) = \sum_{s=0}^{j-1}\sum_{i=s}^{N-j+s}(u^{i+1}-u^i)\\ &= j\sum_{i=0}^{N-1}(u^{i+1}-u^i) - \sum_{s=0}^{j-1}\left\{\sum_{i=0}^{s-1}(u^{i+1}-u^i) + \sum_{i=N-j+s+1}^{N-1}(u^{i+1}-u^i)\right\}\\ &= j(N-(j-1))z,\end{aligned}$$

for $j \in \{2, \dots, K\}$. Hence, we have $\phi_N(z) \geq \sum_{j=2}^K (1-\frac{j-1}{N})\psi_j^{**}(z) + \frac{C}{N}$. Since the right-hand side is convex and lower semicontinuous, we have $\phi_N^{**}(z) \geq \sum_{j=2}^K (1-\frac{j-1}{N})\psi_j^{**}(z) + \frac{C}{N}$. The lower bound follows from the lower semicontinuity of ψ_j^{**} and $\sum_{j=2}^K \psi_j^{**} \equiv J_{CB}^{**}$, see (3.18).

Let us now show the upper bound. In the case $z \leq \gamma$, we have by (3.18) that $J_{CB}^{**}(z) = J_{CB}(z)$. Hence, testing the minimum problem in the definition of ϕ_N, see (3.25), with $u_N = (iz)_{i=0}^N$ yields

$$\begin{aligned}\phi_N^{**}(z) \leq& \phi_N(z) \leq \frac{1}{N}\sum_{j=1}^K\sum_{i=0}^{N-j} J_j(z) = J_{CB}(z) - \frac{1}{N}\sum_{j=2}^K (j-1)J_j(z)\\ =& J_{CB}^{**}(z) - \frac{1}{N}\sum_{j=2}^K (j-1)J_j(z).\end{aligned}$$

Since $\operatorname{dom} J_j = \operatorname{dom} J_1$ for $j \in \{2, \dots, K\}$, this implies the limsup inequality in this case. If $z > \gamma$, we can test the minimum problem in the definition of ϕ_N with u_N satisfying the boundary conditions in (3.25) and being such that $u_N^i = Kz + \gamma(i-K)$ for all $i = K, \dots, N-K-1$. This yields

$$\begin{aligned}\phi_N^{**}(z) \leq& \phi_N(z) \leq \frac{1}{N}\sum_{j=1}^K\sum_{i=K}^{N-K-1-j} J_j(\gamma) + \frac{1}{N}f(z)\\ =& J_{CB}(\gamma) + \frac{1}{N}\left(f(z) - \sum_{j=1}^K (2K+j)J_j(\gamma)\right),\end{aligned}$$

where $f(z)$ is continuous on $\operatorname{dom} J_{CB}$. Hence, the upper bound follows also for $z > \gamma$ and we have $\phi \equiv J_{CB}^{**}$.

It is left to show $\overline{\phi} \equiv J_{CB}^{**}$. Assume on the contrary that there exists $z \in \mathbb{R}$ such that $\overline{\phi}(z) < J_{CB}^{**}(z)$. By the definition of $\overline{\phi}$ and g this implies that there exists $z_1 < z$ such that $J_{CB}^{**}(z_1) < J_{CB}^{**}(z)$. Since $J_{CB}^{**}(x) \geq J_{CB}(\gamma)$ for all $x \in \mathbb{R}$ and $J_{CB}^{**}(x) = J_{CB}(\gamma)$ for $x \geq \gamma$ it must hold $z < \gamma$ and $J_{CB}^{**}(z) > J_{CB}(\gamma)$. Combining $z_1 < z < \gamma$ and $J_{CB}^{**}(\gamma) \leq J_{CB}^{**}(z_1) < J_{CB}^{**}(z)$ yields a contradiction to the convexity of J_{CB}^{**}. □

Remark 3.6. Let us consider the case of Lennard-Jones potentials given by (3.22). For a given C^∞-diffeomorphism u defined on $(0,1)$, the pointwise limit of $(H_n(u))_n$, in the spirit of [6, Theorem 1], is given by

$$H_p(u) = \int_0^1 J_{CB}(u'(x))dx.$$

By standard relaxation arguments, it can be shown that the minimisation problems corresponding to H respectively H_p enjoy the same properties, see also [7, p. 413].

3.2.2 Γ-limit of H_n^ℓ

Let us now study the Γ-limit of the sequence (H_n^ℓ) which takes the boundary conditions (3.3) into account. As mentioned above, we could make use of the convergence result regarding (H_n), see [11, 50]. However, we present here an explicit proof of the corresponding statement, which in particular make no use of the homogenisation formula given in (3.25).

Theorem 3.7. *Suppose that the hypotheses (LJ1)–(LJ5) hold. Let $\ell > 0$ and $u_0^{(1)}$, $u_1^{(1)} \in \mathbb{R}_+^{K-1}$. Then the Γ-limit of (H_n^ℓ) with respect to the $L^1(0,1)$-topology is given by*

$$H^\ell(u) = \begin{cases} \displaystyle\int_0^1 J_{CB}^{**}(u'(x))dx & \text{if } u \in BV^\ell(0,1),\ D^s u \geq 0 \text{ in } [0,1]\ , \\ +\infty & \text{else on } L^1(0,1). \end{cases} \tag{3.26}$$

Moreover, the minimum values of H_n^ℓ and H^ℓ satisfy

$$\lim_{n\to\infty} \inf_u H_n^\ell(u) = \min_u H^\ell(u) = J_{CB}^{**}(\ell). \tag{3.27}$$

Proof. Compactness. Let $(u_n) \subset L^1(0,1)$ be such that $\sup_n H_n^\ell(u_n) < +\infty$. In particular this implies $u_n \in \mathcal{A}_n(0,1)$. Let us show that $\|(u_n')^-\|_{L^1(0,1)}$ is equibounded, where $(u_n')^- := -(u_n' \wedge 0)$. Since J_j is bounded from below for $j \in \{1,\dots,K\}$, we deduce from the equiboundedness of the energy, (3.11) and Jensen's inequality that

$$C \geq \sum_{i:u_n^{i+1}<u_n^i} \lambda_n J_1\left(\frac{u_n^{i+1}-u_n^i}{\lambda_n}\right) \geq d_1 \Psi\left(\int_{\{u_n'<0\}} u_n' dx\right) - d_1,$$

for some $C > 0$ independent of n. By (3.10), we have that $\int_{\{u_n'<0\}} |u_n'| dx \leq C'$ for some constant $C' > 0$ independent of n. Moreover, by using the boundary conditions $u_n(0) = 0$ and $u_n(1) = \ell$, we obtain

$$\int_{\{u_n' \geq 0\}} u_n' dx = \ell - \int_{\{u_n'<0\}} u_n' dx \leq \ell + C'.$$

Since $u_n(0) = 0$, we obtain by the Poincaré-inequality that $\|u_n\|_{W^{1,1}(0,1)}$ is equibounded. Thus, we can extract a subsequence, not relabelled, which weakly* converges in $BV(0,1)$

to some $u \in BV(0,1)$, see Theorem 2.6. Note that in particular this implies $u_n \to u$ in $L^1(0,1)$. It remains to verify that $u \in BV^\ell(0,1)$. This can be done as in [50, Theorem 3.1]: since $u_n(0) = 0$ and $u_n(1) = \ell$ for all n, we can define the function $\tilde{u}_n \in W^{1,\infty}(\mathbb{R})$ as

$$\tilde{u}_n(x) = \begin{cases} 0 & \text{if } x \leq 0, \\ u_n(x) & \text{if } x \in (0,1), \\ \ell & \text{if } x \geq 1. \end{cases} \tag{3.28}$$

Then we have that $\tilde{u}_n$ weakly* converges in $BV(-1,3)$ to the extension $\tilde{u}$ of u and from this we deduce that

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

Liminf inequality. Let $u \in L^1(0,1)$ and (u_n) be a sequence such that $u_n \to u$ in $L^1(0,1)$. We have to show

$$\liminf_{n \to \infty} H_n^\ell(u_n) \geq H^\ell(u).$$

Hence, it is not restrictive to assume that $\lim_{n\to\infty} H_n^\ell(u_n)$ exists in $\mathbb{R}$. By the compactness property, we have $u \in BV^\ell(0,1)$ and $u_n \overset{*}{\rightharpoonup} u$ weakly* in $BV(0,1)$. By (3.7), the definition of $J_{0,j}$ (see (3.8)) and (3.15), we obtain

$$\begin{aligned} H_n^\ell(u_n) &\geq \sum_{j=2}^K \sum_{i=0}^{n-j} \lambda_n \left\{ J_j\left(\frac{u_n^{i+j} - u_n^i}{j\lambda_n}\right) + \frac{c_j}{j} \sum_{s=i}^{i+j-1} J_1\left(\frac{u_n^{s+1} - u_n^s}{\lambda_n}\right)\right\} + C\lambda_n \\ &\geq \sum_{j=2}^K \sum_{i=0}^{n-j} \lambda_n J_{0,j}^{**}\left(\frac{u_n^{i+j} - u_n^i}{j\lambda_n}\right) + C\lambda_n \\ &= \sum_{j=2}^K \frac{1}{j} \sum_{s=0}^{j-1} \sum_{i \in R_{n,j}^s([0,1])} j\lambda_n \psi_j^{**}\left(\frac{u_n^{i+j} - u_n^i}{j\lambda_n}\right) + C\lambda_n \end{aligned} \tag{3.29}$$

where $C = \sum_{j=2}^K c_j(j-1)J_1(\delta_1)$ and

$$R_{n,j}^s([0,1]) = \{i \in s + j\mathbb{Z},\ (i, i+j)\lambda_n \subset [0,1]\}. \tag{3.30}$$

With a slight abuse of notation, we identify in the following u_n with the extension $\tilde{u}_n \in W^{1,\infty}(\mathbb{R})$ defined in (3.28). For given $j \in \{2,\dots,K\}$ and $s \in \{0,\dots,j-1\}$, we define the functions $u_{n,j}^s \in W^{1,\infty}(\mathbb{R})$ as the affine interpolations of u_n with respect to $\lambda_n(s + j\mathbb{Z})$, i.e.

$$u_{n,j}^s(x) = u_n^{s+ji} + \frac{x - (s+ji)\lambda_n}{j\lambda_n}(u_n^{s+j(i+1)} - u_n^{s+ji}), \tag{3.31}$$

for $x \in \lambda_n[s + ji, s + j(i+1))$ with $i \in \mathbb{Z}$.

Fix $j \in \{2,\dots,K\}$ and $s \in \{0,\dots,j-1\}$. Let us show that $u_{n,j}^s \overset{*}{\rightharpoonup} u$ weakly* in $BV(0,1)$. Since $u_n \to u$ in $L^1(0,1)$, it is sufficient to prove that $\sup_n \|{u_{n,j}^s}'\|_{W^{1,1}(0,1)} < +\infty$

and $\lim_{n\to\infty}\|u_n - u^s_{n,j}\|_{L^1(0,1)} = 0$, see Proposition 2.5. Fix $\eta > 0$. For n sufficiently large, we have that

$$\begin{aligned}
\|{u^s_{n,j}}'\|_{L^1(-\eta,1+\eta)} &\leq \sum_{i\in\{s+j\mathbb{Z}\}\cap\lambda_n^{-1}(-2\eta,1+2\eta)} j\lambda_n\left|\frac{u_n^{i+j}-u_n^i}{j\lambda_n}\right| \\
&\leq \sum_{i\in\{s+j\mathbb{Z}\}\cap\lambda_n^{-1}(-2\eta,1+2\eta)} \lambda_n \sum_{s=i}^{i+j-1}\left|\frac{u_n^{s+1}-u_n^s}{\lambda_n}\right| \leq \|u_n'\|_{L^1(0,1)}.
\end{aligned} \tag{3.32}$$

Note that we used for the last inequality that $u_n^{i+1} - u_n^i = 0$ for $i \notin \{0,\dots,n-1\}$. From the compactness proof, we deduce $\sup_n \|u_n'\|_{L^1(0,1)} < +\infty$ and thus that the right-hand side above is equibounded. Hence, we have $\sup_n \|{u^s_{n,j}}'\|_{L^1(-\eta,1+\eta)} < +\infty$. From $u_n(x) = 0$ for $x \leq 0$ and the definition of $u^s_{n,j}$, we obtain that $u^s_{n,j}(-\frac{\eta}{2}) = 0$ for n sufficiently large. Hence, the Poincaré-inequality yields that $\sup_n \|u^s_{n,j}\|_{W^{1,1}(-\eta,1+\eta)} < +\infty$. Let us now estimate $\|u_n - u^s_{n,j}\|_{L^1(0,1)}$. By using $u_n(i\lambda_n) = u^s_{n,j}(i\lambda_n)$ for $i \in \{s + j\mathbb{Z}\}$, we obtain

$$\begin{aligned}
&\int_0^1 |u^s_{n,j} - u_n|dx \\
&\leq \sum_{i\in\{s+j\mathbb{Z}\}\cap\lambda_n^{-1}(-\eta,1+\eta)} \int_{i\lambda_n}^{(i+j)\lambda_n}\left|u_n^i + \int_{i\lambda_n}^x {u^s_{n,j}}'(t)dt - \left(u_n^i + \int_{i\lambda_n}^x u_n'(t)dt\right)\right| dx \\
&\leq \sum_{i\in\{s+j\mathbb{Z}\}\cap\lambda_n^{-1}(-\eta,1+\eta)} \int_{i\lambda_n}^{(i+j)\lambda_n}\left|\int_{i\lambda_n}^x {u^s_{n,j}}'(t)dt - \int_{i\lambda_n}^x u_n'(t)dt\right| dx \\
&\leq \sum_{i\in\{s+j\mathbb{Z}\}\cap\lambda_n^{-1}(-\eta,1+\eta)} \int_{i\lambda_n}^{(i+j)\lambda_n}\left(\int_{i\lambda_n}^{(i+j)\lambda_n} \left|{u^s_{n,j}}'(t)\right| + |u_n'(t)|dt\right) dx \\
&\leq \sum_{i\in\{s+j\mathbb{Z}\}\cap\lambda_n^{-1}(-\eta,1+\eta)} j\lambda_n\left(\int_{i\lambda_n}^{(i+j)\lambda_n} \left|{u^s_{n,j}}'(t)\right| + |u_n'(t)|dt\right) \\
&\leq 2j\lambda_n\int_{-\eta}^{1+2\eta} |u_n'|dx \to 0
\end{aligned} \tag{3.33}$$

as $n \to \infty$. Altogether, we have for $j \in \{2,\dots,K\}$ and $s \in \{0,\dots,j-1\}$ that $u^s_{n,j} \overset{*}{\rightharpoonup} u$ weakly* in $BV(0,1)$.

Fix $j \in \{2,\dots,K\}$ and $s \in \{0,\dots,j-1\}$. By the definition of $u^s_{n,j}$ and $\max\{i : i \in R^s_{n,j}([0,1])\} = \lfloor\frac{n-s-j}{j}\rfloor$, we have

$$\sum_{i\in R^s_{n,j}([0,1])} j\lambda_n\psi_j^{**}\left(\frac{u_n^{i+j}-u_n^i}{j\lambda_n}\right) \geq \int_s^{\lambda_n\lfloor\frac{n-s}{j}\rfloor} \psi_j^{**}\left({u^s_{n,j}}'(x)\right)dx.$$

For every $\frac{1}{2} > \rho > 0$ there exists an $N \in \mathbb{N}$ such that $\lambda_n s < \rho < 1 - \rho < \lambda_n \lfloor \frac{n-s}{j} \rfloor$ for all $n \geq N$. Since γ is the unique minimiser of ψ_j and $\psi_j(\gamma) < 0$, we have

$$\int_{s\lambda_n}^{\lambda_n \lfloor \frac{n-s}{j} \rfloor} \psi_j^{**}\left({u_{n,j}^s}'(x)\right) dx \geq \int_{\rho}^{1-\rho} \psi_j^{**}\left({u_{n,j}^s}'(x)\right) dx + 2\rho\psi_j(\gamma).$$

Since ψ_j^{**} satisfies the assumptions on f in Proposition 2.15 and $u_{n,j}^s$ converges weakly* to u in $BV(\rho, 1-\rho)$, we obtain that

$$\begin{aligned}\liminf_{n\to\infty} \sum_{i\in R_{n,j}^s([0,1])} j\lambda_n \psi_j^{**}\left(\frac{u_n^{i+j} - u_n^i}{j\lambda_n}\right) &\geq \liminf_{n\to\infty} \int_{\rho}^{1-\rho} \psi_j^{**}({u_{n,j}^s}'(x))dx + 2\rho\psi_j(\gamma) \\ &\geq \int_{\rho}^{1-\rho} \psi_j^{**}(u'(x))dx + 2\rho\psi_j(\gamma)\end{aligned}$$

and $D^s u \geq 0$ in $(\rho, 1-\rho)$. By taking the limit $\rho \to 0$, we obtain that $D^s u \geq 0$ in $(0,1)$ and

$$\liminf_{n\to\infty} \sum_{i\in R_{n,j}^s([0,1])} j\lambda_n \psi_j^{**}\left(\frac{u_n^{i+j} - u_n^i}{j\lambda_n}\right) \geq \int_0^1 \psi_j^{**}(u'(x))dx.$$

Altogether, we obtain by (3.29) that

$$\begin{aligned}\liminf_{n\to\infty} H_n^{\ell}(u_n) &\geq \sum_{j=2}^{K} \frac{1}{j} \sum_{s=0}^{j-1} \liminf_{n\to\infty} \sum_{i\in R_{n,j}^s([0,1])} j\lambda_n \psi_j^{**}\left(\frac{u_n^{i+j} - u_n^i}{j\lambda_n}\right) \\ &\geq \sum_{j=2}^{K} \frac{1}{j} \sum_{s=0}^{j-1} \int_0^1 \psi_j^{**}(u'(x))dx \\ &= \int_0^1 \sum_{j=2}^{K} \psi_j^{**}(u'(x))dx = \int_0^1 J_{CB}^{**}(u'(x))dx\end{aligned}$$

and the constraint $D^s u \geq 0$ in $(0,1)$. It is left to show that $D^s u \geq 0$ in $[0,1]$. For this, we argue as in [12, Theorem 4.2]. We set $I = (-1,2)$ and $\mathcal{A}_n(I) = \{u \in C(I) : u \text{ is affine on } (i, i+1)\lambda_n,\ i \in \{-n, \dots, 2n-1\}\}$. Moreover, we define the functional $H_n(u, I) : L^1(I) \to (-\infty, +\infty]$ as

$$H_n(u, I) = \begin{cases} \displaystyle\sum_{i=-n}^{2n-1} J_1\left(\frac{u^{i+1} - u^i}{\lambda_n}\right) & \text{if } u \in \mathcal{A}_n(I), \\ +\infty & \text{else.} \end{cases}$$

From [13, Theorem 3.7], we deduce that $(H_n(\cdot, I))_n$ Γ-converges to $H(\cdot, I)$ with respect to the $L^1_{\mathrm{loc}}(I)$-convergence, where

$$H(u, I) := \begin{cases} \displaystyle\int_I J_1^{**}(u'(x))dx & \text{if } u \in BV_{\mathrm{loc}}(0,1),\ D^s u \geq 0 \text{ in } I, \\ +\infty & \text{otherwise.} \end{cases}$$

For a sequence $(u_n) \subset L^1(0,1)$ satisfying $\sup_n H_n^\ell(u_n) < +\infty$ and $u_n \to u$ in $L^1(0,1)$, we define the auxiliary functions

$$v_n(x) = \begin{cases} u_n(x) & \text{for } x \in [0,1], \\ \ell x & \text{for } x \in \mathbb{R} \setminus (0,1), \end{cases} \qquad v(x) = \begin{cases} u(x) & \text{for } x \in [0,1], \\ \ell x & \text{for } x \in \mathbb{R} \setminus (0,1). \end{cases}$$

Using $v_n \to v$ in $L^1_{\mathrm{loc}}(\mathbb{R})$, $J_j \geq J_j(\delta_j)$ (see (LJ2)) and $v_n' = \ell$ on $(-1,0) \cup (1,2)$, we obtain

$$\begin{aligned} &\liminf_{n\to\infty} H_n^\ell(u_n) + 2J_1(\ell) \\ &\quad \geq \liminf_{n\to\infty} \sum_{i=-n}^{2n-1} \lambda_n J_1\left(\frac{v_n^{i+1} - v_n^i}{\lambda_n}\right) + \liminf_{n\to\infty} \sum_{j=2}^{K} \sum_{i=0}^{n-j} \lambda_n J_j(\delta_j) \\ &\quad \geq \liminf_{n\to\infty} H_n(v_n, I) + \sum_{j=2}^{K} J_j(\delta_j) \geq H(v, I) + \sum_{j=2}^{K} J_j(\delta_j). \end{aligned}$$

Since the left-hand side above is equibounded, we deduce that $D^s v \geq 0$ in $I = (-1,2)$. Since $D^s u$ is the restriction of $D^s v$ to $[0,1]$ it follows that $D^s u \geq 0$ in $[0,1]$. This finishes the proof of the liminf inequality.

Limsup inequality. It remains to show that for every $u \in BV^\ell(0,1)$ with $D^s u \geq 0$ there exists a sequence (u_n) such that $u_n \to u$ in $L^1(0,1)$ and $\limsup_{n\to\infty} H_n^\ell(u_n) \leq H^\ell(u)$. Firstly, we do not take boundary conditions into account and show that

$$\Gamma\text{-}\limsup_{n\to\infty} H_n(u) \leq H(u). \tag{3.34}$$

where H_n is defined in (3.2) and the functional $H : L^1(0,1) \to \mathbb{R} \cup \{+\infty\}$ is defined by

$$H(u) := \begin{cases} \displaystyle\int_0^1 J_{CB}^{**}(u'(x))dx & \text{if } u \in BV(0,1),\ D^s u \geq 0, \\ +\infty & \text{else.} \end{cases}$$

By Proposition 2.15 it is sufficient to show (3.34) for $u \in W^{1,1}(0,1)$.

Let u be such that $u(x) = zx + w$ with $z \leq \gamma$. Then $u \in \mathcal{A}_n(0,1)$ for every $n \in \mathbb{N}$ and it holds

$$H_n(u) = \sum_{j=1}^{K} \sum_{i=0}^{n-j} \lambda_n J_j\left(\frac{u^{i+j} - u^i}{j\lambda_n}\right) = \sum_{j=1}^{K} (n-j+1)\lambda_n J_j(z) \to J_{CB}(z),$$

as $n \to \infty$. Let us now consider u such that $u(x) = zx + w$ with $z > \gamma$. Since $J_{CB}^{**}(z) = J_{CB}(\gamma)$ for all $z > \gamma$, we have to construct a sequence u_n converging to u such that $u_n' \to \gamma$ in measure in $(0,1)$. Let $(N_n) \subset \mathbb{N}$ be such that

$$\lim_{n\to\infty} N_n = +\infty \quad \text{and} \quad \lim_{n\to\infty} \lambda_n N_n \to 0. \tag{3.35}$$

Furthermore, we define the sequence $(r_n) \subset \mathbb{N}$ given by

$$r_n := \sup\{r \in \mathbb{N} : \; rN_n \leq n\}.$$

Clearly, the definition of r_n and N_n yields $\lim_{n\to\infty} \lambda_n r_n N_n = 1$. Set $t_n^i = iN_n$ for $i \in \{0, \dots, r_n - 1\}$ and $t_n^{r_n} = n$. Define $u_n \in \mathcal{A}_n(0,1)$ such that $u_n(x) = u(x)$ for $x \in [\lambda_n t_n^{r_n - 1}, 1]$ and

$$u_n(x) = u(\lambda_n t_n^i) + \gamma(x - \lambda_n t_n^i) \quad \text{for } x \in [t_n^i, t_n^{i+1} - 1]\lambda_n \text{ and } i \in \{0, \dots, r_n - 2\}.$$

By the definition of u_n and u, we have $\|u_n - u\|_{L^\infty(0,1)} \leq \lambda_n N_n |z - \gamma|$ and thus $u_n \to u$ in $L^1(0,1)$. From the definition of u_n, (3.35) and $\lim_n \lambda_n r_n N_n = 1$, we deduce

$$\begin{aligned}
\sum_{j=1}^{K} \sum_{i=0}^{n-j} \lambda_n J_j \left(\frac{u_n^{i+j} - u_n^i}{j\lambda_n} \right) =& \sum_{j=1}^{K} \sum_{m=0}^{r_n - 2} \sum_{i=t_n^m}^{t_n^{m+1}-1} \lambda_n J_j(\gamma) + r(n) \\
=& \sum_{j=1}^{K} N_n(r_n - 1)\lambda_n J_j(\gamma) + r(n) \\
=& J_{CB}(\gamma) + r(n) + o(1),
\end{aligned}$$

where $r(n)$ is defined by

$$r(n) = \sum_{j=2}^{K} \sum_{m=1}^{r_n} \sum_{i=t_n^m - j}^{t_n^m - 1} \lambda_n \left(J_j \left(\frac{u_n^{i+j} - u_n^i}{j\lambda_n} \right) - J_j(\gamma) \right) + \sum_{j=2}^{K} \sum_{i=t_n^{r_n}}^{n-j} \lambda_n J_j \left(\frac{u_n^{i+j} - u_n^i}{j\lambda_n} \right).$$

It is left to show that $r(n)$ tends to zero as n tends to infinity. By construction of u_n it holds $\frac{u_n^{i+1} - u_n^i}{\lambda_n} \geq \gamma$ for all $i \in \{0, \dots, n-1\}$. This implies, using $\gamma > 0$ and (LJ1), that $\sup_n \sum_i J_j \left(\frac{u_n^{i+j} - u_n^i}{j\lambda_n} \right) < +\infty$ for $j \in \{1, \dots, K\}$. Hence, $r(n) = \mathcal{O}(\lambda_n r_n) + \mathcal{O}(\lambda_n N_n) = o(1)$. Indeed, this follows by (3.35) and $0 \leq \lambda_n r_n \leq N_n^{-1} \lambda_n n = N_n^{-1}$.

The above procedure can be applied, up to slight modifications, to any function $u \in C([0,1])$ which is piecewise affine. The statement for $u \in W^{1,1}(0,1)$ follows by usual density and relaxation arguments which we briefly outline in this case: let $u \in W^{1,1}(0,1)$ be such that $H(u) < +\infty$. Let u_N be the piecewise affine interpolation of u with respect to $\frac{1}{N}\mathbb{Z}$ with some $N \in \mathbb{N}$ and set $t_i := \frac{i}{N}$. By Jensen's inequality, we obtain that

$$\begin{aligned} H(u) &= \int_0^1 J_{CB}^{**}(u'(x))dx = \sum_{i=1}^{N} \int_{t_{i-1}}^{t_i} J_{CB}^{**}(u'(x))dx \\ &\geq \sum_{i=1}^{N} \frac{1}{N} J_{CB}^{**}\left(\frac{1}{t_i - t_{i-1}} \int_{t_{i-1}}^{t_i} u'(x)\right) = \int_0^1 J_{CB}^{**}(u_N')dx = H(u_N). \end{aligned}$$

Since $u_N \overset{*}{\rightharpoonup} u$ weakly* in $BV(0,1)$ as $N \to \infty$, the lower semicontinuity of the Γ- $\limsup$ yields

$$\begin{aligned} \Gamma\text{-}\limsup_{n\to\infty} H_n(u) &\leq \liminf_{N\to\infty}\left(\Gamma\text{-}\limsup_{n\to\infty} H_n(u_N)\right) \leq \limsup_{N\to\infty} \int_0^1 J_{CB}^{**}(u_N')dx \\ &\leq \int_0^1 J_{CB}^{**}(u')dx = H(u). \end{aligned}$$

Next, we show that there exists for every $u \in BV^\ell(0,1)$ a sequence (u_n) such that $u_n \to u$ in $L^1(0,1)$ and $\limsup_n H_n^\ell(u_n) \leq H^\ell(u)$. We follow ideas from [12, Theorem 4.2] where the case of nearest neighbour interactions is considered. Let $u \in BV^\ell(0,1)$ be such that $H^\ell(u) < +\infty$, $0 < u(0+)$ and $u(1-) < \ell$. The above arguments provide a sequence (u_n) such that $u_n \to u$ in $L^1(0,1)$ and

$$\limsup_{n\to\infty} \sum_{j=1}^{K} \sum_{i=0}^{n-j} \lambda_n J_j\left(\frac{u_n^{i+j} - u_n^i}{j\lambda_n}\right) \leq \int_0^1 J_{CB}^{**}(u'(x))dx. \tag{3.36}$$

For every $\hat{\varepsilon} > 0$ there exists $0 < \varepsilon < \hat{\varepsilon}$ such that $\varepsilon,\ 1-\varepsilon \notin S_u$, $u_n(\varepsilon) \to u(\varepsilon)$ and $u_n(1-\varepsilon) \to u(1-\varepsilon)$. Indeed, (3.36) is still true if we pass to a subsequence of (u_n) which converges pointwise almost everywhere in $(0,1)$. For $\hat{\varepsilon} > 0$ sufficiently small, we deduce from $0 < u(0+)$ and $u(1-) < \ell$, (3.10) and $D^s u \geq 0$ that $2\varepsilon\gamma < u(\varepsilon)$ and $u(1-\varepsilon) < \ell - 2\varepsilon\gamma$. We define sequences $(h_n^1), (h_n^2) \subset \mathbb{N}$ such that $\varepsilon \in [h_n^1, h_n^1+1)\lambda_n$ and $1-\varepsilon \in (h_n^2-1, h_n^2]\lambda_n$. Let us now define $v_n \in \mathcal{A}_n(0,1)$ by

$$v_n^i = \begin{cases} 0 & \text{if } i = 0, \\ \lambda_n \sum_{s=1}^{i} u_{0,s}^{(1)} & \text{if } 1 \leq i \leq K-1, \\ \lambda_n \sum_{s=1}^{K-1} u_{0,s}^{(1)} + \lambda_n(i-(K-1))\gamma & \text{if } K-1 \leq i < h_n^1, \\ u_n(\varepsilon) - \frac{1}{2}\varepsilon & \text{if } i = h_n^1, \\ u_n^i & \text{if } h_n^1 < i < h_n^2, \\ u_n(1-\varepsilon) + \frac{1}{2}\varepsilon & \text{if } i = h_n^2, \\ \ell - \lambda_n \sum_{s=1}^{K-1} u_{1,s}^{(1)} - \lambda_n(n-K+1-i)\gamma & \text{if } h_n^2 < i \leq n-K+1, \\ \ell - \lambda_n \sum_{s=1}^{n-i} u_{1,s}^{(1)} & \text{if } n-K+1 \leq i \leq n-1, \\ \ell & \text{if } i = n. \end{cases}$$

We observe that v_n satisfies the boundary condition (3.3). Moreover, the sequence (v_n) converges to $u_\varepsilon := u_\gamma \chi_{(0,\varepsilon)} + u\chi_{(\varepsilon,1-\varepsilon)} + (u_\gamma + \ell - \gamma)\chi_{(1-\varepsilon,1)}$ in $L^1(0,1)$, where $u_\gamma(x) = \gamma x$. Let us show that $\limsup_n H_n^\ell(v_n) < +\infty$. Since $u_0^{(1)}, u_1^{(1)} \in \mathbb{R}_+^{K-1}$, $\gamma > 0$, $(0,+\infty) \subset \operatorname{dom} J_j$ and (3.36), it is sufficient to verify that

$$\lim_{n\to\infty} \frac{v_n^{h_n^i+s} - v_n^{h_n^i-1+s}}{\lambda_n} = +\infty \quad \text{for } i \in \{1,2\} \text{ and } s \in \{0,1\}. \tag{3.37}$$

We show (3.37) only for $i = 1$. The case $i = 2$ can be done in a similar way. Using $u_n(\varepsilon) \to u(\varepsilon) \geq 2\varepsilon\gamma$ as $n \to \infty$, we obtain that

$$v_n^{h_n^1} - v_n^{h_n-1} = u_n(\varepsilon) - \frac{1}{2}\varepsilon - h_n^1\lambda_n\gamma + \mathcal{O}(\lambda_n) \geq \frac{1}{2}\varepsilon\gamma + \mathcal{O}(\lambda_n) + o(1)$$

as $n \to \infty$. Moreover, we have, using $u_n(\varepsilon) = u_n^{h_n} + \frac{\varepsilon - h_n\lambda_n}{\lambda_n}(u_n^{h_n^1+1} - u_n^{h_n^1})$, that

$$v_n^{h_n^1+1} - v_n^{h_n} = (u_n^{h_n^1+1} - u_n^{h_n^1})\left(1 - \frac{\varepsilon - \lambda_n h_n^1}{\lambda_n}\right) + \frac{\varepsilon}{4} \geq \frac{\varepsilon}{4} + o(1)$$

as $n \to \infty$. For the last inequality, we used (3.36) and the superlinear growth of J_1 at $-\infty$. More precisely: assume there exists $c > 0$ such that $u_n^{h_n^1+1} - u_n^{h_n} \leq -c$ for all n sufficiently large. From (3.10) and (3.11), we deduce

$$\lambda_n J_1\left(\frac{u_n^{h_n+1} - u_n^{h_n}}{\lambda_n}\right) \geq d_1 c \inf_{z \leq -c} \frac{1}{n|z|}\Psi(nz) + \mathcal{O}(\lambda_n) \to +\infty \quad \text{as } n \to \infty.$$

This is a contradiction to (3.36) and $H^\ell(u) < +\infty$. Altogether, we have shown (3.37) for $i = 1$. Combining the fact that u_n satisfies (3.36) and the definition of v_n implies

$$\limsup_{n\to\infty} H_n^\ell(v_n) \leq \int_\varepsilon^{1-\varepsilon} J_{CB}^{**}(u'(x))dx + 2\varepsilon J_{CB}(\gamma) = H^\ell(u_\varepsilon).$$

We can apply the above arguments to a sequence $(\varepsilon_k) \subset (0,1)$ with $\varepsilon_k \to 0$ as $k \to +\infty$. Then we obtain by the lower semicontinuity of the Γ-$\limsup$ and $u_{\varepsilon_k} \to u$ in $L^1(0,1)$ as $k \to \infty$:

$$\begin{aligned}\Gamma\text{-}\limsup_{n\to\infty} H_n^\ell(u) &\leq \liminf_{k\to\infty}\left(\Gamma\text{-}\limsup_{n\to\infty} H_n^\ell(u_{\varepsilon_k})\right)\\ &\leq \limsup_{k\to\infty}\left(\int_{\varepsilon_k}^{1-\varepsilon_k} J_{CB}^{**}(u'(x))dx + 2\varepsilon_k J_{CB}(\gamma)\right) = H^\ell(u).\end{aligned}$$

Let us now consider $u \in BV^\ell(0,1)$ such that $H^\ell(u) < +\infty$ and $u(0+) = 0$ or $u(1-) = \ell$. Since $\ell > 0$, there exists a sequence (u_N) such that $u_N \to u$ weakly* in $BV(0,1)$ such that

$$\int_0^1 J_{CB}^{**}(u_N'(x))dx \to \int_0^1 J_{CB}^{**}(u'(x))dx,\ 0 < u_N(0+), \quad u_N(1-) < \ell, \quad D^s u_N \geq 0,$$

see [12, Theorem 4.1]. By the previous step, we have $\Gamma\text{-}\limsup_{n\to\infty} H_n^\ell(u_N) \leq H^\ell(u_N)$ for every N. Passing with $N \to \infty$, we obtain $\Gamma\text{-}\limsup_{n\to\infty} H_n^\ell(u) \leq H^\ell(u)$. Hence, the limsup inequality is proven.

Convergence of minimum values. The convergence follows directly from the coercivity of H_n^ℓ and the Γ-convergence result. Combining J_{CB}^{**} is decreasing, Jensen's inequality and $D^s u \geq 0$ yield

$$\min H^\ell(u) \geq J_{CB}^{**}\left(\int_0^1 u' dx\right) \geq J_{CB}^{**}\left(Du([0,1])\right) = J_{CB}^{**}\left(\ell\right).$$

The reverse inequality follows by testing with $u(x) = \ell x$ if $\ell \leq \gamma$ and $u(0) = 0$ and $u(x) = \gamma x + \ell - \gamma$ if $\ell > \gamma$. □

3.3 Γ-limit of first order

In this section, we provide the first-order Γ-limit of H_n^ℓ. That is, for given $\ell > 0$, we derive the Γ-limit of the sequence $(H_{1,n}^\ell)$, where $H_{1,n}^\ell$ is defined by

$$H_{1,n}^\ell(u) := \frac{H_n^\ell(u) - \min H^\ell}{\lambda_n}. \tag{3.38}$$

In the case of nearest and next-to-nearest neighbour interactions ($K = 2$) this was done in [50, Theorem 4.1, Theorem 4.2] (see also [11]).

It will be useful to rearrange the terms in the energy (3.38) in a suitable way. For given $\ell > 0$ and $u_0^{(1)}, u_1^{(1)} \in \mathbb{R}_+^{K-1}$ let $u \in \mathcal{A}_n(0,1)$ be such that the boundary conditions (3.3) are satisfied. Using $\min_u H^\ell(u) = J_{CB}^{**}(\ell) = \sum_{j=2}^K \psi_j^{**}(\ell)$ and (3.7), we can rewrite the energy (3.38) by

$$\begin{aligned} H_{1,n}^\ell(u) =& \sum_{j=1}^K \sum_{i=0}^{n-j} J_j\left(\frac{u_n^{i+j} - u_n^i}{j\lambda_n}\right) - \frac{J_{CB}^{**}(\ell)}{\lambda_n} \\ =& \sum_{j=2}^K \sum_{i=0}^{n-j} \left\{ J_j\left(\frac{u^{i+j} - u^i}{j\lambda_n}\right) + \frac{c_j}{j} \sum_{s=i}^{i+j-1} J_1\left(\frac{u^{s+1} - u^s}{\lambda_n}\right) - \psi_j^{**}(\ell) \right\} \\ &+ \sum_{j=2}^K c_j \sum_{s=1}^{j-1} \frac{j-s}{j} \left(J_1(u_{0,s}^{(1)}) + J_1(u_{1,s}^{(1)})\right) - \sum_{j=2}^K (j-1)\psi_j^{**}(\ell). \end{aligned} \tag{3.39}$$

In the case $\ell \geq \gamma$ the terms in the curly brackets in (3.39) are non-negative. Indeed this follows by the definition of $J_{0,j}$, see (3.8), (3.12) and (3.15). Fix $j \in \{2, \dots, K\}$. For $u \in \mathcal{A}_n(0,1)$ which satisfies the boundary conditions (3.3), we obtain by similar calculations as in (3.6) that

$$\begin{aligned}
\sum_{i=0}^{n-j}\left(u^{i+j}-u^{i}\right) &= \sum_{i=0}^{n-j}\sum_{s=0}^{j-1}\left(u^{i+s+1}-u^{i+s}\right) = \sum_{s=0}^{j-1}\sum_{i=s}^{n-j+s}\left(u^{i+1}-u^{i}\right) \\
&= \sum_{s=0}^{j-1}\left\{\sum_{i=0}^{n-1}(u^{i+1}-u^{i}) - \sum_{i=0}^{s-1}(u^{i+1}-u^{i}) - \sum_{i=n-j+s+1}^{n-1}(u^{i+1}-u^{i})\right\} \\
&= \sum_{s=0}^{j-1}\left(\ell - \sum_{i=1}^{s}\lambda_n u_{0,i}^{(1)} - \sum_{i=1}^{j-s-1}\lambda_n u_{1,i}^{(1)}\right) = j\ell - \lambda_n\sum_{i=1}^{j-1}(j-i)\left(u_{0,i}^{(1)}+u_{1,i}^{(1)}\right).
\end{aligned}$$

Hence, we have

$$\begin{aligned}
\sum_{i=0}^{n-j}\left(\frac{u^{i+j}-u^{i}}{j\lambda_n}-\ell\right) &= -\sum_{s=1}^{j-1}\frac{j-s}{j}\left(u_{0,s}^{(1)}+u_{1,s}^{(1)}\right)+(j-1)\ell \\
&= -\sum_{s=1}^{j-1}\frac{j-s}{j}\left(u_{0,s}^{(1)}+u_{1,s}^{(1)}-2\ell\right). \qquad (3.40)
\end{aligned}$$

Let $(u_n) \subset L^1(0,1)$ be such that $u_n \in \mathcal{A}_n(0,1)$ and u_n satisfies the boundary conditions (3.3). By adding and subtracting the term $\sum_{j=2}^{K}\sum_{i=0}^{n-j}(\psi_j^{**})'(\ell)(\frac{u_n^{i+j}-u_n^{i}}{j\lambda_n}-\ell)$ to $H_{1,n}^{\ell}(u_n)$, we obtain that

$$\begin{aligned}
H_{1,n}^{\ell}(u_n) = &\sum_{j=2}^{K}\sum_{i=0}^{n-j}\sigma_{j,n}^{i}(\ell) + \sum_{j=2}^{K}c_j\sum_{s=1}^{j-1}\frac{j-s}{j}\left(J_1(u_{0,s}^{(1)})+J_1(u_{1,s}^{(1)})\right) \\
&-\sum_{j=2}^{K}(\psi_j^{**})'(\ell)\sum_{s=1}^{j-1}\frac{j-s}{j}\left(u_{0,s}^{(1)}+u_{1,s}^{(1)}-2\ell\right)-\sum_{j=2}^{K}(j-1)\psi_j^{**}(\ell) \qquad (3.41)
\end{aligned}$$

where for $j \in \{2,\dots,K\}$ and $i \in \{0,\dots,n-j\}$, we define

$$\begin{aligned}
\sigma_{j,n}^{i}(\ell) :=& J_j\left(\frac{u_n^{i+j}-u_n^{i}}{j\lambda_n}\right) + \frac{c_j}{j}\sum_{s=i}^{i+j-1}J_1\left(\frac{u_n^{s+1}-u_n^{s}}{\lambda_n}\right) \\
&-(\psi_j^{**})'(\ell)\left(\frac{u_n^{i+j}-u_n^{i}}{j\lambda_n}-\ell\right)-\psi_j^{**}(\ell). \qquad (3.42)
\end{aligned}$$

By the definition of $J_{0,j}$ (see (3.8)) and (3.15), we have

$$\sigma_{j,n}^{i}(\ell) \geq J_{0,j}\left(\frac{u_n^{i+j}-u_n^{i}}{j\lambda_n}\right)-(\psi_j^{**})'(\ell)\left(\frac{u_n^{i+j}-u_n^{i}}{j\lambda_n}-\ell\right)-\psi_j^{**}(\ell) \geq 0. \qquad (3.43)$$

Note that the last inequality follows from $J_{0,j}(z) \geq J_{0,j}^{**}(z) = \psi_j^{**}(z)$ and the convexity of ψ_j^{**}. Furthermore, we show in the following lemma that, under the hypotheses (LJ1)–(LJ5), it holds $\sigma_{j,n}^{i}(\ell) = 0$ if and only if $u_n^{s+1}-u_n^{s} = \lambda_n\min\{\ell,\gamma\}$ for all $s \in \{i,\dots,i+j-1\}$. For $d \in \mathbb{N}$, we denote by $|\cdot|_\infty$ the norm on $\mathbb{R}^d$ given by $|z|_\infty = \max_{1\leq i\leq d}|z_i|$, for $z \in \mathbb{R}^d$.

Lemma 3.8. *Let $\ell > 0$ and let $J_1, \dots, J_K$ satisfy (LJ1)–(LJ5). For given $j \in \{2, \dots, K\}$, the function $F_j^\ell : \mathbb{R}^j \to [0, +\infty]$ is defined for $z = (z_1, \dots, z_j) \in \mathbb{R}^j$ by*

$$F_j^\ell(z) := J_j\left(\sum_{s=1}^j \frac{z_s}{j}\right) + \frac{c_j}{j}\sum_{s=1}^j J_1(z_s) - (\psi_j^{**})'(\ell)\left(\sum_{s=1}^j \frac{z_s}{j} - \ell\right) - \psi_j^{**}(\ell). \tag{3.44}$$

Then it holds $F_j^\ell(z) = 0$ if and only if $z_s = \min\{\ell, \gamma\}$ for $s \in \{1, \dots, j\}$. Moreover, for every $\varepsilon > 0$ there exists $\eta = \eta(\varepsilon) > 0$ such that

$$\inf\left\{F_j^\ell(z) : \ z \in \mathbb{R}^j \text{ such that } |z - \min\{\ell, \gamma\}e|_\infty \geq \varepsilon\right\} \geq \eta > 0 \tag{3.45}$$

where $e := (1, \dots, 1) \in \mathbb{R}^j$

Proof. Fix $j \in \{2, \dots, K\}$. For given $z \in \mathbb{R}^j$, we have by the definition of $J_{0,j}$, see (3.8) that

$$F_j^\ell(z) \geq J_{0,j}\left(\sum_{s=1}^j \frac{z_s}{j}\right) - (\psi_j^{**})'(\ell)\left(\sum_{s=1}^j \frac{z_s}{j} - \ell\right) - \psi_j^{**}(\ell) =: f_j^\ell\left(\frac{1}{j}\sum_{s=1}^j z_s\right).$$

Firstly, we observe that $f_j^\ell(x) \geq 0$ for all $x \in \mathbb{R}$ and $f_j^\ell(x) = 0$ if and only if $x = \min\{\ell, \gamma\}$. If $\ell \geq \gamma$ this follows from $(\psi_j^{**})'(\ell) = 0$ and $\psi_j^{**}(\ell) = J_{0,j}(\gamma)$ where γ is the unique minimiser of $J_{0,j}$. Let us fix $0 < \ell < \gamma$. For $z \leq \gamma$ the claim follows from $J_{0,j}(z) = \psi_j(z)$, (3.15) and the strict convexity of ψ_j on $(-\infty, \gamma]$. For $z > \gamma$, we use the same estimate and $J_{0,j}(z) - \psi_j'(\ell)(z - \gamma) > J_{0,j}(\gamma)$ (note $\psi_j'(\ell) < 0$). Hence, we have, using (LJ4), that $F_j^\ell(z) \geq 0$ for all $z \in \mathbb{R}^j$ and $F_j^\ell(z) = 0$ if and only if $z_s = \min\{\ell, \gamma\}e$.

Fix $\varepsilon > 0$. We want to show the existence of $\eta = \eta(\varepsilon) > 0$ such that (3.45) holds true. Therefore, it is not restrictive to assume that $\varepsilon < \gamma^c - \gamma$, where γ^c is defined in assumption (LJ4). For given $z \in \mathbb{R}^j$, we set $\bar{z}(z) := \frac{1}{j}\sum_{s=1}^j z_s$. Let us now distinguish between the cases when $\bar{z}(z)$ is close to $\bar{\ell} := \min\{\ell, \gamma\}$ and when it is not. Firstly, we assume that $|\bar{z}(z) - \bar{\ell}| \geq \frac{\varepsilon}{2}$. Combining $J_{0,j}(z) = \psi_j(z)$ for $z \leq \gamma$ with (3.10) and (3.11) yields $\lim_{x\to-\infty} f_j^\ell(x) = +\infty$. Since $(\psi_j^{**})'(\ell) < 0$ if $\ell < \gamma$ and $J_{0,j}$ is bounded from below it holds $\lim_{x\to+\infty} f_j^\ell(x) = +\infty$. In the case $\ell \geq \gamma$, the assumption (3.16) yields

$$\liminf_{x\to\infty} f_j^\ell(x) \geq \liminf_{x\to\infty} J_{0,j}(x) - \psi_j(\gamma) > 0.$$

Hence, there exist $\eta_1 > 0$ and $R > 0$ such that $f_j^\ell(x) \geq \eta_1 > 0$ for $|x| \geq R$. By the lower semicontinuity of J_j there exists x^ε such that

$$f_j^\ell(x) \geq f_j^\ell(x^\varepsilon) =: \eta_2(\varepsilon) > 0,$$

for all $x \in \mathbb{R}$ such that $|x - \bar{\ell}| \geq \frac{\varepsilon}{2}$ and $|x| \leq R$. By the last estimates, we have that $F_j^\ell(z) \geq \min\{\eta_1, \eta_2(\varepsilon)\}$ for all $z \in \mathbb{R}^j$ such that $|z - \bar{\ell}e|_\infty \geq \varepsilon$ and $|\bar{z}(z) - \bar{\ell}| \geq \frac{\varepsilon}{2}$.
Let us now consider the case $|\bar{z}(z) - \bar{\ell}\}| \leq \frac{\varepsilon}{2}$. We define the function $G_{j,\varepsilon}^\ell : \mathbb{R}^d \to [0, +\infty]$

by

$$G^{\ell}_{j,\varepsilon}(z) := F^{\ell}_j(z) + \bar{\chi}_{A^\varepsilon}(z),$$

where $A^\varepsilon := \{z \in \mathbb{R}^j : \ |z - \bar{\ell}e|_\infty \geq \varepsilon \text{ and } |\frac{1}{j}\sum_{s=1}^j z_s - \bar{\ell}| \leq \frac{\varepsilon}{2}\}$. Clearly $G^{\ell}_{j,\varepsilon}$ is lower semicontinuous and using the growth conditions (3.10) and (3.11) it admits a minimiser. We denote by $z^\varepsilon \in \mathbb{R}^j$ this minimiser. Using the definition of $J_{0,j}$, $f^{\ell}_j(z) \geq 0$ and (LJ4), we obtain

$$F^{\ell}_j(z^\varepsilon) \geq J_{0,j}\left(\sum_{s=1}^{j}\frac{z^\varepsilon_s}{j}\right) - (\psi^{**}_j)'(\ell)\left(\sum_{s=1}^{j}\frac{z^\varepsilon_s}{j} - \ell\right) - \psi^{**}_j(\ell) + \eta_3(\varepsilon) \geq \eta_3(\varepsilon),$$

with $\eta_3(\varepsilon) := c_j(\frac{1}{j}\sum_{s=1}^j J_1(z^\varepsilon_s) - J_1(\sum_{s=1}^j \frac{z^\varepsilon_s}{j})) > 0$. Note that we have used $\bar{z}(z^\varepsilon) \leq \gamma + \frac{\varepsilon}{2} < \gamma^c$ and by $|z^\varepsilon - \bar{\ell}e|_\infty \geq \varepsilon$ there exists $i \in \{1,\dots,j\}$ such that $|z^\varepsilon_i - \bar{z}(z^\varepsilon)| \geq \frac{\varepsilon}{2}$, thus (LJ4) yields $\eta_3(\varepsilon) > 0$.
Altogether, we have shown that for all $z \in \mathbb{R}^j$ with $|z - \bar{\ell}e|_\infty \geq \varepsilon$ it holds

$$F(z) \geq \eta(\varepsilon)$$

with $\eta(\varepsilon) = \min\{\eta_1, \eta_2(\varepsilon), \eta_3(\varepsilon)\} > 0$. Taking the infimum over all those $z \in \mathbb{R}^j$ yields the assertion. □

We are now in position to state a compactness result for sequences (u_n) with equi-bounded energy $H^{\ell}_{1,n}(u_n)$. This extends a previous result obtained in [50, Proposition 4.1], see also [11, Proposition 4.2], for nearest and next-to-nearest neighbour interactions, i.e. $K = 2$, to the case of finite range interactions of Lennard–Jones type.

Proposition 3.9. *Let $\ell > 0$, $u^{(1)}_0, u^{(1)}_1 \in \mathbb{R}^{K-1}_+$ and suppose that hypotheses (LJ1)–(LJ5) hold. Let (u_n) be a sequence of functions such that*

$$\sup_n H^{\ell}_{1,n}(u_n) < +\infty. \tag{3.46}$$

(1) If $\ell \leq \gamma$, then, up to subsequences, $u_n \to u$ in $L^\infty(0,1)$ with $u(x) = \ell x$, $x \in [0,1]$.

(2) In the case $\ell > \gamma$, 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) $[u] \geq 0$ in $[0,1]$,

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

Remark 3.10. Recall that $u \in SBV^\ell(0,1)$ and condition (ii) imply $u(0+) \geq 0$ and $u(1-) \leq \ell$; see Section 2.1.1.

Proof of Proposition 3.9. Let $(u_n) \subset L^1(0,1)$ satisfy (3.46). With the same arguments, as in the proof of Theorem 3.7, we have the existence of $u \in BV^\ell(0,1)$ such that, up to subsequences, $u_n \overset{*}{\rightharpoonup} u$ weakly* in $BV(0,1)$.

Let us now show $u_n' \to \min\{\ell,\gamma\}$ in measure in $(0,1)$. For $\varepsilon > 0$, we define

$$I_n^\varepsilon := \left\{ i \in \{0,\dots,n-1\} : \left| \frac{u_n^{i+1}-u_n^i}{\lambda_n} - \min\{\ell,\gamma\} \right| > \varepsilon \right\}.$$

By the definition of $\sigma_{j,n}^i(\ell)$, see (3.42), and Lemma 3.8, we deduce the existence of $\eta = \eta(\varepsilon) > 0$ such that $\sigma_{j,n}^i(\ell) \geq \eta$ for $i \in I_n^\varepsilon$ and $j \in \{2,\dots,K\}$. Moreover, we obtain from (3.41), (3.46), $\sigma_{j,n}^i(\ell) \geq 0$ for $j \in \{2,\dots,K\}$, and J_j is bounded from below that there exists a constant $C > 0$ such that

$$C \geq \sum_{j=2}^{K} \sum_{i=0}^{n-j} \sigma_{j,n}^i \geq \sum_{i=0}^{n-2} \sigma_{n,2}^i(\ell) \geq \# I_n^\varepsilon \eta.$$

Hence, by using $|\{x : |u_n'(x) - \min\{\ell,\gamma\}| > \varepsilon\}| = \lambda_n \# I_n^\varepsilon \leq \lambda_n \frac{C}{\eta}$ it follows that $u_n' \to \min\{\ell,\gamma\}$ in measure. Moreover, we can use the above argument in the following way: we define the set

$$Q_n := \left\{ i \in \{0,\dots,n-2\} : \frac{u_n^{i+1}-u_n^i}{\lambda_n} > 2\gamma \right\}.$$

As above, Lemma 3.8 ensures $\sigma_{n,2}^i(\ell) \geq \eta$ for $i \in Q_n$ and some $\eta > 0$. From (3.46), we deduce the equiboundedness of $\# Q_n$. We define the sequence $(v_n) \subset SBV(0,1)$ as

$$v_n(x) = \begin{cases} u_n(x), & \text{if } x \in (i,i+1)\lambda_n, i \notin Q_n, \\ u_n(i\lambda_n), & \text{if } x \in (i,i+1)\lambda_n, i \in Q_n. \end{cases}$$

The sequence (v_n) is constructed such that $\lim_n \|u_n - v_n\|_{L^1(0,1)} = 0$ and $\|v_n\|_{BV(0,1)} \leq \|u_n\|_{W^{1,1}(0,1)}$. Thus we can assume, by passing to a subsequence, that (v_n) weakly* converges in $BV(0,1)$ to u. By definition of v_n, we have $\# S_{v_n} = \# Q_n$ and thus there exists a constant $C > 0$ such that $\sup_n \# S_{v_n} \leq C$. Using $v_n'(x) \leq 2\gamma$ a.e., (3.10) and (3.11), and (3.46), the sequence (v_n) satisfies all assumptions of Theorem 2.8 and we conclude that $u \in SBV^\ell(0,1)$, $v_n' \rightharpoonup u'$ weakly in $L^1(0,1)$, $+\infty > \# S_u$ and $D^j v_n \overset{*}{\rightharpoonup} D^j u$ weakly* in the sense of measures. By the construction of (v_n), we have $[v_n] > 0$ on S_{v_n} and we conclude, by the weak* convergence of the jump part in $(0,1)$, that $[u] \geq 0$ in $(0,1)$. To prove (ii) it is left to show $0 \leq u(0+)$ and $u(1-) \leq \ell$. For this, we can repeat the above argument for the extensions $\tilde{u}, \tilde{u}_n, \tilde{v}_n \in BV_{\mathrm{loc}}(\mathbb{R})$ of u, u_n, v_n with $\tilde{u}(x) = u_n(x) = \tilde{v}_n(x) = 0$ for $x \leq 0$ and $\tilde{u}(x) = u_n(x) = \tilde{v}_n(x) = \ell$ for $1 \leq x$. From this, we deduce that $D^j \tilde{u}$ is a positive measure in $\mathbb{R}$. Since $D^j u$ is the restriction of $D^j \tilde{u}$ to $[0,1]$ the assertion (ii) follows.

Note that (v_n) is defined such that $|\{x : u_n'(x) \neq v_n'(x)\}| \leq \# S_{v_n} \lambda_n$, which implies $v_n' \to \min\{\ell,\gamma\}$ in measure in $(0,1)$. Combining this with $v_n' \rightharpoonup u'$ in $L^1(0,1)$, we show $u' = \min\{\ell,\gamma\}$ a.e. in $(0,1)$. Indeed, by the Dunford-Pettis theorem, we deduce from the relative compactness of $(v_n') \subset L^1(0,1)$ in the weak $L^1(0,1)$-topology that (v_n') is equi-integrable. By extracting a subsequence, we can assume that $v_n' \to \min\{\ell,\gamma\}$ pointwise a.e. in $(0,1)$ and by Vitali's convergence theorem it follows $v_n' \to \min\{\ell,\gamma\}$ strongly in

$L^1(0,1)$. Thus $u' = \min\{\ell, \gamma\}$ a.e. in $(0,1)$. Thus the assertion for $\ell > \gamma$ is proven. In the case $0 < \ell \leq \gamma$, we have, up to subsequences, $u_n \to u$ in $L^1(0,1)$ with $u \in SBV^\ell(0,1)$, $u' = \ell$ a.e. in $(0,1)$ and $[u] > 0$ on S_u. This implies $u(x) = \ell x$ on $[0,1]$. It is left to show: $u_n \to u$ in $L^\infty(0,1)$. Note that for the above defined sequence (v_n) it holds $u_n' = v_n' + w_n$ a.e. on $(0,1)$ with $w_n \in L^1(0,1)$ and $w_n(x) \geq 0$. Using $v_n' \to \ell$ in $L^1(0,1)$, we deduce from

$$\ell = \int_0^1 u_n'(x)dx = \int_0^1 v_n'(x)dx + \int_0^1 w_n(x)dx$$

that $w_n \to 0$ in $L^1(0,1)$ (using $w_n \geq 0$). Altogether, we have $u_n' = v_n' + w_n \to \ell$ in $L^1(0,1)$ and thus $u_n \to u$ in $W^{1,1}(0,1)$ with $u(x) = \ell x$. Hence, the assertion follows from the Sobolev inequality on intervals. □

To simplify the notation, we define for $\ell > \gamma$ the set

$$SBV_c^\ell(0,1) := \big\{u \in SBV^\ell(0,1)\text{: conditions (i)-(iii) of Proposition 3.9 are satisfied}\big\}, \tag{3.47}$$

as in [50].

Proposition 3.9 tells us that a sequence of deformations (u_n) with equibounded energy converges in $L^1(0,1)$ to a deformation u which has a constant gradient almost everywhere. In the following lemma, we prove a local convergence result for the discrete gradients of sequences (u_n) with equibounded energy. This turns out to be crucial in the proof of the first-order Γ-limit.

Lemma 3.11. *Suppose that hypotheses (LJ1)–(LJ5) hold. Let* $\ell > 0$ *and* $u_0^{(1)}, u_1^{(1)} \in \mathbb{R}_+^{K-1}$. *Let* (u_n) *be a sequence of functions such that (3.46) is satisfied. Then there exists for every* $x \in [0,1]$ *a sequence* $(h_n) \subset \mathbb{N}$ *with* $0 \leq h_n \leq n - K$ *and* $\lim_{n\to\infty} \lambda_n h_n = x$ *such that , up to subsequences,*

$$\lim_{n\to\infty} \frac{u_n^{h_n+s+1} - u_n^{h_n+s}}{\lambda_n} = \min\{\ell, \gamma\} \quad \textit{for } s \in \{0, \dots, K-1\}.$$

Proof. Let us define the set I_n as

$$I_n := \left\{ i \in \{0, \dots, n-K\} : \sigma_{n,K}^i(\ell) > \frac{1}{\sqrt{n}} \right\}.$$

By (3.46) there exists $C > 0$ such that

$$C \geq \sup_n \sum_{j=2}^{K} \sum_{i=0}^{n-j} \sigma_{j,n}^i(\ell) \geq \sup_n \sum_{i=0}^{n-K} \sigma_{n,K}^i(\ell) = \sup_n \frac{\#I_n}{\sqrt{n}}.$$

This yields $\#I_n = \mathcal{O}(\sqrt{n})$.

Now let $i \notin I_n$. By using the definition of $J_{0,K}$ and $J_{0,K}(z) \geq \psi_K^{**}(z) \geq (\psi_K^{**})'(\ell)(z - \ell) + \psi_K^{**}(\ell)$, we deduce from $0 \leq \sigma_{n,K}^i(\ell) \leq \frac{1}{\sqrt{n}}$ that

$$0 \leq J_K\left(\frac{u_n^{i+K} - u_n^i}{K\lambda_n}\right) + \frac{c_K}{K}\sum_{s=i}^{i+K-1} J_1\left(\frac{u_n^{s+1} - u_n^s}{\lambda_n}\right) - J_{0,K}\left(\frac{u_n^{i+K} - u_n^i}{K\lambda_n}\right) \leq \frac{1}{\sqrt{n}}, \quad (3.48)$$

$$0 \leq J_{0,K}\left(\frac{u_n^{i+K} - u_n^i}{K\lambda_n}\right) - \psi_K^{**}(\ell) - (\psi_K^{**})'(\ell)\left(\frac{u_n^{i+K} - u_n^i}{K\lambda_n} - \ell\right) \leq \frac{1}{\sqrt{n}}. \quad (3.49)$$

Fix $x \in [0,1]$. From $\#I_n = \mathcal{O}(\sqrt{n})$, we deduce the existence of a sequence $(h_n) \subset \mathbb{N}$ such that $h_n \in \{0, \dots, n-K\}$, $h_n \notin I_n$ and $\lim_{n\to\infty} \lambda_n h_n = x$. By using the fact that $J_{0,K}(z) = \psi_K^{**}(\ell) + (\psi_K^{**})'(\ell)(z - \ell)$ if and only if $z = \min\{\ell, \gamma\}$, we conclude from (3.49) that

$$\frac{u_n^{h_n+K} - u_n^{h_n}}{K\lambda_n} \to \min\{\ell, \gamma\} \quad \text{as } n \to \infty.$$

Combining this with (3.48) and assumption (LJ4), we deduce

$$\lim_{n\to\infty} \frac{u_n^{h_n+s+1} - u_n^{h_n+s}}{\lambda_n} = \min\{\ell, \gamma\} \qquad \text{for } s \in \{0, \dots, K-1\},$$

which proves the assertion. □

3.3.1 The case $\ell \leq \gamma$

As in [50], we distinguish between the cases $\ell \leq \gamma$ and $\ell > \gamma$, where ℓ denotes the boundary condition on the last atom in the chain and γ is given in (3.12). In the case of $\ell \leq \gamma$ no fracture occurs by Proposition 3.9. For any $0 < \ell \leq \gamma$ and $\theta = (\theta_s)_{s=1}^{K-1} \in \mathbb{R}_+^{K-1}$, we define the boundary layer energy $B(\theta, \ell)$ as

$$\begin{aligned} B(\theta,\ell) = \inf_{\substack{N\in\mathbb{N}\\ N\geq K-1}} \min\Bigg\{ & \sum_{j=2}^{K} c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1\left(v^s - v^{s-1}\right) + \sum_{j=2}^{K}\sum_{i\geq 0}\Bigg\{ J_j\left(\frac{v^{i+j} - v^i}{j}\right) \\ & + \frac{c_j}{j}\sum_{s=i}^{i+j-1} J_1\left(v^{s+1} - v^s\right) - \psi_j'(\ell)\left(\frac{v^{i+j} - v^i}{j} - \ell\right) - \psi_j(\ell)\Bigg\} : \ v : \mathbb{N}_0 \to \mathbb{R}, \\ & v^0 = 0,\ v^s - v^{s-1} = \theta_s \text{ if } 1 \leq s \leq K-1,\ v^{i+1} - v^i = \ell \text{ if } i \geq N\Bigg\}. \end{aligned} \quad (3.50)$$

In what follows we often refer to $B(\theta, \ell)$ as the *elastic boundary layer energy.* The term $B(\theta, \ell)$ show up in the Γ-limit below with $\theta = u_0^{(1)}$ and $\theta = u_1^{(1)}$, so the constraint $v^s - v^{s-1} = \theta_s$ if $1 \leq s \leq K-1$ in (3.50) is due to the boundary conditions imposed on the first and on the last K atoms of the chain, respectively. The terms in the infinite sum have the same structure as $\sigma_{j,n}^i(\ell)$ defined in (3.42) and are always non-negative, see also Lemma 3.8. Moreover, we note that the infinite sum in (3.50) is actually a finite sum from $i = 1$ to $i = N-1$. Indeed, for $i \geq N$ the terms in the infinite sum reads $J_j(\ell) + c_j J_1(\ell) - \psi_j(\ell) = 0$, see (3.14).

Let us remark that in the case of nearest and next-to-nearest neighbour interactions, i.e. $K = 2$, the definition of $B(\theta, \ell)$ matches exactly the definition of the elastic boundary layer energy given in [50, eq. (4.13)].

Theorem 3.12. *Suppose that $J_1, \dots, J_K$ satisfy the assumptions (LJ1)–(LJ5). Let $0 < \ell \leq \gamma$ and $u_0^{(1)}, u_1^{(1)} \in \mathbb{R}_+^{K-1}$. Then $(H_{1,n}^\ell)$ Γ-converges with respect to the $L^1(0,1)$-convergence and the $L^\infty(0,1)$-convergence to the functional H_1^ℓ defined by*

$$H_1^\ell(u) := \begin{cases} B(u_0^{(1)}, \ell) + B(u_1^{(1)}, \ell) - \sum_{j=2}^{K} (j-1)\psi_j(\ell) \\ \quad - \sum_{j=2}^{K} \psi_j'(\ell) \sum_{s=1}^{j-1} \frac{j-s}{j} \left(u_{0,s}^{(1)} + u_{1,s}^{(1)} - 2\ell \right) & \text{if } u(x) = \ell x, \\ +\infty & \text{else,} \end{cases} \tag{3.51}$$

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

Proof. We adapt the proof of [50, Theorem 4.1] where the case of nearest and next-to-nearest neighbour interactions is considered.

Liminf inequality. Let $(u_n) \subset L^1(0,1)$ be a sequence satisfying $\sup_n H_{1,n}^\ell(u_n) < +\infty$ and $u_n \to u$ in $L^1(0,1)$. From Proposition 3.9, we deduce that $u_n \to u$ in $L^\infty(0,1)$ and $u(x) = \ell x$ for $x \in [0,1]$. Moreover, Lemma 3.11 ensures that we find sequences $(T_n^0), (T_n^1) \subset \mathbb{N}$ such that $\lim_{n\to\infty} \lambda_n T_n^0 = 0$, $\lim_{n\to\infty} \lambda_n T_n^1 = 1$ and

$$\lim_{n\to\infty} \frac{u_n^{T_n^i+s+1} - u_n^{T_n^i+s}}{\lambda_n} = \ell \quad \text{for } i \in \{0,1\} \text{ and } 0 \leq s \leq K-1. \tag{3.52}$$

From (3.41) and $\sigma_{j,n}^i(\ell) \geq 0$, we deduce

$$\begin{aligned} H_{1,n}^\ell(u_n) \geq & \sum_{j=2}^{K} \left\{ \sum_{i=0}^{T_n^0} \sigma_{j,n}^i(\ell) + c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(u_{0,s}^{(1)}) + \sum_{i=T_n^1}^{n-j} \sigma_{j,n}^i(\ell) + c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(u_{1,s}^{(1)}) \right\} \\ & - \sum_{j=2}^{K} (j-1)\psi_j(\ell) - \sum_{j=2}^{K} \psi_j'(\ell) \sum_{s=1}^{j-1} \frac{j-s}{j} \left(u_{0,s}^{(1)} + u_{1,s}^{(1)} - 2\ell \right). \end{aligned} \tag{3.53}$$

Let us define the sequence $v_n : \mathbb{N}_0 \to \mathbb{R}$ as

$$v_n^i = \begin{cases} \frac{u_n^i}{\lambda_n} & \text{if } 0 \leq i \leq T_n^0 + K, \\ \ell\left(i - (T_n^0 + K)\right) + \frac{u_n^{T_n^0+K}}{\lambda_n} & \text{if } i \geq T_n^0 + K. \end{cases} \tag{3.54}$$

Fix $j \in \{2, \dots, K\}$. In terms of v_n, we have that

$$\begin{aligned}\sum_{i=0}^{T_n^0} \sigma_{j,n}^i(\ell) =& \sum_{i=0}^{T_n^0} \Bigg\{ J_j \left(\frac{v_n^{i+j} - v_n^i}{j} \right) + \frac{c_j}{j} \sum_{s=i}^{i+j-1} J_1 \left(v_n^{s+1} - v_n^s \right) \\ &- \psi_j'(\ell) \left(\frac{v_n^{i+j} - v_n^i}{j} - \ell \right) - \psi_j(\ell) \Bigg\} \\ =& \sum_{i \geq 0} \Bigg\{ J_j \left(\frac{v_n^{i+j} - v_n^i}{j} \right) + \frac{c_j}{j} \sum_{s=i}^{i+j-1} J_1 \left(v_n^{s+1} - v_n^s \right) \\ &- \psi_j'(\ell) \left(\frac{v_n^{i+j} - v_n^i}{j} - \ell \right) - \psi_j(\ell) \Bigg\} - \omega_j(n),\end{aligned}$$

where

$$\begin{aligned}\omega_j(n) = \sum_{i=T_n^0+1}^{T_n^0+K-1} &\Bigg\{ J_j \left(\frac{v_n^{i+j} - v_n^i}{j} \right) + \frac{c_j}{j} \sum_{s=i}^{i+j-1} J_1 \left(v_n^{s+1} - v_n^s \right) \\ &- \psi_j'(\ell) \left(\frac{v_n^{i+j} - v_n^i}{j} - \ell \right) - \psi_j(\ell) \Bigg\} \to 0 \quad \text{as } n \to \infty.\end{aligned}$$

Indeed, by the definition of v_n in (3.54), we have $v_n^{i+1} - v_n^i = \ell$ for $i \geq T_n^0 + K$. Thus, for $i \geq T_n^0 + K$ the terms in the infinite sum are given by $J_j(\ell) + c_j J_1(\ell) - \psi_j(\ell) = 0$, see (3.14). Moreover, we have by (3.52) for $1 \leq s \leq K - 1$ that

$$\lim_{n\to\infty} (v_n^{T_n^0+s+1} - v_n^{T_n^0+s}) = \lim_{n\to\infty} \frac{u_n^{T_n^0+1+s} - u_n^{T_n^0+s}}{\lambda_n} = \ell.$$

Combining this with $v_n^{i+1} - v_n^i = \ell$ for $i \geq T_n^0 + K$ and the definition of ψ_j, see (3.14), yields $\lim_{n\to\infty} \omega_j(n) = 0$. Since u_n satisfies (3.3), we have $v_n^0 = \frac{u_n^0}{\lambda_n} = 0$, $v_n^s - v_n^{s-1} = \frac{1}{\lambda_n}(u_n^s - u_n^{s-1}) = u_{0,s}^{(1)}$ for $s \in \{1, \dots, K-1\}$ and $v_n^{i+1} - v_n^i = \ell$ for $i \geq T_n^0 + K$. Hence, v_n is a competitor for the minimum problem defining $B(u_0^{(1)}, \ell)$, see (3.50). Therefore

$$\begin{aligned}&\sum_{j=2}^{K} \Bigg\{ c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(u_{0,s}^{(1)}) + \sum_{i=0}^{T_n^0} \sigma_{j,n}^i(\ell) \Bigg\} \\ &= \sum_{j=2}^{K} \Bigg\{ c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(u_{0,s}^{(1)}) + \sum_{i\geq 0} \Bigg\{ J_j \left(\frac{v_n^{i+j} - v_n^i}{j} \right) + \frac{c_j}{j} \sum_{s=i}^{i+j-1} J_1 \left(v_n^{s+1} - v_n^s \right) \\ &\quad - \psi_j'(\ell) \left(\frac{v_n^{i+j} - v_n^i}{j} - \ell \right) - \psi_j(\ell) \Bigg\} - \omega_j(n) \Bigg\} \geq B(u_0^{(1)}, \ell) - \sum_{j=2}^{K} \omega_j(n). \qquad (3.55)\end{aligned}$$

Let us define $w_n : \mathbb{N}_0 \to \mathbb{R}$ as

$$w_n^m = \begin{cases} \frac{\ell - u_n^{n-m}}{\lambda_n} & \text{if } 0 \le m \le n - T_n^1, \\ \ell\left(m - (n - T_n^1)\right) + \frac{\ell - u_n^{T_n^1}}{\lambda_n} & \text{if } n - T_n^1 \le m. \end{cases} \tag{3.56}$$

For fixed $j \in \{2, \dots, K\}$, we have that

$$\begin{aligned} \sum_{i=T_n^1}^{n-j} \sigma_{j,n}^i(\ell) = \sum_{m=0}^{n-T_n^1-j} \Bigg\{ & J_j\left(\frac{u_n^{n-m} - u_n^{n-m-j}}{j\lambda_n}\right) + \frac{c_j}{j}\sum_{s=m}^{m+j-1} J_1\left(\frac{u_n^{n-s} - u_n^{n-s-1}}{\lambda_n}\right) \\ & - \psi_j'(\ell)\left(\frac{u_n^{n-m} - u_n^{n-m-j}}{j\lambda_n} - \ell\right) - \psi_j(\ell)\Bigg\} \\ = \sum_{m \ge 0} \Bigg\{ & J_j\left(\frac{w_n^{m+j} - w_n^m}{j}\right) + \frac{c_j}{j}\sum_{s=m}^{m+j-1} J_1(w_n^{s+1} - w_n^s) \\ & - \psi_j'(\ell)\left(\frac{w_n^{m+j} - w_n^m}{j} - \ell\right) - \psi_j(\ell)\Bigg\} - \hat{\omega}_j(n), \end{aligned}$$

where $\hat{\omega}_j(n) \to 0$ for $n \to \infty$ and $j \in \{2, \dots, K\}$. Indeed, by (3.56) and (3.14) the terms in the infinite sum vanish for $m \ge n - T_n^1$. Hence, $\hat{\omega}_j(n)$ is given by

$$\begin{aligned} \hat{\omega}_j(n) = \sum_{m=n-T_n^1-j+1}^{n-T_n^1-1} \Bigg\{ & J_j\left(\frac{w_n^{m+j} - w_n^m}{j}\right) + \frac{c_j}{j}\sum_{s=m}^{m+j-1} J_1(w_n^{s+1} - w_n^s) \\ & - \psi_j'(\ell)\left(\frac{w_n^{m+j} - w_n^m}{j} - \ell\right) - \psi_j(\ell)\Bigg\}. \end{aligned}$$

By the definition of w_n, see (3.56), and (3.52) it holds for $s \in \{1, \dots, K-1\}$ that

$$\lim_{n\to\infty} (w_n^{n-T_n^1-K+s+1} - w_n^{n-T_n^1-K+s}) = \lim_{n\to\infty} \frac{u_n^{T_n^1+K-s} - u_n^{T_n^1+K-s-1}}{\lambda_n} = \ell.$$

Combining this with $w_n^{i+1} - w_n^i = \ell$ for $i \ge n - T_n^1$ and the definition of $\psi_j(\ell)$, we obtain $\lim_{n\to\infty} \hat{\omega}_j(n) = 0$. Since u_n satisfies (3.3), we have $w_n^0 = 0$ and $w_n^s - w_n^{s-1} = \frac{1}{\lambda_n}(u_n^{n-s+1} - u_n^{n-s}) = u_{1,s}^{(1)}$ for $s \in \{1, \dots, K-1\}$. Hence, w_n is a competitor for the infimum problem defining $B(u_1^{(1)}, \ell)$ and we obtain as in (3.55) that

$$\sum_{j=2}^{K} \left\{ c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(u_{1,s}^{(1)}) + \sum_{i=T_n^1+1}^{n-j} \sigma_{j,n}^i(\ell) \right\} \ge B(u_1^{(1)}, \ell) - \sum_{j=2}^{K} \hat{\omega}_j(n). \tag{3.57}$$

Combining (3.53) with (3.55), (3.57) and $\omega_j(n), \hat{\omega}_j(n) \to 0$ as $n \to \infty$ for $j \in \{2, \dots, K\}$ proves the liminf inequality.

Limsup inequality. Since $H_1^\ell(u)$ is finite if and only if $u(x) = \ell x$ for all $x \in [0,1]$ it is sufficient to consider this case only. We construct a sequence (u_n) such that $u_n \to u$ in $L^\infty(0,1)$ (and thus also in L^1) and

$$\begin{aligned}\limsup_{n\to\infty} H^\ell_{1,n}(u_n) \leq & B(u_0^{(1)},\ell) + B(u_1^{(1)},\ell) - \sum_{j=2}^K (j-1)\psi_j(\ell) \\ & - \sum_{j=2}^K \psi_j'(\ell) \sum_{s=1}^{j-1} \frac{j-s}{j}\left(u_{0,s}^{(1)} + u_{1,s}^{(1)} - 2\ell\right).\end{aligned}$$

The following construction of (u_n) is similar to the recovery sequence in [50, Theorem 4.2] for the case $K=2$. Fix $\eta > 0$. By the definition of $B(\theta,\ell)$, see (3.50), there exist a function $v : \mathbb{N}_0 \to \mathbb{R}$ and an $N_1 \in \mathbb{N}$ such that $v^0 = 0$, $v^s - v^{s-1} = u_{0,s}^{(1)}$ for $s \in \{1,\dots,K-1\}$, $v^{i+1} - v^i = \ell$ for $i \geq N_1$ and

$$\begin{aligned}&\sum_{j=2}^K c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1\left(v^s - v^{s-1}\right) + \sum_{j=2}^K \sum_{i\geq 0} \Bigg\{ J_j\left(\frac{v^{i+j}-v^i}{j}\right) \\ &\quad + \frac{c_j}{j}\sum_{s=i}^{i+j-1} J_1\left(v^{s+1}-v^s\right) - \psi_j'(\ell)\left(\frac{v^{i+j}-v^i}{j} - \ell\right) - \psi_j(\ell)\Bigg\} \\ &\quad \leq B(u_0^{(1)},\ell) + \eta. \end{aligned} \tag{3.58}$$

From $v^{i+1} - v^i = \ell$ for $i \geq N_1$, we deduce that the sum over $i \geq 0$ can replaced by a sum over $0 \leq i \leq N_1$ without changing the estimate. Furthermore, there exist a function $w : \mathbb{N}_0 \to \mathbb{R}$ and an $N_2 \in \mathbb{N}$ with $w^0 = 0$, $w^s - w^{s-1} = u_{1,s}^{(1)}$ for $s \in \{1,\dots,K-1\}$, $w^{i+1} - w^i = \ell$ for $i \geq N_2$ and

$$\begin{aligned}&\sum_{j=2}^K c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1\left(w^s - w^{s-1}\right) + \sum_{j=2}^K \sum_{i\geq 0} \Bigg\{ J_j\left(\frac{w^{i+j}-w^i}{j}\right) \\ &\quad + \frac{c_j}{j}\sum_{s=i}^{i+j-1} J_1\left(w^{s+1}-w^s\right) - \psi_j'(\ell)\left(\frac{w^{i+j}-w^i}{j} - \ell\right) - \psi_j(\ell)\Bigg\} \\ &\quad \leq B(u_1^{(1)},\ell) + \eta. \end{aligned} \tag{3.59}$$

As in the estimate corresponding to $B(u_0^{(1)},\ell)$, we can replace the infinite sum by the sum over $0 \leq i \leq N_2$. We construct a recovery sequence (u_n) for u by means of v and w:

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

By the definition of u_n, v, and w, we have $u_n^0 = 0$ and $u_n^n = \ell$. Moreover, it holds

$$u_n^{s+1} - u_n^s = \lambda_n(v^s - v^{s-1}) = \lambda_n u_{0,s}^{(1)},$$
$$u_n^{n+1-s} - u_n^{n-s} = -\lambda_n(w^{s-1} - w^s) = \lambda_n u_{1,s}^{(1)},$$

for $i \in \{1, \dots, K-1\}$. Hence, we have that u_n satisfies the boundary conditions (3.3). Let us show that $\limsup_{n\to\infty} H_{1,n}^\ell(u_n) \le H_1^\ell(u) + 2\eta$. From (3.58), (3.59) and the definition of u_n we deduce:

$$\begin{aligned}
&\sum_{j=2}^K c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1\left(\frac{u_n^s - u_n^{s-1}}{\lambda_n}\right) + \sum_{j=2}^K \sum_{i=0}^{N_1} \sigma_{j,n}^i(\ell) \\
&= \sum_{j=2}^K c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1\left(v^s - v^{s-1}\right) + \sum_{j=2}^K \sum_{i=0}^{N_1} \Bigg\{ J_j\left(\frac{v^{i+j} - v^i}{j}\right) \\
&+ \frac{c_j}{j} \sum_{s=i}^{i+j-1} J_1(v^{s+1} - v^s) - \psi_j'(\ell)\left(\frac{v^{i+j} - v^i}{j} - \ell\right) - \psi_j(\ell)\Bigg\} \le B(u_0^{(1)}, \ell) + \eta. \qquad (3.60)
\end{aligned}$$

Similarly, we obtain

$$\begin{aligned}
&\sum_{j=2}^K c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1\left(\frac{u_n^{n+1-s} - u_n^{n-s}}{\lambda_n}\right) + \sum_{j=2}^K \sum_{i=n-N_2-K}^{n-j} \sigma_{j,n}^i(\ell) \\
&= \sum_{j=2}^K c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1\left(w^s - w^{s-1}\right) + \sum_{j=2}^K \sum_{i=0}^{N_2+K-j} \Bigg\{ J_j\left(\frac{w^{i+j} - w^i}{j}\right) \\
&+ \frac{c_j}{j} \sum_{s=i}^{i+j-1} J_1(w^{s+1} - w^s) - \psi_j'(\ell)\left(\frac{w^{i+j} - w^i}{j} - \ell\right) - \psi_j(\ell)\Bigg\} \le B(u_1^{(1)}, \ell) + \eta. \qquad (3.61)
\end{aligned}$$

Thus it remains to show that

$$\lim_{n\to\infty} \sum_{j=2}^K \sum_{i=N_1+1}^{n-N_2-K-1} \sigma_{j,n}^i = 0.$$

For $N_1 + K \le i \le n - N_2 - K - 1$, we have

$$\begin{aligned}
\frac{u_n^{i+1} - u_n^i}{\lambda_n} =& \frac{\ell - \lambda_n(w^{N_2+K} + v^{N_1+K})}{\lambda_n(n - N_1 - N_2 - 2K)} \\
=& \ell + \lambda_n \frac{\ell(N_1 - N_2 - 2K) - (w^{N_2+K} + v^{N_1+K})}{1 - \lambda_n(N_1 + N_2 + 2K)} = \ell + \frac{c + d_n}{n}, \qquad (3.62)
\end{aligned}$$

with some constant c independent of n and a sequence (d_n) such that $\lim_{n\to\infty} d_n = 0$ (notice: $\frac{a}{n-b} - \frac{a}{n} = \frac{ba}{n(n-b)}$). Fix $j \in \{2, \dots, K\}$. For $N_1 + K \le i \le n - N_2 - K - j$, we have

$$\begin{aligned}\sigma^i_{j,n}(\ell) =& J_j\left(\ell+\frac{c+d_n}{n}\right)+c_jJ_1\left(\ell+\frac{c+d_n}{n}\right)-\psi_j(\ell)-\psi_j'(\ell)\frac{c+d_n}{n}\\ =&\psi_j\left(\ell+\frac{c+d_n}{n}\right)-\psi_j(\ell)-\psi_j'(\ell)\frac{c+d_n}{n}\\ =&(\psi_j'(\xi_{j,n})-\psi_j'(\ell))\frac{c+d_n}{n}\end{aligned}$$

with $\xi_{j,n}\in[\ell,\ell+\frac{c+d_n}{n}]$. By combining the above estimates with the Hölder continuity of J_j, see (LJ1), we deduce that there exist $\tilde{c}>0$ and $\alpha\in(0,1)$ such that

$$\begin{aligned}\sum_{j=2}^{K}\sum_{i=N_1+K}^{n-N_2-K-j}\sigma^i_{j,n}(\ell)\leq&\sum_{j=2}^{K}\sum_{i=N_1+K}^{n-N_2-K-j}|\sigma^i_{j,n}(\ell)|\\ \leq& K\sum_{i=N_1+K}^{n-N_2-K-j}\frac{\tilde{c}}{n^{1+\alpha}}=\mathcal{O}\left(\frac{1}{n^\alpha}\right)\to 0 \text{ as } n\to\infty.\end{aligned}$$

Thus, it is left to estimate the terms $\sigma^i_{j,n}(\ell)$ with $j\in\{2,\dots,K\}$ and $i\in\{N_1+1,\dots,N_1+K-1\}\cup\{n-N_2-K-j+1,\dots,n-N_2-K-1\}$. By the definition of v and w, we have that $u_n^{i+1}-u_n^i=\lambda_n\ell$ for $i\in\{N_1,\dots,N_1+K-1\}\cup\{n-N_2-K,\dots,n-N_2-1\}$. Combining this with (3.62) and (3.14), we obtain that $\sigma^i_{j,n}\to 0$ as $n\to\infty$ for $i\in\{N_1+1,\dots,N_1+K-1\}\cup\{N_2-K-j+1,\dots,n-N_2-K-1\}$. This proves the convergence of the energy. It is left to show that $u_n\to u$ in $L^\infty(0,1)$. Using (3.62) and the definition of u_n, we obtain that $u_n'\to\ell$ in $L^1(0,1)$. Since $u_n(0)=0$ for all n this yields $u_n\to u$ in $L^\infty(0,1)$ and the assertion is proven. □

Remark 3.13. For given $\theta\in\mathbb{R}^{K-1}_+$, we have

$$B(\theta,\gamma)\geq\sum_{j=2}^{K}c_j\sum_{s=1}^{j-1}\frac{j-s}{j}J_1(\theta_s).$$

Note that we used here that the terms in the infinite sum of the definition of $B(\theta,\ell)$, see (3.50), are non-negative. In the special case $0<\ell\leq\gamma$ and $\theta^\ell=(\theta^\ell_s)_{s=1}^{K-1}$ with $\theta^\ell_s=\ell$ for $1\leq s<K$, the above lower bound for $B(\theta^\ell,\ell)$ is attained by $u^i=\ell i$ for $i\geq 0$. Hence,

$$B(\theta^\ell,\ell)=\sum_{j=2}^{K}c_j\sum_{s=1}^{j-1}\frac{j-s}{j}J_1(\ell)=\frac{1}{2}J_1(\ell)\sum_{j=2}^{K}(j-1)c_j. \tag{3.63}$$

The following corollary is a direct consequence of Theorem 3.12 and (3.63).

Corollary 3.14. *Suppose that hypotheses (LJ1)–(LJ5) are satisfied. Let $0<\ell\leq\gamma$ and let $u_0^{(1)},u_1^{(1)}\in\mathbb{R}^{K-1}_+$ be such that $u_{0,s}^{(1)}=u_{1,s}^{(1)}=\ell$ for all $s\in\{1,\dots,K-1\}$. Then the*

Γ-limit H_1^ℓ, see (3.51), of $(H_{1,n}^\ell)$ is given by

$$H_1^\ell(u) = \begin{cases} -\sum_{j=2}^K (j-1)J_j(\ell) & \text{if } u(x) = \ell x, \\ +\infty & \text{else} \end{cases}$$

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

Proof. From (3.14), (3.51) and (3.63), we obtain for $u_0^{(1)}, u_1^{(1)} \in \mathbb{R}_+^{K-1}$ such that $u_{0,s}^{(1)} = u_{1,s}^{(1)} = \ell$ for $1 \le s < K$ that

$$H_1^\ell(u) = J_1(\ell)\sum_{j=2}^K (j-1)c_j - \sum_{j=2}^K (j-1)(J_j(\ell) + c_j J_1(\ell)) = -\sum_{j=2}^K (j-1)J_j(\ell),$$

if $u(x) = \ell x$, and $+\infty$ otherwise. This finishes the proof. □

Next, we show that the energy H_1^ℓ given in Theorem 3.12 is independent of $c = (c_j)_{j=2}^K$.

Proposition 3.15. *Let $J_1, \dots, J_K$ satisfy (LJ1)–(LJ5). Let $0 < \ell \le \gamma$ and $u_0^{(1)}, u_1^{(1)} \in \mathbb{R}_+^{K-1}$. Then the functional H_1^ℓ, given in (3.51), reads*

$$H_1^\ell(u) = \begin{cases} \widetilde{B}(u_0^{(1)}, \ell) + \widetilde{B}(u_1^{(1)}, \ell) - \sum_{j=2}^K (j-1)J_j(\ell) & \text{if } u(x) = \ell x, \\ +\infty & \text{otherwise,} \end{cases}$$

where for $0 < \ell \le \gamma$ and $\theta \in \mathbb{R}_+^{K-1}$ the boundary layer energy $\widetilde{B}(\theta, \ell)$ is given by

$$\begin{aligned} \widetilde{B}(\theta,\ell) := \inf_{\substack{N\in\mathbb{N}\\ N \ge K-1}} \min \Bigg\{ & \sum_{i \ge 0}\sum_{j=1}^K \left\{ J_j\left(\frac{u^{i+j}-u^i}{j}\right) - J_j(\ell) - J_j'(\ell)\left(\frac{u^{i+j}-u^i}{j} - \ell\right)\right\} \\ & - \sum_{j=2}^K \sum_{s=1}^{j-1} \frac{j-s}{j} J_j'(\ell)\,(\theta_s - \ell) : u : \mathbb{N}_0 \to \mathbb{R},\ u^0 = 0, \\ & u^s - u^{s-1} = \theta_s \text{ if } 1 \le s \le K-1,\ u^{i+1} - u^i = \ell \text{ if } i \ge N \Bigg\}. \end{aligned} \tag{3.64}$$

Proof. For given $0 < \ell \le \gamma$ and $\theta \in \mathbb{R}_+^{K-1}$, we prove that

$$B(\theta,\ell) - \frac{1}{2}J_1(\ell)\sum_{j=2}^K (j-1)c_j - \sum_{j=2}^K\sum_{s=1}^{j-1}\frac{j-s}{j}\psi_j'(\ell)(\theta_s - \ell) = \widetilde{B}(\theta,\ell), \tag{3.65}$$

where $B(\theta,\ell)$ is given in (3.50). The combination of (3.65), $\psi_j(\ell) = J_j(\ell) + c_j J_1(\ell)$, see (3.14), and the definition of H_1^ℓ (see (3.51)) implies the assertion.

Fix $0 < \ell \leq \gamma$ and $\theta \in \mathbb{R}_+^{K-1}$. Let us show (3.65). To simplify the notation, we define for $j \in \{1, \dots, K\}$ the functions $\Phi_j^\ell : \mathbb{R} \to \mathbb{R} \cup \{+\infty\}$ by

$$\Phi_j^\ell(z) := J_j(z) - J_j(\ell) - J_j'(\ell)(z - \ell). \tag{3.66}$$

Let $u : \mathbb{N}_0 \to \mathbb{R}$ be a candidate for the minimum problems defining $B(\theta, \ell)$ and $\widetilde{B}(\theta, \ell)$, i.e. $u^0 = 0$, $u^s - u^{s-1} = \theta_s$ if $s \in \{1, \dots, K-1\}$ and there exists an $N \in \mathbb{N}$ such that $u^{i+1} - u^i = \ell$ for $i \geq N$. We show that

$$\begin{aligned}
&\sum_{j=2}^{K} \sum_{i \geq 0} \left\{ J_j\left(\frac{u^{i+j} - u^i}{j}\right) + \frac{c_j}{j} \sum_{s=i}^{i+j-1} J_1\left(u^{s+1} - u^s\right) - \psi_j(\ell) - \psi_j'(\ell)\left(\frac{u^{i+j} - u^i}{j} - \ell\right) \right\} \\
&\quad + \sum_{j=2}^{K} c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(\theta_s) - \frac{1}{2} J_1(\ell) \sum_{j=2}^{K} (j-1) c_j - \sum_{j=2}^{K} \sum_{s=1}^{j-1} \frac{j-s}{j} \psi_j'(\ell)(\theta_s - \ell) \\
&= \sum_{i \geq 0} \sum_{j=1}^{K} \Phi_j^\ell\left(\frac{u^{i+j} - u^i}{j}\right) - \sum_{j=2}^{K} \sum_{s=1}^{j-1} \frac{j-s}{j} J_j'(\ell)(\theta_s - \ell).
\end{aligned} \tag{3.67}$$

This finishes the proof of the proposition. Indeed, by the definition of $B(\theta, \ell)$, $\widetilde{B}(\theta, \ell)$ and Φ_j^ℓ, see (3.50), (3.64) and (3.66), and the arbitrariness of the test function u, the equality (3.67) implies (3.65) and thus the assertion is proven.

By the definition of Φ_j^ℓ, see (3.66), it holds $\Phi_j^\ell(\ell) = 0$. Hence, using (3.14), $u^{i+1} - u^i = \ell$ for $i \geq N$ and $\frac{u^{i+j} - u^i}{j} - \ell = \frac{1}{j} \sum_{s=i}^{i+j-1} (u^{s+1} - u^s - \ell)$ for $j \in \{2, \dots, K\}$, we can rewrite the infinite sum on the left-hand side in (3.67) in terms of Φ_j^ℓ as follows

$$\begin{aligned}
&\sum_{j=2}^{K} \sum_{i \geq 0} \left\{ J_j\left(\frac{u^{i+j} - u^i}{j}\right) + \frac{c_j}{j} \sum_{s=i}^{i+j-1} J_1\left(u^{s+1} - u^s\right) - \psi_j(\ell) - \psi_j'(\ell)\left(\frac{u^{i+j} - u^i}{j} - \ell\right) \right\} \\
&= \sum_{j=2}^{K} \sum_{i=0}^{N-1} \left\{ \Phi_j^\ell\left(\frac{u^{i+j} - u^i}{j}\right) + \frac{c_j}{j} \sum_{s=i}^{i+j-1} \Phi_1^\ell\left(u^{s+1} - u^s\right) \right\} \\
&= \sum_{i=0}^{N-1} \sum_{j=2}^{K} \Phi_j^\ell\left(\frac{u^{i+j} - u^i}{j}\right) + \sum_{j=2}^{K} \frac{c_j}{j} \sum_{i=0}^{N-1} \sum_{s=i}^{i+j-1} \Phi_1^\ell\left(u^{s+1} - u^s\right).
\end{aligned} \tag{3.68}$$

The nearest neighbour terms on the right-hand side above can be rewritten as

$$\begin{aligned}
&\sum_{j=2}^{K} \frac{c_j}{j} \sum_{i=0}^{N-1} \sum_{s=i}^{i+j-1} \Phi_1^\ell\left(u^{s+1} - u^s\right) = \sum_{j=2}^{K} \frac{c_j}{j} \sum_{s=0}^{j-1} \sum_{i=s}^{N+s-1} \Phi_1^\ell\left(u^{i+1} - u^i\right) \\
&= \sum_{j=2}^{K} \frac{c_j}{j} \sum_{s=0}^{j-1} \left\{ \sum_{i=0}^{N-1} \Phi_1^\ell\left(u^{i+1} - u^i\right) - \sum_{i=0}^{s-1} \Phi_1^\ell\left(u^{i+1} - u^i\right) + \sum_{i=N}^{N+s-1} \Phi_1^\ell\left(u^{i+1} - u^i\right) \right\} \\
&= \sum_{j=2}^{K} c_j \sum_{i=0}^{N-1} \Phi_1^\ell\left(u^{i+1} - u^i\right) - \sum_{j=2}^{K} \frac{c_j}{j} \sum_{s=0}^{j-1} \sum_{i=0}^{s-1} \Phi_1^\ell\left(u^{i+1} - u^i\right).
\end{aligned}$$

Note that we used $u^{i+1}-u^i=\ell$ and thus $\Phi_1^\ell(u^{i+1}-u^i)=0$ for $i\geq N$. Since $u^i-u^{i-1}=\theta_i$ for $i\in\{1,\ldots,K-1\}$, we obtain that

$$\sum_{j=2}^{K}\frac{c_j}{j}\sum_{s=0}^{j-1}\sum_{i=0}^{s-1}\Phi_1^\ell\left(u^{i+1}-u^i\right)=\sum_{j=2}^{K}\frac{c_j}{j}\sum_{i=0}^{j-2}\sum_{s=i+1}^{j}\Phi_1^\ell\left(u^{i+1}-u^i\right)=\sum_{j=2}^{K}c_j\sum_{i=1}^{j-1}\frac{j-i}{j}\Phi_1^\ell\left(\theta_i\right).$$

Hence, using $\sum_{j=2}^K c_j=1$ and the definition of Φ_1^ℓ, the right-hand side of (3.68) reads

$$\sum_{i=0}^{N-1}\sum_{j=1}^{K}\Phi_j^\ell\left(\frac{u^{i+j}-u^i}{j}\right)-\sum_{j=2}^{K}c_j\sum_{i=1}^{j-1}\frac{j-i}{j}\left(J_1(\theta_i)-J_1(\ell)-J_1'(\ell)(\theta_i-\ell)\right).$$

Altogether, we have

$$\begin{aligned}
&\sum_{j=2}^{K}\sum_{i\geq 0}\left\{J_j\left(\frac{u^{i+j}-u^i}{j}\right)+\frac{c_j}{j}\sum_{s=i}^{i+j-1}J_1\left(u^{s+1}-u^s\right)-\psi_j(\ell)-\psi_j'(\ell)\left(\frac{u^{i+j}-u^i}{j}-\ell\right)\right\}\\
&\quad+\sum_{j=2}^{K}c_j\sum_{s=1}^{j-1}\frac{j-s}{j}J_1\left(\theta_s\right)-\frac{1}{2}J_1(\ell)\sum_{j=2}^{K}(j-1)c_j-\sum_{j=2}^{K}\sum_{s=1}^{j-1}\frac{j-s}{j}\psi_j'(\ell)(\theta_s-\ell)\\
&=\sum_{i=0}^{N-1}\sum_{j=1}^{K}\Phi_j^\ell\left(\frac{u^{i+j}-u^i}{j}\right)+\sum_{j=2}^{K}c_j\sum_{s=1}^{j-1}\frac{j-s}{j}\left(J_1(\ell)+J_1'(\ell)(\theta_s-\ell)\right)\\
&\quad-\frac{1}{2}J_1(\ell)\sum_{j=2}^{K}(j-1)c_j-\sum_{j=2}^{K}\sum_{s=1}^{j-1}\frac{j-s}{j}\left(J_j'(\ell)+c_jJ_1'(\ell)\right)(\theta_s-\ell)\\
&=\sum_{i=0}^{N-1}\sum_{j=1}^{K}\Phi_j^\ell\left(\frac{u^{i+j}-u^i}{j}\right)-\sum_{j=2}^{K}\sum_{s=1}^{j-1}\frac{j-s}{j}J_j'(\ell)(\theta_s-\ell)\\
&=\sum_{i\geq 0}\sum_{j=1}^{K}\Phi_j^\ell\left(\frac{u^{i+j}-u^i}{j}\right)-\sum_{j=2}^{K}\sum_{s=1}^{j-1}\frac{j-s}{j}J_j'(\ell)(\theta_s-\ell),
\end{aligned}$$

which proves (3.67). □

Remark 3.16. Note that in the special case $\ell=\gamma$, the terms involving $J_j'(\ell)$ in the definition of $\widetilde{B}(\theta,\ell)$ cancel out. Thus for given $\theta\in\mathbb{R}_+^{K-1}$, we have

$$\begin{aligned}
\widetilde{B}(\theta,\gamma)=\inf_{\substack{N\in\mathbb{N}\\ N\geq K-1}}\min\Bigg\{&\sum_{i\geq 0}\left\{\sum_{j=1}^{K}J_j\left(\frac{v^{i+j}-v^i}{j}\right)-J_{CB}(\gamma)\right\}:\ v:\mathbb{N}_0\to\mathbb{R},\\
&v^0=0,\ v^s-v^{s-1}=\theta_i\text{ if }1\leq s<K,\ v^{i+1}-v^i=\gamma\text{ if }i\geq N\Bigg\}.
\end{aligned}\tag{3.69}$$

By the definition $J_{CB}\equiv\sum_{j=1}^K J_j$, we only have to show that the terms involving $J_j'(\ell)$ in the definition (3.64) vanish if $\ell=\gamma$. Indeed, let u be a test function for the infimum problem in the definition of $\widetilde{B}(\theta,\gamma)$, i.e. $u^0=0$, $u^s-u^{s-1}=\theta_s$ if $1\leq s\leq K-1$ and there exists an $N \in \mathbb{N}$ such that $u^{i+1} - u^i = \gamma$ for $i \geq N$. Then we have

$$\begin{aligned}
-\sum_{i\geq 0}\sum_{j=1}^{K} J_j'(\gamma)\left(\frac{u^{i+j}-u^i}{j}-\gamma\right) &= -\sum_{j=1}^{K}\sum_{i=0}^{N-1} J_j'(\gamma)\frac{1}{j}\sum_{s=0}^{j-1}\left(u^{s+i+1}-u^{s+i}-\gamma\right)\\
&= -\sum_{j=1}^{K}\frac{1}{j}J_j'(\gamma)\sum_{s=0}^{j-1}\sum_{i=s}^{N-1+s}(u^{i+1}-u^i-\gamma)\\
&= -\sum_{j=1}^{K}J_j'(\gamma)\sum_{i=0}^{N-1}(u^{i+1}-u^i-\gamma)+\sum_{j=1}^{K}\frac{1}{j}J_j'(\gamma)\sum_{s=0}^{j-1}\sum_{i=0}^{s-1}(u^{i+1}-u^i-\gamma)\\
&= \sum_{j=2}^{K}\sum_{i=1}^{j-1}\frac{j-i}{j}J_j'(\gamma)(\theta_i-\gamma),
\end{aligned}$$

where we used $u^i - u^{i-1} = \theta_i$ for $1 \leq i \leq K-1$ and $\sum_{j=1}^{K} J_j'(\gamma) = J_{CB}'(\gamma) = 0$. Combining the above calculation with the definition of $\widetilde{B}(\theta,\gamma)$ in (3.64), we obtain that $\widetilde{B}(\theta,\gamma)$ is given as in (3.69).

3.3.2 The case $\ell > \gamma$

In analogy to [11, 50], we have fracture in the case $\ell > \gamma$, cf. Proposition 3.9. The presence of fracture yields additional boundary layer energies. These energies are generalisations of the boundary layer energies provided in [50] for the case of nearest and next-to-nearest neighbour interactions. For given $\theta \in \mathbb{R}_+^{K-1}$, we define

$$\begin{aligned}
B_b(\theta) := \inf_{\substack{k\in\mathbb{N}\\ k\geq K-1}} \min\Bigg\{ &\sum_{j=2}^{K} c_j \sum_{s=1}^{j-1}\frac{j-s}{j}J_1\left(v^s - v^{s-1}\right) + \sum_{j=2}^{K}\sum_{i=0}^{k-j}\Bigg\{J_j\left(\frac{v^{i+j}-v^i}{j}\right)\\
&+\frac{c_j}{j}\sum_{s=i}^{i+j-1}J_1\left(v^{s+1}-v^s\right) - \psi_j(\gamma)\Bigg\} :\ v:\mathbb{N}_0\to\mathbb{R}, v^k = 0,\\
&v^{k+1-s}-v^{k-s} = \theta_s \text{ if } s\in\{1,\dots,K-1\}\Bigg\}. \qquad (3.70)
\end{aligned}$$

Remark 3.17. The boundary layer energy $B_b(\theta)$ can be interpreted as follows: if fracture occurs at the boundary on a macroscopic scale then $B_b(\theta)$ yields the optimal distance from the boundary on a microscopic scale. By (3.8) and since γ denotes the unique minimum point of $J_{0,j}$ with $J_{0,j}(\gamma) = \psi_j(\gamma)$, we have that the terms in the sum from $i = 0$ to $i = k - j$ are non-negative. In the case of nearest and next-to-nearest neighbour interactions, the definition of $B_b(\theta)$ coincides with the boundary layer energy given in [50, eq. (4.27)].

Next, we introduce the boundary layer energy of a free boundary $B(\gamma)$, defined by

$$B(\gamma) := \inf_{N\in\mathbb{N}_0} \min\Big\{ \sum_{j=2}^{K} c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1\left(u^s - u^{s-1}\right) + \sum_{j=2}^{K}\sum_{i\geq 0} \Big\{ J_j\left(\frac{u^{i+j}-u^i}{j}\right) + \frac{c_j}{j}\sum_{s=i}^{i+j-1} J_1\left(u^{s+1}-u^s\right) - \psi_j(\gamma)\Big\} :\ u:\mathbb{N}_0\to\mathbb{R}, u^0 = 0, u^{i+1}-u^i = \gamma \text{ if } i\geq N\Big\}. \tag{3.71}$$

Remark 3.18. The same arguments as above yield that the terms in the infinite sum over $i \geq 0$ are non-negative. In the case of nearest and next-to-nearest neighbour interactions the definition of $B(\gamma)$ coincides with the boundary layer energies, also denoted by $B(\gamma)$ in [11, 50].

Before we state the Γ-convergence result for $H^\ell_{1,n}$, we note that the definition of the elastic boundary layer energy $B(\theta,\gamma)$ in (3.50) reads

$$B(\theta,\gamma) = \inf_{\substack{N\in\mathbb{N}\\ N\geq K-1}} \min\Big\{ \sum_{j=2}^{K} c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1\left(v^s - v^{s-1}\right) + \sum_{j=2}^{K}\sum_{i\geq 0} \Big\{ J_j\left(\frac{v^{i+j}-v^i}{j}\right) + \frac{c_j}{j}\sum_{s=i}^{i+j-1} J_1\left(v^{s+1}-v^s\right) - \psi_j(\gamma)\Big)\Big\} :\ v:\mathbb{N}_0\to\mathbb{R},\ v^0=0, v^s - v^{s-1} = \theta_i \text{ if } s\in\{1,\dots,K-1\},\, v^{i+1}-v^i = \gamma \text{ if } i\geq N\Big\}, \tag{3.72}$$

for $\theta \in \mathbb{R}^{K-1}_+$, where we have used $\psi_j'(\gamma) = 0$.

Theorem 3.19. *Suppose that hypotheses (LJ1)–(LJ5) hold. Let $\ell > \gamma$ and $u_0^{(1)}, u_1^{(1)} \in \mathbb{R}^{K-1}_+$. Then $(H^\ell_{1,n})$ Γ-converges with respect to the $L^1(0,1)$-topology to the functional H^ℓ_1 defined by*

$$H_1^\ell(u) = \begin{cases} B(u_0^{(1)},\gamma)(1-\#(S_u\cap\{0\})) + B_{BJ}(u_0^{(1)})\#(S_u\cap\{0\}) \\ \quad + B_{IJ}\#(S_u\cap(0,1)) + B_{BJ}(u_1^{(1)})\#(S_u\cap\{1\}) \\ \quad + B(u_1^{(1)},\gamma)(1-\#(S_u\cap\{1\})) - \sum_{j=2}^{K}(j-1)\psi_j(\gamma) & \text{if } u\in SBV^\ell_c(0,1), \\ +\infty & \text{else} \end{cases} \tag{3.73}$$

on $L^1(0,1)$, where, for $\theta\in\mathbb{R}^{K-1}_+$,

$$B_{BJ}(\theta) = \sum_{j=2}^{K} c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(\theta_s) + B_b(\theta) + B(\gamma) - \sum_{j=2}^{K} j\psi_j(\gamma) \tag{3.74}$$

is the boundary layer energy due to a jump at the boundary and

$$B_{IJ} = 2B(\gamma) - \sum_{j=2}^{K} j\psi_j(\gamma) \tag{3.75}$$

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

Remark 3.20. Note that in the case $K = 2$, the limiting functional H_1^ℓ coincides with the one which is derived in [50, Theorem 4.2].

Proof. Liminf inequality. As in the proof of [50, Theorem 4.2] for the case $K = 2$, we assume, without loss of generality, that there exists only one jump point. By symmetry it is sufficient to distinguish between a jump in 0 or $(0, 1)$.

Jump at 0. Let u and (u_n) be such that $S_u = \{0\}$ and $u_n \to u$ in $L^1(0, 1)$ with $\sup_n H_{1,n}^\ell(u_n) < \infty$. By Proposition 3.9, we have

$$u(x) = \begin{cases} 0 & \text{if } x = 0, \\ \gamma x + (\ell - \gamma) & \text{if } x \in (0, 1]. \end{cases} \tag{3.76}$$

We prove that

$$\begin{aligned} \liminf_{n\to\infty} H_{1,n}^\ell(u_n) \geq & \sum_{j=2}^{K} c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(u_{0,s}^{(1)}) + B_b(u_0^{(1)}) + B(\gamma) \\ & + B(u_1^{(1)}, \gamma) - \sum_{j=2}^{K} (2j-1)\psi_j(\gamma). \end{aligned} \tag{3.77}$$

From (3.41), $\psi_j^{**}(\ell) = \psi_j(\gamma)$ and $\psi_j'(\ell) = 0$ for $\ell \geq \gamma$, we deduce that

$$H_{1,n}^\ell(u_n) = \sum_{j=2}^{K} \sum_{i=0}^{n-j} \sigma_{j,n}^i(\gamma) + \sum_{j=2}^{K} c_j \sum_{s=1}^{j-1} \frac{j-s}{j} \left(J_1(u_{0,s}^{(1)}) + J_1(u_{1,s}^{(1)}) \right) - \sum_{j=2}^{K} (j-1)\psi_j(\gamma). \tag{3.78}$$

By Lemma 3.11 there exist $(T_n^0), (T_n^1) \subset \mathbb{N}$ such that $\lim_{n\to\infty} \lambda_n T_n^0 = 0$, $\lim_{n\to\infty} \lambda_n T_n^1 = 1$ and

$$\lim_{n\to\infty} \frac{u_n^{T_n^i+1+s} - u_n^{T_n^i+s}}{\lambda_n} = \gamma, \quad \text{for } i \in \{0, 1\} \text{ and } 0 \leq s \leq K-1. \tag{3.79}$$

Let us first show the estimate regarding the elastic boundary layer energy at 1. This can be done exactly as in proof of Theorem 3.12. We define w_n as

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

In the same way as (3.57), we prove that

$$\liminf_{n\to\infty}\sum_{j=2}^{K}\left\{c_j\sum_{s=1}^{j-1}\frac{j-s}{j}J_1(u_{1,s}^{(1)})+\sum_{i=T_n^1+1}^{n-j}\sigma_{j,n}^i(\gamma)\right\}\geq B(u_1^{(1)},\gamma). \tag{3.80}$$

By (3.78), $\sigma_{j,n}^i(\gamma)\geq 0$, and the definition of $B_{BJ}(u_0^{(1)})$, it is left to show that

$$\liminf_{n\to\infty}\sum_{j=2}^{K}\sum_{i=0}^{T_n^0}\sigma_{j,n}^i(\gamma)\geq B_b(u_0^{(1)})+B(\gamma)-\sum_{j=2}^{K}j\psi_j(\gamma).$$

As in the proof of [50, Theorem 4.2], we deduce from $u_n\to u$ that there exists $(h_n)\subset\mathbb{N}$ with $\lambda_n h_n\to 0$ such that

$$\lim_{n\to\infty}\frac{u_n^{h_n+1}-u_n^{h_n}}{\lambda_n}=+\infty. \tag{3.81}$$

Indeed, since u_n converges to u almost everywhere, there exists for every $\varepsilon_0>0$ an $\varepsilon\in(0,\varepsilon_0)$ such that $u_n(\varepsilon)\to u(\varepsilon)=\varepsilon\gamma+\ell-\gamma$, see (3.76). Let us define the sequence $(q_n)\subset\mathbb{N}$ such that $\varepsilon\in\lambda_n[q_n,q_n+1)$. Using $u_n(0)=0$ for all $n\in\mathbb{N}$ and $\gamma>0$, we obtain for n sufficiently large

$$\ell-\gamma\leq\int_0^\varepsilon u_n'(x)dx=\sum_{i=0}^{q_n-1}\lambda_n\frac{u_n^{i+1}-u_n^i}{\lambda_n}+(\varepsilon-q_n\lambda_n)\frac{u_n^{q_n+1}-u_n^{q_n}}{\lambda_n}.$$

With a slight abuse of notation we set $u_n^{q_n+1}:=\max\{u_n^{q_n+1},u_n^{q_n}\}$. The above estimate and $\varepsilon-q_n\lambda_n\leq\lambda_n$ imply that there exists $0\leq i_n\leq q_n$ such that

$$\frac{u_n^{i_n+1}-u_n^{i_n}}{\lambda_n}\geq\frac{1}{q_n+1}\sum_{i=0}^{q_n}\frac{u_n^{i+1}-u_n^i}{\lambda_n}\geq\frac{\ell-\gamma}{\lambda_n(q_n+1)}\geq\frac{\ell-\gamma}{2\varepsilon_0}.$$

By $\ell-\gamma>0$ and the arbitrariness of $\varepsilon_0>0$, we deduce the existence of $(h_n)\subset\mathbb{N}$ such that $\lambda_n h_n\to 0$ and (3.81) is satisfied.

From $\sup_n H_{1,n}^\ell(u_n)<+\infty$ and $\lim_{z\to-\infty}J_j(z)=+\infty$, $J_j(z)\geq J_j(\delta_j)\in\mathbb{R}$ for $j\in\{1,\dots,K\}$, see (LJ2), we deduce the existence of $C\in\mathbb{R}$ with $\inf_n\frac{u_n^{i+1}-u_n^i}{\lambda_n}\geq C$. Thus, (3.81) implies

$$\frac{u_n^{h_n+j+s}-u_n^{h_n+s}}{j\lambda_n}\geq\frac{u_n^{h_n+1}-u_n^{h_n}}{j\lambda_n}+\frac{j-1}{j}C\to+\infty\quad\text{as } n\to\infty,$$

for $j\in\{2,\dots,K\}$ and $s\in\{0,\dots,j-1\}$. Hence, (3.9) yields $\lim_{n\to\infty}r_1(n)=0$, where $r_1(n)$ is defined by

$$r_1(n)=\sum_{j=1}^{K}\sum_{s=-j+1}^{0}J_j\left(\frac{u_n^{h_n+j+s}-u_n^{h_n+s}}{j\lambda_n}\right).$$

It is useful to rewrite the terms which involve $u_n^{h_n+1} - u_n^{h_n}$ as follows:

$$\begin{aligned}
&\sum_{j=2}^{K} \sum_{i=h_n-j+1}^{h_n} \sigma_{j,n}^i(\gamma) \\
&= \sum_{j=2}^{K} \sum_{i=h_n-j+1}^{h_n} \left\{ \frac{c_j}{j} \sum_{\substack{s=i \\ s\neq h_n}}^{i+j-1} J_1\left(\frac{u_n^{s+1}-u_n^s}{\lambda_n}\right) - \psi_j(\gamma) \right\} + r_1(n) \\
&= \sum_{k=2}^{K} c_j \sum_{s=1}^{j-1} \frac{j-s}{j} \left\{ J_1\left(\frac{u_n^{h_n+1-s}-u_n^{h_n-s}}{\lambda_n}\right) + J_1\left(\frac{u_n^{h_n+s+1}-u_n^{h_n+s}}{\lambda_n}\right) \right\} \\
&\quad - \sum_{j=2}^{K} j\psi_j(\gamma) + r_1(n) \qquad (3.82)
\end{aligned}$$

Note that the second equality follows from:

$$\begin{aligned}
\sum_{i=h_n-j+1}^{h_n} \sum_{\substack{s=i \\ s\neq h_n}}^{i+j-1} a_s &= \sum_{i=1-j}^{0} \left\{ \sum_{s=i}^{-1} a_{h_n+s} + \sum_{s=1}^{i+j-1} a_{h_n+s} \right\} = \sum_{i=1-j}^{0} \left\{ \sum_{s=1}^{-i} a_{h_n-s} + \sum_{s=1}^{i+j-1} a_{h_n+s} \right\} \\
&= \sum_{s=1}^{j-1} \left\{ \sum_{i=1-j}^{-s} a_{h_n-s} + \sum_{i=s-j+1}^{0} a_{h_n+s} \right\} = \sum_{s=1}^{j-1} (j-s)(a_{h_n-s} + a_{h_n+s})
\end{aligned}$$

with $a_s = J_1(\frac{u_n^{s+1}-u_n^s}{\lambda_n})$. Hence, we have by (3.82) that

$$\begin{aligned}
\sum_{j=2}^{K} \sum_{i=0}^{T_n^0} \sigma_{j,n}^i(\gamma) = \sum_{j=2}^{K} \Bigg\{ &\sum_{i=0}^{h_n-j} \sigma_{j,n}^i(\gamma) + c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1\left(\frac{u_n^{h_n-s+1}-u_n^{h_n-s}}{\lambda_n}\right) \\
&+ \sum_{i=h_n+1}^{T_n^0} \sigma_{j,n}^i(\gamma) + c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1\left(\frac{u_n^{h_n+s+1}-u_n^{h_n+s}}{\lambda_n}\right) \Bigg\} - \sum_{j=2}^{K} j\psi_j(\gamma) + r_1(n). \qquad (3.83)
\end{aligned}$$

It remains to show the following inequalities:

$$\sum_{j=2}^{K} \left\{ \sum_{i=0}^{h_n-j} \sigma_{j,n}^i(\gamma) + c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1\left(\frac{u_n^{h_n+1-s}-u_n^{h_n-s}}{\lambda_n}\right) \right\} \geq B_b(u_0^{(1)}), \qquad (3.84)$$

$$\sum_{j=2}^{K} \left\{ \sum_{i=h_n+1}^{T_n^0} \sigma_{j,n}^i(\gamma) + c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1\left(\frac{u_n^{h_n+s+1}-u_n^{h_n+s}}{\lambda_n}\right) \right\} \geq B(\gamma) - \omega(n), \qquad (3.85)$$

with $\lim_{n\to\infty} \omega(n) = 0$. Let us first prove inequality (3.84). We define for $0 \leq m \leq h_n$

$$\hat{w}_n^m = -\frac{1}{\lambda_n} u_n^{h_n-m}.$$

We can now rewrite the sum involving the $\sigma^i_{j,n}(\gamma)$ terms on the left-hand side of (3.84) in terms of $\hat{w}^m_n$ and obtain that

$$\begin{aligned}
&\sum_{j=2}^{K}\sum_{i=0}^{h_n-j}\sigma^i_{j,n}(\gamma)\\
&=\sum_{j=2}^{K}\sum_{m=0}^{h_n-j}\left\{J_j\left(\frac{u_n^{h_n-m}-u_n^{h_n-m-j}}{j\lambda_n}\right)+\frac{c_j}{j}\sum_{s=m}^{m+j-1}J_1\left(\frac{u_n^{h_n-s}-u_n^{h_n-s-1}}{\lambda_n}\right)-\psi_j(\gamma)\right\}\\
&=\sum_{j=2}^{K}\sum_{m=0}^{h_n-j}\left\{J_j\left(\frac{\hat{w}^{m+j}-\hat{w}^m_n}{j}\right)+\frac{c_j}{j}\sum_{s=m}^{m+j-1}J_1\left(\hat{w}^{s+1}_n-\hat{w}^s_n\right)-\psi_j(\gamma)\right\}
\end{aligned}$$

Hence, we have for the left-hand side of (3.84)

$$\begin{aligned}
&\sum_{j=2}^{K}\left\{\sum_{i=0}^{h_n-j}\sigma^i_{j,n}(\gamma)+c_j\sum_{s=1}^{j-1}\frac{j-s}{j}J_1\left(\frac{u_n^{h_n+1-s}-u_n^{h_n-s}}{\lambda_n}\right)\right\}\\
&=\sum_{j=2}^{K}\left\{c_j\sum_{s=1}^{j-1}\frac{j-s}{j}J_1\left(\hat{w}^s_n-\hat{w}^{s-1}_n\right)+\sum_{m=0}^{h_n-j}\left(J_j\left(\frac{\hat{w}^{m+j}-\hat{w}^m_n}{j}\right)\right.\right.\\
&\qquad\left.\left.+\frac{c_j}{j}\sum_{s=m}^{m+j-1}J_1\left(\hat{w}^{s+1}_n-\hat{w}^s_n\right)-\psi_j(\gamma)\right)\right\}.
\end{aligned}$$

Furthermore, it holds $\hat{w}^{h_n}_n=\frac{1}{\lambda_n}u^0_n=0$ and $\hat{w}^{h_n+1-s}_n-\hat{w}^{h_n-s}_n=\frac{1}{\lambda_n}(u^s_n-u^{s-1}_n)=u^{(1)}_{0,s}$ for $s\in\{1,\dots,K-1\}$. Hence, $\hat{w}_n$ is an admissible test function for $B_b(u^{(1)}_0)$ and thus (3.84) holds true. Let us prove (3.85). Define for $i\geq 0$:

$$\tilde{u}^i_n=\begin{cases}\frac{u_n^{h_n+1+i}-u_n^{h_n+1}}{\lambda_n} & \text{if } 0\leq i\leq T^0_n-h_n+K-1,\\ \gamma\left(i-(T^0_n-h_n+K-1)\right)+\frac{u_n^{T^0_n+K}-u_n^{h_n+1}}{\lambda_n} & \text{if } i\geq T^0_n-h_n+K-1.\end{cases}$$

We can now rewrite the left-hand side of (3.85) in terms of $\tilde{u}^i_n$:

$$\begin{aligned}
&\sum_{j=2}^{K}\left\{\sum_{i=h_n+1}^{T^0_n}\sigma^i_{j,n}(\gamma)+c_j\sum_{s=1}^{j-1}\frac{j-s}{j}J_1\left(\frac{u_n^{h_n+s+1}-u_n^{h_n+s}}{\lambda_n}\right)\right\}\\
&=\sum_{j=2}^{K}\left\{c_j\sum_{s=1}^{j-1}\frac{j-s}{j}J_1\left(\tilde{u}^s_n-\tilde{u}^{s-1}_n\right)+\sum_{i=0}^{T^0_n-h_n-1}\left\{J_j\left(\frac{\tilde{u}^{i+j}_n-\tilde{u}^i_n}{j}\right)\right.\right.\\
&\qquad\left.+\frac{c_j}{j}\sum_{s=i}^{i+j-1}J_1\left(\tilde{u}^{s+1}_n-\tilde{u}^s_n\right)-\psi_j(\gamma)\right\}
\end{aligned}$$

$$= \sum_{j=2}^{K} \Bigg\{ c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1\left(\tilde{u}_n^s - \tilde{u}_n^{s-1}\right) + \sum_{i \geq 0} \Bigg\{ J_j \left(\frac{\tilde{u}_n^{i+j} - \tilde{u}_n^i}{j} \right) + \frac{c_j}{j} \sum_{s=i}^{i+j-1} J_1\left(\tilde{u}_n^{s+1} - \tilde{u}_n^s\right) - \psi_j(\gamma) \Bigg\} \Bigg\} - \omega(n) \tag{3.86}$$

with

$$\omega(n) = \sum_{j=2}^{K} \sum_{i=T_n^0-h_n}^{T_n^0-h_n+K-2} \left\{ J_j \left(\frac{\tilde{u}_n^{i+j} - \tilde{u}_n^i}{j} \right) + \frac{c_j}{j} \sum_{s=i}^{i+j-1} J_1\left(\tilde{u}_n^{s+1} - \tilde{u}_n^s\right) - \psi_j(\gamma) \right\}.$$

Indeed, by the definition of $\tilde{u}_n$ and $J_j(\gamma) + c_j J_1(\gamma) = \psi_j(\gamma)$ the terms in the infinite sum over $i \geq 0$ in (3.86) vanish identically for $i \geq T_n^0 - h_n + K - 1$. Moreover, we deduce from (3.79) and the definition of $\tilde{u}_n$ that

$$\lim_{n\to\infty} (\tilde{u}_n^{T_n^0-h_n+s} - \tilde{u}_n^{T_n^0-h_n+s-1}) = \lim_{n\to\infty} \frac{u_n^{T_n^0+1+s} - u_n^{T_n^0+s}}{\lambda_n} = \gamma$$

for $s \in \{1, \dots, K-1\}$. Combining this with $\tilde{u}_n^{i+1} - \tilde{u}_n^i = \gamma$ for $i \geq T_n^0 - h_n + K - 1$ and the definition of ψ_j implies $\lim_{n\to\infty} \omega(n) = 0$. Thus inequality (3.85) is proven. Altogether, we deduce from (3.78), (3.80), (3.83)–(3.85) the assertion (3.77).

Internal jump. Assume that $S_u = \{\bar{t}\}$ with $\bar{t} \in (0,1)$. Let (u_n) be a sequence converging to u in $L^1(0,1)$ such that $\sup_n H_{1,n}^\ell(u_n) < +\infty$. Then Proposition 3.9 implies

$$u(t) = \begin{cases} \gamma x & \text{if } 0 \leq x < \bar{t}, \\ \gamma x + \ell - \gamma & \text{if } \bar{t} < x \leq 1. \end{cases} \tag{3.87}$$

We prove that

$$\liminf_{n\to\infty} H_{1,n}^\ell(u_n) \geq B(u_0^{(1)}, \gamma) + B(u_1^{(1)}, \gamma) + 2B(\gamma) - \sum_{j=2}^{K} (2j-1)\psi_j(\gamma). \tag{3.88}$$

From Lemma 3.11, we deduce the existence of sequences $(T_n^0), (T_n^1) \subset \mathbb{N}$ such that $\lim_{n\to\infty} \lambda_n T_n^0 = 0$, $\lim_{n\to\infty} \lambda_n T_n^1 = 1$ satisfying (3.79). As in the elastic case, see (3.55) and (3.57), we obtain:

$$\liminf_{n\to\infty} \sum_{j=2}^{K} \left(c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(u_{0,s}^{(1)}) + \sum_{i=0}^{T_n^0} \sigma_{j,n}^i(\gamma) \right) \geq B(u_0^{(1)}, \gamma), \tag{3.89}$$

$$\liminf_{n\to\infty} \sum_{j=2}^{K} \left(c_j \sum_{s=1}^{j} \frac{j-s}{j} J_1(u_{1,s}^{(1)}) + \sum_{i=T_n^1+1}^{n-j} \sigma_{j,n}^i(\gamma) \right) \geq B(u_1^{(1)}, \gamma). \tag{3.90}$$

Furthermore, as in the case of a jump in 0 there exists a sequence $(h_n) \subset \mathbb{N}$ such that $\lim_{n\to\infty} \lambda_n h_n = \bar{t}$ and

$$\lim_{n\to\infty} \frac{u_n^{h_n+1} - u_n^{h_n}}{\lambda_n} = +\infty. \tag{3.91}$$

Indeed, we can apply a similar argument as for a jump in 0. We only give a sketch of the reasoning here. Fix $\varepsilon > 0$. Since $u_n \to u$ almost everywhere there exist t_1, t_2 with $t_1 \in (\bar{t}-\varepsilon, \bar{t})$ and $t_2 \in (\bar{t}, \bar{t}+\varepsilon)$ such that $u_n(t_1) \to u(t_1) = \gamma t_1$ and $u_n(t_2) \to u(t_2) = \gamma t_2 + \ell - \gamma$, see (3.87). Thus, we have for n sufficiently large that $u_n(t_1) \le \gamma \bar{t}$ and $u_n(t_2) \ge \gamma \bar{t} + \ell - \gamma$. Hence, we have

$$\ell - \gamma \le u_n(t_2) - u_n(t_1) = \int_{t_1}^{t_2} u_n'(x)dx.$$

Now we can rewrite the above inequality in terms of the discrete derivatives of u_n and obtain that there exists i_n with $\lambda_n i_n \in (t-\varepsilon, t+\varepsilon)$ such that

$$\frac{\ell - \gamma}{4\varepsilon} \le \frac{u_n^{i_n+1} - u_n^{i_n}}{\lambda_n}.$$

The claim follows from $\ell - \gamma > 0$ and the arbitrariness of $\varepsilon > 0$.

From (3.91) and similar calculations as in (3.82) and (3.83), we obtain that

$$\begin{aligned}\sum_{j=2}^{K} \sum_{i=T_n^0+1}^{T_n^1} \sigma_{j,n}^i(\gamma) = \sum_{j=2}^{K} \Bigg\{ &\sum_{i=T_n^0+1}^{h_n-j} \sigma_{j,n}^i(\gamma) + c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1\left(\frac{u_n^{h_n-s+1} - u_n^{h_n-s}}{\lambda_n}\right) \\ &+ \sum_{h_n+1}^{T_n^1} \sigma_{j,n}^i(\gamma) + c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1\left(\frac{u_n^{h_n+s+1} - u_n^{h_n+s}}{\lambda_n}\right)\Bigg\} - \sum_{j=2}^{K} j\psi_j(\gamma) + r(n),\end{aligned} \tag{3.92}$$

where

$$r(n) = \sum_{j=1}^{K} \sum_{s=-j+1}^{0} J_j\left(\frac{u_n^{h_n+j+s} - u_n^{h_n+s}}{j\lambda_n}\right) \to 0 \quad \text{as } n \to \infty.$$

Thus, it remains to prove that

$$\sum_{j=2}^{K} \Bigg\{ \sum_{i=T_n^0+1}^{h_n-j} \sigma_{j,n}^i(\gamma) + c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1\left(\frac{u_n^{h_n-s+1} - u_n^{h_n-s}}{\lambda_n}\right)\Bigg\} \ge B(\gamma) - r_1(n), \tag{3.93}$$

$$\sum_{j=2}^{K} \Bigg\{ \sum_{i=h_n+1}^{T_n^1} \sigma_{j,n}^i(\gamma) + c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1\left(\frac{u_n^{h_n+s+1} - u_n^{h_n+s}}{\lambda_n}\right)\Bigg\} \ge B(\gamma) - r_2(n), \tag{3.94}$$

with $r_1(n), r_2(n) \to 0$ as $n \to \infty$. Since inequality (3.94) can be proven exactly as (3.85), we only show (3.93). Note that also this estimate follows by very similar arguments as we have used to show (3.85). We define for $i \geq 0$

$$\tilde{u}_n^i = \begin{cases} \frac{u_n^{h_n} - u_h^{h_n - i}}{\lambda_n} & \text{if } 0 \leq i \leq h_n - T_n^0 - 1, \\ \gamma(i - h_n + T_n^0 + 1) + \frac{u_n^{h_n} - u_n^{T_n^0+1}}{\lambda_n} & \text{if } i \geq h_n - T_n^0 - 1. \end{cases} \tag{3.95}$$

Now we rewrite the left-hand side in (3.93) in terms of $\tilde{u}_n$

$$\begin{aligned}
&\sum_{j=2}^{K} \Bigg\{ \sum_{i=T_n^0+1}^{h_n-j} \sigma_{j,n}^i(\gamma) + c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1\left(\frac{u_n^{h_n-s+1} - u_n^{h_n-s}}{\lambda_n}\right) \Bigg\} \\
&= \sum_{j=2}^{K} c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(\tilde{u}_n^s - \tilde{u}_n^{s-1}) + \sum_{j=2}^{K} \sum_{i=0}^{h_n-j-T_n^0-1} \Bigg\{ J_j\left(\frac{u_n^{h_n-i} - u_n^{h_n-i-j}}{j\lambda_n}\right) \\
&\quad + \frac{c_j}{j} \sum_{s=i}^{i+j-1} J_1\left(\frac{u_n^{h_n-s} - u_n^{h_n-s-1}}{\lambda_n}\right) - \psi_j(\gamma) \Bigg\} \\
&= \sum_{j=2}^{K} c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(\tilde{u}_n^s - \tilde{u}_n^{s-1}) + \sum_{j=2}^{K} \sum_{i\geq 0} \Bigg\{ J_j\left(\frac{\tilde{u}_n^{i+j} - \tilde{u}_n^i}{j}\right) \\
&\quad + \frac{c_j}{j} \sum_{s=i}^{i+j-1} J_1(\tilde{u}_n^{s+1} - u_n^s) - \psi_j(\gamma) \Bigg\} - r_1(n),
\end{aligned}$$

where

$$r_1(n) = \sum_{j=2}^{K} \sum_{i=h_n-j-T_n^0}^{h_n-T_n^0-2} \Bigg\{ J_j\left(\frac{\tilde{u}_n^{i+j} - \tilde{u}_n^i}{j}\right) + \frac{c_j}{j} \sum_{s=i}^{i+j-1} J_1(\tilde{u}_n^{s+1} - u_n^s) - \psi_j(\gamma) \Bigg\}.$$

Indeed, by definition of $\tilde{u}_n$ and (3.14) the terms in the infinite sum over i with $i \geq h_n - T_n^0 - 1$ vanish identically. Furthermore, by the choice of T_n^0, see (3.79), we have for $s \in \{0, \ldots, K-2\}$ that

$$\lim_{n\to\infty} (\tilde{u}_n^{h_n - T_n^0 - K + s + 1} - \tilde{u}_n^{h_n - T_n^0 - K + s}) = \lim_{n\to\infty} \frac{u_n^{T_n^0 + K - s} - u_n^{T_n^0 + K - s - 1}}{\lambda_n} = \gamma.$$

Hence, we have $r_1(n) \to 0$ as $n \to \infty$. Combining (3.89), (3.90) and (3.92)–(3.94) proves the assertion (3.88).

Limsup inequality. As for the lower bound, we distinguish between a jump at 0 and a jump in $(0, 1)$.
Jump in 0. Let $u \in SBV_c^\ell(0, 1)$ be given as in (3.76). We have to show that there exists

a sequence (u_n) with $u_n \to u$ in $L^1(0,1)$ and

$$\limsup_{n\to\infty} H^\ell_{1,n}(u_n) \le \sum_{j=2}^K c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(u^{(1)}_{0,s}) + B_b(u^{(1)}_0) + B(\gamma) + B(u^{(1)}_1,\gamma) - \sum_{j=2}^K (2j-1)\psi_j(\gamma). \tag{3.96}$$

Let us fix $\eta > 0$. By the definition of $B(\gamma)$, we can find a function $\tilde u : \mathbb{N}_0 \to \mathbb{R}$ and an $\tilde N \in \mathbb{N}$ such that $\tilde u^0 = 0$, $\tilde u^{i+1} - \tilde u^i = \gamma$ if $i \ge \tilde N$ and

$$\sum_{j=2}^K c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1\left(\tilde u^s - \tilde u^{s-1}\right) + \sum_{j=2}^K \sum_{i\ge 0} \left\{ J_j\left(\frac{\tilde u^{i+j} - \tilde u^i}{j}\right) + \frac{c_j}{j} \sum_{s=i}^{i+j-1} J_1\left(\tilde u^{s+1} - \tilde u^s\right) - \psi_j(\gamma) \right\} \le B(\gamma) + \eta. \tag{3.97}$$

Analogously, by the definition of $B_b(\theta)$ given in (3.70), there exist $\hat w : \mathbb{N}_0 \to \mathbb{R}$ and a $\hat k_0 \in \mathbb{N}$, $\hat k_0 \ge K-1$ such that $\hat w^{\hat k_0} = 0$, $\hat w^{\hat k_0+1-s} - \hat w^{\hat k_0 - s} = u^{(1)}_{0,s}$ for $s = 1, \dots, K-1$ and

$$\sum_{j=2}^K c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1\left(\hat w^s - \hat w^{s-1}\right) + \sum_{j=2}^K \sum_{i=0}^{\hat k_0 - j} \left\{ J_j\left(\frac{\hat w^{i+j} - \hat w^i}{j}\right) + \frac{c_j}{j} \sum_{s=i}^{i+j-1} J_1\left(\hat w^{s+1} - \hat w^s\right) - \psi_j(\gamma) \right\} \le B_b(u^{(1)}_0) + \eta. \tag{3.98}$$

Moreover, we find a function $w : \mathbb{N}_0 \to \mathbb{R}$ and an $N_2 \in \mathbb{N}$ with $w^0 = 0$, $w^s - w^{s-1} = u^{(1)}_{1,s}$ for $s \in \{1, \dots, K-1\}$, $w^{i+1} - w^i = \gamma$ for $i \ge N_2$ such that

$$\sum_{j=2}^K c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1\left(w^s - w^{s-1}\right) + \sum_{j=2}^K \sum_{i\ge 0} \left\{ J_j\left(\frac{w^{i+j} - w^i}{j}\right) + \frac{c_j}{j} \sum_{s=i}^{i+j-1} J_1\left(w^{s+1} - w^s\right) - \psi_j(\gamma) \right\} \le B(u^{(1)}_1,\gamma) + \eta. \tag{3.99}$$

Let (T^1_n) be a sequence of integers such that

$$T^1_n - (\hat k_0 + K) \ge \tilde N \text{ and } T^1_n + K \le n - N_2 \text{ for all } n \in \mathbb{N} \text{ large enough.} \tag{3.100}$$

We construct a recovery sequence (u_n) by means of the functions $\tilde u$, w and $\hat w$:

$$u^i_n = \begin{cases} -\lambda_n \hat w^{\hat k_0 - i} & \text{if } 0 \le i \le \hat k_0, \\ \ell + \lambda_n(\tilde u^{i-(\hat k_0+1)} - w^{n-(T^1_n+1)} - \tilde u^{T^1_n+1-(\hat k_0+1)}) & \text{if } \hat k_0 + 1 \le i \le T^1_n + 1, \\ \ell - \lambda_n w^{n-i} & \text{if } T^1_n + 1 \le i \le n. \end{cases}$$

The definition of u_n, $\hat{w}$, and w implies that $u_n^0 = 0$ and $u_n^n = \ell$. Moreover, we have that

$$u_n^s - u_n^{s-1} = \lambda_n(\hat{w}^{k_0-s+1} - \hat{w}^{k_0-s}) = \lambda_n u_{0,s}^{(1)},$$
$$u_n^{n+1-s} - u_n^{n-s} = \lambda_n(w^s - w^{s-1}) = \lambda_n u_{1,s}^{(1)},$$

for $s \in \{1, \ldots, K-1\}$. Thus, u_n satisfies the boundary conditions (3.3). Furthermore, it holds $u_n^{i+1} - u_n^i = \lambda_n\gamma$ for $\tilde{N} + \hat{k}_0 + 1 \le i \le n - 1 - N_2$ by definition. Let us show:

$$\lim_{n\to\infty}(u_n^{\hat{k}_0+1} - u_n^{\hat{k}_0}) = \ell - \gamma. \tag{3.101}$$

For this, we use that $\tilde{u}^{i+1} - \tilde{u}^i = \gamma$ for $i \ge \tilde{N}$ and $w^{i+1} - w^i = \gamma$ if $i \ge N_2$:

$$\begin{aligned}
u_n^{\hat{k}_0+1} - u_n^{\hat{k}_0} =& \ell + \lambda_n(\tilde{u}^0 - w^{n-(T_n^1+1)} - \tilde{u}^{T_n^1+1-(\hat{k}_0+1)} + \hat{w}^0)\\
=&\ell + \lambda_n(w^{N_2} - w^{n-(T_n^1+1)} + \tilde{u}^{\tilde{N}} - \tilde{u}^{T_n^1-\hat{k}_0} - w^{N_2} - \tilde{u}^{\tilde{N}} + \hat{w}^0)\\
=&\ell + \lambda_n(\gamma(N_2 - n + T_n^1 + 1 + \tilde{N} - T_n^1 + \hat{k}_0) - w^{N_2} - \tilde{u}^{\tilde{N}} + \hat{w}^0)\\
=&\ell - \gamma + \lambda_n(\gamma(N_2 + \tilde{N} + \hat{k}_0 + 1) - w^{N_2} - \tilde{u}^{\tilde{N}} + \hat{w}^0) \;\to\; \ell - \gamma \quad \text{as } n \to \infty.
\end{aligned}$$

Hence, we have $u_n \to u$ in $L^1(0,1)$. Indeed, the above calculations imply $\lim_{n\to\infty} u_n^{\hat{k}_0+1} = \ell-\gamma$ and we deduce from the definition of u_n that $u_n^{\hat{k}_0+\tilde{N}+1} - u_n^{\hat{k}_0+1} = \lambda_n\tilde{u}^{\tilde{N}} \to 0$ as $n \to \infty$. Since u_n is equibounded in $L^\infty(0,1)$ and $u^{i+1} - u^i = \lambda_n\gamma$ for $i \in \{\tilde{N}+\hat{k}_0+1, \ldots, n-1-N_2\}$, we have

$$\begin{aligned}
&\int_0^1 |u_n - u|dx\\
&= \int_{\lambda_n(\hat{k}_0+\tilde{N}+1)}^{\lambda_n(n-N_2)} |u_n^{\hat{k}_0+1+\tilde{N}} + \gamma(x - \lambda_n(\hat{k}_0 + \tilde{N} + 1)) - (\ell - \gamma + \gamma x)|dx + o(1)\\
&= \int_{\lambda_n(\hat{k}_0+\tilde{N}+1)}^{\lambda_n(n-N_2)} |u_n^{\hat{k}_0+1+\tilde{N}} - \gamma\lambda_n(\hat{k}_0 + \tilde{N} + 1) - (\ell - \gamma)|dx + o(1) \to 0
\end{aligned}$$

as $n \to \infty$. By the definition of u_n and (3.101) it holds for $j \in \{1, \ldots, K\}$ and $s \in \{0, \ldots, j-1\}$ that

$$\frac{u_n^{\hat{k}_0+j-s} - u_n^{\hat{k}_0-s}}{\lambda_n} = \frac{\ell - \gamma}{\lambda_n} + \mathcal{O}(1) \to +\infty \quad \text{as } n \to \infty.$$

Hence, we obtain similarly to (3.82) that

$$\begin{aligned}
\sum_{j=2}^{K}\sum_{i=0}^{T_n^1} \sigma_{j,n}^i(\gamma) =& \sum_{j=2}^{K}\Bigg\{\sum_{i=0}^{\hat{k}_0-j} \sigma_{j,n}^i(\gamma) + c_j\sum_{s=1}^{j-1}\frac{j-s}{j}J_1\left(\frac{u_n^{\hat{k}_0-s+1} - u_n^{\hat{k}_0-s}}{\lambda_n}\right)\\
&+ \sum_{i=\hat{k}_0+1}^{T_n^1} \sigma_{j,n}^i(\gamma) + c_j\sum_{s=1}^{j-1}\frac{j-s}{j}J_1\left(\frac{u_n^{\hat{k}_0+s+1} - u_n^{\hat{k}_0+s}}{\lambda_n}\right)\Bigg\} - \sum_{j=2}^{K} j\psi_j(\gamma) + r(n)
\end{aligned} \tag{3.102}$$

with

$$r(n)=\sum_{j=1}^{K}\sum_{s=-j+1}^{0}J_j\left(\frac{u_n^{\hat{k}_0+j+s}-u_n^{\hat{k}_0+s}}{j\lambda_n}\right)\to 0 \quad \text{as } n\to\infty. \tag{3.103}$$

By the definition of u_n and $\hat{w}$, we have

$$\begin{aligned}&\sum_{j=2}^{K}\left\{\sum_{i=0}^{\hat{k}_0-j}\sigma_{j,n}^{i}(\gamma)+c_j\sum_{s=1}^{j-1}\frac{j-s}{j}J_1\left(\frac{u_n^{\hat{k}_0-s+1}-u_n^{\hat{k}_0-s}}{\lambda_n}\right)\right\}\\&=\sum_{j=2}^{K}\sum_{i=0}^{\hat{k}_0-j}\left\{J_j\left(\frac{\hat{w}^{i+j}-\hat{w}^{i}}{j}\right)+\frac{c_j}{j}\sum_{s=i}^{i+j-1}J_1(\hat{w}^{s+1}-\hat{w}^{s})-\psi_j(\gamma)\right\}\\&\quad+\sum_{j=2}^{K}c_j\sum_{s=1}^{j-1}\frac{j-s}{j}J_1(\hat{w}^{s}-\hat{w}^{s-1})\leq B_b(u_0^{(1)})+\eta.\end{aligned} \tag{3.104}$$

Furthermore, we have

$$\begin{aligned}&\sum_{j=2}^{K}\left\{\sum_{i=\hat{k}_0+1}^{T_n^1+1-j}\sigma_{j,n}^{i}(\gamma)+c_j\sum_{s=1}^{j-1}\frac{j-s}{j}J_1\left(\frac{u_n^{\hat{k}_0+s+1}-u_n^{\hat{k}_0+s}}{\lambda_n}\right)\right\}\\&=\sum_{j=2}^{K}\sum_{i=0}^{T_n^1-\hat{k}_0-j}\left\{J_j\left(\frac{\tilde{u}^{i+j}-\tilde{u}^{i}}{j}\right)+\frac{c_j}{j}\sum_{s=i}^{i+j-1}J_1(\tilde{u}^{s+1}-\hat{u}^{s})-\psi_j(\gamma)\right\}\\&\quad+\sum_{j=2}^{K}c_j\sum_{s=1}^{j-1}\frac{j-s}{j}J_1\left(\tilde{u}^{\hat{s}}-\tilde{u}^{\hat{s}-1}\right)\leq B(\gamma)+\eta.\end{aligned} \tag{3.105}$$

Note that we used that $\tilde{u}^{i+1}-\tilde{u}^{i}=\gamma$ for $i\geq\tilde{N}$ and $T_n^1-(\hat{k}_0+K-1)\geq\tilde{N}$ for n large enough (see (3.100)).

From the assumption on $\tilde{u}$ and w it follows for n sufficiently large such that (3.100) holds $u_n^{i+1}-u_n^{i}=\lambda_n\gamma$ for $i=T_n^1+2-K,\ldots,T_n^1+K$. Hence, $\sigma_{j,n}^{i}(\gamma)=0$ for $i=T_n^1+2-K,\ldots,T_n^1$. In the same way as in the elastic case, we obtain

$$\sum_{j=2}^{K}\sum_{i=T_n^1+1}^{n-j}\sigma_n^{i}(\gamma)+\sum_{j=2}^{K}c_j\sum_{s=1}^{j-1}\frac{j-s}{j}J_1(u_{1,s}^{(1)})\leq B(u_1^{(1)},\gamma)+\eta \tag{3.106}$$

Combining (3.102) with (3.104)-(3.106), and $\sigma^i_{j,n}(\gamma) = 0$ for $i \in \{T^1_n + 2 - K, \dots, T^1_n\}$, we have for n sufficiently large that

$$\begin{aligned} H^\ell_{1,n}(u_n) = &\sum_{j=2}^K c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(u^{(1)}_{0,s}) \\ &+ \sum_{j=2}^K \left\{ \sum_{i=0}^{\hat{k}_0 - j} \sigma^i_{j,n}(\gamma) + c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1\left(\frac{u_n^{\hat{k}_0 - s + 1} - u_n^{\hat{k}_0 - s}}{\lambda_n} \right) \right\} \\ &+ \sum_{j=2}^K \left\{ \sum_{i=\hat{k}_0+1}^{T^1_n + 1 - j} \sigma^i_{j,n}(\gamma) + c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1\left(\frac{u_n^{\hat{k}_0 + s + 1} - u_n^{\hat{k}_0 + s}}{\lambda_n} \right) \right\} \\ &+ \sum_{j=2}^K \left\{ \sum_{i=T^1_n+1}^{n-j} \sigma^i_n(\gamma) + c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(u^{(1)}_{1,s}) \right\} + r(n) - \sum_{j=2}^K (2j-1)\psi_j(\gamma) \\ \le &\sum_{j=2}^K c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(u^{(1)}_{0,s}) + B_b(u^{(1)}_0) + B(\gamma) + B(u^{(1)}_1, \gamma) \\ &- \sum_{j=2}^K (2j-1)\psi_j(\gamma) + 3\eta + r(n), \end{aligned}$$

with $r(n)$ as in (3.103). By the arbitrariness of $\eta > 0$ this proves the assertion (3.96).

Internal jump. Consider $u \in SBV^\ell_c(0,1)$ with $S_u = \{t\}$, $t \in (0,1)$. We prove the existence of a sequence (u_n) converging to u in $L^1(0,1)$, such that

$$\limsup_{n\to\infty} H^\ell_{1,n}(u_n) \le B(u^{(1)}_0, \gamma) + B(u^{(1)}_1, \gamma) + 2B(\gamma) - \sum_{j=2}^K (2j-1)\psi_j(\gamma). \tag{3.107}$$

Fix $\eta > 0$. As in the elastic case, we find $v : \mathbb{N}_0 \to \mathbb{R}$ and $N_1 \in \mathbb{N}$ such that $v^0 = 0$, $v^s - v^{s-1} = u^{(1)}_{0,s}$ for $s \in \{1, \dots, K-1\}$ and $v^{i+1} - v^i = \gamma$ for $i \ge N_1$ such that it holds

$$\begin{aligned} &\sum_{j=2}^K c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1\left(v^s - v^{s-1}\right) + \sum_{j=2}^K \sum_{i\ge 0} \left\{ J_j\left(\frac{v^{i+j} - v^i}{j} \right) \right. \\ &\quad \left. + \frac{c_j}{j} \sum_{s=i}^{i+j-1} J_1\left(v^{s+1} - v^s\right) - \psi_j(\gamma) \right\} \le B(u^{(1)}_0, \gamma) + \eta. \end{aligned} \tag{3.108}$$

Analogously, there exist a function $w : \mathbb{N}_0 \to \mathbb{R}$ and an $N_2 \in \mathbb{N}$ such that (3.99) holds. Finally, by definition of $B(\gamma)$, we can find as in the previous case $\tilde{u} : \mathbb{N}_0 \to \mathbb{R}$ and $\tilde{N} \in \mathbb{N}$ such that (3.97) holds. Let T^0_n, T^1_n, h_n be sequences of integers such that $\lim_{n\to\infty} h_n\lambda_n = t$ and

$$T^0_n \ge N_1 + K, \quad T^1_n + K \le n - N_2, \quad \tilde{N} + K \le \min\{h_n - T^0_n - 1, T^1_n - h_n - 1\} \tag{3.109}$$

for n large enough. We construct the recovery sequence by means of v, w and $\tilde{u}$:

$$u_n^i = \begin{cases} \lambda_n v^i & \text{if } 0 \le i \le T_n^0, \\ \lambda_n (v^{T_n^0} - \tilde{u}^{h_n - i} + \tilde{u}^{h_n - T_n^0}) & \text{if } T_n^0 \le i \le h_n, \\ \ell + \lambda_n (\tilde{u}^{i-(h_n+1)} - \tilde{u}^{T_n^1 - h_n} - w^{n-(T_n^1+1)}) & \text{if } h_n + 1 \le i \le T_n^1 + 1, \\ \ell - \lambda_n w^{n-i} & \text{if } T_n^1 + 1 \le i \le n. \end{cases}$$

By the definition of v and w, we observe that u_n satisfies the boundary conditions (3.3). Moreover, we have $u_n^{i+1} - u_n^i = \lambda_n \gamma$ for $i \in \{N_1, \dots, h_n - \tilde{N} - 1\} \cup \{h_n + \tilde{N} + 1, \dots, n - N_2 - 1\}$. Next, we show

$$\lim_{n \to \infty} (u_n^{h_n+1} - u_n^{h_n}) = \ell - \gamma. \tag{3.110}$$

Therefore, we use that $w^{i+1} - w^i = \gamma$ for $i \ge N_2$, $v^{i+1} - v^i = \gamma$ for $i \ge N_1$ and $\tilde{u}^{i+1} - \tilde{u}^i = \gamma$ for $i \ge \tilde{N}$:

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

Similarly as in the previous case, we can deduce that $u_n \to u$ in $L^1(0,1)$. As in the case of a jump in 0 we have that

$$\begin{aligned} \sum_{j=2}^{K} \sum_{i=T_n^0}^{T_n^1} \sigma_{j,n}^i(\gamma) =& \sum_{j=2}^{K} \Bigg\{ \sum_{i=T_n^0}^{h_n - j} \sigma_{j,n}^i(\gamma) + c_j \sum_{s=1}^{j} \frac{j-s}{j} J_1 \left(\frac{u_n^{h_n+1-s} - u_n^{h_n - s}}{\lambda_n} \right) \\ & + c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1 \left(\frac{u_n^{h_n+s+1} - u_n^{h_n+s}}{\lambda_n} \right) + \sum_{i=h_n+1}^{T_n^1} \sigma_{j,n}^i(\gamma) \Bigg\} - \sum_{j=2}^{K} j \psi_j(\gamma) + r(n) \end{aligned}$$

with $r(n) \to 0$ as $n \to \infty$. In order to estimate the energy $H_{1,n}^{\ell}(u_n)$ it is useful to rewrite it as follows:

$$\begin{aligned} H_{1,n}^{\ell}(u_n) =& \sum_{j=2}^{K} \Bigg\{ c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(u_{0,s}^{(1)}) + \sum_{i=0}^{T_n^0 - 1} \sigma_{j,n}^i(\gamma) + \sum_{i=T_n^0}^{h_n - j} \sigma_{j,n}^i(\gamma) \\ & + c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1 \left(\tilde{u}^s - \tilde{u}^{s-1} \right) + \sum_{i=h_n+1}^{T_n^1} \sigma_{j,n}^i(\gamma) + c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1 \left(\tilde{u}_n^s - \tilde{u}^{s-1} \right) \\ & + \sum_{i=T_n^1+1}^{n-j} \sigma_{j,n}^i(\gamma) + c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(u_{1,s}^{(1)}) \Bigg\} - \sum_{j=2}^{K} (2j-1) \psi_j(\gamma) + r(n). \end{aligned}$$

Using (3.108), (3.99) and (3.97), we obtain

$$\limsup_{n\to\infty} H^\ell_{1,n}(u_n) \le B(u_0^{(1)},\gamma) + B(u_0^{(1)},\gamma) - \sum_{j=2}^K (2j-1)\psi_j(\gamma) + 2B(\gamma) + 4\eta,$$

which proves, by the arbitrariness of $\eta > 0$, the assertion (3.107). □

In analogy to Proposition 3.15, we reformulate the functional H_1^ℓ without the explicit dependence on $c = (c_j)_{j=2}^K$ in the case $\ell > \gamma$. To this end, we introduce the following boundary layer energies

$$\widetilde{B}_b(\theta) := \inf_{\substack{k\in\mathbb{N}\\ k\ge K-1}} \min\left\{ \sum_{j=1}^K \sum_{i=0}^{k-j} \left\{ J_j\left(\frac{v^{i+j}-v^i}{j}\right) - J_j(\gamma)\right\} : v:\mathbb{N}_0\to\mathbb{R}, v^k = 0,\ v^{k+1-s} - v^{k-s} = \theta_s \text{ if } 1 \le s \le K-1 \right\}, \tag{3.111}$$

$$\widetilde{B}(\gamma) := \inf_{N\in\mathbb{N}_0} \min\left\{ \sum_{i\ge 0} \left\{ \sum_{j=1}^K J_j\left(\frac{u^{i+j}-u^i}{j}\right) - J_{CB}(\gamma)\right\} : u:\mathbb{N}_0\to\mathbb{R},\ u^0 = 0,\ u^{i+1}-u^i = \gamma \text{ if } i \ge N \right\}. \tag{3.112}$$

Proposition 3.21. *Suppose that hypotheses (LJ1)–(LJ5) hold. Let $\ell > \gamma$ and $u_0^{(1)}, u_1^{(1)} \in \mathbb{R}_+^{K-1}$. Let $\widetilde{B}(\theta,\gamma)$, $\widetilde{B}_b(\theta)$ and $\widetilde{B}(\gamma)$ are as* (3.64)*,* (3.111) *and* (3.112)*, respectively. Then the functional $H^\ell_{1,n}$, given in* (3.73)*, reads*

$$H_1^\ell(u) = \begin{cases} \widetilde{B}(u_0^{(1)},\gamma) + \widetilde{B}(u_1^{(1)},\gamma) + \beta_{BJ}(u_0^{(1)})\#(S_u\cap\{0\}) \\ \quad + \beta_{IJ}\#(S_u\cap(0,1)) + \beta_{BJ}(u_1^{(1)})\#(S_u\cap\{1\}) \\ \quad - \sum_{j=2}^K (j-1)J_j(\gamma) & \text{if } u \in SBV_c^\ell(0,1) \\ +\infty & \text{else} \end{cases} \tag{3.113}$$

on $L^1(0,1)$, where, for $\theta \in \mathbb{R}_+^{K-1}$,

$$\beta_{BJ}(\theta) := \widetilde{B}_b(\theta) + \widetilde{B}(\gamma) - \sum_{j=1}^K jJ_j(\gamma) - \widetilde{B}(\theta,\gamma), \quad \beta_{IJ} := 2\widetilde{B}(\gamma) - \sum_{j=1}^K jJ_j(\gamma). \tag{3.114}$$

Proof. By (3.73) and (3.14), it is sufficient to prove that $B_{IJ} = \beta_{IJ}$ and that for any $\theta \in \mathbb{R}_+^{K-1}$ the following equalities hold true:

$$B(\theta,\gamma) - \frac{1}{2}J_1(\gamma)\sum_{j=2}^{K}(j-1)c_j = \widetilde{B}(\theta,\gamma),$$

$$B_{BJ}(\theta) - \frac{1}{2}J_1(\gamma)\sum_{j=2}^{K}(j-1)c_j = \beta_{BJ}(\theta) + \widetilde{B}(\theta,\gamma).$$

The equality regarding the elastic boundary layer energies $B(\theta,\gamma)$ and $\widetilde{B}(\theta,\gamma)$ follows from (3.65) and $\psi_j'(\gamma) = 0$. Next, we show that

$$B(\gamma) - \frac{1}{2}J_1(\gamma)\sum_{j=2}^{K}(j-1)c_j = \widetilde{B}(\gamma), \tag{3.115}$$

where $B(\gamma)$ is given in (3.71). This equality implies $B_{IJ} = \beta_{IJ}$. Indeed, we have by (3.75), (3.14) and $\sum_{j=2}^{K} c_j = 1$ that

$$\begin{aligned} B_{IJ} =& 2B(\gamma) - \sum_{j=2}^{K} j(J_j(\gamma) + c_j J_1(\gamma)) = 2B(\gamma) - \sum_{j=2}^{K}(j-1)c_j J_1(\gamma) - \sum_{j=1}^{K} jJ_j(\gamma) \\ =& 2\widetilde{B}(\gamma) - \sum_{j=1}^{K} jJ_j(\gamma) = \beta_{IJ}. \end{aligned}$$

Let $u : \mathbb{N}_0 \to \mathbb{R}$ be a candidate for the minimum problems defining $B(\gamma)$ and $\widetilde{B}(\gamma)$, i.e. $u^0 = 0$ and $u^{i+1} - u^i = \gamma$ for $i \geq N$ for some $N \in \mathbb{N}_0$. Then it holds for the infinite sum in the definition of $B(\gamma)$ that

$$\begin{aligned} &\sum_{j=2}^{K}\sum_{i\geq 0}\left\{J_j\left(\frac{u^{i+j}-u^i}{j}\right) + \frac{c_j}{j}\sum_{s=i}^{i+j-1} J_1\left(u^{s+1}-u^s\right) - \psi_j(\gamma)\right\} \\ &= \sum_{i=0}^{N-1}\left\{\sum_{j=2}^{K} J_j\left(\frac{u^{i+j}-u^i}{j}\right) - \sum_{j=2}^{K}\psi_j(\gamma)\right\} + \sum_{j=2}^{K}\frac{c_j}{j}\sum_{i=0}^{N-1}\sum_{s=i}^{i+j-1} J_1\left(u^{s+1}-u^s\right). \end{aligned}$$

The nearest neighbour terms on the right-hand side above can be rewritten as

$$\begin{aligned} &\sum_{j=2}^{K}\frac{c_j}{j}\sum_{i=0}^{N-1}\sum_{s=i}^{i+j-1} J_1\left(u^{s+1}-u^s\right) = \sum_{j=2}^{K}\frac{c_j}{j}\sum_{s=0}^{j-1}\sum_{i=s}^{N+s-1} J_1\left(u^{i+1}-u^i\right) \\ &= \sum_{j=2}^{K} c_j \sum_{i=0}^{N-1} J_1\left(u^{i+1}-u^i\right) - \sum_{j=2}^{K}\frac{c_j}{j}\sum_{s=0}^{j-1}\left\{\sum_{i=0}^{s-1} J_1\left(u^{i+1}-u^i\right) - \sum_{i=N}^{N+s-1} J_1\left(u^{i+1}-u^i\right)\right\}. \end{aligned}$$

Using $u^{i+1} - u^i = \gamma$ for $i \geq N$, we obtain

$$\sum_{j=2}^{K} \frac{c_j}{j} \sum_{s=0}^{j-1} \sum_{i=0}^{s-1} J_1\left(u^{i+1} - u^i\right) = \sum_{j=2}^{K} c_j \sum_{i=1}^{j-1} \frac{j-i}{j} J_1\left(u^i - u^{i-1}\right),$$

$$\sum_{j=2}^{K} \frac{c_j}{j} \sum_{s=0}^{j-1} \sum_{i=N}^{N+s-1} J_1\left(u^{i+1} - u^i\right) = \frac{1}{2} \sum_{j=2}^{K} c_j (j-1) J_1(\gamma).$$

Altogether, we showed that

$$\begin{aligned}
&\sum_{j=2}^{K} \sum_{i \geq 0} \left\{ J_j\left(\frac{u^{i+j} - u^i}{j}\right) + \frac{c_j}{j} \sum_{s=i}^{i+j-1} J_1\left(u^{s+1} - u^s\right) - \psi_j(\gamma) \right\} \\
&+ \sum_{j=2}^{K} c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1\left(u^s - u^{s-1}\right) - \frac{1}{2} \sum_{j=2}^{K} (j-1) c_j J_1(\gamma) \\
&= \sum_{i=0}^{N-1} \left\{ \sum_{j=2}^{K} J_j\left(\frac{u^{i+j} - u^i}{j}\right) - \sum_{j=2}^{K} \psi_j(\gamma) \right\} + \sum_{i=0}^{N-1} J_1\left(u^{i+1} - u^i\right) \\
&= \sum_{i \geq 0} \left\{ \sum_{j=1}^{K} J_j\left(\frac{u^{i+j} - u^i}{j}\right) - J_{CB}(\gamma) \right\},
\end{aligned}$$

where we applied again $\sum_{j=2}^{K} c_j = 1$ and $u^{i+1} - u^i = \gamma$ for $i \geq N$. By the arbitrariness of $u : \mathbb{N}_0 \to \mathbb{R}$ and $N \in \mathbb{N}_0$ with $u^0 = 0$ and $u^{i+1} - u^i = \gamma$ for $i \geq N$ and the definition of $B(\gamma)$ and $\widetilde{B}(\gamma)$, see (3.71) and (3.112), the equality (3.115) is proven.

It is left to show that for any $\theta \in \mathbb{R}_+^{K-1}$ it holds

$$\sum_{j=2}^{K} c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(\theta_s) + B_b(\theta) - J_1(\gamma) \sum_{j=2}^{K} (j-1) c_j = \widetilde{B}_b(\theta), \tag{3.116}$$

where $B_b(\theta)$ is defined in (3.70). Note that (3.115) and (3.116) imply that $B_{BJ}(\theta) - \frac{1}{2} J_1(\gamma) \sum_{j=2}^{K} (j-1) c_j = \beta_{BJ}(\theta) + \widetilde{B}(\theta, \gamma)$. Indeed, we have, using (3.14), (3.74), (3.114)–(3.116) and $\sum_{j=2}^{K} c_j = 1$, that

$$\begin{aligned}
&B_{BJ}(\theta) - \frac{1}{2} J_1(\gamma) \sum_{j=2}^{K} (j-1) c_j \\
&= \sum_{j=2}^{K} c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(\theta_s) + B_b(\theta) + B(\gamma) - \sum_{j=1}^{K} j J_j(\gamma) - \frac{3}{2} J_1(\gamma) \sum_{j=2}^{K} (j-1) c_j \\
&= \widetilde{B}_b(\theta) + \widetilde{B}(\gamma) - \sum_{j=1}^{K} j J_j(\gamma) = \beta_{BJ}(\theta) + \widetilde{B}(\theta, \gamma).
\end{aligned}$$

To show (3.116), we follow the same line of arguments as we used to prove (3.65) and (3.115). Let $\theta \in \mathbb{R}_+^{K-1}$ be fixed. Let $v : \mathbb{N}_0 \to \mathbb{R}$ be a candidate for the minimum problems defining $B_b(\theta)$ and $\widetilde{B}_b(\theta)$, i.e. $v^0 = 0$ and $v^{k+1-s} - v^{k-s} = \theta_s$ if $1 \leq s \leq K-1$ for some $k \geq K-1$. Then we have that

$$\begin{aligned}
&\sum_{j=2}^{K}\sum_{i=0}^{k-j}\left\{J_j\left(\frac{v^{i+j}-v^i}{j}\right)+\frac{c_j}{j}\sum_{s=i}^{i+j-1}J_1\left(v^{s+1}-v^s\right)-\psi_j(\gamma)\right\}\\
&=\sum_{j=2}^{K}\sum_{i=0}^{k-j}\left\{J_j\left(\frac{v^{i+j}-v^i}{j}\right)-J_j(\gamma)-c_jJ_1(\gamma)\right\}+\sum_{j=2}^{K}\frac{c_j}{j}\sum_{i=0}^{k-j}\sum_{s=i}^{i+j-1}J_1\left(v^{s+1}-v^s\right).
\end{aligned}$$

By similar calculations as before, we can rewrite the nearest neighbour terms on the right-hand side above as

$$\begin{aligned}
&\sum_{j=2}^{K}\frac{c_j}{j}\sum_{i=0}^{k-j}\sum_{s=i}^{i+j-1}J_1\left(v^{s+1}-v^s\right)=\sum_{j=2}^{K}\frac{c_j}{j}\sum_{s=0}^{j-1}\sum_{i=s}^{k+s-j}J_1\left(v^{i+1}-v^i\right)\\
&\quad=\sum_{i=0}^{k-1}J_1\left(v^{i+1}-v^i\right)-\sum_{j=2}^{K}c_j\sum_{i=1}^{j-1}\frac{j-i}{j}\left\{J_1\left(v^i-v^{i-1}\right)+J_1(v^{k+1-i}-v^{k-i})\right\}.
\end{aligned}$$

Since $v^{k+1-s} - v^{k-s} = \theta_s$ for $1 \leq s \leq K-1$, we have that

$$\begin{aligned}
&\sum_{j=2}^{K}\sum_{i=0}^{k-j}\left\{J_j\left(\frac{v^{i+j}-v^i}{j}\right)+\frac{c_j}{j}\sum_{s=i}^{i+j-1}J_1\left(v^{s+1}-v^s\right)-\psi_j(\gamma)\right\}\\
&+\sum_{j=2}^{K}c_j\sum_{s=1}^{j-1}\frac{j-s}{j}J_1\left(v^s-v^{s-1}\right)+\sum_{j=2}^{K}c_j\sum_{s=1}^{j-1}\frac{j-s}{j}J_1(\theta_s)-\sum_{j=2}^{K}(j-1)c_jJ_1(\gamma)\\
&=\sum_{j=2}^{K}\sum_{i=0}^{k-j}\left\{J_j\left(\frac{v^{i+j}-v^i}{j}\right)-J_j(\gamma)\right\}+\sum_{i=0}^{k-1}J_1\left(v^{i+1}-v^i\right)-\sum_{j=2}^{K}c_jkJ_1(\gamma)\\
&=\sum_{j=1}^{K}\sum_{i=0}^{k-j}\left\{J_j\left(\frac{v^{i+j}-v^i}{j}\right)-J_j(\gamma)\right\}.
\end{aligned}$$

By the arbitrariness of $v : \mathbb{N}_0 \to \mathbb{R}$ and $k \geq K-1$ with $v^0 = 0$ and $v^{k+1-s} - v^{k-s} = \theta_s$ for $s \in \{1, \dots, K-1\}$ and the definition of $B_b(\theta)$ and $\widetilde{B}_b(\theta)$, see (3.70) and (3.111), the equality (3.116) is proven.

□

3.4 Properties of the boundary layer energies

In this section, we study the different boundary layer energies which we have derived in Section 3.3 in more detail. In particular we look for the location of fracture. This is similar to the analysis presented in [50, Section 5] for the case $K = 2$.

3.4.1 Boundary layer energies and location of fracture

Let us prove some relations between the different boundary layer energies which show up in the last section; that is the elastic boundary layer energy $B(\theta,\gamma)$, see (3.72), $B(\gamma)$ defined in (3.71), and $B_b(\theta)$ which is defined in (3.70). These relations are proven in [50, Lemma 5.1] in the case $K = 2$.

Lemma 3.22. *Suppose that the hypotheses (LJ1)–(LJ5) hold true. Set $e = (1,\dots,1) \in \mathbb{R}^{K-1}$. Then*

(1) $\frac{1}{2}J_1(\delta_1)\sum_{j=2}^K (j-1)c_j \le B(\gamma) \le \frac{1}{2}J_1(\gamma)\sum_{j=2}^K (j-1)c_j$;

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

(3) $B(\gamma e,\gamma) = \frac{1}{2}J_1(\gamma)\sum_{j=2}^K (j-1)c_j$;

(4) For every $\theta \in \mathbb{R}_+^{K-1}$ *it holds* $\frac{1}{2}J_1(\delta_1)\sum_{j=2}^K (j-1)c_j \le B_b(\theta)$ *and*

$$B_b(\theta) \le \sum_{j=1}^{K-1}\sum_{i=1}^{K-j} J_j\left(\frac{1}{j}\sum_{s=i}^{i+j-1}\theta_s\right) - \sum_{j=2}^K c_j \sum_{s=1}^{j-1}\frac{j-s}{j}J_1(\theta_s) - \sum_{j=2}^K (K-j)\psi_j(\gamma).$$

Moreover, it holds

$$B(\theta,\gamma) \ge \sum_{j=1}^{K-1}\sum_{i=1}^{K-j} J_j\left(\frac{1}{j}\sum_{s=i}^{i+j-1}\theta_s\right) - \sum_{j=2}^K c_j \sum_{s=1}^{j-1}\frac{j-s}{j}J_1(\theta_{K-s}) - \sum_{j=2}^K (K-j)\psi_j(\gamma),$$

and the inequality is strict if $\theta \neq \gamma e$.

(5) For all $\alpha > 0$ *it holds that* $B_b(\alpha e) \le B(\alpha e,\gamma)$.

Proof. (1) Since all the terms in the infinite sum in the definition of $B(\gamma)$ in (3.71) are non-negative and δ_1 is the unique minimiser of J_1 (see (LJ2)), we have that

$$B(\gamma) \ge \sum_{j=2}^K c_j \sum_{s=1}^{j-1}\frac{j-s}{j}J_1(\delta_1) = \frac{1}{2}J_1(\delta_1)\sum_{j=2}^K (j-1)c_j.$$

The upper bound of $B(\gamma)$ follows by testing the infimum problem in the definition of $B(\gamma)$ with $u : \mathbb{N}_0 \to \mathbb{R}$ such that $u^i = \gamma i$ for $i \ge 0$:

$$B(\gamma) \le \sum_{j=2}^K \left\{ c_j \sum_{s=1}^{j-1}\frac{j-s}{j}J_1(\gamma) + \sum_{i\ge 0}(J_j(\gamma) + c_jJ_1(\gamma) - \psi_j(\gamma))\right\} = \frac{1}{2}J_1(\gamma)\sum_{j=2}^K (j-1)c_j.$$

Note that we used $\psi_j(\gamma) = J_j(\gamma) + c_jJ_1(\gamma)$, see (3.14).
(2) Follows directly from the definition $B_b(\theta)$ and $B(\gamma)$, see (3.70) and (3.71).
(3) See Remark 3.13.
(4) The lower bound on $B_b(\theta)$ follows from (3.70) in the same way as the lower bound

for $B(\gamma)$ in (1). Next, we show the upper bound for $B_b(\theta)$. Let $v : \mathbb{N}_0 \to \mathbb{R}$ be such that $v^{K-1} = 0$, $v^{K-i} - v^{K-i-1} = \theta_i$ for $i \in \{1, \dots, K-1\}$. Clearly, the function v is a competitor for the infimum problem in the definition of $\widetilde{B}_b(\theta)$, see (3.111). Hence,

$$\begin{aligned}
\widetilde{B}_b(\theta) \leq & \sum_{j=1}^{K} \sum_{i=0}^{K-1-j} \left\{ J_j\left(\frac{v^{i+j} - v^i}{j}\right) - J_j(\gamma)\right\} \\
= & \sum_{j=1}^{K-1} \sum_{i=1}^{K-j} \left\{ J_j\left(\frac{v^{K-i} - v^{K-i-j}}{j}\right) - J_j(\gamma)\right\} \\
= & \sum_{j=1}^{K-1} \sum_{i=1}^{K-j} J_j\left(\sum_{s=i}^{i+j-1} \frac{\theta_s}{j}\right) - \sum_{j=2}^{K-1} (K-j)\psi_j(\gamma) - J_1(\gamma) \sum_{j=2}^{K} (j-1)c_j,
\end{aligned}$$

where we used (3.14) and $\sum_{j=2}^{K} c_j = 1$ in the last line. The assertion for $B_b(\theta)$ follows directly by (3.116).

Next, we show the lower bound for $B(\theta, \gamma)$. Let $v : \mathbb{N}_0 \to \mathbb{R}$ be test function for (3.50). Since the terms in the infinite sum in the definition of $B(\theta, \gamma)$ are non-negative and $v^s - v^{s-1} = \theta_s$ for $s \in \{1, \dots, K-1\}$, we have

$$\begin{aligned}
B(\theta, \gamma) \geq & \sum_{j=2}^{K} c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(\theta_s) + \sum_{j=2}^{K} \sum_{i\geq 0} \left\{ J_j\left(\frac{v^{i+j} - v^i}{j}\right)\right. \\
& \left. + \frac{c_j}{j} \sum_{s=i}^{i+j-1} J_1\left(v^{s+1} - v^s\right) - \psi_j(\gamma)\right\} \\
\geq & \sum_{j=2}^{K} c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(\theta_s) + \sum_{j=2}^{K-1} \sum_{i=1}^{K-j} \left\{ J_j\left(\frac{1}{j} \sum_{s=i}^{i+j-1} \theta_s\right) + \frac{c_j}{j} \sum_{s=i}^{i+j-1} J_1(\theta_s) - \psi_j(\gamma)\right\}.
\end{aligned}$$

Moreover, we have that

$$\begin{aligned}
\sum_{j=2}^{K-1} \frac{c_j}{j} \sum_{i=1}^{K-j} \sum_{s=i}^{i+j-1} J_1(\theta_s) = & \sum_{j=2}^{K-1} \frac{c_j}{j} \sum_{s=0}^{j-1} \sum_{i=1+s}^{K-j+s} J_1(\theta_i) \\
= & \sum_{j=2}^{K-1} c_j \sum_{i=1}^{K-1} J_1(\theta_i) - \sum_{j=2}^{K-1} \frac{c_j}{j} \sum_{s=0}^{j-1} \left\{ \sum_{i=1}^{s} J_1(\theta_i) + \sum_{i=K-j+s+1}^{K-1} J_1(\theta_i)\right\} \\
= & \sum_{j=2}^{K} c_j \sum_{i=1}^{K-1} J_1(\theta_i) - \sum_{j=2}^{K} \frac{c_j}{j} \left\{ \sum_{i=1}^{j-1} (j-i) J_1(\theta_i) + \sum_{i=K-j+1}^{K-1} (j+i-K) J_1(\theta_i)\right\} \\
= & \sum_{i=1}^{K-1} J_1(\theta_i) - \sum_{j=2}^{K} c_j \sum_{i=1}^{j-1} \frac{j-i}{j} \left\{ J_1(\theta_i) + J_1(\theta_{K-i})\right\}.
\end{aligned}$$

Note that we added and subtracted $c_K \sum_{i=1}^{K-1} J_1(\theta_i)$ in the third line above. Thus,

$$B(\theta,\gamma) \geq \sum_{j=2}^{K-1} \sum_{i=1}^{K-j} J_j \left(\frac{1}{j} \sum_{s=i}^{i+j-1} \theta_s \right) - \sum_{j=2}^{K} c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(\theta_{K-s}) - \sum_{j=2}^{K-1} (K-j)\psi_j(\gamma).$$

By taking the infimum over v, we prove the lower bound for $B(\theta,\gamma)$. If $\theta \neq \gamma e$ the term corresponding to $j = K$ and $i = 0$ in the infinite sum in (3.72) is, using Lemma 3.8, bounded from below by a constant $c = c(\theta) > 0$ if $\theta \neq \gamma e$. Thus the inequality is strict in this case.
(5) Follows directly from the upper bound on $B_b(\theta)$ and the lower bound on $B(\theta,\gamma)$ in (4). □

Now we present further estimates for the boundary layer energies in H_1^ℓ, see (3.73).

Lemma 3.23. *Let (LJ1)–(LJ5) be satisfied. Then*

$$B(\theta,\gamma) \leq B_{BJ}(\theta) \leq B(\theta,\gamma) + B_{IJ} \qquad \forall \theta \in \mathbb{R}_+^{K-1}, \tag{3.117}$$

and $B_{IJ} > 0$, where $B(\theta,\gamma)$, $B_{BJ}(\theta)$, and B_{IJ} are defined as in (3.72), (3.74), *and* (3.75).

Proof. Let $\ell > \gamma$ and $u_0^{(1)} = u_1^{(1)} = \theta \in \mathbb{R}_+^{K-1}$. The assertion follows from the lower semicontinuity of H_1^ℓ. Indeed, by the properties of the Γ-limit, we deduce that H_1^ℓ is lower semicontinuous with respect to the strong $L^1(0,1)$-topology, see e.g. [9, Proposition 1.28]. Let $u \in SBV_c^\ell(0,1)$ (see (3.47)) be such that $S_u = \{0\}$. Furthermore, let $(u_n), (v_n) \subset SBV_c^\ell(0,1)$ be such that $S_{u_n} = \left\{\frac{1}{n}\right\}$ and $S_{v_n} \subset \{0,1\}$ with $[v_n](1) = \frac{\ell-\gamma}{n}$. Note that the functions u, u_n and v_n are uniquely defined for $n \geq 1$. Since, (u_n) and (v_n) converge strongly in $L^1(0,1)$ to u, we deduce from the lower semicontinuity of H_1^ℓ:

$$H_1^\ell(u) \leq \liminf_{n\to\infty} H_1^\ell(u_n) \leq 2B(\theta,\gamma) + B_{IJ} - \sum_{j=2}^{K} (j-1)\psi_j(\gamma),$$
$$H_1^\ell(u) \leq \liminf_{n\to\infty} H_1^\ell(v_n) \leq 2B_{BJ}(\theta) - \sum_{j=2}^{K} (j-1)\psi_j(\gamma).$$

The combination of the above inequalities with

$$H_1^\ell(u) = B(\theta,\gamma) + B_{BJ}(\theta) - \sum_{j=2}^{K} (j-1)\psi_j(\gamma)$$

proves the inequality (3.117).

Let us show $B_{IJ} > 0$. Consider u with $u(x) = \ell x$ and $\ell > \gamma$. For given $N \in \mathbb{N}$, we set $t_i := \frac{i}{N}$ and define $w_N \in SBV_c^\ell(0,1)$ such that $S_{w_N} = \{t_i, i \in \{0,\dots,N\}\}$ and $w_N(t_i+) = \ell t_i$ for $i \in \{0,\dots,N\}$. Clearly, we have that $w_N \to u$ in $L^1(0,1)$. If we assume that $B_{IJ} \leq 0$, we have $\sup_N H_1^\ell(w_N) \leq C$ but $H_1^\ell(u) = +\infty$ since $u \notin SBV_c^\ell(0,1)$ for $\ell > \gamma$, which is a contradiction to the lower semicontinuity of H_1^ℓ. Thus $B_{IJ} > 0$. □

As a direct consequence of Lemma 3.23, we have the following result about the minimisers and minimal energies of H_1^ℓ, which extends in some sense the results of [50, Theorem 5.1]. We prove that there exists no choice for $u_0^{(1)}, u_1^{(1)} > 0$ such that an internal jump has strictly less energy than a jump at the boundary. However, we note that for special values of $u_0^{(1)}, u_1^{(1)} > 0$ the energies can be the same.

Proposition 3.24. *Suppose that hypotheses (LJ1)–(LJ5) hold. Let $\ell > \gamma$. For any $u_0^{(1)}, u_1^{(1)} \in \mathbb{R}_+^{K-1}$ it holds*

$$\begin{aligned}\min_u H_1^\ell(u) =& \min\left\{B_{BJ}(u_0^{(1)}) + B(u_1^{(1)},\gamma), B_{BJ}(u_1^{(1)}) + B(u_0^{(1)},\gamma)\right\} \\ & - \sum_{j=2}^K (j-1)\psi_j(\gamma). \end{aligned} \tag{3.118}$$

Furthermore, it holds $B_{BJ}(\theta) = B(\theta,\gamma) + B_{IJ}$ for $\theta = \gamma e$ and $B_{BJ}(\theta) < B(\theta,\gamma) + B_{IJ}$ for $\theta = \delta_1 e$, where $e = (1,\dots,1) \in \mathbb{R}^{K-1}$. Hence, for $u_0^{(1)} = u_1^{(1)} = \gamma e$ fracture can appear indifferently in $[0,1]$. If instead $u_0^{(1)} = \delta_1 e$ or $u_1^{(1)} = \delta_1 e$ and $\delta_1 \neq \gamma$ a jump in $\{0,1\}$ is energetically favourable.

Proof. From $B_{BJ}(\theta) \leq B(\theta,\gamma) + B_{IJ}$ for all $\theta \in \mathbb{R}_+^{K-1}$, see Lemma 3.23 and the formula for H_1^ℓ in (3.73), it follows that no internal jump can has strictly less energy than a jump at the boundary. Hence,

$$\min\left\{H_1^\ell(u) : u \in SBV_c^\ell(0,1)\right\} = \min\left\{H_1^\ell(u) : u \in SBV_c^\ell(0,1), S_u \subset \{0,1\}\right\},$$

which proves, using $B(\theta,\gamma) \leq B_{BJ}(\theta)$ (see (3.117)), the assertion (3.118), cf. (3.73).

Let us now show that $B_{BJ}(\gamma e) = B(\gamma e,\gamma) + B_{IJ}$. By the definition of B_{BJ} and Lemma 3.22 (2) and (3), we have that

$$\begin{aligned} B_{BJ}(\gamma e) - B(\gamma e,\gamma) =& \frac{1}{2}J_1(\gamma)\sum_{j=2}^K (j-1)c_j + B_b(\gamma e) + B(\gamma) - \sum_{j=2}^K j\psi_j(\gamma) - B(\gamma e,\gamma) \\ =& 2B(\gamma) - \sum_{j=2}^K j\psi_j(\gamma) = B_{IJ}. \end{aligned} \tag{3.119}$$

Let us now show $B_{BJ}(\delta_1 e) < B_{IJ} + B(\delta_1 e,\gamma)$. From Lemma 3.22 (1) and (5), we deduce

$$\begin{aligned} \sum_{j=2}^K c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(\delta_1) + B_b(\delta_1 e) <& \frac{1}{2}J_1(\delta_1)\sum_{j=2}^K (j-1)c_j + B(\delta_1 e,\gamma) \\ <& B(\gamma) + B(\delta_1 e,\gamma), \end{aligned}$$

which proves by the definition of $B_{BJ}(\delta_1 e)$ and B_{IJ} the assertion. □

Remark 3.25. Let us consider the special case $\ell > \gamma$ and $u_0^{(1)}, u_1^{(1)} \in \mathbb{R}^{K-1}$ such that $u_{0,s}^{(1)} = u_{1,s}^{(1)} = \gamma$ for $1 \leq s < K$. From Lemma 3.22 (3), we deduce $2B(\gamma,\gamma) - \sum_{j=2}^K (j -$

$1)\psi_j(\gamma) = -\sum_{j=2}^K (j-1)J_j(\gamma)$. Hence, using (3.119), the first-order Γ-limit H_1^ℓ given in Theorem 3.19 reads:

$$H_1^\ell(u) = \begin{cases} B_{IJ}\#(S_u \cap [0,1]) - \sum_{j=2}^K (j-1)J_j(\gamma) & \text{if } u \in SBV_c^\ell(0,1), \\ +\infty & \text{otherwise.} \end{cases} \tag{3.120}$$

3.4.2 Non-accuracy of the Γ-expansion

In this section, we point out a non-accuracy of the development by Γ-convergence which we have presented in Section 3.2 and 3.3. This issue was already discussed in [20, 51] for the cases $K = 1, 2$; we follow their arguments here.

For given $\ell > 0$, we consider $u_0^{(1)}, u_1^{(1)} \in \mathbb{R}_+^{K-1}$ such that $u_{0,s}^{(1)} = u_{1,s}^{(1)} = \min\{\ell, \gamma\}$ for $1 \le s < K$. We recall that $m^{(0)}(\ell) := \min H^\ell = J_{CB}^{**}(\ell)$, see (3.27). For the minimum $m^{(1)}(\ell)$ of the first-order Γ-limit H_1^ℓ, given in the Theorems 3.12 and 3.19, we deduce that

$$m^{(1)}(\ell) := \begin{cases} -\sum_{j=2}^K (j-1)J_j(\ell) & \text{if } \ell \le \gamma, \\ -\sum_{j=2}^K (j-1)J_j(\gamma) + B_{IJ} & \text{if } \ell > \gamma, \end{cases} \tag{3.121}$$

see Corollary 3.14 and Remark 3.25. In the case $\ell \le \gamma$, the (unique) minimiser of the first-order Γ-limit is given by the continuous function $u_\ell(x) = \ell x$, $x \in [0,1]$. For $\ell > \gamma$ the minimisers of H_1^ℓ are functions in SBV_c^ℓ with only one jump point. Indeed, this is a consequence of (3.120) and $B_{IJ} > 0$, see Lemma 3.23.

The Γ-expansion yields the following approximation of the minimum values $m_n(\ell) := \min_u H_n^\ell(u)$ of the discrete energy:

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

Direct computations of the exact values of $m_n(\ell)$ yield that the function $\ell \mapsto m_n(\ell)$ is continuous (see e.g. [60]). In the case $\ell = \gamma$ and $u_{0,s}^{(1)} = u_{1,s}^{(1)} = \gamma$, for $1 \le s < K$, we can calculate the minima $m_n(\gamma)$ explicitly. Indeed, we obtain from (3.7), the definition of $J_{0,j}$, (3.12) and $J_{0,j}(\gamma) = J_j(\gamma) + c_j J_1(\gamma)$ (see (LJ4)) that

$$\begin{aligned} H_n^\gamma(u) \ge& \sum_{j=2}^K \sum_{i=0}^{n-j} \lambda_n J_{0,j}(\gamma) + 2\sum_{j=2}^K c_j \sum_{s=1}^{j-1} \frac{j-s}{j} \lambda_n J_1(\gamma) \\ =& \sum_{j=2}^K J_{0,j}(\gamma) - \lambda_n \sum_{j=2}^K (j-1)J_{0,j}(\gamma) + \lambda_n J_1(\gamma) \sum_{j=2}^K (j-1)c_j \\ =& J_{CB}(\gamma) - \lambda_n \sum_{j=2}^K (j-1)J_j(\gamma). \end{aligned}$$

By taking the infimum over u, we obtain $m_n(\gamma) \ge J_{CB}(\gamma) - \lambda_n (j-1)J_j(\gamma)$. The reverse inequality follows since $H_n^\gamma(u_\gamma) = J_{CB}(\gamma) - \lambda_n (j-1)J_j(\gamma)$, where $u_\gamma(x) = \gamma x$, $x \in [0,1]$.

Thus $m_n(\gamma) = J_{CB}(\gamma) - \lambda_n \sum_{j=2}^{K}(j-1)J_j(\gamma)$. Formally, we have

$$\lim_{\ell\to\gamma+}\Big(m^{(0)}(\ell) + \lambda_n m^{(1)}(\ell) - m_n(\ell)\Big) = \lambda_n B_{IJ},$$

from which one can deduce that the Γ-expansion is not accurate close to the point $\ell = \gamma$.

As it is pointed out in [20, 51], the physical reason for this is the crack nucleation at $\ell = \gamma$. This breaks the separation of scales and thus we have to consider a simultaneous limit $\ell \to \gamma$ and $n \to \infty$ to obtain a more accurate approximation of $m_n(\ell)$ for ℓ close to γ. This is the subject of Section 3.5 and Section 3.6.

3.4.3 Exponential decay of $B(\gamma)$ for second neighbour interactions

Next, we investigate the boundary layer energy $B(\gamma)$, see (3.71), in more detail. Therefore, we restrict ourselves to the case of nearest and next-to-nearest neighbour interaction, i.e. the case $K = 2$. Recall that in this case, we have

$$J_0(z) := J_{0,2}(z) = J_2(z) + \frac{1}{2}\inf\{J_1(z_1) + J_1(z_2) :\ z_1 + z_2 = 2z\}$$

and $\psi_2(z) \equiv J_{CB} \equiv J_1 + J_2$. Throughout this subsection, we assume that J_1 and J_2 satisfy the assumptions (LJ1)–(LJ5) (for $K = 2$). We make the following additionally assumptions on J_1 and J_2:

(1) The functions J_1 and J_2 are of class C^2 in their domain.

(2) There exist constants z_c^1 and z_c^2 with $z_c^1 > \delta_1 > \gamma > z_c^2 > \delta_2$ such that J_1 is strictly convex on $(-\infty, z_c^1) \cap \operatorname{dom} J_1$ and J_2 is strictly concave on $(z_c^2, +\infty)$, where $\delta_1, \delta_2, \gamma$ denote the unique minimisers of J_1, J_2, J_0, see (LJ2), (LJ4).

(3) There exist constants $\alpha, \beta, z_c^3 > 0$ with $z_c^1 \geq z_c^3 > \gamma$ such that $J_{CB}''(z) \geq \alpha$, $J_1''(z) \geq \beta$ for $z \in (-\infty, z_c^3) \cap \operatorname{dom} J_1$.

(4) The function J_i is decreasing on $(-\infty, \delta_i)$ and increasing on $(\delta_i, +\infty)$ for $i = 1, 2$.

(5) It holds: $J_1'(z_c^2) + \sup_z J_2'(z) < 0$

Remark 3.26. Our main example, the Lennard-Jones potentials, satisfy the above assumptions. Assumption (1) and (4) are clear. Let us briefly discuss the remaining assumptions. Recall that $J_1(z) = k_1 z^{-12} - k_2 z^{-6}$ for $z > 0$, $J_1(z) = +\infty$ for $z \leq 0$ and $J_2(z) = J_1(2z)$. From the calculations of Proposition 3.2, we have

$$\delta_j = \frac{1}{j}\left(\frac{2k_1}{k_2}\right)^{\frac{1}{6}} \quad \text{for } j = 1, 2 \quad \text{and} \quad \gamma = \left(\frac{1 + 2^{-12}}{1 + 2^{-6}}\right)^{\frac{1}{6}} \delta_1 < \delta_1.$$

The function J_1 has exactly one inflection point z_c^1, given by

$$z_c^1 = \left(\frac{26k_1}{7k_2}\right)^{\frac{1}{6}} = \left(\frac{13}{7}\right)^{\frac{1}{6}} \delta_1 > \delta_1.$$

It holds that J_1 is convex on $(0, z_c^1)$ and concave on $(z_c^1, +\infty)$. The same hold true for J_2 and $z_c^2 := \frac{1}{2}z_c^1$. Note that $\delta_2 = \frac{1}{2}\delta_1 < z_c^2 = \frac{1}{2}z_c^1 < \gamma$. Hence, (2) is satisfied. The assumption (3) is satisfied with $z_c^3 = \delta_1$. Indeed, J_{CB} is given by $J_{CB}(z) = k_1(1 + 2^{-12})\frac{1}{z^{12}} - k_2(1+2^{-6})\frac{1}{z^6}$ for $z > 0$ and $J_{CB} = +\infty$ for $z \leq 0$. Hence, it is also a Lennard-Jones potential. The inflection point of J_{CB} is given by $z = \left(\frac{13}{7}\right)^{\frac{1}{6}}\gamma = (\frac{13}{7})^{\frac{1}{6}}(\frac{1+2^{-12}}{1+2^{-6}})^{\frac{1}{6}}\delta_1 > \delta_1$. Note that we used that γ is the minimiser of J_{CB}. It is left to show (5). Note that $\sup_z J_2'(z) = J_2'(z_c^2)$, where z_c^2 is the inflection point of J_2. Hence,

$$J_1'\left(z_c^2\right) + J_2'\left(z_c^2\right) = J_{CB}'(z_c^2) < 0,$$

which shows that (5) is satisfied. Note that we used $0 < z_c^2 < \gamma$ and J_{CB} is strictly decreasing on $(0, \gamma)$.

A similar reasoning can be applied to Morse potentials, see (3.24), in a certain parameter regime. Let us choose δ_1 such that $\gamma = 1$, i.e.

$$\delta_1 = \frac{1}{k_2}\ln\left(\frac{e^{-k_2} + 2e^{-2k_2}}{e^{-2k_2} + 2e^{-4k_2}}\right).$$

By a direct calculation, we obtain that $k_2 > 1 + \sqrt{3}$ ensures $z_c^2 < 1 = \gamma$, see also [36, p. 112]. With this restriction on k_2, we can show the assumptions (1)–(5) in a similar manner as in the case of Lennard-Jones potentials (we can choose $z_c^3 = \delta_1$ to show (3)).

We prove under these assumptions an exponential decay of the boundary layer $B(\gamma)$ in the sense of Proposition 3.30. Therefore, we rely on a similar result by Hudson in [35]. In [35], the author considers a one-dimensional discrete system with nearest and next-to-nearest neighbour interaction. The interaction potential J_1 for the nearest neighbour interaction is assumed to be convex with quadratic growth at $+\infty$, and the interaction potential for the next-to-nearest neighbour interaction J_2 is assumed to be concave. Under certain additional assumptions decay estimates are proven for similar boundary layer energies as our $B(\gamma)$. In order to use the techniques provided in [35], we have to show that functions $v : \mathbb{N}_0 \to \mathbb{R}$ which almost minimises the functional in the definition of $B(\gamma)$ are such that the nearest neighbours are in the 'convex region' of J_1 and the next-to-nearest neighbours are in the 'concave region' of J_2.

First, we recall the definition of $B(\gamma)$, see (3.71), in the case of only nearest and next-to-nearest neighbour interactions

$$B(\gamma) = \inf_{N \in \mathbb{N}_0} \min\left\{\frac{1}{2}J_1\left(u^1 - u^0\right) + \sum_{i \geq 0}\left\{J_2\left(\frac{u^{i+2} - u^i}{2}\right) + \frac{1}{2}\sum_{s=i}^{i+1} J_1\left(u^{s+1} - u^s\right) - J_{CB}(\gamma)\right\} : u : \mathbb{N}_0 \to \mathbb{R}, u^0 = 0, u^{i+1} - u^i = \gamma \text{ if } i \geq N\right\}.$$

Next, we rewrite $B(\gamma)$ in a suitable variational framework. Let us define the function $F:\mathbb{R}^2\to\mathbb{R}\cup\{+\infty\}$ by

$$F(a,b) := J_2\left(\gamma+\frac{a+b}{2}\right)+\frac{1}{2}J_1(\gamma+a)+\frac{1}{2}J_1(\gamma+b)-J_{CB}(\gamma).$$

Since J_1 and J_2 satisfy (LJ1)–(LJ5), we have $F\geq 0$ and $F(a,b)=0$ if and only if $a=b=0$. Note that $F(a,b)=F_2^\gamma(\gamma+a,\gamma+b)$, where F_2^γ is as in (3.44) with $K=2$. For $(r^i)_{i=1}^\infty\in\ell^\infty(\mathbb{N})$, we define the functional $B_\gamma:\ell^\infty(\mathbb{N})\to\mathbb{R}\cup\{+\infty\}$ by

$$B_\gamma(r)=\frac{1}{2}J_1\left(\gamma+r^1\right)+\sum_{i=1}^\infty F\left(r^i,r^{i+1}\right). \tag{3.122}$$

By setting $\gamma+r^i=u^i-u^{i-1}$, we can rewrite $B(\gamma)$ as

$$B(\gamma)=\inf_{N\in\mathbb{N}}\min\{B_\gamma(r):\ r\in c_0(N)\},$$

where, we denote by $c_0(N)$ the space of sequences $(a^i)_{i\in\mathbb{N}}\subset\mathbb{R}$ such that $a^i=0$ for $i\geq N$.

Lemma 3.27. *It holds*

$$B(\gamma)=\inf\{B_\gamma(r):\ r\in c_0(\mathbb{N})\}, \tag{3.123}$$

where $c_0(\mathbb{N})$ *denotes the space of sequences converging to* 0.

Proof. Let us denote the right-hand side of (3.123) by $\tilde{B}_\gamma$. The inequality $\tilde{B}_\gamma\leq B(\gamma)$ is obvious since every $r\in c_0(N)$ for some $N\in\mathbb{N}$ satisfies $r\in c_0(\mathbb{N})$. Let us show the reverse inequality. For every $\eta>0$ there exists $r\in c_0(\mathbb{N})$ such that

$$\tilde{B}_\gamma\geq B_\gamma(r)-\eta. \tag{3.124}$$

By the continuity of J_1 and J_2 there exists $\varepsilon>0$ such that

$$\omega(\varepsilon)=\max_{j\in\{1,2\}}\sup\{|J_j(z_1)-J_j(z_2)|:|\gamma-z_i|<\varepsilon\text{ for }i\in\{1,2\}\}<\eta.$$

Since $r\in c_0(\mathbb{N})$ there exists an $N\in\mathbb{N}$ such that $|r^i|<\varepsilon$ for $i\geq N$. Let us define $\tilde{r}\in c_0(\mathbb{N})$ by

$$\tilde{r}^i:=\begin{cases} r^i & \text{for } i\leq N,\\ 0 & \text{for } i\geq N+1.\end{cases}$$

Clearly $\tilde{r} \in c_0(N+1)$. By the definition of $r, \tilde{r}$ and since $F \geq 0$ and $F(0,0) = 0$, we have

$$\begin{aligned} B_\gamma(r) - B_\gamma(\tilde{r}) =& F(r^N, r^{N+1}) - F(r^N, 0) + \sum_{i \geq N+1} F(r^i, r^{i+1}) \\ \geq& J_2\left(\gamma + \frac{r^N + r^{N+1}}{2}\right) - J_2\left(\gamma + \frac{r^N}{2}\right) + \frac{1}{2}\left(J_1(\gamma + r^{N+1}) - J_1(\gamma)\right) \\ \geq& -\frac{3}{2}\eta. \end{aligned} \tag{3.125}$$

Combining (3.124) and (3.125) with the fact that $\tilde{r}$ is a competitor for the infimum problem in the definition of $B(\gamma)$ yields

$$\tilde{B}_\gamma \geq B_\gamma(r) - \eta \geq B_\gamma(\tilde{r}) - \frac{5}{2}\eta \geq B(\gamma) - \frac{5}{2}\eta,$$

and the claim follows by the arbitrariness of $\eta > 0$. □

Let us now show that the infimum in (3.123) is attained.

Lemma 3.28. *There exists a minimiser $\bar{r} \in \ell^2(\mathbb{N})$ of* (3.123). *Moreover, if $r \in \ell^2(\mathbb{N})$ is a minimiser of* (3.123) *then r satisfies the following equilibrium equations*

$$0 = J_1'(\gamma + r^1) + \frac{1}{2}J_2'\left(\gamma + \frac{r^1 + r^2}{2}\right), \tag{3.126}$$

$$0 = \frac{1}{2}J_2'\left(\gamma + \frac{r^{i-1} + r^i}{2}\right) + J_1'(\gamma + r^i) + \frac{1}{2}J_2'\left(\gamma + \frac{r^i + r^{i+1}}{2}\right) \quad \textit{for all } i \geq 2. \tag{3.127}$$

Proof. By Lemma 3.22, we have the following bounds for $B(\gamma)$:

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

Let $(r_n) \subset c_0(\mathbb{N})$ be a sequence such that $\lim_{n\to\infty} B_\gamma(r_n) = \inf_r B_\gamma(r)$. We show that $\|r_n\|_{\ell^2(\mathbb{N})}$ is equibounded. Therefore, we first prove the equiboundedness of (r_n) in $\ell^\infty(\mathbb{N})$. Since $\lim_{z\to-\infty} J_1(z) = +\infty$ and $F \geq 0$, there exists $C_{low} > 0$ such that $\inf_{n\in\mathbb{N}} \inf_{i\in\mathbb{N}} r_n^i > -C_{low}$. Let us assume that $r_n^i > 2\delta_1 + 2\delta_2 + C_{low}$ for some $i \in \mathbb{N}$. Then, we can always decrease $B_\gamma(r_n)$ by reducing r_n^i. Indeed, this follows from the monotonicity of J_i on $(\delta_i, +\infty)$, the fact that $\delta_1, \delta_2, \gamma > 0$, and that $\gamma + r_n^i > \delta_1$ and $\gamma + \frac{1}{2}(r_n^{i-1} + r_n^i), \gamma + \frac{1}{2}(r_n^{i+1} + r_n^i) > \delta_2$. Since (r_n) is a minimising sequence, we can assume that there exists $N \in \mathbb{N}$ such that $\sup_i r_n^i \leq 2\delta_1 + 2\delta_2 + C_{low}$ for $n \geq N$. Hence, $\|r_n\|_{\ell^\infty(\mathbb{N})}$ is equibounded. Let us now show the equiboundedness in $\ell^2(\mathbb{N})$. Let $\varepsilon > 0$ be such that $(\gamma - \varepsilon, \gamma + \varepsilon) \subset (z_c^2, z_c^3)$, cf. assumptions (2), (3). We define the set $I_n = \{i \in \mathbb{N} : |r_n^i| > \varepsilon\}$. From Lemma 3.8, we deduce that there exists $\eta = \eta(\varepsilon) > 0$ such that $F(r^i, r^{i+1}) > \eta$ for $i \in I_n$. This implies $B_\gamma(r_n) \geq \frac{1}{2}J_1(\delta_1) + \eta\#I_n$. Thus there exists a constant $M \in \mathbb{N}$ such that $\sup_n \#I_n \leq M$.

For $i \in \mathbb{N}$ such that $i, i+1 \notin I_n$, we deduce from the concavity of J_2 on $(z_c^2, +\infty)$ that

$$J_2\left(\gamma + \frac{r_n^i + r_n^{i+1}}{2}\right) \geq \frac{1}{2}\left(J_2(\gamma + r_n^i) + J_2(\gamma + r_n^{i+1})\right).$$

A combination of the above inequality with $J_{CB}'(\gamma) = 0$ and (3) yields

$$\begin{aligned} C \geq& \sum_{i \in \mathbb{N}: i, i+1 \notin I_n} \left\{ J_2\left(\gamma + \frac{r_n^{i+1} + r_n^i}{2}\right) + \frac{1}{2} J_1(\gamma + r_n^i) + \frac{1}{2} J_1(\gamma + r_n^{i+1}) - J_{CB}(\gamma) \right\} \\ \geq& \sum_{i \in \mathbb{N}: i, i+1 \notin I_n} \frac{1}{2}\left\{ J_{CB}(\gamma + r_n^i) + J_{CB}(\gamma + r_n^{i+1}) - 2J_{CB}(\gamma) \right\} \\ \geq& \sum_{i \in \mathbb{N}: i, i+1 \notin I_n} \frac{1}{4}\alpha\left((r_n^i)^2 + (r_n^{i+1})^2\right). \end{aligned}$$

Combining this with $\sup \# I_n \leq M$ and $\sup_n \|r_n\|_{\ell^\infty(\mathbb{N})} < +\infty$, we deduce $\sup_n \|r_n\|_{\ell^2(\mathbb{N})} < +\infty$. Hence, there exist a subsequence (r_{n_k}) and $\bar{r} \in \ell^2(\mathbb{N})$ such that $r_{n_k} \rightharpoonup \bar{r}$ in $\ell^2(\mathbb{N})$.
To apply the direct method of the calculus of variations it is left to show that B_γ is lower semicontinuous with respect to the weak convergence of $\ell^2(\mathbb{N})$. Let $r \in \ell^2(\mathbb{N})$ be such that $B_\gamma(r)$ is finite. Since $F(r^i, r^{i+1}) \geq 0$ for all $i \in \mathbb{N}$ there exists for every $\varepsilon > 0$ a constant $N \in \mathbb{N}$ such that

$$B_\gamma(r) \leq \frac{1}{2} J_1\left(r^1\right) + \sum_{i=1}^{N} F\left(r^i, r^{i+1}\right) + \varepsilon.$$

Let $(r_n) \subset \ell^2(\mathbb{N})$ be such that $r_n \rightharpoonup r$ in $\ell^2(\mathbb{N})$. From $r_n \rightharpoonup r$ in $\ell^2(\mathbb{N})$, we deduce that $r_n^i \to r^i$ for every $i \in \mathbb{N}$. Hence, by the continuity of J_1, J_2 and $F \geq 0$, we obtain that

$$\begin{aligned} \liminf_{n \to \infty} B_\gamma(r_n) =& \liminf_{n \to \infty} \left\{ \frac{1}{2} J_1\left(r_n^1\right) + \sum_{i=1}^{N} F_\gamma\left(r_n^i, r_n^{i+1}\right) + \sum_{i \geq N+1} F_\gamma\left(r_n^i, r_n^{i+1}\right) \right\} \\ \geq& \frac{1}{2} J_1\left(r^1\right) + \sum_{i=1}^{N} F\left(r^i, r^{i+1}\right) \geq B_\gamma(r) - \varepsilon. \end{aligned}$$

This proves the lower semicontinuity since $\varepsilon > 0$ can be arbitrarily small. Hence, we have the existence of a minimiser $r \in \ell^2(\mathbb{N})$ of B_γ.
We obtain the equilibrium equations, see (3.126), (3.127), for minimisers $r \in \ell^2(\mathbb{N})$ of B_γ in the same way as it was done in [35, Proposition 6]. We just repeat the argument here. Let $e_i \in \ell^2(\mathbb{N})$ be defined by

$$e_i^j = \begin{cases} 1 & \text{if } j = i, \\ 0 & \text{else.} \end{cases}$$

Let r be the minimiser of B_γ. For $i \geq 2$ and $t > 0$ sufficiently small, it holds

$$\begin{aligned}0 \leq & \frac{B_\gamma(r + te_i) - B_\gamma(r)}{t} \\ = & \int_0^1 \frac{1}{2} J_2' \left(\gamma + \frac{r^{i-1} + r^i + st}{2} \right) + J_1'(\gamma + r^i + st) + \frac{1}{2} J_2' \left(\gamma + \frac{r^i + r^{i+1} + st}{2} \right) ds.\end{aligned}$$

The dominated convergence theorem for $t \to 0+$ and the same argument for $t < 0$ yield

$$\frac{1}{2} J_2' \left(\gamma + \frac{r^{i-1} + r^i}{2} \right) + J_1'(\gamma + r^i) + \frac{1}{2} J_2' \left(\gamma + \frac{r^i + r^{i+1}}{2} \right) = 0,$$

which matches (3.127). The same argument applied to $i = 1$ yields (3.126). $\square$

Next, we prove that every minimiser r of B_γ satisfy that $\gamma + r^i$ is in the 'convex region' of J_1 and the 'concave region' of J_2 for all $i \in \mathbb{N}$.

Lemma 3.29. *Suppose $r \in \ell^2(\mathbb{N})$ is a minimiser of B_γ. Then it holds $r^i \geq r^{i+1} \geq 0$ and $\gamma + r^i \in (z_c^2, z_c^3)$ for all $i \in \mathbb{N}$.*

Proof. Let $r \in \ell^2(\mathbb{N})$ be a minimiser of B_γ. We show that $\gamma + r^i \in (z_c^2, z_c^3)$ for all $i \in \mathbb{N}$. From $B_\gamma(r) = B(\gamma) \leq \frac{1}{2} J_1(\gamma)$ and $\gamma < \delta_1$, we deduce $r^1 \geq 0$, see (3.122). Note that we used (4) and $F \geq 0$. Assume on the contrary that $\gamma + r^i \leq z_c^2$ for some $i \geq 2$. By (4) and $z_c^2 < \delta_1$ this yields $J_1'(\gamma + r^i) \leq J_1'(z_c^2)$. Using assumption (5), we have that

$$\frac{1}{2} J_2' \left(\gamma + \frac{r^{i-1} + r^i}{2} \right) + J_1'(\gamma + r^i) + \frac{1}{2} J_2' \left(\gamma + \frac{r^i + r^{i+1}}{2} \right) \leq J_1'(z_c^2) + \sup_z J_2'(z) < 0.$$

Hence, r does not solve (3.127) and cannot be a minimiser of (3.123). Thus we have that $\gamma + r^i \geq z_c^2 > \delta_2$ for all $i \in \mathbb{N}$. This and (4) imply that $J_2'(\gamma + \frac{r^i + r^{i+1}}{2}) \geq 0$ for all $i \in \mathbb{N}$. Hence, (3.127) implies that $J_1'(\gamma + r^i) \leq 0$ for all $i \geq 2$. This implies $\gamma + r^i \leq \delta_1 < z_c^3$ for every $i \in \mathbb{N}$. Altogether, we have shown that a minimiser $r \in \ell^2(\mathbb{N})$ of (3.123) satisfies $r^1 \geq 0$ and $\gamma + r^i \in (z_c^2, z_c^3)$ for every $i \in \mathbb{N}$.

To conclude the proof, we next follow the proof of [35, Corollary 1]: Consider $i \geq 2$ such that r^i is a local maximum, i.e. $r^i = \max\{r^{i-1}, r^i, r^{i+1}\}$. The concavity of J_2 on $(z_c^2, +\infty)$, (3.127) and (3) implies

$$\begin{aligned}0 = & \frac{1}{2} J_2' \left(\gamma + \frac{r^{i-1} + r^i}{2} \right) + J_1'(\gamma + r^i) + \frac{1}{2} J_2' \left(\gamma + \frac{r^i + r^{i+1}}{2} \right) \\ \geq & J_1'(\gamma + r^i) + J_2'(\gamma + r^i) = J_{CB}'(\gamma + r^i) - J_{CB}'(\gamma) \geq \alpha r^i\end{aligned}$$

and thus $r^i \leq 0$. Next, we consider $r^i = \min\{r^{i-1}, r^i, r^{i+1}\}$. Then, (3.127) and the concavity of J_2 on $(z_c^2, +\infty)$ yields

$$0 \leq J_{CB}'(\gamma + r^i) = J_{CB}''(\xi) r^i$$

for some $\xi \in [\gamma, \gamma + r^i]$. Since $\gamma + r^i < z_c^3$, we have $J''_{CB}(\xi) \geq \alpha > 0$ and thus $r^i \geq 0$.
Let us on the contrary assume that there exists $M \in \mathbb{N}$ such that $r^M < 0$ and $r^M = \max\{r^{M-1}, r^M, r^{M+1}\}$. Then, it follows $r^{M+1} \leq r^M < 0$. Hence, r^{M+1} cannot be a local minimiser and thus $r^{M+2} \leq r^{M+1}$. By induction, we obtain $r^j \leq r^M < 0$ for all $j \geq i$, which contradicts $r \in \ell^2(\mathbb{N})$. By the same argument there does not exist an $m \geq 2$ such that $r^m > 0$ and $r^m = \min\{r^{m-1}, r^m, r^{m+1}\}$.
Consider $M > 0$ such that $r^M = 0$ and $r^M = \max\{r^{M-1}, r^M, r^{M+1}\}$. If $r^{M+1} < 0$ or $r^{M+1} > 0$ the previous arguments lead to a contradiction. Thus $r^{M+1} = 0$. Then r^{M+1} is either a local minimum or a local maximum. Using again the previous arguments yield a contradiction if $r^{M+2} \neq 0$.
Altogether, we have shown that a minimiser of (3.123) does not contain an internal local extremum r^i unless $r^j = 0$ for $j \geq i$. This implies that r^i is monotone and from $r^1 \geq 0$ and $\lim_{i\to\infty} r^i = 0$ the claim follows. □

Now we are in position to prove the exponential decay of minimisers of (3.123).

Proposition 3.30. *Let $C > 0$ be such that for all $t \in (0, r^1)$,*

$$0 \geq J''_2(\gamma + t) \geq -C.$$

Define $\lambda := \frac{C}{\alpha+C}$ with C as above and $\alpha > 0$ as in assumption (3). Then, we have $\lambda \in (0, 1)$ and

$$0 \leq r^i \leq \lambda^{i-1} r^1.$$

Proof. Let r be a minimiser of B_γ. Since we have already shown that $\gamma + r^i \in (z_c^2, z_c^3)$ we can use the same proof as [35, Proposition 15]. The equation (3.127) can be rewritten, using $J'_{CB}(\gamma) = 0$, as

$$\begin{aligned} 0 =& \frac{1}{2} J'_2\left(\gamma + \frac{r^{i-1} + r^i}{2}\right) + \frac{1}{2} J'_2\left(\gamma + \frac{r^i + r^{i+1}}{2}\right) + J'_{CB}(\gamma + r^i) - J'_2(\gamma + r^i) \\ =& \int_{r^i}^{r^{i-1}} J''_2\left(\gamma + \frac{r^i + t}{2}\right) dt + \int_{r^i}^{r^{i+1}} J''_2\left(\gamma + \frac{r^i + t}{2}\right) dt + \int_0^{r^i} J''_{CB}(\gamma + t) dt. \end{aligned}$$

By Lemma 3.29, we have $r^{i-1} \geq r^i \geq r^{i+1} \geq 0$. The definition of C, α, see (3), and the fact that $J''_2 \leq 0$ on $[\gamma, +\infty)$ imply that

$$\begin{aligned} 0 =& \int_{r^i}^{r^{i-1}} J''_2\left(\gamma + \frac{r^i + t}{2}\right) dt - \int_{r^{i+1}}^{r^i} J''_2\left(\gamma + \frac{r^i + t}{2}\right) dt + \int_0^{r^i} J''_{CB}(\gamma + t) dt \\ \geq& - C(r^{i-1} - r^i) + \alpha r^i. \end{aligned}$$

Hence, it follows

$$r^i \leq \frac{C}{C + \alpha} r^{i-1}$$

for every $i \geq 2$. The claim follows by $\alpha, C > 0$. □

Notice that in [36, Section 2.3] exponential decay for a similar boundary layer is proven for a linearised Morse potential model. In Proposition 3.30, we provide the corresponding result for the nonlinear model.

3.5 Analysis of rescaled functionals

As we have outlined in Section 3.4.2, the formal development by Γ-convergence may not yield a good approximation for the minima of H_n^ℓ for ℓ close to γ. Hence, we present a refined analysis in this section. For this, we consider the behaviour of the sequence of functionals $(H_n^{\ell_n})$ for some sequence $(\ell_n) \subset \mathbb{R}$ instead of (H_n^ℓ) with fixed $\ell > 0$. More precisely, we consider sequences $(\ell_n) \subset \mathbb{R}$ satisfying $\ell_n \geq \gamma$ for all $n \in \mathbb{N}$ and $\ell_n \to \gamma$ such that

$$\delta_n := \frac{\ell_n - \gamma}{\sqrt{\lambda_n}} \to \delta \geq 0 \quad \text{as } n \to \infty. \tag{3.128}$$

For fixed $u_0^{(1)}, u_1^{(1)} \in \mathbb{R}_+^{K-1}$, we consider the analogous boundary conditions to (3.3) where ℓ is replaced by ℓ_n:

$$\begin{aligned} &u^0 = 0, \ u^s - u^{s-1} = \lambda_n u_{0,s}^{(1)}, \\ &u^n = \ell_n, \ u^{n+1-s} - u^{n-s} = \lambda_n u_{1,s}^{(1)} \quad \text{for } 1 \leq s \leq K-1. \end{aligned} \tag{3.129}$$

For $u \in \mathcal{A}_n(0,1)$ satisfying (3.129), we define $v := \frac{1}{\sqrt{\lambda_n}}(u - u_\gamma) \in \mathcal{A}_n(0,1)$, where $u_\gamma(x) = \gamma x$ for $x \in [0,1]$. The definition of v implies that $v^i = \frac{1}{\sqrt{\lambda_n}}(u^i - \lambda_n \gamma i)$ for $i \in \{0, \dots, n\}$, and

$$\begin{aligned} &v^0 = 0, \ v^s - v^{s-1} = \sqrt{\lambda_n}(u_{0,s}^{(1)} - \gamma), \\ &v^n = \delta_n, \ v^{n+1-s} - v^{n-s} = \sqrt{\lambda_n}(u_{1,s}^{(1)} - \gamma), \quad \text{for } 1 \leq s \leq K-1. \end{aligned} \tag{3.130}$$

We can rewrite $H_{1,n}^{\ell_n}(u)$ in terms of the displacement v instead of the deformation u by

$$E_n^{\delta_n}(v) = H_{1,n}^{\ell_n}(u), \quad \text{with} \quad E_n^{\delta_n}(v) := H_{1,n}^{\ell_n}(u_\gamma + \sqrt{\lambda_n} v).$$

The functional $E_n^{\delta_n} : L^1(0,1) \to (-\infty, +\infty]$ is given by

$$E_n^{\delta_n}(v) := \begin{cases} E_n(v) & \text{if } v \in \mathcal{A}_n(0,1) \text{ satisfies (3.130)}, \\ +\infty & \text{else}, \end{cases} \tag{3.131}$$

where E_n is defined by

$$E_n(v) := \sum_{j=1}^{K} \sum_{i=0}^{n-j} J_j \left(\gamma + \frac{v^{i+j} - v^i}{j\sqrt{\lambda_n}} \right) - nJ_{CB}(\gamma). \tag{3.132}$$

Note that we have used that $J_{CB}^{**}(\ell_n) = J_{CB}(\gamma)$ since $\ell_n \geq \gamma$ by assumption.

The remainder of this section is devoted to a Γ-convergence analysis of the sequence of functionals $(E_n^{\delta_n})$ as n tends to infinity. In addition to the assumptions (LJ1)–(LJ5), we state further assumptions on the potentials J_j with $j \in \{1, \dots, K\}$:

(LJ6) The functions $J_1, \dots, J_K$ are C^2 on their domain.

(LJ7) For given $j \in \{2, \dots, K\}$ there exist $\eta > 0$ and $C > 0$ such that

$$\frac{1}{j}\sum_{s=1}^{j} J_1(z_s) \geq J_1(z) + C\sum_{s=1}^{j}(z_s - z)^2 \tag{3.133}$$

whenever $\sum_{s=1}^{j} z_s = jz$ and $\sum_{s=1}^{j}|z_s - z| + |z - \gamma| \leq \eta$. Moreover, it holds that $\psi_j''(\gamma) > 0$, were γ and ψ_j are given in (3.12) and (3.14).

Remark 3.31. The additional assumptions (LJ6) and (LJ7) are satisfied by our main example of the Lennard-Jones potentials given in (3.22). Indeed, the regularity is clear by the definition. Moreover, we have shown in Proposition 3.2 that $\gamma < \delta_1$ and $\psi_j''(\gamma) > 0$ for $j \in \{2, \dots, K\}$. We only have to show that there exist $\eta, C > 0$ such that (3.133) holds true. Fix $j \in \{2, \dots, K\}$. For z and z_s such that $jz = \sum_{s=1}^{j} z_s$, we make the following expansion:

$$\sum_{s=1}^{j} J_1(z_s) = jJ_1(z) + J_1'(z)\sum_{s=1}^{j}(z_s - z) + \frac{1}{2}\sum_{s=1}^{j} J_1''(z + \xi_s)(z_s - z)^2$$

with $|\xi_s| \leq |z_s - z|$. The second term on the right-hand side vanishes since $\sum_{s=1}^{j} z_s = jz$. For $\eta > 0$ sufficiently small, e.g. $\eta < \frac{1}{2}|\gamma - \delta_1|$, we have for z with $|z - \gamma| < \eta$ that $J_1''(z + \xi_s) \geq \inf_{0<z\leq\delta_1} J_1''(z) > 0$, which proves the assertion.

As in the analysis of the first-order Γ-limit in Section 3.3 it is useful to rewrite the energy E_n, as $H_{1,n}^{\ell}$ in (3.41), in a suitable way:

$$\begin{aligned}
E_n(v) =& \sum_{j=1}^{K}\sum_{i=0}^{n-j} J_j\left(\gamma + \frac{v^{i+j} - v^i}{j\sqrt{\lambda_n}}\right) - nJ_{CB}(\gamma)\\
=& \sum_{j=2}^{K} c_j \sum_{s=1}^{j-1}\frac{j-s}{j} J_1\left(\gamma + \frac{v^s - v^{s-1}}{\sqrt{\lambda_n}}\right) + \sum_{j=2}^{K}\sum_{i=0}^{n-j}\left\{J_j\left(\gamma + \frac{v^{i+j} - v^i}{j\sqrt{\lambda_n}}\right)\right.\\
&\left. + \frac{c_j}{j}\sum_{s=i}^{i+j-1} J_1\left(\gamma + \frac{v^{s+1} - v^s}{\sqrt{\lambda_n}}\right) - \psi_j(\gamma)\right\}\\
&+ \sum_{j=2}^{K} c_j \sum_{s=1}^{j-1}\frac{j-s}{j} J_1\left(\gamma + \frac{v^{n+1-s} - v^{n-s}}{\sqrt{\lambda_n}}\right) - \sum_{j=2}^{K}(j-1)\psi_j(\gamma)
\end{aligned}$$

Note that, we used here $J_{CB}(\gamma) = \sum_{j=2}^{K} \psi_j(\gamma)$. For a sequence of functions (v_n) satisfying $v_n \in \mathcal{A}_n(0,1)$ and (3.130) the energy $E_n^{\delta_n}(v_n)$ reads

$$E_n^{\delta_n}(v_n) = \sum_{j=2}^{K} \left\{ \sum_{i=0}^{n-j} \zeta_{j,n}^i + c_j \sum_{s=1}^{j-1} \frac{j-s}{j} \left(J_1(u_{0,s}^{(1)}) + J_1(u_{1,s}^{(1)}) \right) - (j-1)\psi_j(\gamma) \right\} \tag{3.134}$$

where $\zeta_{j,n}^i$ is defined as

$$\zeta_{j,n}^i := J_j \left(\gamma + \frac{v_n^{i+j} - v_n^i}{j\sqrt{\lambda_n}} \right) + \frac{c_j}{j} \sum_{s=i}^{i+j-1} J_1 \left(\gamma + \frac{v_n^{s+1} - v_n^s}{\sqrt{\lambda_n}} \right) - \psi_j(\gamma), \tag{3.135}$$

for $j \in \{2, \dots, K\}$ and $i \in \{0, \dots, n-j\}$. By the definition of $J_{0,j}$, see (3.8), γ and ψ_j (see (LJ4)), we have that $\zeta_{j,n}^i \geq J_{0,j}(\gamma + \frac{v_n^{i+j} - v_n^i}{j\sqrt{\lambda_n}}) - \psi_j(\gamma) \geq 0$. The following lemma is similar to [17, Remark 4] and will give us a finer estimate of terms of the form as $\zeta_{j,n}^i$.

Lemma 3.32. *Let $J_1, \dots, J_K$ satisfy the assumptions (LJ1)–(LJ7). For $\eta_1 > 0$ sufficiently small there exists $C_1 > 0$ such that*

$$J_j \left(\sum_{s=1}^{j} \frac{z_s}{j} \right) + \frac{c_j}{j} \sum_{s=1}^{j} J_1(z_s) - \psi_j(\gamma) \geq C_1 \sum_{s=1}^{j} (z_s - \gamma)^2 \tag{3.136}$$

if $\sum_{s=1}^{j} |z_s - \gamma| \leq \eta_1$.

Proof. Fix $j \in \{2, \dots, K\}$. If $\sum_{s=1}^{j} z_s = j\gamma$ the claim follows from assumption (LJ7). Let η denotes the same constant as in assumption (LJ7). Since $\psi_j \in C^2(0, +\infty)$ (see (LJ1) and (LJ6)), $\gamma > 0$ and $\psi_j''(\gamma) > 0$ there exists $\eta_1 > 0$ such that $\sum_{s=1}^{j} |z_s - \gamma| \leq \eta_1$ implies $\sum_{s=1}^{j} |z_s - z| + |z - \gamma| \leq \eta$ for $\sum_{s=1}^{j} z_s = jz$ and that there exists $\delta > 0$ such that $\psi_j'' \geq \delta$ on $[\gamma - \eta_1, \gamma + \eta_1]$.

Assume by contradiction that there exist $\hat{z}_s$, $s = 1, \dots, j$ and $\hat{z} = \sum_{s=1}^{j} \frac{\hat{z}_s}{j}$ such that $\sum_{s=1}^{j} |\hat{z}_s - \gamma| < \eta_1$ and for all $N > 2$ it holds

$$J_j(\hat{z}) + \frac{c_j}{j} \sum_{s=1}^{j} J_1(\hat{z}_s) - \psi_j(\gamma) \leq \frac{C}{N} \sum_{s=1}^{j} (\hat{z}_s - \gamma)^2,$$

where C is the same constant as in (3.133). By the choice of η_1, we have $\sum_{s=1}^{j} |\hat{z}_s - \hat{z}| + |\hat{z} - \gamma| \leq \eta$ and thus by (3.133) it holds

$$\begin{aligned} J_j(\hat{z}) + \frac{c_j}{j} \sum_{s=1}^{j} J_1(\hat{z}_s) - \psi_j(\gamma) &\leq \frac{C}{N} \sum_{s=1}^{j} (\hat{z}_s - \gamma)^2 \leq \frac{2C}{N} \sum_{s=1}^{j} (\hat{z}_s - \hat{z})^2 + \frac{2Cj}{N} (\hat{z} - \gamma)^2 \\ &\leq \frac{2}{N} \left(J_j(\hat{z}) + \frac{c_j}{j} \sum_{s=1}^{j} J_1(\hat{z}_s) - \psi_j(\hat{z}) \right) + \frac{2Cj}{N} (\hat{z} - \gamma)^2. \end{aligned}$$

In the last inequality, we used (3.133) and the definition of ψ_j, see (3.14). For $\eta_1 > 0$ sufficiently small, such that $\hat{z} < \gamma^c$ (see (LJ4)), we have by the definition of $J_{0,j}$ and $J_{0,j}(\hat{z}) = \psi_j(\hat{z})$ that

$$\psi_j(\hat{z}) - \psi_j(\gamma) \leq J_j(\hat{z}) + \frac{c_j}{j}\sum_{s=1}^{j} J_1(\hat{z}_s) - \psi_j(\gamma) \leq \frac{2jC}{N-2}(\hat{z}-\gamma)^2.$$

Clearly, this is, for N sufficiently large, a contradiction to

$$\psi_j(\hat{z}) - \psi_j(\gamma) = \frac{1}{2}\int_\gamma^{\hat{z}} \psi_j''(s)(s-\gamma)ds \geq \frac{1}{4}\delta(\hat{z}-\gamma)^2,$$

where we used $\psi_j'(\gamma) = 0$. □

Next, we state a compactness result for functions with equibounded energy $E_n^{\delta_n}$.

Lemma 3.33. *Assume that $J_1, \dots, J_K$ satisfy the assumptions (LJ1)–(LJ7). Let $u_0^{(1)}$, $u_1^{(1)} \in \mathbb{R}_+^{K-1}$ and $\delta_n \to \delta$ such that* (3.128) *is satisfied. Let (v_n) be a sequence of functions such that*

$$\sup_n E_n^{\delta_n}(v_n) < +\infty. \tag{3.137}$$

Then there exist a subsequence (v_{n_k}) and $v \in SBV^\delta(0,1)$ such that $v_{n_k} \to v$ in $L^1(0,1)$. The function v satisfies

$$v' \in L^2(0,1), \quad \#S_v < +\infty, \quad [v] \geq 0 \text{ in } [0,1]. \tag{3.138}$$

Moreover, there exists a finite set $S \subset [0,1]$ such that $v_{n_k} \rightharpoonup v$ locally weakly in $H^1((0,1)\setminus S)$.

Proof. Let (v_n) be such that (3.137) is satisfied. By $\{\gamma\} = \arg\min_z J_{0,j}(z)$ and by Lemma 3.32, there exist constants $K_1, K_2 > 0$ such that for all $i \in \{0,\dots,n-j\}$ it holds

$$\zeta_{n,j}^i \geq \left\{K_1 \sum_{s=i}^{i+j-1}\left(\frac{v_n^{s+1}-v_n^s}{\sqrt{\lambda_n}}\right)^2\right\} \wedge K_2. \tag{3.139}$$

Hence, we deduce from (3.134) that

$$\begin{aligned} E_n^{\delta_n}(v_n) &\geq \sum_{j=2}^{K}\sum_{i=0}^{n-j}\left\{\lambda_n K_1 \sum_{s=i}^{i+j-1}\left(\frac{v_n^{s+1}-v_n^s}{\lambda_n}\right)^2\right\} \wedge K_2 + K_3 \\ &\geq \sum_{i=0}^{n-1}\left\{\lambda_n K_1\left(\frac{v_n^{i+1}-v_n^i}{\lambda_n}\right)^2 \wedge K_2\right\} + K_3, \end{aligned} \tag{3.140}$$

with

$$K_3 := \sum_{j=2}^{K} c_j \sum_{s=1}^{j-1} \frac{j-s}{j} \left(J_1(u_{0,s}^{(1)}) + J_1(u_{1,s}^{(1)}) \right) - \sum_{j=2}^{K} (j-1)\psi_j(\gamma). \tag{3.141}$$

Next, we show that $\sup_n \|v_n\|_{W^{1,1}(0,1)} < +\infty$. Therefore, we define the sets I_n^- and I_n^{--} by

$$\begin{aligned} I_n^- &:= \left\{ i \in \{0, \dots, n-1\} : v_n^{i+1} < v_n^i \right\}, \\ I_n^{--} &:= \left\{ i \in I_n^- : K_1 \lambda_n \left(\frac{v_n^{i+1} - v_n^i}{\lambda_n} \right)^2 \geq K_2 \right\}. \end{aligned}$$

From (3.140), we deduce that

$$\begin{aligned} E_n^{\delta_n}(v_n) &\geq \sum_{i \in I_n^-} \left(\lambda_n K_1 \left(\frac{v_n^{i+1} - v_n^i}{\lambda_n} \right)^2 \wedge K_2 \right) + K_3 \\ &\geq \sum_{i \in I_n^- \setminus I_n^{--}} \lambda_n K_1 \left(\frac{v_n^{i+1} - v_n^i}{\lambda_n} \right)^2 + K_2 \# I_n^{--} + K_3. \end{aligned}$$

Thus, we obtain from $\sup_n E_n^{\delta_n}(v_n) < +\infty$ and $K_2 > 0$ that $I^{--} := \sup_n \# I_n^{--} < +\infty$. Moreover, we deduce from the equiboundedness of the energy, $\lim_{z \to -\infty} J_j(z) = +\infty$, $\zeta_{n,j}^i \geq 0$, and the fact that J_j is bounded from below for $j \in \{1, \dots, K\}$, that there exists a constant $M \geq 0$ such that

$$\gamma + \frac{v_n^{i+1} - v_n^i}{\sqrt{\lambda_n}} \geq -M \quad \Rightarrow \quad \frac{v_n^{i+1} - v_n^i}{\lambda_n} \geq -\frac{M + \gamma}{\sqrt{\lambda_n}}, \tag{3.142}$$

for all n and $i \in \{0, \dots, n-1\}$. Hence, using Hölder's inequality and $\# I_n^- \leq n$, we have for $(v_n')^- := -(v_n' \wedge 0)$ that

$$\begin{aligned} &\|(v_n')^-\|_{L^1(0,1)} \leq \sum_{i \in I_n^-} \lambda_n \left| \frac{v_n^{i+1} - v_n^i}{\lambda_n} \right| \\ &\leq \sum_{i \in I_n^- \setminus I_n^{--}} \lambda_n \left| \frac{v_n^{i+1} - v_n^i}{\lambda_n} \right| + \sqrt{\lambda_n} \# I_n^{--} |M + \gamma| \\ &\leq \left(\sum_{i \in I_n^- \setminus I_n^{--}} \lambda_n \left| \frac{v_n^{i+1} - v_n^i}{\lambda_n} \right|^2 \right)^{\frac{1}{2}} + \left(\sum_{i \in I_n^- \setminus I_n^{--}} \lambda_n \right)^{\frac{1}{2}} + \sqrt{\lambda_n} \# I_n^{--} |M + \gamma| \\ &\leq \left(\frac{1}{K_1} E_n^{\delta_n}(v_n) - K_3 \right)^{\frac{1}{2}} + 1 + I^{--} |M + \gamma|. \end{aligned}$$

Thus there exists $C > 0$ such that $\|(v_n')^-\|_{L^1(0,1)} < C$. Using the boundary conditions $v_n(0) = 0$ and $v_n(1) = \delta_n$, we obtain that

$$\int_{\{v_n'\geq 0\}} v_n'(x)dx = \delta_n - \int_{\{v_n'<0\}} v_n'(x)dx \leq \delta_n + C.$$

Thus, v_n' is equibounded in $L^1(0,1)$. The Poincaré-inequality and $v_n(0) = 0$ for all $n \in \mathbb{N}$ yield that $\sup_n \|v_n\|_{W^{1,1}(0,1)} < +\infty$. By the equiboundedness of the $W^{1,1}$-norm, there exists $v \in BV(0,1)$ such that, up to subsequences, (v_n) weakly* converges in $BV(0,1)$ to v. A similar argument as in the compactness proof in Theorem 3.7 yields $v \in BV^\delta(0,1)$.

Next, we show that $v \in SBV^\delta(0,1)$ and v satisfies (3.138). Let us define the set

$$I_n := \left\{ i \in \{0,\dots,n-1\} : K_1\lambda_n \left(\frac{v_n^{i+1} - v_n^i}{\lambda_n}\right)^2 \geq K_2 \right\}.$$

Moreover, we define the sequence $(\tilde{v}_n) \subset SBV(0,1)$ by $\tilde{v}_n(1) = \delta_n$ and

$$\tilde{v}_n(x) := \begin{cases} v_n(x) & \text{if } x \in \lambda_n[i,i+1),\ i \notin I_n, \\ v_n(i\lambda_n) & \text{if } x \in \lambda_n[i,i+1),\ i \in I_n. \end{cases}$$

The construction of $\tilde{v}_n$ implies $\lim_{n\to\infty} \|\tilde{v}_n - v_n\|_{L^1(0,1)} = 0$, $\|\tilde{v}_n\|_{BV(0,1)} \leq \|v_n\|_{W^{1,1}(0,1)}$ and thus $\tilde{v}_n \overset{*}{\rightharpoonup} v$ in $BV(0,1)$. Moreover, it holds $\#S_{\tilde{v}_n} = \#I_n$ and

$$\begin{aligned} +\infty > E_n^{\delta_n}(v_n) &\geq \sum_{\substack{i=0\\ i\notin I_n}}^{n-1} K_1\lambda_n \left(\frac{v_n^{i+1} - v_n^i}{\lambda_n}\right)^2 + K_2\#I_n + K_3 \\ &\geq \min\{K_1, K_2\} \left(\int_0^1 |\tilde{v}_n'(x)|^2 dx + \#S_{\tilde{v}_n}\right) + K_3. \end{aligned} \tag{3.143}$$

Hence, we obtain by the closure theorem for SBV functions that $v \in SBV(0,1)$, $\tilde{v}_n' \rightharpoonup v'$ in $L^1(0,1)$, $+\infty > \liminf_{n\to\infty} \#S_{v_n} \geq \#S_v$ and $D^j\tilde{v}_n \overset{*}{\rightharpoonup} D^jv$ weakly* in the sense of measures, see Theorem 2.8. Moreover, we deduce that $\tilde{v}_n' \rightharpoonup v' \in L^2(0,1)$ in $L^2(0,1)$ from $\sup_n \|\tilde{v}_n'\|_{L^2(0,1)} < +\infty$ (see (3.143)).

Let us now show that there exists a finite set $S \subset [0,1]$ such that $v_n \rightharpoonup v$ locally weakly in $H^1((0,1)\setminus S)$. Here, we use similar arguments as in [10, Lemma 2.4]. The estimate (3.143), yields the existence of $x_1^n, \dots, x_m^n \in [0,1]$, with m independent of n, such that

$$S_{\tilde{v}_n} \subset \{x_i^n :\ i \in \{1,\dots,m\}\}.$$

Up to subsequences, we have that $x_i^n \to x_i \in [0,1]$ for $i \in \{1,\dots,m\}$. We set $S = \{x_1,\dots,x_m\}$. Fix $\eta > 0$ and define $S_\eta := \bigcup_{i=1}^m (x_i - \eta, x_i + \eta)$. Then there exists a constant $N \in \mathbb{N}$ such that $v_n \equiv \tilde{v}_n$ on $(0,1)\setminus S_\eta$ for $n \geq N$ and by (3.143) that $\sup_{n\geq N} \|v_n'\|_{L^2((0,1)\setminus S_\eta)} < +\infty$. We already have shown that v_n is equibounded in $L^1(0,1)$. Thus, we can apply the Poincaré inequality on every connected subset of $(0,1)\setminus S_\eta$ and obtain that the L^2-norm of v_n is equibounded in $(0,1) \setminus S_\eta$. Indeed, we have for every connected subset Ω of $(0,1) \setminus S_\eta$ that

$$\int_\Omega v_n^2 dx \leq \int_\Omega (v_n - \fint_\Omega v_n dt)^2 + 2v_n(\fint_\Omega v_n dt) dx \leq C\|v_n'\|_{L^2(\Omega)} + \frac{2}{|\Omega|}\|v_n\|^2_{L^1(0,1)}.$$

Hence, $v_n \rightharpoonup v$ in $H^1((0,1) \setminus S_\eta)$. By the arbitrariness of $\eta > 0$, we have that $v_n \rightharpoonup v$ locally weakly in $H^1((0,1) \setminus S)$.

It is left to show that $[v] \geq 0$ in $[0,1]$, i.e. $[v](x) > 0$ on S_v. Recall that we set $v(0-) = 0$ and $v(1+) = \delta$ for $v \in SBV^\delta(0,1)$. The assumptions (LJ2) and (LJ5) imply

$$\liminf_{z \to +\infty} J_{0,j}(z) > J_{0,j}(\gamma) = \psi_j(\gamma), \quad \liminf_{z \to -\infty} J_{0,j}(z) = +\infty. \tag{3.144}$$

Hence, we infer as in [17] that there exist constants $C_1, C_2, C_3 > 0$ such that

$$J_{0,2}(z) - \psi_2(\gamma) \geq \Psi(z - \gamma) := \begin{cases} C_1(z-\gamma)^2 \wedge C_2 & \text{if } z \geq \gamma, \\ C_1(z-\gamma)^2 \wedge C_3 & \text{if } z \leq \gamma. \end{cases} \tag{3.145}$$

From (3.144), we deduce that

$$\sup\{C_3 : (3.145) \text{ holds for some } C_1 \text{ and } C_2\} = +\infty. \tag{3.146}$$

We find, using $\zeta_{j,n}^i \geq 0$, (3.8), (3.134) and (3.145), the following lower bound for $E_n^{\delta_n}(v_n)$:

$$\begin{aligned} E_n^{\delta_n}(v_n) - K_3 &\geq \sum_{j=2}^{K} \sum_{i=0}^{n-j} \zeta_{j,n}^i \geq \sum_{i=0}^{n-2} \zeta_{2,n}^i \geq \sum_{i=0}^{n-2} \left\{ J_{0,2}\left(\gamma + \frac{v_n^{i+2} - v_n^i}{2\sqrt{\lambda_n}}\right) - \psi_2(\gamma) \right\} \\ &\geq \sum_{i=0}^{n-2} \Psi\left(\frac{v_n^{i+2} - v_n^i}{2\sqrt{\lambda_n}}\right) \geq \sum_{\substack{i=0 \\ i \text{ even}}}^{n-2} \Psi\left(\frac{v_n^{i+2} - v_n^i}{2\sqrt{\lambda_n}}\right), \end{aligned} \tag{3.147}$$

where K_3 is given in (3.141).

In order to capture the boundary behaviour of v, we introduce, as in Theorem 3.7, the following auxiliary functions

$$w(x) := \begin{cases} 0 & \text{for } x \leq 0, \\ v(x) & \text{for } 0 < x < 1, \\ \delta & \text{for } 1 \leq x, \end{cases} \qquad w_n(x) := \begin{cases} 0 & \text{for } x \leq 0, \\ v_n(x) & \text{for } 0 < x < 1, \\ \delta_n & \text{for } 1 \leq x. \end{cases} \tag{3.148}$$

Let us fix constants $a < 0$ and $1 < b$. We observe that $w_n \overset{*}{\rightharpoonup} w$ in $BV(a,b)$. As in Theorem 3.7, we denote by $v_{n,2}^0$ the piecewise affine interpolation of w_n with respect to $2\mathbb{Z}$, see (3.31). To shorten the notation, we drop the superscript '0' and set $v_{n,2} := v_{n,2}^0$. Similar calculations as in (3.32) and (3.33) yield $v_{n,2} \overset{*}{\rightharpoonup} w$ in $BV(a,b)$.

In analogy to [9, Theorem 8.8], we define the sets

$$\tilde{I}_n^+ := \left\{ i \in \{0,\dots,n-2\} \cap 2\mathbb{Z} : \; v_n^{i+2} > v_n^i \text{ and } C_1(v_n^{i+2}-v_n^i)^2 \geq 4C_2\lambda_n \right\},$$
$$\tilde{I}_n^- := \left\{ i \in \{0,\dots,n-2\} \cap 2\mathbb{Z} : \; v_n^{i+2} < v_n^i \text{ and } C_1(v_n^{i+2}-v_n^i)^2 \geq 4C_3\lambda_n \right\}.$$

Note that $\sup_n \#(\tilde{I}_n^+ \cup \tilde{I}_n^-) < +\infty$ by (3.137), (3.145) and (3.147). By (3.146) it is not restrictive to choose $C_1, C_2, C_3 > 0$ such that $C_3 > C_1(M+\gamma)^2$, where $M \geq 0$ is such that (3.142) holds true for all n and $i \in \{0,\dots,n-1\}$. We claim that $\tilde{I}_n^- = \emptyset$ for this choice. Assume by contradiction that there exists $i \in \tilde{I}_n^-$. Let us additionally assume that $v_n^{i+1} \leq v_n^i$ and $v_n^{i+2} \leq v_n^{i+1}$. By (3.142), we obtain

$$C_1(v_n^{i+2}-v_n^i)^2 \leq 2C_1((v_n^{i+2}-v_n^{i+1})^2 + (v_n^{i+1}-v_n^i)^2) \leq 4C_1(M+\gamma)^2\lambda_n < 4C_3\lambda_n,$$

which is a contradiction to $i \in \tilde{I}_n^-$. The same argument works also without the additional assumption since $(v_n^{i+2}-v_n^i)^2 \leq (v_n^{i+2}-v_n^{i+1})^2$ if $v^{i+1} \geq v^i$ and $(v_n^{i+2}-v_n^i)^2 \leq (v_n^{i+1}-v_n^i)^2$ if $v^{i+2} \geq v^{i+1}$. Hence, $C_3 > C_1(M+\gamma)^2$ yields $\tilde{I}_n^- = \emptyset$.

For $C_1, C_2, C_3 > 0$ such that (3.145) and $\tilde{I}_n^- = \emptyset$ hold true, we define the sequence $(\tilde{v}_{n,2}) \subset SBV(a,b)$ by

$$\tilde{v}_{n,2}(x) := \begin{cases} v_{n,2}(x) & \text{if } x \in \lambda_n[i,i+2),\; i \in 2\mathbb{Z}\setminus \tilde{I}_n^+, \\ v_{n,2}(i\lambda_n) & \text{if } x \in \lambda_n[i,i+2),\; i \in \tilde{I}_n^+. \end{cases}$$

The definition of $(\tilde{v}_{n,2})$ and $\sup_n \#\tilde{I}_n^+ < +\infty$ yield that $\lim_{n\to\infty} \|\tilde{v}_{n,2} - v_{n,2}\|_{L^1(a,b)} = 0$ and $\|\tilde{v}_{n,2}\|_{BV(a,b)} \leq \|v_{n,2}\|_{W^{1,1}(a,b)}$. Thus, $\tilde{v}_{n,2} \overset{*}{\rightharpoonup} w$ weakly* in $BV(a,b)$. Moreover, $\tilde{v}_{n,2}$ has only positive jumps, i.e. $D^j\tilde{v}_{n,2} \geq 0$ in (a,b), by definition. By (3.145) and the choice of $C_1, C_2, C_3 > 0$, we obtain in analogy to [9, Theorem 8.8] that

$$\begin{aligned}\sum_{\substack{i=0\\ i \text{ even}}}^{n-2} \Psi\left(\frac{v_n^{i+2}-v_n^i}{2\sqrt{\lambda_n}}\right) &= \sum_{\substack{i=0\\ i \text{ even}}}^{n-2} C_1\lambda_n \left(\frac{v_n^{i+2}-v_n^i}{2\lambda_n}\right)^2 \wedge C_2 \\ &\geq \frac{C_1}{2}\int_0^{2\lambda_n\lfloor n/2\rfloor} |\tilde{v}_{n,2}'(x)|^2 dx + C_2 \# S_{\tilde{v}_{n,2}} \\ &\geq \frac{C_1}{2}\int_a^b |\tilde{v}_{n,2}'(x)|^2 dx + C_2 \# S_{\tilde{v}_{n,2}} - \frac{C_1}{4}(u_{1,1}^{(1)}-\gamma)^2. \end{aligned} \tag{3.149}$$

For the last inequality, we used that $\tilde{v}_{n,2}' = 0$ a.e. on $(a,b)\setminus(0,1)$ for n even and $\tilde{v}_{n,2}' = 0$ a.e. on $(a,b)\setminus(0,1+\lambda_n)$ for n odd and $\tilde{v}_{n,2}' = \frac{w_n(1+\lambda_n)-w_n(1-\lambda_n)}{2\lambda_n} = \frac{1}{2\sqrt{\lambda_n}}(u_{1,1}^{(1)}-\gamma)$ on $(1-\lambda_n, 1+\lambda_n)$ in this case. Note that we used $w_n(x) = \delta_n$ for $x \geq 1$ and $w_n(1) - w_n(1-\lambda_n) = v^n - v^{n-1} = \sqrt{\lambda_n}(u_{1,1}^{(1)}-\gamma)$ (see (3.130)).

Since the left-hand side in (3.149) is equibounded and $\tilde{v}_{n,2} \overset{*}{\rightharpoonup} w$ in $BV(a,b)$, we have $D^j\tilde{v}_{n,2} \overset{*}{\rightharpoonup} D^j w$ in $\mathcal{M}(a,b)$, cf. Theorem 2.8, and since $D^j\tilde{v}_{n,2} \geq 0$ in (a,b) we have $D^j w \geq 0$ in (a,b). The measure $D^j v$ is the restriction of $D^j w$ to $[0,1]$ and thus $D^j v \geq 0$ in $[0,1]$. This yields the assertion $[v] \geq 0$ in $[0,1]$ and finishes the proof. □

We define the set

$$SBV_e^\delta(0,1) := \Big\{ v \in SBV^\delta(0,1) : \ v \text{ satisfies } (3.138) \Big\}. \tag{3.150}$$

We are now in position to prove a Γ-convergence result for the sequence of functionals $(E_n^{\delta_n})$.

Theorem 3.34. *Assume that $J_1, \dots, J_K$ satisfy the assumptions (LJ1)–(LJ7). Let $u_0^{(1)}$, $u_1^{(1)} \in \mathbb{R}_+^{K-1}$ and $\delta_n \to \delta$ such that* (3.128) *is satisfied. Let $\alpha := \frac{1}{2} J''_{CB}(\gamma)$, and $B(\theta,\gamma)$, $B_{BJ}(\theta)$ and B_{IJ} as in* (3.72), (3.74) *and* (3.75), *respectively. Then the sequence $(E_n^{\delta_n})$ Γ-converges with respect to the $L^1(0,1)$-topology to the functional E^δ defined by*

$$E^\delta(v) = \begin{cases} \alpha \displaystyle\int_0^1 |v'|^2 dx + B(u_0^{(1)},\gamma)(1 - \#(S_v \cap \{0\})) \\ \quad + B_{BJ}(u_0^{(1)})\#(S_v \cap \{0\}) + B_{IJ}\#(S_v \cap (0,1)) \\ \quad + B_{BJ}(u_1^{(1)})\#(S_v \cap \{1\}) + B(u_1^{(1)},\gamma)\,(1 - \#(S_v \cap \{1\})) \\ \quad - \sum_{j=2}^K (j-1)\psi_j(\gamma) & \text{if } v \in SBV_e^\delta(0,1), \\ +\infty & \text{else} \end{cases} \tag{3.151}$$

on $L^1(0,1)$. Moreover, if $\delta > 0$ it holds

$$\lim_{n\to\infty} \inf_v E_n^{\delta_n}(v) = \min\{\alpha\delta^2, \beta_{\min}\} + B(u_0^{(1)},\gamma) + B(u_1^{(1)},\gamma) - \sum_{j=2}^K (j-1)\psi_j(\gamma), \tag{3.152}$$

with

$$\beta_{\min} := \min\Big\{ B_{BJ}(u_0^{(1)}) - B(u_0^{(1)},\gamma), B_{BJ}(u_1^{(1)}) - B(u_1^{(1)},\gamma) \Big\}.$$

Before we proceed with the proof of Theorem 3.34, let us recall that by the same calculations as in Proposition 3.21 we can rewrite E^δ above independent of $c = (c_j)_{j=2}^K$:

Corollary 3.35. *Assume that $J_1, \dots, J_K$, $u_0^{(1)}, u_1^{(1)}, \delta_n$, δ and α are as in Theorem 3.34. Let $\widetilde{B}(\theta,\gamma)$, β_{BJ} and β_{IJ} as in* (3.64) *and* (3.114), *respectively. Then the functional E^δ, given in* (3.151), *reads*

$$E^\delta(v) = \begin{cases} \alpha \displaystyle\int_0^1 |v'|^2 dx + \widetilde{B}(u_0^{(1)},\gamma) + \widetilde{B}(u_1^{(1)},\gamma) \\ \quad + \beta_{BJ}(u_0^{(1)})\#(S_v \cap \{0\}) + \beta_{IJ}\#(S_v \cap (0,1)) \\ \quad + \beta_{BJ}(u_1^{(1)})\#(S_v \cap \{1\}) - \sum_{j=2}^K (j-1)J_j(\gamma) & \text{if } v \in SBV_e^\delta(0,1), \\ +\infty & \text{else} \end{cases} \tag{3.153}$$

on $L^1(0,1)$.

Proof of Theorem 3.34. Liminf inequality. Let $v \in L^1(0,1)$ and let (v_n) be a sequence of functions such that $\sup_n E_n^{\delta_n}(v_n) < +\infty$ and $v_n \to v$ in $L^1(0,1)$. By Lemma 3.33, we have that $v \in SBV_e^\ell(0,1)$. Moreover, we can assume that there exists a finite set $S = \{x_1, \dots, x_N\}$ such that $v_n \rightharpoonup v$ locally weakly in $H^1((0,1) \setminus S)$. We have to show that

$$\begin{aligned}\liminf_{n\to\infty} E_n^{\delta_n}(v_n) \geq & \alpha \int_0^1 |v'|^2 dx + B(u_0^{(1)},\gamma)(1 - \#(S_u \cap \{0\})) + B_{BJ}(u_0^{(1)})\#(S_u \cap \{0\}) \\ & + B_{IJ}\#(S_u \cap (0,1)) + B_{BJ}(u_1^{(1)})\#(S_u \cap \{1\}) \\ & + B(u_1^{(1)},\gamma)\,(1 - \#(S_u \cap \{1\})) - \sum_{j=2}^K (j-1)\psi_j(\gamma). \end{aligned} \tag{3.154}$$

The plan of the proof is as follows: first we estimate the terms which contribute to the elastic integral term. Next, we consider the terms which contribute to the boundary layer energies at 0 and 1. Here we have to distinguish between the case $x \notin S_v$ and the case $x \in S_v$ with $x \in \{0,1\}$. Finally, we estimate possible boundary layer energies due to jumps in the interior $(0,1)$.

Step 1. Let us estimate the elastic part. Let $\rho > 0$ be such that $|x_i - x_j| > 4\rho$ for all $x_i, x_j \in S$, $i \neq j$. We define the set $S_\rho = \bigcup_{i=1}^N (x_i - \rho, x_i + \rho)$ and the set $Q_n(\rho)$ as

$$Q_n(\rho) := \{i \in \{0, \dots, n-1\} : \ (i, i+K)\lambda_n \subset (\rho, 1-\rho) \setminus S_\rho\}\,. \tag{3.155}$$

We show that

$$\liminf_{n\to\infty} \sum_{j=2}^K \sum_{i \in Q_n(\rho)} \zeta_{j,n}^i \geq \alpha \int_{(2\rho, 1-2\rho)\setminus S_{2\rho}} |v'|^2 dx. \tag{3.156}$$

Therefore, we use a Taylor expansion of $J_{0,j}$ at γ:

$$J_{0,j}(\gamma + z) = J_{0,j}(\gamma) + \alpha_j z^2 + \eta_j(z)$$

with $\alpha_j := \frac{1}{2} J''_{0,j}(\gamma) = \frac{1}{2}\psi''_j(\gamma)$ (see (LJ4), (LJ6)) and $\eta_j(z)/|z|^2 \to 0$ as $|z| \to 0$. Note that we have

$$\sum_{j=2}^K \sum_{i \in Q_n(\rho)} \zeta_{j,n}^i = \sum_{j=2}^K \sum_{s=0}^{j-1} \sum_{i \in Q_n(\rho)\cap\{s+j\mathbb{Z}\}} \zeta_{j,n}^i.$$

For given $j \in \{2, \dots, K\}$ and $s \in \{0, \dots, j-1\}$, we define the set

$$I_{n,j}^s = \left\{ i \in \{0, \dots, n-j\} \cap \{s + j\mathbb{Z}\} : \ \left| \frac{v_n^{i+j} - v_n^i}{j\lambda_n} \right| > \lambda_n^{-\frac{1}{4}} \right\}.$$

Fix $j' \in \{2, \dots, K\}$. From the equiboundedness of $E_n^{\delta_n}(v_n)$, $\zeta_{j,n}^i \geq 0$ and (3.140), we deduce that there exists $C > 0$ such that for n sufficiently large it holds

$$C \geq \sum_{j=2}^{K} \sum_{i=0}^{n-j} \zeta_{j,n}^i \geq \sum_{i \in I_{n,j'}^s} \zeta_{j',n}^i \geq \# I_{n,j'}^s \sqrt{\lambda_n} K_1.$$

Hence, $\# I_{n,j}^s = \mathcal{O}(\sqrt{\lambda_n}^{-1})$ and thus $|\{x \in (0,1) : \chi_{n,j}^s(x) \neq 1\}| \leq j\lambda_n \# I_{n,j}^s \to 0$ as $n \to \infty$, where $\chi_{n,j}^s$ is defined by

$$\chi_{n,j}^s(x) := \begin{cases} 1 & \text{if } x \in [i, i+j)\lambda_n \text{ and } i \in \{s + j\mathbb{Z}\} \setminus I_{n,j}^s, \\ 0 & \text{if } x \in [i, i+j)\lambda_n \text{ and } i \in I_{n,j}^s. \end{cases} \tag{3.157}$$

Thus $\chi_{n,j}^s \to 1$ bounded in measure in $(0,1)$.

In the following, we identify v_n with the function $w_n \in W^{1,\infty}(\mathbb{R})$ given in (3.148). As in the proof of Theorem 3.7, we denote by $v_{n,j}^s$ the piecewise affine interpolation of v_n with respect to $s + j\mathbb{Z}$, see (3.31). From $\sup_n E_n^{\delta_n}(v_n) < +\infty$, we deduce by Lemma 3.33 that $\sup_n \|v_n\|_{W^{1,1}(0,1)}$ and thus, as in the proof of Theorem 3.7, that $v_{n,j}^s \to v$ in $L^1(0,1)$ for all $j \in \{2, \dots, K\}$ and $s \in \{0, \dots, j-1\}$. Furthermore, we define $\omega_j(t) := \sup_{|z| \leq t} |\eta_j(z)|$ and $\chi_{n,j}^{s,i} = \chi_{j,n}^s(i\lambda_n)$. A Taylor expansion of $J_{0,j}$ at γ yields:

$$\begin{aligned}
\sum_{i \in Q_n(\rho) \cap \{s+j\mathbb{Z}\}} \zeta_{j,n}^i &\geq \sum_{i \in Q_n(\rho) \cap \{s+j\mathbb{Z}\}} \left\{ J_{0,j}\left(\gamma + \frac{v_n^{i+j} - v_n^i}{j\sqrt{\lambda_n}}\right) - \psi_j(\gamma) \right\} \\
&\geq \sum_{i \in Q_n(\rho) \cap \{s+j\mathbb{Z}\}} \chi_{n,j}^{s,i} \left\{ J_{0,j}\left(\gamma + \frac{v_n^{i+j} - v_n^i}{j\sqrt{\lambda_n}}\right) - \psi_j(\gamma) \right\} \\
&\geq \sum_{i \in Q_n(\rho) \cap \{s+j\mathbb{Z}\}} \chi_{n,j}^{s,i} \left\{ \alpha_j \left| \frac{v_n^{i+j} - v_n^i}{j\sqrt{\lambda_n}} \right|^2 - \omega_j\left(\left| \frac{v_n^{i+j} - v_n^i}{j\sqrt{\lambda_n}} \right| \right) \right\} \\
&= \frac{1}{j} \sum_{i \in Q_n(\rho) \cap \{s+j\mathbb{Z}\}} j\lambda_n \left\{ \alpha_j \chi_{n,j}^{s,i} \left| \frac{v_n^{i+j} - v_n^i}{j\lambda_n} \right|^2 - \frac{\chi_{n,j}^{s,i}}{\lambda_n} \omega_j \left(\left| \frac{v_n^{i+j} - v_n^i}{j\sqrt{\lambda_n}} \right| \right) \right\} \\
&\geq \frac{\alpha_j}{j} \int_{(2\rho, 1-2\rho) \setminus S_{2\rho}} |\chi_{n,j}^s {v_{n,j}^s}'|^2 dx - \int_{(\rho, 1-\rho) \setminus S_\rho} \chi_{n,j}^s \lambda_n^{-1} \omega_j \left(\sqrt{\lambda_n} |{v_{n,j}^s}'| \right) dx
\end{aligned} \tag{3.158}$$

for n sufficiently large. Let us show that the second term in the last line above vanishes as n tends to infinity. From $v_n \rightharpoonup v$ locally weakly in $H^1((0,1) \setminus S)$, we deduce that

${v^s_{n,j}}' \rightharpoonup v'$ in $L^2((\rho,1-\rho)\setminus S_\rho)$. Indeed, we have for n sufficiently large that

$$\begin{aligned}\|{v^s_{n,j}}'\|_{L^2((\rho,1-\rho)\setminus S_\rho)} &\leq \sum_{i\in Q_n(\frac{\rho}{2})\cap\{s+j\mathbb{Z}\}} j\lambda_n \left|\frac{v_n^{i+j}-v_n^i}{j\lambda_n}\right|^2\\ &\leq \sum_{i\in Q_n(\frac{\rho}{2})\cap\{s+j\mathbb{Z}\}} \lambda_n \sum_{s=i}^{i+j-1}\left|\frac{v_n^{s+1}-v_n^s}{\lambda_n}\right|^2 \leq j\|v_n'\|_{L^2((\frac{\rho}{2},1-\frac{\rho}{2})\setminus S_{\frac{\rho}{2}})}.\end{aligned}$$

Since (v_n) converges locally weakly in $H^1((0,1)\setminus S)$, we have $\sup_n\|v_n'\|_{L^2((\frac{\rho}{2},1-\frac{\rho}{2})\setminus S_{\frac{\rho}{2}})} < +\infty$. From $v^s_{n,j}\to v$ in $L^1(0,1)$ and $\sup_n\|{v^s_{n,j}}'\|_{L^2((\rho,1-\rho)\setminus S_\rho)} < +\infty$, we deduce that ${v^s_{n,j}}' \rightharpoonup v'$ in $L^2((\rho,1-\rho)\setminus S_\rho)$. Furthermore, it holds $\sqrt{\lambda_n}|{v^s_{n,j}}'|\leq \lambda_n^{1/4}$ if $\chi^s_{n,j}$ is nonzero and thus

$$|{v^s_{n,j}}'|^2\cdot\chi^s_{n,j}\omega_j\left(\sqrt{\lambda_n}|{v^s_{n,j}}'|\right)/(\lambda_n|{v^s_{n,j}}'|^2)$$

is the product of a sequence equibounded in $L^1((\rho,1-\rho)\setminus S_\rho)$ and a sequence converging to zero in $L^\infty((\rho,1-\rho)\setminus S_\rho)$. Note that we have used $\eta_j(z)/|z|^2\to 0$ as $z\to 0$ by definition. Hence, using $\chi^s_{n,j}{v^s_{n,j}}' \rightharpoonup v'$ in $L^2((\rho,1-\rho)\setminus S_\rho)$ it follows

$$\begin{aligned}\liminf_{n\to\infty}\sum_{i\in Q_n(\rho)\cap\{s+j\mathbb{Z}\}}\zeta^i_{j,n} \geq& \liminf_{n\to\infty}\frac{\alpha_j}{j}\int_{(2\rho,1-2\rho)\setminus S_{2\rho}}|\chi^s_{n,j}{v^s_{n,j}}'|^2dx\\ \geq&\frac{\alpha_j}{j}\int_{(2\rho,1-2\rho)\setminus S_{2\rho}}|v'|^2dx\end{aligned}$$

for $j\in\{2,\dots,K\}$ and $s\in\{0,\dots,j-1\}$. Hence,

$$\begin{aligned}\liminf_{n\to\infty}\sum_{j=2}^K\sum_{i\in Q_n(\rho)}\zeta^i_{j,n} \geq& \sum_{j=2}^K\sum_{s=0}^{j-1}\liminf_{n\to\infty}\sum_{i\in Q_n(\rho)\cap\{s+j\mathbb{Z}\}}\zeta^i_{j,n}\\ \geq&\sum_{j=2}^K\sum_{s=0}^{j-1}\frac{\alpha_j}{j}\int_{(2\rho,1-2\rho)\setminus S_{2\rho}}|v'|^2dx\\ =&\sum_{j=2}^K\alpha_j\int_{(2\rho,1-2\rho)\setminus S_{2\rho}}|v'|^2dx\\ =&\alpha\int_{(2\rho,1-2\rho)\setminus S_{2\rho}}|v'|^2dx,\end{aligned}$$

and assertion (3.156) is proven. Note, that we used

$$\alpha=\frac{1}{2}J''_{CB}(\gamma)=\frac{1}{2}\left(\sum_{j=2}^K J''_j(\gamma)+c_jJ''_1(\gamma)\right)=\frac{1}{2}\psi''_j(\gamma)=\sum_{j=2}^K\alpha_j$$

which follows from $\sum_{j=2}^K c_j=1$ and the definition of ψ_j, see (3.14).

Step 2. Let us now estimate the boundary layer energies in 0 and 1. By the assumptions on $\rho > 0$ it holds $\#((0,\rho) \cap S_v) \leq 1$ and $\#((1-\rho,1) \cap S_v) \leq 1$. Hence, there exist intervals $J_1 \subset (0,\rho)$ and $J_2 \subset (1-\rho,1)$ with $|J_1| = |J_2| = \frac{\rho}{2}$ and $J_1 \cap S_v = J_2 \cap S_v = \emptyset$. Without loss of generality, we can assume that $J_1 = (\frac{\rho}{2},\rho)$ and $J_2 = (1-\rho, 1-\frac{\rho}{2})$. This yields the existence of sequences $(T_n^0),(T_n^1) \subset \mathbb{N}$ with $\frac{\rho}{2} \leq \lambda_n(T_n^0+s) \leq \rho$ and $1-\rho \leq \lambda_n(T_n^1+s) \leq 1-\frac{\rho}{2}$ for all $s \in \{1,\dots,K\}$ such that

$$\lim_{n\to\infty} \frac{v_n^{T_n^i+s+1} - v_n^{T_n^i+s}}{\sqrt{\lambda_n}} = 0, \quad \text{for } i \in \{0,1\} \text{ and } s \in \{1,\dots,K\}. \tag{3.159}$$

Let us show the existence of $(T_n^0) \subset \mathbb{N}$ with the above properties, the existence of (T_n^1) can be proven similarly. To this end, we assume by contradiction that there exists $c > 0$ such that for all $i \in \mathbb{N}$ with $\frac{\rho}{2} \leq \lambda_n(i+s) \leq \rho$ with $s \in \{1,\dots,K\}$ there exists an $\hat{s} \in \{1,\dots,K\}$ such that $|\frac{v_n^{i+\hat{s}+1} - v_n^{i+\hat{s}}}{\sqrt{\lambda_n}}| \geq c$. Let $i_n^\rho, j_n^\rho \subset \mathbb{N}$ be such such that $\frac{\rho}{2} \in (i_n^\rho - 1, i_n^\rho]\lambda_n$ and $\rho \in (j_n^\rho, j_n^\rho+1]\lambda_n$. We have by $\sup_n E_n^{\delta_n}(v_n) < +\infty$ and (3.140) that there exists $C > 0$ such that

$$C \geq \sum_{i=i_n^\rho+1}^{j_n^\rho-K} \zeta_{n,K}^i \geq \sum_{i=i_n^\rho+1}^{j_n^\rho-K} K_1c^2 \wedge K_2 \geq \big(K_1c^2 \wedge K_2\big)\,(j_n^\rho - i_n^\rho - K) \to +\infty$$

as $n \to \infty$, which is a contradiction to $\sup_n E_n^{\delta_n}(v_n) < +\infty$. Note that we have used $j_n^\rho - i_n^\rho \geq \frac{\rho}{2\lambda_n} - 2$ for n sufficiently large. From $0 \leq \lambda_n(T_n^0+1) < \rho$ and $1-\rho \leq \lambda_n(T_n^1+1) < 1$, we deduce that

$$\big(\{0,\dots,T_n^0\} \cup \{T_n^1+1,\dots,n-1\}\big) \cap Q_n(\rho) = \emptyset.$$

We have to show that

$$\begin{aligned}
&\liminf_{n\to\infty} \sum_{j=2}^{K} \left\{ c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(u_{0,s}^{(1)}) + \sum_{i=0}^{T_n^0} \zeta_{j,n}^i \right\} \\
&\qquad \geq B(u_0^{(1)},\gamma) + \Big(B_{BJ}(u_0^{(1)}) - B(u_0^{(1)},\gamma)\Big)\,\#(S_v \cap \{0\}), \qquad (3.160) \\
&\liminf_{n\to\infty} \sum_{j=2}^{K} \left\{ c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(u_{1,s}^{(1)}) + \sum_{i=T_n^1+1}^{n-j} \zeta_{j,n}^i \right\} \\
&\qquad \geq B(u_1^{(1)},\gamma) + \Big(B_{BJ}(u_1^{(1)}) - B(u_1^{(1)},\gamma)\Big)\,\#(S_v \cap \{1\}). \qquad (3.161)
\end{aligned}$$

We prove only (3.160). The estimate (3.161) can be proven in a similar way.

Let us first consider the case $S_v \cap \{0\} = \emptyset$. We define the sequence $\hat{v}_n : \mathbb{N}_0 \to \mathbb{R}$ as

$$\hat{v}_n^i := \begin{cases} \frac{v_n^i}{\sqrt{\lambda_n}} + i\gamma & \text{if } 0 \leq i \leq T_n^0 + K, \\ \frac{v_n^{T_n^0+K}}{\sqrt{\lambda_n}} + i\gamma & \text{if } i \geq T_n^0 + K. \end{cases} \tag{3.162}$$

Using the fact that v_n satisfies (3.130), we have $\hat{v}_n^0 = 0$, $\hat{v}^s - \hat{v}^{s-1} = \frac{v_n^s - v_n^{s-1}}{\sqrt{\lambda_n}} + \gamma = u_{0,s}^{(1)}$ for $s \in \{1, \dots, K-1\}$ and $\hat{v}^{i+1} - \hat{v}^i = \gamma$ for $i \geq T_n^0 + K$. Hence, $\hat{v}_n$ is a competitor for the minimum problem defining $B(u_0^{(1)}, \gamma)$, see (3.72). Thus we obtain that

$$
\begin{aligned}
\sum_{j=2}^{K} \left\{ c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(u_{0,s}^{(1)}) + \sum_{i=0}^{T_n^0} \zeta_{j,n}^i \right\} &= \sum_{j=2}^{K} c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(u_{0,s}^{(1)}) \\
&+ \sum_{j=2}^{K} \sum_{i \geq 0} \left\{ J_j \left(\frac{\hat{v}^{i+j} - \hat{v}^i}{j} \right) + \frac{c_j}{j} \sum_{s=i}^{i+j-1} J_1(\hat{v}^{s+1} - \hat{v}^s) - \psi_j(\gamma) \right\} - r_2(n) \\
&\geq B(u_0^{(1)}, \gamma) - r_2(n), \qquad (3.163)
\end{aligned}
$$

with

$$
r_2(n) = \sum_{j=2}^{K} \sum_{i=T_n^0+1}^{T_n^0+K-1} \left\{ J_j \left(\frac{\hat{v}^{i+j} - \hat{v}^i}{j} \right) + \frac{c_j}{j} \sum_{s=i}^{i+j-1} J_1(\hat{v}^{s+1} - \hat{v}^s) - \psi_j(\gamma) \right\} \to 0
$$

as $n \to \infty$. Indeed, from $\hat{v}_n^{i+1} - \hat{v}_n^i = \gamma$ for $i \geq T_n^0 + K$ and the definition of ψ_j we deduce that the terms in the infinite sum in (3.163) vanish identically for $i \geq T_n^0 + K$. By (3.159) it holds

$$
\lim_{n \to \infty} (\hat{v}_n^{T_n^0+1+s} - \hat{v}_n^{T_n^0+s}) = \lim_{n \to \infty} \frac{v_n^{T_n^0+1+s} - v_n^{T_n^0+s}}{\sqrt{\lambda_n}} + \gamma = \gamma,
$$

for $s \in \{1, \dots, K\}$, and thus we obtain $\lim_{n \to \infty} r_2(n) = 0$. From (3.163), we deduce the assertion (3.160) in the case $S_v \cap \{0\} = \emptyset$.

Let us now consider the case $0 \in S_v$. From $v_n \to v$ in $L^1(0,1)$ and $0 \in S_v$, we deduce, in analogy to [17, eq. (117)], that there exists $(h_n) \subset \mathbb{N}$ with $\lambda_n h_n \to 0$ such that

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

Indeed, otherwise v_n' would be equibounded in L^2 in a neighbourhood of 0. For given $j \in \{2, \dots, K\}$ and $s \in \{0, \dots, j-1\}$, we deduce from (3.9) that some terms in $\zeta_{j,n}^{h_n - j}$ vanish as n tends to infinity. We collect them in the function $r_1(n)$ defined by

$$
r_1(n) = \sum_{j=1}^{K} \sum_{s=h_n-j+1}^{h_n} J_j \left(\gamma + \frac{v_n^{s+j} - v_n^s}{j\sqrt{\lambda_n}} \right) \to 0 \quad \text{as } n \to \infty.
$$

As in the proof of Theorem 3.19, see (3.82), it is useful to rewrite the terms which involve $v_n^{h_n+1} - v_n^{h_n}$ as follows:

$$\sum_{j=2}^{K} \sum_{i=h_n-j+1}^{h_n} \zeta_{j,n}^i = \sum_{j=2}^{K} c_j \sum_{s=1}^{j-1} \frac{j-s}{j} \Big\{ J_1 \left(\gamma + \frac{v_n^{h_n-s+1} - v_n^{h_n-s}}{\sqrt{\lambda_n}} \right) + J_1 \left(\gamma + \frac{v_n^{h_n+s+1} - v_n^{h_n+s}}{\sqrt{\lambda_n}} \right) \Big\} - \sum_{j=2}^{K} j\psi_j(\gamma) + r_1(n).$$

Hence, we have

$$\sum_{j=2}^{K} \sum_{i=0}^{T_n^0} \zeta_{j,n}^i = \sum_{j=2}^{K} \Big\{ \sum_{i=0}^{h_n-j} \zeta_{j,n}^i + c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1 \left(\gamma + \frac{v_n^{h_n-s+1} - v_n^{h_n-s}}{\sqrt{\lambda_n}} \right) + \sum_{i=h_n+1}^{T_n^0} \zeta_{j,n}^i + c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1 \left(\gamma + \frac{v_n^{h_n+s+1} - v_n^{h_n+s}}{\sqrt{\lambda_n}} \right) \Big\} - \sum_{j=2}^{K} j\psi_j(\gamma) + r_1(n). \quad (3.164)$$

Thus, it remains to prove that

$$\sum_{j=2}^{K} \Big\{ \sum_{i=0}^{h_n-j} \zeta_{j,n}^i + c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1 \left(\gamma + \frac{v_n^{h_n-s+1} - v_n^{h_n-s}}{\sqrt{\lambda_n}} \right) \Big\} \geq B_b(u_0^{(1)}), \quad (3.165)$$

$$\sum_{j=2}^{K} \Big\{ \sum_{i=h_n+1}^{T_n^0} \zeta_{j,n}^i + c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1 \left(\gamma + \frac{v_n^{h_n+s+1} - v_n^{h_n+s}}{\sqrt{\lambda_n}} \right) \Big\} \geq B(\gamma) - r_2(n), \quad (3.166)$$

with $r_2(n) \to 0$ as $n \to \infty$. The inequality (3.165) can be proven in a similar way as inequality (3.84) in the proof of Theorem 3.19. We define for $m \in \{0, \dots, h_n\}$

$$\hat{w}_n^m = -\frac{v_n^{h_n-m}}{\sqrt{\lambda_n}} - (h_n - m)\gamma.$$

Now we rewrite the left-hand side in (3.165) in terms of $\hat{w}_n^m$:

$$\begin{aligned}
&\sum_{j=2}^{K} \Big\{ \sum_{i=0}^{h_n-j} \zeta_{j,n}^i + c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1 \left(\gamma + \frac{v_n^{h_n-s+1} - v_n^{h_n-s}}{\sqrt{\lambda_n}} \right) \Big\} \\
&= \sum_{j=2}^{K} \Big\{ \sum_{i=0}^{h_n-j} \zeta_{j,n}^{h_n-j-i} + c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1 \left(\gamma + \frac{v_n^{h_n-s+1} - v_n^{h_n-s}}{\sqrt{\lambda_n}} \right) \Big\} \\
&= \sum_{j=2}^{K} c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(\hat{w}_n^s - \hat{w}_n^{s-1}) + \sum_{j=2}^{K} \sum_{i=0}^{h_n-j} \Big\{ J_j \left(\frac{\hat{w}_n^{i+j} - \hat{w}_n^i}{j} \right) \\
&\quad + \frac{c_j}{j} \sum_{s=i}^{i+j-1} J_1(\hat{w}_n^{s+1} - \hat{w}_n^s) - \psi_j(\gamma) \Big\}.
\end{aligned}$$

Since v_n satisfies the boundary conditions (3.130), we have $\hat{w}_n^{h_n} = 0$, $\hat{w}_n^{h_n+1-s} - \hat{w}_n^{h_n-s} =$

$u_{0,s}^{(1)}$. Thus $\hat{w}_n$ is an admissible test for $B_b(u_0^{(1)})$ with h_n playing the role of k, cf. (3.70). Thus (3.165) holds true.

The proof of (3.166) is similar to the proof of inequality (3.85) in Theorem 3.19. We define for $i \geq 0$:

$$\tilde{u}_n^i = \begin{cases} \gamma i + \frac{v_n^{h_n+1+i} - v_n^{h_n+1}}{\sqrt{\lambda_n}} & \text{if } 0 \leq i \leq T_n^0 - h_n + K - 1, \\ \gamma i + \frac{v_n^{T_n^0+K} - v_n^{h_n+1}}{\sqrt{\lambda_n}} & \text{if } i \geq T_n^0 - h_n + K - 1. \end{cases}$$

We can now rewrite the left-hand side of (3.166) in terms of $\tilde{u}_n^i$:

$$\begin{aligned}
&\sum_{j=2}^{K} \left\{ \sum_{i=h_n+1}^{T_n^0} \zeta_{n,j}^i(\gamma) + c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1\left(\gamma + \frac{v_n^{h_n+s+1} - v_n^{h_n+s}}{\sqrt{\lambda_n}}\right) \right\} \\
&= \sum_{j=2}^{K} c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1\left(\tilde{u}_n^s - \tilde{u}_n^{s-1}\right) + \sum_{j=2}^{K} \sum_{i=0}^{T_n^0-h_n-1} \left\{ J_j\left(\frac{\tilde{u}_n^{i+j} - \tilde{u}_n^i}{j}\right) \right. \\
&\quad \left. + \frac{c_j}{j} \sum_{s=i}^{i+j-1} J_1\left(\tilde{u}_n^s - \tilde{u}_n^{s-1}\right) - \psi_j(\gamma) \right\} \\
&= \sum_{j=2}^{K} c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1\left(\tilde{u}_n^s - \tilde{u}_n^{s-1}\right) + \sum_{j=2}^{K} \sum_{i\geq 0} \left\{ J_j\left(\frac{\tilde{u}_n^{i+j} - \tilde{u}_n^i}{j}\right) \right. \\
&\quad \left. + \frac{c_j}{j} \sum_{s=i}^{i+j-1} J_1\left(\tilde{u}_n^{s+1} - \tilde{u}_n^s\right) - \psi_j(\gamma) \right\} - r_2(n),
\end{aligned}$$

where

$$r_2(n) = \sum_{j=2}^{K} \sum_{i=T_n^0-h_n}^{T_n^0-h_n+K-2} \left\{ J_j\left(\frac{\tilde{u}_n^{i+j} - \tilde{u}_n^i}{j}\right) + \frac{c_j}{j} \sum_{s=i}^{i+j-1} J_1\left(\tilde{u}_n^{s+1} - \tilde{u}_n^s\right) - \psi_j(\gamma) \right\}.$$

Indeed, by definition of $\tilde{u}_n$, we have $\tilde{u}_n^{i+1} - \tilde{u}_n^i = \gamma$ for $i \geq T_n^0 - h_n + K - 1$ and thus the terms in the infinite sum over i with $i \geq T_n^0 - h_n + K - 1$ vanish identically. Furthermore, we have by the definition of $\tilde{u}_n$ and (3.159):

$$\lim_{n\to\infty} \left(\tilde{u}_n^{T_n^0-h_n+s} - \tilde{u}_n^{T_n^0-h_n-1+s}\right) = \gamma + \lim_{n\to\infty} \frac{v_n^{T_n^0+1+s} - v_n^{T_n^0+s}}{\sqrt{\lambda_n}} = \gamma$$

for $s \in \{1, \ldots, K\}$. Hence, we have $r_2(n) \to 0$ as $n \to \infty$. Note that $\tilde{u}_n^0 = 0$ and $\tilde{u}_n^{i+1} - \tilde{u}_n^i = \gamma$ for $i \geq T_n^0 - h_n + K - 1$. Thus $\tilde{u}_n$ is an admissible test function in the definition of $B(\gamma)$, see (3.71), and we obtain (3.166). Combining (3.164)–(3.166) yields (3.160) in the case $0 \in S_v$.

Step 3. Let us now consider the boundary layer energy due to a jump in $(0, 1)$. Assume there exists $t \in (0, 1)$ such that $t \in S_v$. By the choice of $\rho > 0$, we have that $S \cap (t - \rho, t + \rho) = \{t\}$. Similar arguments as in the case of a jump in 0 provide us the existence of sequences $(k_n^{1,t}),(h_n),(k_n^{2,t})\subset\mathbb{N}$ with

$$t-\rho\leq\lambda_n(k_n^{1,t}+s)\leq t-\frac{\rho}{2},\quad t+\frac{\rho}{2}\leq\lambda_n(k_n^{2,t}+s)\leq t+\rho$$

for $s\in\{1,\dots,K\}$ and $\lambda_n h_n\to t$ such that

$$\frac{v_n^{h_n+1}-v_n^{h_n}}{\sqrt{\lambda_n}}\to+\infty,\quad \frac{v_n^{k_n^{i,t}+s+1}-v_n^{k_n^{i,t}+s}}{\sqrt{\lambda_n}}\to 0 \text{ for } i\in\{1,2\} \text{ and } s\in\{1,\dots,K\} \tag{3.167}$$

as $n\to\infty$. The choice of the sequences $(k_n^{1,t})$, $(k_n^{2,t})$ and the definition of $Q_n(\rho)$, see (3.155), yield that $\{k_n^{1,t}+1,\dots,k_n^{2,t}\}\cap Q_n(\rho)=\emptyset$. We have to show that

$$\liminf_{n\to\infty}\sum_{j=2}^{K}\sum_{i=k_n^{1,t}+1}^{k_n^{2,t}}\zeta_{j,n}^i\geq 2B(\gamma)-\sum_{j=1}^{K}j\psi_j(\gamma). \tag{3.168}$$

As in the case of a jump in 0 (see (3.164)), we have that

$$\begin{aligned}\sum_{j=2}^{K}\sum_{i=k_n^{1,t}+1}^{k_n^{2,t}}\zeta_{j,n}^i=&\sum_{j=2}^{K}\Bigg\{\sum_{i=k_n^{1,t}}^{h_n-j}\zeta_{j,n}^i+c_j\sum_{s=1}^{j-1}\frac{j-s}{j}J_1\left(\gamma+\frac{v_n^{h_n-s+1}-v_n^{h_n-s}}{\sqrt{\lambda_n}}\right)+\sum_{i=h_n+1}^{k_n^{2,t}}\zeta_{j,n}^i\\&+c_j\sum_{s=1}^{j-1}\frac{j-s}{j}J_1\left(\gamma+\frac{v_n^{h_n+s+1}-v_n^{h_n+s}}{\sqrt{\lambda_n}}\right)\Bigg\}-\sum_{j=2}^{K}j\psi_j(\gamma)+r_1(n),\end{aligned}$$

with

$$r_1(n)=\sum_{j=1}^{K}\sum_{s=0}^{j-1}J_j\left(\gamma+\frac{v_n^{h_n+j-s}-v_n^{h_n-s}}{j\sqrt{\lambda_n}}\right)\to 0\quad\text{as } n\to\infty.$$

Thus it remains to prove that

$$\sum_{j=2}^{K}\Bigg\{\sum_{i=k_n^{1,t}+1}^{h_n-j}\zeta_{j,n}^i+c_j\sum_{s=1}^{j-1}\frac{j-s}{j}J_1\left(\gamma+\frac{v_n^{h_n-s+1}-v_n^{h_n-s}}{\sqrt{\lambda_n}}\right)\Bigg\}\geq B(\gamma)-r_2(n) \tag{3.169}$$

$$\sum_{j=2}^{K}\Bigg\{\sum_{i=h_n+1}^{k_n^{2,t}}\zeta_{j,n}^i+c_j\sum_{s=1}^{j-1}\frac{j-s}{j}J_1\left(\gamma+\frac{v_n^{h_n+s+1}-v_n^{h_n+s}}{\sqrt{\lambda_n}}\right)\Bigg\}\geq B(\gamma)-r_3(n) \tag{3.170}$$

with $\lim_{n\to\infty}r_i(n)=0$ for $i\in\{2,3\}$. The inequality (3.170) can be proven in exactly the same way as (3.166). Moreover, a straightforward adaption of the proof of inequality (3.94) to the rescaled situation yields (3.169). Hence, it holds (3.168). Clearly the above arguments can be applied to every $t\in S_v\cap(0,1)$.

Hence, combining (3.134), the estimates (3.53), (3.160), (3.161) and (3.168) yields

$$\begin{aligned}\liminf_{n\to\infty} E_n^{\delta_n}(v_n) \geq& \alpha \int_{(2\rho,1-2\rho)\setminus S_{2\rho}} |v'|^2 dx + B(u_0^{(1)},\gamma) + B(u_1^{(1)},\gamma)\\ &+ \Big(B_{BJ}(u_0^{(1)}) - B(u_0^{(1)},\gamma)\Big)\#(S_v\cap\{0\}) + B_{IJ}\#(S_v\cap(0,1))\\ &+ \Big(B_{BJ}(u_1^{(1)}) - B(u_1^{(1)},\gamma)\Big)\#(S_v\cap\{1\}) - \sum_{j=2}^{K}(j-1)\psi_j(\gamma).\end{aligned}$$

By taking $\rho\to 0$ and using the fact that $v'\in L^2(0,1)$, we obtain (3.154). This proves the liminf inequality.

Limsup inequality. To complete the Γ-convergence proof it is left to show that for every $v\in SBV_e^\delta(0,1)$ there exists a sequence (v_n) such that $v_n\to v$ in $L^1(0,1)$ and $\limsup_n E_n^{\delta_n}(v_n)\leq E^\delta(v)$. As in the proof of Theorem 3.19, we consider the case $\#S_v=1$ and distinguish between having a jump at the boundary or in the interior. Similarly, as in [17] and [51], it is enough to consider functions v which are sufficiently smooth and locally constant on both sides of S_v. The claim follows by density and relaxation arguments.

Jump in 0. Let $v\in SBV_e^\delta(0,1)$ with $S_v=\{0\}$ be such that $v\in C^2(0,1)$, $v(0)=0$ and $v(1)=\delta$. Moreover, let $v\equiv v(0+)$ on $(0,\rho)$ and $v\equiv\delta$ on $(1-\rho,1)$ for some (small) $\rho>0$. Since $E^\delta(v)=+\infty$ if $[v](t)<0$ for some $t\in S_v$, we can assume that $v(0+)>0$.

Let us recall some sequences which were introduced in the proof of Theorem 3.19. Fix $\eta>0$. By the definition of $B(\gamma)$, we can find a function $\tilde u:\mathbb{N}_0\to\mathbb{R}$ and an $\tilde N\in\mathbb{N}$ such that $\tilde u^0=0$, $\tilde u^{i+1}-\tilde u^i=\gamma$ if $i\geq\tilde N$ and (3.97) is satisfied. Analogously, by the definition of $B_b(\theta)$ given in (3.70), there exist $\hat w:\mathbb{N}_0\to\mathbb{R}$ and $\hat k_0\in\mathbb{N}$, $\hat k_0\geq K-1$ such that $\hat w^{k_0}=0$, $\hat w^{k_0+1-s}-\hat w^{k_0-s}=u_{0,s}^{(1)}$ for $s=1,\dots,K-1$ and it holds (3.98). Finally the definition of $B(\theta,\gamma)$ yields the existence of a function $w:\mathbb{N}_0\to\mathbb{R}$ and natural number $N_2\in\mathbb{N}$ with $w^0=0$, $w^s-w^{s-1}=u_{1,s}^{(1)}$ for $s\in\{1,\dots,K-1\}$, $w^{i+1}-w^i=\gamma$ for $i\geq N_2$ such that (3.99) is satisfied.

Let $(T_n^0),(T_n^1)\subset\mathbb{N}$ be such that $\frac{\rho}{2}\in\lambda_n[T_n^0,T_n^0+1)$ and $1-\frac{\rho}{2}\in\lambda_n[T_n^1,T_n^1+1)$. For n sufficiently large it holds

$$\hat k_0+\tilde N+K+1\leq T_n^0\leq\frac{\rho}{\lambda_n}-K-1 \quad\text{and}\quad \frac{1-\rho}{\lambda_n}+K\leq T_n^1\leq n-N_2-K. \tag{3.171}$$

Indeed, since $\rho>0$ the statement regarding T_n^0 follows by $\hat k_0+\tilde N+K+1\leq\frac{\rho}{2\lambda_n}-1\leq T_n^0\leq\frac{\rho}{2\lambda_n}\leq\frac{\rho}{\lambda_n}-K-1$ for n large enough. The inequalities regarding T_n^1 follow analogously. For n sufficiently large such that (3.171) holds, we define a recovery sequence (v_n) for v

by means of the functions v, $\tilde{u}$, w and $\hat{w}$ by

$$v_n^i = \begin{cases} -\sqrt{\lambda_n}(\hat{w}^{\hat{k}_0-i}+\gamma i) & \text{if } 0 \le i \le \hat{k}_0, \\ v(0+)+\delta_n-\delta+\sqrt{\lambda_n}(\tilde{u}^{i-\hat{k}_0-1}-\tilde{u}^{\tilde{N}}-w^{N_2+1}) & \\ -\sqrt{\lambda_n}\gamma(i-\hat{k}_0-2-\tilde{N}-N_2) & \text{if } \hat{k}_0+1 \le i \le T_n^0+1, \\ v(i\lambda_n)+\delta_n-\delta-\sqrt{\lambda_n}(w^{N_2+1}-\gamma(N_2+1)) & \text{if } T_n^0+1 \le i \le T_n^1+1, \\ \delta_n-\sqrt{\lambda_n}(w^{n-i}-\gamma(n-i)) & \text{if } T_n^1+1 \le i \le n. \end{cases}$$

By the definition of v_n, $\hat{w}$ and w, we have $v_n(0)=v_n^0=0$, $v_n(1)=v^n=\delta_n$, and

$$v_n^s - v_n^{s-1} = \sqrt{\lambda_n}(\hat{w}^{\hat{k}_0+1-s}-\hat{w}^{\hat{k}_0-s}-\gamma) = \sqrt{\lambda_n}(u_{0,s}^{(1)}-\gamma),$$
$$v_n^{n+1-s} - v_n^{n-s} = \sqrt{\lambda_n}(w^s-w^{s-1}-\gamma) = \sqrt{\lambda_n}(u_{1,s}^{(1)}-\gamma),$$

for $s \in \{1,\dots,K\}$. Thus v_n satisfies the boundary conditions (3.130). Let us show that v_n is uniquely defined for $i \in \{T_n^0+1, T_n^1+1\}$. The definition of T_n^0 yields $0 < \lambda_n T_n^0 \le \frac{\varrho}{2}$ and thus $v(\lambda_n(T_n^0+1)) = v(0+)$. By $\tilde{u}^{i+1}-\tilde{u}^i=\gamma$ for $i \ge \tilde{N}$, it holds for $i \in \{\hat{k}_0+\tilde{N}+2,\dots,T_n^0+1\} \neq \emptyset$ (by (3.171)) that

$$\tilde{u}_n^{i-\hat{k}_0-1} - \tilde{u}^{\tilde{N}} - \gamma(i-\hat{k}_0-2-\tilde{N}-N_2) = N_2+1. \tag{3.172}$$

Hence, v_n^i is well defined for $i=T_n^0+1$. Similarly, $\lambda_n(T_n^1+1) \ge 1-\frac{\varrho}{2}$ implies $v(\lambda_n(T_n^1+1))=\delta$ and $n-T_n^1 \ge N_2+K$ implies $w^{n-T_n^1-1}-\gamma(n-T_n^1-1) = w^{N_2+1}-\gamma(N_2+1)$. Thus v_n^i is uniquely defined for $i=T_n^1+1$.

Next, we show that $v_n \to v$ in $L^1(0,1)$. Let us denote by $\tilde{v}_n$ the piecewise affine interpolation of v with respect to $\lambda_n\mathbb{N}$, i.e. $\tilde{v}_n \in \mathcal{A}_n(0,1)$ and $\tilde{v}_n^i = v(i\lambda_n)$. The sequence $(\tilde{v}_n)$ converges to v strongly in L^1. Hence, it is sufficient to show that $(v_n-\tilde{v}_n) \to 0$ in $L^1(0,1)$. We prove the L^1 convergence only on the interval $(0,\frac{\varrho}{2})$, since similar arguments yield the convergence on the intervals $(\frac{\varrho}{2},1-\frac{\varrho}{2})$ and $(1-\frac{\varrho}{2},1)$. Note that $\tilde{v}_n$ and v_n are equibounded in $L^\infty(0,\frac{\varrho}{2})$ for n sufficiently large. Indeed, $\|\tilde{v}_n\|_{L^\infty(0,\frac{\varrho}{2})} \le v(0+)$ by the definition $\tilde{v}_n$ and v. Using $v_n \in \mathcal{A}_n$, (3.172) and $\frac{\varrho}{2} \le \lambda_n(T_n^0+1)$, we obtain

$$\begin{aligned}\|v_n\|_{L^\infty(0,\frac{\varrho}{2})} \le \sup_{i\in\{0,\dots,T_n^0+1\}} |v_n^i| \le \max_{i\in\{0,\dots,\hat{k}_0\}} \sqrt{\lambda_n}|\hat{w}^{\hat{k}_0-i}+\gamma i| + |v(0+)+\delta_n-\delta| \\ + \max_{i\in\{\hat{k}_0+1,\dots,\hat{k}_0+\tilde{N}+2\}} \sqrt{\lambda_n}(\tilde{u}^{i-\hat{k}_0-1}-\gamma i+c_1))|,\end{aligned}$$

with $c_1 = \gamma(\hat{k}_0+2+\tilde{N}+N_2)-\tilde{u}^{\tilde{N}}-w^{N_2+1}$. Moreover, we have for $i \in \{\hat{k}_0+\tilde{N}+2,\dots,T_n^0+1\}$ that

$$|v_n^i - \tilde{v}_n^i| \le |\delta_n-\delta| + \sqrt{\lambda_n}|(w^{N_2+1}-\gamma(N_2+1)| =: r(n).$$

Note that $\delta_n \to \delta$ yields $r(n) \to 0$ as $n \to \infty$. Hence, we deduce from the previous calculations, $\frac{\rho}{2} \le \lambda_n(T_n^0+1)$ and $v_n, \tilde{v}_n \in \mathcal{A}_n(0,1)$ that

$$\begin{aligned}
\|v_n - \tilde{v}_n\|_{L^1(0,\frac{\rho}{2})} \le & \sum_{i=0}^{T_n^0} \int_{i\lambda_n}^{(i+1)\lambda_n} |v_n - \tilde{v}_n| dx \\
\le & \lambda_n(\hat{k}_0 + \tilde{N} + 2)\|v_n - \tilde{v}_n\|_{L^\infty(0,\frac{\rho}{2})} + \sum_{i=\hat{k}_0+\tilde{N}+2}^{T_n^0} \int_{i\lambda_n}^{(i+1)\lambda_n} |v_n - \tilde{v}_n| dx \\
\le & \mathcal{O}(\lambda_n) + \sum_{i=\hat{k}_0+\tilde{N}+2}^{T_n^0} \int_{i\lambda_n}^{(i+1)\lambda_n} r(n) + 2r(n)\frac{x - i\lambda_n}{\lambda_n} dx \\
\le & \mathcal{O}(\lambda_n) + 2(T_n^0+1)\lambda_n r(n) \le \mathcal{O}(\lambda_n) + 2\rho r(n),
\end{aligned}$$

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

Let us now show that v_n is indeed a recovery sequence for v. To this end, we split the sum over $\zeta_{j,n}^i$ as follows

$$\begin{aligned}
\sum_{j=2}^{K}\sum_{i=0}^{n-j} \zeta_{j,n}^i = & \sum_{j=2}^{K} \Bigg\{ \sum_{i=0}^{T_n^0+1-K} \zeta_{j,n}^i + \sum_{i=T_n^0+2-K}^{T_n^0} \zeta_{j,n}^i + \sum_{i=T_n^0+1}^{T_n^1+1-K} \zeta_{j,n}^i + \sum_{i=T_n^1+2-K}^{T_n^1} \zeta_{j,n}^i \\
& + \sum_{i=T_n^1+1}^{n-j} \zeta_{j,n}^i \Bigg\}.
\end{aligned} \tag{3.173}$$

We show that $v_n^{i+1} - v_n^i = 0$ for $i \in \{T_n^0+2-K, \dots, T_n^0+K-1\} \cup \{T_n^1+2-K, \dots, T_n^1+K-1\}$. This implies $\zeta_{j,n}^i = 0$ for $i \in \{T_n^0+2-K, \dots, T_n^0\} \cup \{T_n^1+2-K, \dots, T_n^1\}$ and $j \in \{2, \dots, K\}$. Since $T_n^0 + 1 - K - k_0 \ge \tilde{N}$ it holds $v_n^{i+1} - v_n^i = \sqrt{\lambda_n}(\tilde{u}^{i-\hat{k}_0} - \tilde{u}^{i-\hat{k}_0-1} - \gamma) = 0$ for $i \in \{T_n^0 + 2 - K, \dots, T_n^0\}$. Moreover, we deduce from $\lambda_n(T_n^0 + K) < \rho$ and $v \equiv v(0^+)$ on $(0, \rho)$ that $v_n^{i+1} - v_n^i = v((i+1)\lambda_n) - v(i\lambda_n) = 0$ for $i \in \{T_n^0 + 1, \dots, T_n^0 + K - 1\}$. Similar calculations combined with $v \equiv \delta$ on $(1-\rho, 1)$, $\lambda_n(T_n^1 - K + 1) > 1 - \rho$ and $n - T_n^1 \ge N_2 + K$ yields $v_n^{i+1} - v_n^i = 0$ for $i \in \{T_n^1 + 2 - K, \dots, T_n^1 + K - 1\}$. Hence, we have

$$\sum_{j=2}^{K} \left\{ \sum_{i=T_n^0+2-K}^{T_n^0} \zeta_{j,n}^i + \sum_{i=T_n^1+2-K}^{T_n^1} \zeta_{j,n}^i \right\} = 0. \tag{3.174}$$

Let us now estimate the sum from $i = 0$ to $i = T_n^0 + 1 - K$ of (3.173). This contributes to the jump energy $B_{BJ}(u_0^{(1)})$. The definition of v_n and $\delta_n \to \delta$ imply that

$$\frac{v_n^{\hat{k}_0+j-s} - v_n^{\hat{k}_0-s}}{\sqrt{\lambda_n}} = \frac{v(0+) + \delta_n - \delta}{\sqrt{\lambda_n}} + \mathcal{O}(1) \to +\infty \quad \text{as } n \to +\infty,$$

for $j \in \{1, \dots, K\}$ and $s \in \{0, \dots, j-1\}$. Hence, we obtain similarly to (3.164) that

$$\sum_{j=2}^{K}\sum_{i=0}^{T_n^0}\zeta_{j,n}^i = \sum_{j=2}^{K}\Bigg\{\sum_{i=0}^{\hat{k}_0-j}\zeta_{j,n}^i + c_j\sum_{s=1}^{j-1}\frac{j-s}{j}J_1\left(\gamma + \frac{v_n^{\hat{k}_0-s+1}-v_n^{\hat{k}_0-s}}{\sqrt{\lambda_n}}\right) + \sum_{i=\hat{k}_0+1}^{T_n^0}\zeta_{n,j}^i$$
$$+ c_j\sum_{s=1}^{j-1}\frac{j-s}{j}J_1\left(\frac{v_n^{\hat{k}_0+s+1}-v_n^{\hat{k}_0+s}}{\lambda_n}\right)\Bigg\} - \sum_{j=2}^{K} j\psi_j(\gamma) + r(n), \qquad (3.175)$$

with

$$r(n) = \sum_{j=1}^{K}\sum_{s=-j+1}^{0} J_j\left(\gamma + \frac{v_n^{\hat{k}_0+j+s}-v_n^{\hat{k}_0+s}}{j\sqrt{\lambda_n}}\right) \to 0 \quad \text{as } n \to \infty.$$

By the definition of v_n and $\hat{w}$, we obtain

$$\sum_{j=2}^{K}\left\{\sum_{i=0}^{\hat{k}_0-j}\zeta_{j,n}^i + c_j\sum_{s=1}^{j-1}\frac{j-s}{j}J_1\left(\gamma + \frac{v_n^{\hat{k}_0-s+1}-v_n^{\hat{k}_0-s}}{\sqrt{\lambda_n}}\right)\right\}$$
$$= \sum_{j=2}^{K}\sum_{i=0}^{\hat{k}_0-j}\left\{J_j\left(\frac{\hat{w}^{i+j}-\hat{w}^i}{j}\right) + \frac{c_j}{j}\sum_{s=i}^{i+j-1}J_1(\hat{w}^{s+1}-\hat{w}^s) - \psi_j(\gamma)\right\} \leq B_b(u_0^{(1)}) + \eta. \qquad (3.176)$$

Note that this is essentially the same calculation as in (3.104). Moreover, we obtain from the definition of v_n, $\tilde{u}$ and (3.105) that

$$\sum_{j=2}^{K}\left\{\sum_{i=\hat{k}_0+1}^{T_n^0+1-K}\zeta_{j,n}^i + c_j\sum_{s=1}^{j-1}\frac{j-s}{j}J_1\left(\gamma + \frac{v_n^{\hat{k}_0-s+1}-v_n^{\hat{k}_0-s}}{\sqrt{\lambda_n}}\right)\right\} \leq B(\gamma) + \eta. \qquad (3.177)$$

The estimate for the elastic boundary layer energy at 1 can be treated as in the first-order Γ-limit result. By the definition of v_n, w and (3.106) it holds

$$\sum_{j=2}^{K}\left\{\sum_{i=T_n^1+1}^{n-j}\zeta_{j,n}^i + c_j\sum_{s=1}^{j-1}\frac{j-s}{j}J_1(u_{1,s}^{(1)})\right\} \leq B(u_1^{(1)},\gamma) + \eta. \qquad (3.178)$$

Next, we show that the term

$$\sum_{j=2}^{K}\sum_{i=T_n^0+1}^{T_n^1+1-K}\zeta_{j,n}^i$$

in (3.173) yields the elastic integral term in the limit as n tends to infinity. By the definition of (T_n^0) and (T_n^1) it holds $\lambda_n T_n^0 > \frac{\varrho}{4}$ and $\lambda_n(T_n^1+K) < 1-\frac{\varrho}{4}$ for n sufficiently large. Thus, we deduce from $v \in C^2(0,1)$ that

$$\left|\frac{v((i+1)\lambda_n)-v(i\lambda_n)}{\sqrt{\lambda_n}}\right| = \sqrt{\lambda_n}\left|\frac{v((i+1)\lambda_n)-v(i\lambda_n)}{\lambda_n}\right| \leq \sqrt{\lambda_n}\|v\|_{C^2([\frac{\varrho}{4},1-\frac{\varrho}{4}])} \qquad (3.179)$$

for $i \in \{T_n^0, \dots, T_n^1 + K - 1\}$. Clearly, the right-hand side in (3.179) tends to zero as n tend to infinity. A Taylor expansion of J_j at γ yields:

$$J_j(\gamma + z) = J_j(\gamma) + J_j'(\gamma)z + \frac{1}{2}J_j''(\gamma)z^2 + \eta_j(z)$$

with $\frac{\eta_j(z)}{|z|^2} \to 0$ as $z \to 0$ for $j \in \{1, \dots, K\}$. Hence, using the definition of $\psi_j(z) = J_j(z) + c_j J_1(z)$, $\psi_j'(\gamma) = 0$ and $\alpha_j = \frac{1}{2}\psi_j''(\gamma)$, we have for $z = \frac{1}{j}\sum_{s=1}^j z_s$ and $\omega(z) := \sup_{|t|\le z}|\eta_j(t)| + j\sup_{|t|\le z}|\eta_1(t)|$ that

$$\begin{aligned}
&J_j(\gamma + z) + \frac{c_j}{j}\sum_{s=1}^{j} J_1(\gamma + z_s) - \psi_j(\gamma) \\
&\le \frac{1}{2}\left\{J_j''(\gamma)\left(\frac{1}{j}\sum_{s=1}^{j} z_s\right)^2 + c_j J_1''(\gamma)\frac{1}{j}\sum_{s=1}^{j} z_s^2\right\} + \omega(\max_{1\le s\le j}|z_s|) \\
&= \frac{\alpha_j}{j}\sum_{s=1}^{j} z_s^2 - \frac{1}{2j^2}J_j''(\gamma)\sum_{s=1}^{j-1}\sum_{m=s+1}^{j}(z_s - z_m)^2 + \omega(\max_{1\le s\le j}|z_s|)
\end{aligned}$$

where we used the following identity in the last step:

$$\left(\sum_{s=1}^{j} a_s\right)^2 = \sum_{s=1}^{j} a_s^2 + 2\sum_{s=1}^{j-1}\sum_{m=s+1}^{j} a_s a_m = j\sum_{s=1}^{j} a_s^2 - \sum_{s=1}^{j-1}\sum_{m=s+1}^{j}(a_s - a_m)^2.$$

Hence, for $i \in \{T_n^0, \dots, T_n^1 + 1 - j\}$ and n sufficiently large such that (3.171) holds, we have the following estimate:

$$\begin{aligned}
\zeta_{j,n}^i =& J_j\left(\gamma + \sqrt{\lambda_n}\frac{v_n^{i+j} - v_n^i}{j\lambda_n}\right) + \sum_{s=i}^{i+j-1} J_1\left(\gamma + \sqrt{\lambda_n}\frac{v_n^{s+1} - v_n^s}{\lambda_n}\right) - \psi_j(\gamma) \\
\le& \lambda_n \Bigg\{\frac{\alpha_j}{j}\sum_{s=i}^{i+j-1}\left(\frac{v_n^{s+1} - v_n^s}{\lambda_n}\right)^2 - \frac{1}{2j^2}J_j''(\gamma)\sum_{s=i}^{i+j-2}\sum_{m=s+1}^{i+j-1}\left(\frac{v_n^{s+1} - v_n^s - (v_n^{m+1} - v_n^m)}{\lambda_n}\right)^2 \\
&+ \frac{1}{\lambda_n}\omega\left(\max_{i\le s\le i+j-1}\left|\frac{v_n^{s+1} - v_n^s}{\sqrt{\lambda_n}}\right|\right)\Bigg\} \\
=& \lambda_n\left\{\frac{\alpha_j}{j}\sum_{s=i}^{i+j-1}\left(\frac{v_n^{s+1} - v_n^s}{\lambda_n}\right)^2 + o(1)\right\}
\end{aligned}$$

as $n \to \infty$. Indeed, from the definition of v_n and $v \in C^2(0,1)$ we deduce for $i \in \{T_n^0, \dots, T_n^1 + 1 - j\}$ and $s, m \in \mathbb{N}$ with $i \le s < m \le i + j - 1$ that:

$$\begin{aligned}
\frac{v_n^{s+1} - v_n^{m+1} - (v_n^s - v_n^m)}{\lambda_n} =& \frac{v((s+1)\lambda_n) - v((m+1)\lambda_n) - (v(s\lambda_n) - v(m\lambda_n))}{\lambda_n} \\
=& (v'((m+1)\lambda_n) - v'(m\lambda_n))(s - m) + o(1) \to 0
\end{aligned}$$

as $n \to \infty$. Hence, the second term in the brackets on the right-hand side of the estimate for $\zeta_{j,n}^i$ is of order $o(1)$. It remains to estimate the third term. If $\max_{i \leq s \leq i+j-1} |v_n^{s+1} - v_n^s| = 0$ nothing is to be shown since $\omega(0) = 0$. Let us consider the case that $\max_{i \leq s \leq i+j-1} |v_n^{s+1} - v_n^s| > 0$. Then we have for $i \in \{T_n^0, \dots, T_n^1 + 1 - j\}$ that

$$\max_{i \leq s \leq i+j-1} \frac{v_n^{s+1} - v_n^s}{\lambda_n} = \max_{T_n^0 \leq i \leq T_n^1} \frac{v((i+1)\lambda_n) - v(i\lambda_n)}{\lambda_n} \leq \|v\|_{C^2((0,1))}.$$

Let us fix $i \in \{T_n^0, \dots, T_n^1 + 1 - K\}$. By the definition of ω and by $\eta_j(z)/z^2 \to 0$ as $|z| \to 0$, and (3.179), we have that

$$\frac{1}{\lambda_n}\omega\left(\max_{i \leq s \leq i+j-1}\left|\frac{v_n^{s+1} - v_n^s}{\sqrt{\lambda_n}}\right|\right)$$
$$= \max_{i \leq s \leq i+j-1}\left(\frac{v_n^{s+1} - v_n^s}{\lambda_n}\right)^2 \cdot \frac{\omega\left(\max_{i \leq s \leq i+j-1}\left|\frac{v_n^{s+1} - v_n^s}{\sqrt{\lambda_n}}\right|\right)}{\max_{i \leq s \leq i+j-1}\left(\frac{v_n^{s+1} - v_n^s}{\sqrt{\lambda_n}}\right)^2} \to 0$$

as $n \to \infty$. Hence, we have for n large enough such that (3.171) holds that

$$\begin{aligned}
\sum_{j=2}^{K}\sum_{i=T_n^0+1}^{T_n^1+1-K} \zeta_{j,n}^i &\leq \sum_{j=2}^{K}\frac{\alpha_j}{j}\lambda_n \sum_{i=T_n^0+1}^{T_n^1+1-K}\left\{\sum_{s=i}^{i+j-1}\left(\frac{v_n^{s+1} - v_n^s}{\lambda_n}\right)^2 + o(1)\right\} \\
&= \sum_{j=2}^{K}\alpha_j\lambda_n \sum_{i=T_n^0+1}^{T_n^1+1-K}\left(\frac{v((i+1)\lambda_n) - v(i\lambda_n)}{\lambda_n}\right)^2 + o(1) \\
&= \sum_{j=2}^{K}\alpha_j\lambda_n \sum_{i=T_n^0+1}^{T_n^1+1-K} v'(i\lambda_n)^2 + o(1) \\
&= \sum_{j=2}^{K}\alpha_j \int_0^1 |v'|^2 dx + o(1) = \alpha\int_0^1 |v'|^2 dx + o(1). \qquad (3.180)
\end{aligned}$$

Note that we used $v \equiv v(0^+)$ on $\lambda_n[T_n^0, T_n^0 + K]$, and $v \equiv \delta$ on $\lambda_n[T_n^1 - K, T_n^1]$ for n sufficiently large. The left Riemann sum converges to the integral since v' is continuous. Altogether, we obtain from (3.174),(3.176)-(3.178) and (3.180) that

$$\begin{aligned}
\limsup_{n\to\infty} E_n^{\delta_n}(v_n) \leq &\alpha\int_0^1 |v'|^2 dx + \sum_{j=2}^{K} c_j \sum_{s=1}^{j-1}\frac{j-s}{j}J_1(u_{0,s}^{(1)}) + B_b(u_0^{(1)}) + B(\gamma) \\
&+ B(u_1^{(1)}, \gamma) - \sum_{j=2}^{K}(2j-1)\psi_j(\gamma) + 3\eta
\end{aligned}$$

and the assertion follows by the arbitrariness of $\eta > 0$.

Internal jump. Let us now consider the case $S_v = \{t\}$ with $t \in (0,1)$. As in the case of a jump in 0 it is not restrictive to assume that $v \in C^2([0,1] \setminus \{t\})$, $v \equiv 0$ on $[0,\rho)$, $v \equiv v(t-)$ on $(t-\rho,t)$, $v \equiv v(t+)$ on $(t,t+\rho)$ and $v \equiv \delta$ on $(1-\rho,1]$ for some $\rho > 0$ with $\rho < \frac{1}{2}\min\{t,1-t\}$. Since $E^\delta(v) = +\infty$ if $v(t+) < v(t-)$, we can assume $v(t+) > v(t-)$. Fix $\eta > 0$. By the definition of the boundary layer energy $B(u_0^{(1)},\gamma)$, we can find $\hat{v} : \mathbb{N}_0 \to \mathbb{R}$ and $N_1 \in \mathbb{N}$ such that $\hat{v}^0 = 0$, $\hat{v}^s - \hat{v}^{s-1} = u_{0,s}^{(1)}$ for $s \in \{1,\dots,K-1\}$, $\hat{v}^{i+1} - \hat{v}^i = \gamma$ if $i \geq N_1$ and it holds (3.108) (with v replaced by $\hat{v}$). Moreover, let $\tilde{u} : \mathbb{N}_0 \to \mathbb{R}$ and $\tilde{N} \in \mathbb{N}$ be such that $\tilde{u}^0 = 0$, $\tilde{u}^{i+1} - \tilde{u}^i$ if $i \geq \tilde{N}$ and (3.97) holds. By the definition of $B(u_1^{(1)},\gamma)$, we find a sequence $\hat{w} : \mathbb{N}_0 \to \mathbb{R}$ and a natural number $N_2 \in \mathbb{N}$ with $w^0 = 0$, $w^s - w^{s-1} = u_{1,s}^{(1)}$ for $i \in \{1,\dots,K-1\}$, $w^{i+1} - w^i = \gamma$ for $i \geq N_2$ such that (3.99) be satisfied.

Let the sequences $(T_n^0), (k_n^1), (h_n), (k_n^2), (T_n^1) \subset \mathbb{N}$ be such that $\frac{\rho}{2} \in \lambda_n[T_n^0, T_n^0+1)$, $t-\frac{\rho}{2} \in \lambda_n[k_n^1,k_n^1+1)$, $t \in \lambda_n[h_n,h_n+1)$, $t+\frac{\rho}{2} \in \lambda_n[k_n^2,k_n^2+1)$, and $1-\frac{\rho}{2} \in \lambda_n[T_n^1,T_n^1+1)$. Thus, for n sufficiently large it hold

$$\begin{gathered} N_1 + K \leq T_n^0 \leq \frac{\rho}{\lambda_n} - K, \quad \frac{1-\rho}{\lambda_n} \leq T_n^1 \leq n - N_2 - K, \\ \frac{t-\rho}{\lambda_n} < k_n^1 \leq h_n - K, \quad h_n + 1 + K + \tilde{N} \leq k_n^2 \leq \frac{t+\rho}{\lambda_n} - K. \end{gathered} \tag{3.181}$$

For n sufficiently large such that (3.181) holds, we define a recovery sequence (v_n) by means of the functions $v, \hat{v}, \tilde{u}$ and w as

$$v_n^i = \begin{cases} \sqrt{\lambda_n}(\hat{v}^i - \gamma i) & \text{if } 0 \leq i \leq T_n^0, \\ v(i\lambda_n) + \sqrt{\lambda_n}(\hat{v}^{N_1} - \gamma N_1) & \text{if } T_n^0 \leq i \leq k_n^1, \\ v(t-) - \sqrt{\lambda_n}(\tilde{u}^{h_n-i} - \tilde{u}^{\tilde{N}} - \hat{v}^{N_1} & \\ \qquad +\gamma(i - h_n + \tilde{N} + N_1)) & \text{if } k_n^1 \leq i \leq h_n, \\ v(t+) + \delta_n - \delta + \sqrt{\lambda_n}(\tilde{u}^{i-(h_n+1)} - \tilde{u}^{\tilde{N}} - w^{N_2+1} & \\ \qquad -\gamma(i - h_n - 2 - \tilde{N} - N_2)) & \text{if } h_n + 1 \leq i \leq k_n^2 + 1, \\ v(i\lambda_n) + \delta_n - \delta - \sqrt{\lambda_n}(w^{N_2+1} - \gamma(N_2+1)) & \text{if } k_n^2 + 1 \leq i \leq T_n^1 + 1, \\ \delta_n - \sqrt{\lambda_n}(w^{n-i} - \gamma(n-i)) & \text{if } T_n^1 + 1 \leq i \leq n. \end{cases}$$

By the definition of $\hat{v}$, w and v the boundary conditions (3.130) are satisfied. The assumptions on v and (3.181) yield $v(T_n^0\lambda_n) = 0$, $v(k_n^1\lambda_n) = v(t-)$, $v((k_n^2+1)\lambda_n) = v(t+)$ and $v((T_n^1+1)\lambda_n) = \delta$. Thus, v_n^i is by the definition of $\hat{v}$, $\tilde{u}$ and w uniquely defined for $i \in \{T_n^0, k_n^1, k_n^2+1, T_n^1+1\}$. The definition of v_n yields $v_n \to v$ in $L^1(0,1)$, which can be proven in a similar way as for the case of a jump in 0.

Moreover, the definition of v_n, $v(t+) > v(t-)$ and $\lim_{n\to\infty}\delta_n = \delta$ yield

$$\frac{v_n^{h_n-s+j} - v_n^{h_n-s}}{\sqrt{\lambda_n}} = \frac{v(t+) - v(t-) + \delta_n - \delta}{\sqrt{\lambda_n}} + \mathcal{O}(1) \to +\infty \quad \text{as } n \to \infty,$$

for $j \in \{1, \dots, K\}$ and $s \in \{0, \dots, j-1\}$. Let us now show that v_n is a recovery for v. Firstly, we decompose the sum over the $\zeta^i_{j,n}$ terms in (3.134) as

$$\sum_{j=2}^{K}\sum_{i=0}^{n-j} = \sum_{j=2}^{K}\Bigg\{ \sum_{i=0}^{T_n^0-K} \zeta^i_{j,n} + \sum_{i=T_n^0-K+1}^{T_n^0-1} \zeta^i_{j,n} + \sum_{i=T_n^0}^{k_n^1-K} \zeta^i_{j,n} + \sum_{i=k_n^1-K+1}^{k_n^1-1} \zeta^i_{j,n} + \sum_{i=k_n^1}^{k_n^2+1-K} \zeta^i_{j,n} + \sum_{i=k_n^2+2-K}^{k_n^2} \zeta^i_{j,n} + \sum_{i=k_n^2+1}^{T_n^1+1-K} \zeta^i_{j,n} + \sum_{i=T_n^1+2-K}^{T_n^1} \zeta^i_{j,n} + \sum_{i=T_n^1+1}^{n-j} \zeta^i_{j,n}\Bigg\}.$$

The definition of $\hat{v}, \tilde{u}, w$ and v_n, combined with similar calculations as for the case of a jump in 0 and for a jump in $(0,1)$ in the proof of Theorem 3.19 yield that

$$\begin{aligned}
&\sum_{j=2}^{K}\left\{ c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(u^{(1)}_{0,s}) + \sum_{i=0}^{T_n^0-K} \zeta^i_{j,n} \right\} \le B(u^{(1)}_0, \gamma) + \eta,\\
&\sum_{j=2}^{K}\sum_{i=k_n^1}^{k_n^2+1-K} \zeta^i_{j,n} \le 2B(\gamma) - \sum_{j=2}^{K} j\psi_j(\gamma) + 2\eta + r(n),\\
&\sum_{j=2}^{K}\left\{ c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(u^{(1)}_{1,s}) + \sum_{i=T_n^1+1}^{n-j} \zeta^i_{j,n} \right\} \le B(u^{(1)}_1, \gamma) + \eta,
\end{aligned}$$

where $r(n) \to 0$ as $n \to \infty$. For given $j \in \{2, \dots, K\}$, the definition of v, v_n, $\hat{v}, \tilde{u}$, w and (3.181) imply that

$$\begin{aligned}
\zeta^i_{j,n} = 0 \quad \text{for} \quad & i \in \{T_n^0 - K + 1, \dots, T_n^0 - 1\} \cup \{k_n^1 - K + 1, \dots, k_n^1 - 1\}\\
\text{and} \quad & i \in \{k_n^2 + 2 - K, \dots, k_n^2\} \cup \{T_n^1 + 2 - K, \dots, T_n^1\}.
\end{aligned}$$

We show that $\zeta^i_{j,n} = 0$ for $i \in \{T_n^0 - K + 1, \dots, T_n^0 - 1\}$ the other cases can be proven in a similar way. It is sufficient to show that $v_n^{i+1} - v_n^i = 0$ for $i \in \{T_n^0 - K + 1, \dots, T_n^0 + K - 1\}$. By the properties of $\hat{v}$ and $N_1 \le T_n^0 - K$ it holds $v_n^{i+1} - v_n^i = \sqrt{\lambda_n}(\gamma - \gamma) = 0$ for $i \in \{T_n^0 - K + 1, \dots, T_n^0 - 1\}$. Since $\lambda_n(T_n + K) < \rho$ it holds $\tilde{v}(i\lambda_n) = 0$ for $i \in \{T_n^0, \dots, T_n^0 + K\}$ and thus $v_n^{i+1} - v_n^i = 0$ for $i \in \{T_n^0, \dots, T_n^0 + K - 1\}$.
Moreover, we obtain in a similar fashion as in the case of a jump in 0 that

$$\limsup_{n\to\infty} \sum_{j=2}^{K}\left\{ \sum_{i=T_n^0}^{k_n^1-K} \zeta^i_{j,n} + \sum_{i=k_n^2+1}^{T_n^1+1-K} \zeta^i_{j,n} \right\} \le \alpha \int_0^t |v'|^2 dx + \int_t^1 |v'|^2 dx.$$

Altogether, we deduce from the above estimates and (3.134) that

$$\begin{aligned}\limsup_{n\to\infty} E_n^{\delta_n}(v_n) \leq& \alpha \int_0^1 |v'|^2 dx + B(u_0^{(1)},\gamma) + B(u_1^{(1)},\gamma) \\ &+ 2B(\gamma) + \sum_{j=2}^{K}(2j-1)\psi_j(\gamma) + 4\eta,\end{aligned}$$

which proves the assertion since $\eta > 0$ can be chosen arbitrarily small.

No jump. It remains to provide a recovery sequence for functions $v \in SBV_e^\delta(0,1)$ with $S_v = \emptyset$. As before it is sufficient to consider $v \in C^2(0,1)$ and $v \equiv 0$ on $[0,\rho)$ and $v \equiv \delta$ on $(1-\rho,1]$. For fixed $\eta > 0$ the functions $\hat{v}, w : \mathbb{N}_0 \to \mathbb{R}$ and the natural numbers $N_1, N_2 \in \mathbb{N}$ are defined as in the previous case. Moreover, let the sequences $(T_n^0), (T_n^1) \subset \mathbb{N}$ be such that $\frac{\rho}{2} \in [T_n^0, T_n^0+1)$ and $1-\frac{\rho}{2} \in \lambda_n[T_n^1, T_n^1+1)$. Let us define the sequence (v_n) by

$$v_n^i = \begin{cases} \sqrt{\lambda_n}(\hat{v}^i - \gamma i) & \text{if } 0 \leq i \leq T_n^0, \\ v(i\lambda_n) + \sqrt{\lambda_n}(\hat{v}^{N_1} - \gamma N_1) & \\ -\frac{\sqrt{\lambda_n}(\hat{v}^{N_1}-\gamma N_1 + w^{N_2} - \gamma N_2) - \delta_n + \delta}{T_n^1 - T_n^0}(i - T_n^0) & \text{if } T_n^0 \leq i \leq T_n^1, \\ \delta_n - \sqrt{\lambda_n}(w^{n-i} - \gamma(n-i)) & \text{if } T_n^1 \leq i \leq n. \end{cases}$$

By the definition of $\hat{v}$ and w, the function v_n satisfies the boundary condition (3.130). The function v_n^i is uniquely defined for $i \in \{T_n^0, T_n^1\}$. Let us denote the additional affine term in the definition of v_n^i by z_n^i, i.e.

$$z_n^i := \frac{\sqrt{\lambda_n}(\hat{v}^{N_1} - \gamma N_1 + w^{N_2} - \gamma N_2) - \delta_n + \delta}{T_n^1 - T_n^0}(i - T_n^0),$$

for $i \in \{T_n^0, \ldots, T_n^1\}$. From $\delta_n \to \delta$, we deduce that $\lim_n \sup_i |z_n^i| = 0$. Thus, we have as in the previous cases that $v_n \to v$ in $L^1(0,1)$. The definition of $\hat{v}$ and w yields

$$\begin{aligned}\lim_{n\to\infty} \sum_{j=2}^{K} \left\{ c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(u_{0,s}^{(1)}) + \sum_{i=0}^{T_n^0 - K} \zeta_{j,n}^i \right\} \leq B(u_0^{(1)},\gamma) + \eta, \\ \lim_{n\to\infty} \sum_{j=2}^{K} \left\{ c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(u_{1,s}^{(1)}) + \sum_{i=T_n^1}^{n-j} \zeta_{j,n}^i \right\} \leq B(u_1^{(1)},\gamma) + \eta. \qquad (3.182)\end{aligned}$$

For $i \in \{T_n^0, \ldots, T_n^1 - 1\}$, we have

$$\left| \frac{z_n^{i+1} - z_n^i}{\lambda_n} \right| \leq \frac{|\hat{v}^{N_1} - \gamma N_1 + w^{N_2} - \gamma N_2|}{\sqrt{\lambda_n}(T_n^1 - T_n^0)} + \frac{|\delta_n - \delta|}{\lambda_n(T_n^1 - T_n^0)} =: \omega(n). \qquad (3.183)$$

Since $\lambda_n(T_n^1 - T_n^0) \geq 1 - \rho - 2\lambda_n$ and $\lim_n \delta_n = \delta$, the right-hand side above tends to 0 as $n \to \infty$. Thus, we have that

$$\sup_{i \in \{T_n^0, \dots, T_n^1 - 1\}} \left| \frac{v_n^{i+1} - v_n^i}{\lambda_n} - \frac{v((i+1)\lambda_n) - v(i\lambda_n)}{\lambda_n} \right| \leq r(n) \to 0 \quad \text{as } n \to \infty.$$

Hence, we can use similar arguments as in the case of a jump in 0 to prove the convergence of the elastic part, i.e. that

$$\lim_{n\to\infty} \sum_{j=2}^{K} \sum_{i=T_n^0}^{T_n^1 - K} \zeta_{j,n}^i = \alpha \int_0^1 |v'|^2 dx. \tag{3.184}$$

Using $\lambda_n(T_n^0 + K) \leq \frac{\rho}{2}$, $\lambda_n T_n^1 - K + 1 \geq 1 - \frac{\rho}{2}$ and (3.183), we obtain that $\frac{1}{\sqrt{\lambda_n}}(v_n^{i_n} - v_n^{i_n}) \to 0$ for all $(i_n) \subset \mathbb{N}$ with $i_n \in \{T_n^0 - K + 1, \dots, T_n^0 + K - 1\} \cup \{T_n^1 - K + 1, \dots, T_n^1 + K - 1\}$. Hence

$$\lim_{n\to\infty} \sum_{j=2}^{K} \left\{ \sum_{i=T_n^0 - K + 1}^{T_n^0 - 1} \zeta_{j,n}^i + \sum_{i=T_n^1 - K + 1}^{T_n^1 - 1} \zeta_{j,n}^i \right\} = 0. \tag{3.185}$$

Combining (3.182), (3.184) and (3.185) yields the assertion in the case of no jump.

Convergence of minimisation problems. The convergence of minima follows from the coerciveness of $E_n^{\delta_n}$ and the Γ-convergence result. To verify (3.152), we can argue precisely as in [51, Theorem 6.1]. Fix $\delta > 0$ and consider $\min_v E^\delta(v)$. We distinguish between $S_v = \emptyset$ and $S_v \neq \emptyset$. Let v be such that $E^\delta(v) < +\infty$ and $S_v = \emptyset$. That is, $v \in W^{1,1}(0,1)$ satisfying $v(0) = 0$ and $v(1) = \delta$. Hence,

$$E^\delta(v) = \alpha \int_0^1 |v'|^2 dx + B(u_0^{(1)}, \gamma) + B(u_1^{(1)}, \gamma) - \sum_{j=2}^{K} (j-1)\psi_j(\gamma)$$

and the minimiser is given by $v(x) = \delta x$. Using $\alpha > 0$ and Proposition 3.24, we have that

$$\min_{v: S_v \neq \emptyset} E^\delta(v) \geq \min \left\{ B_{BJ}(u_0^{(1)}) + B(u_1^{(1)}, \gamma), B_{BJ}(u_1^{(1)}) + B(u_0^{(1)}, \gamma) \right\} - \sum_{j=2}^{K} (j-1)\psi_j(\gamma),$$

which finishes the proof. □

Remark 3.36. For the limiting analysis of $(E_n^{\delta_n})$, we used several times results from [17], where a similar result is proven for periodic boundary conditions and multibody potentials with finite range, see [17, Theorem 4]. Let us now briefly discuss that this result is not directly applicable for Lennard-Jones systems with $K > 2$. In [17], a lower-bound comparison potential is defined, which is in our notation given by

$$\Phi_{-}(z) = \inf\left\{\sum_{j=1}^{K}\sum_{i=1}^{K-j+1}\frac{1}{K-j+1}J_j\left(\frac{1}{j}\sum_{s=i}^{i+j-1}z_s\right) : \sum_{s=1}^{K}z_s = Kz\right\},$$

cf. [17, eq. (8)]. It is assumed that Φ_- has a unique minimiser $z_{\min}$ and the infimum in the definition of $\Phi_-(z_{\min})$ is attained for $z_s = z_{\min}$ for $s = 1, \dots, K$. This is in general not satisfied by Lennard-Jones potentials (3.22) for $K > 2$. For simplicity, we consider $K = 3$. In this case the term in the infimum problem in the definition of $\Phi_-(z_{\min})$ reads

$$\frac{1}{3}\left\{J_1(z_1) + J_1(z_2) + J_1(z_3)\right\} + \frac{1}{2}\left\{J_2\left(\frac{z_1+z_2}{2}\right) + J_2\left(\frac{z_1+z_2}{2}\right)\right\} + J_3\left(z_{\min}\right),$$

where $z_1 + z_2 + z_3 = 3z_{\min}$. Assume by contradiction that the infimum is attained for $z_1 = z_2 = z_3 = z_{\min}$. The optimality conditions yield that there exists $\lambda \in \mathbb{R}$ such that $\frac{1}{3}J_1'(z_{\min}) + \frac{1}{4}J_2'(z_{\min}) = \lambda$ (condition for $z_1 = z_3 = z_{\min}$) and $\frac{1}{3}J_1'(z_{\min}) + \frac{1}{2}J_2'(z_{\min}) = \lambda$ (condition for $z_2 = z_{\min}$). Hence, $J_2'(z_{\min}) = 0$ and thus $z_{\min} = \delta_2$, where δ_2 denotes the unique minimiser of J_2. In Proposition 3.2, we showed that $\gamma > \delta_2$, where γ is the unique minimiser of J_{CB}. By the definition of Φ_-, it holds $\Phi_-(z) \le J_{CB}(z)$, and by assumption we have $\inf_{z\in\mathbb{R}}\Phi_-(z) = \Phi_-(\delta_2) = J_{CB}(\delta_2)$. Hence,

$$\Phi_-(\gamma) \le J_{CB}(\gamma) < J_{CB}(\delta_2) = \Phi_-(\delta_2) = \inf_{z\in\mathbb{R}}\Phi_-(z) \le \Phi_-(\gamma),$$

which is a contradiction. Hence, the Lennard-Jones potentials do not satisfy the assumptions on Φ_- in the case $K = 3$. This argument can be adapted for all $K > 2$.

To end this section, we give a similar result as Theorem 3.34 for the case of periodic boundary conditions. This was obtained in [56]. Here, we present the theorem without a proof. We set

$$\mathcal{A}_n(\mathbb{R}) := \big\{u \in C(\mathbb{R}) : u \text{ is affine on } (i, i+1)\lambda_n \text{ for all } i \in \mathbb{Z}\big\}.$$

Let us define the functional $E_n^{\#,\delta} : \mathcal{A}_n(\mathbb{R}) \to [0, +\infty]$ by

$$E_n^{\#,\delta}(v) = \begin{cases} \displaystyle\sum_{j=1}^{K}\sum_{i=0}^{n-1}J_j\left(\gamma + \frac{v^{i+j}-v^i}{j\sqrt{\lambda_n}}\right) - nJ_{CB}(\gamma) & \text{if } v \in \mathcal{A}_n^{\#,\delta}(0,1) \text{ and } v(0) = 0,\\ +\infty & \text{otherwise,}\end{cases}$$

where $\mathcal{A}_n^{\#,\delta}(0,1) = \{v \in \mathcal{A}_n(\mathbb{R}) : x \mapsto v(x) - \delta x \text{ is 1-periodic}\}$. Note that $v \in \mathcal{A}_n^{\#,\delta}(0,1)$ implies that $v(1) = \delta$. Adapting the arguments of Lemma 3.33 and Theorem 3.34, it is possible to show the following Γ-convergence result for the sequence (E_n^{δ}); see [56, Theorem 4.2] for a complete proof.

Theorem 3.37. *Let the hypotheses (LJ1)–(LJ7) be satisfied. Let $\delta > 0$. Then the sequence $(E_n^{\#,\delta})$ Γ-converges with respect to L^1_{loc}-topology to the functional $E^{\#,\delta}$ defined on piecewise-H^1 functions satisfying $v - \delta x$ is 1-periodic, $v(0+) \geq 0$ and $v(1-) \leq \delta$, by*

$$E^{\#,\delta}(v) = \begin{cases} \alpha \int_0^1 |v'|^2 dx + B_{IJ}\#(S_v \cap [0,1)) & \text{if } [v] > 0 \text{ on } S_v, \\ +\infty & \text{otherwise,} \end{cases}$$

where $\alpha = \frac{1}{2} J''_{CB}(\gamma)$ and B_{IJ} is defined as in (3.75).

3.6 Equivalence by Γ-convergence

In the last section, we have shown that the sequence $(E_n^{\delta_n})$ defined in (3.131) Γ-converges to a one-dimensional version of Griffith's model for fracture. In this section, we come back to our original discrete energy H_n^ℓ and link it to a nonlinear model for fracture. To this end, we use the notion of *equivalence* by Γ-convergence due to Braides and Truskinovsky, see [20]. Scardia, Schlömerkemper and Zanini [51] consider a sequence of functionals which allow for homogeneous elastic deformations or fractured deformations only, i.e. $u(x) = \ell x$ for all $x \in [0,1]$ or $u \in SBV_c^\ell(0,1)$ (see (3.47)), and show that this sequence is *uniformly* Γ*-equivalent* at first order to the discrete model H_n^ℓ in the case $K = 2$ (see Remark 3.41 (b)). Here, we study functionals which are more flexible with respect to the allowed deformations and have the same Γ-development up to the first order as the discrete energy for a particular choice of $u_0^{(1)}, u_1^{(1)}$ in the boundary conditions (3.3). Next, we recall the definition of Γ-equivalence as it is stated in [11].

Definition 3.38. [11, Definition 6.1] Let $\mathcal{L}$ be a set of parameters. For $\ell \in \mathcal{L}$ let (F_n^ℓ) and (G_n^ℓ) be sequences of functionals. We say that $(F_n^\ell)_n$ and $(G_n^\ell)_n$ are Γ-equivalent up to the first order if

$$\text{(i)} \quad \text{for all } \ell \in \mathcal{L} \quad \Gamma\text{-}\lim_{n\to\infty} F_n^\ell = \Gamma\text{-}\lim_{n\to\infty} G_n^\ell =: F_0^\ell,$$

$$\text{(ii)} \quad \text{for all } \ell \in \mathcal{L} \quad \Gamma\text{-}\lim_{n\to\infty} \frac{F_n^\ell - \min F_0^\ell(u)}{\lambda_n} = \Gamma\text{-}\lim_{n\to\infty} \frac{G_n^\ell - \min F_0^\ell(u)}{\lambda_n}.$$

Let $J_1, \dots, J_K$ satisfy the hypotheses (LJ1)–(LJ7). We define $G_n^\ell : L^1(0,1) \to \mathbb{R} \cup \{+\infty\}$ by

$$G_n^\ell(u) := \begin{cases} \int_0^1 W(u')dx + \lambda_n \left(B_{IJ}\#(S_u \cap [0,1]) + r(\ell)\right) & \text{if } u \in \mathcal{A}^\ell(0,1), \\ +\infty & \text{otherwise,} \end{cases} \tag{3.186}$$

where the elastic energy density W is given by

$$W(z) := \begin{cases} J_{CB}(z) & \text{if } z \leq \gamma, \\ J_{CB}(\gamma) + \frac{1}{2}J''_{CB}(\gamma)(z-\gamma)^2 & \text{if } z \geq \gamma, \end{cases} \tag{3.187}$$

the jump energy B_{IJ} is given in (3.75), the set of admissible functions $\mathcal{A}^\ell(0,1)$ is defined by

$$\mathcal{A}^\ell(0,1) := \{u \in SBV^\ell(0,1) : \ u' > 0 \text{ in } (0,1), \, [u] \geq 0 \text{ in } [0,1], \, \#S_u < +\infty\}, \tag{3.188}$$

and the term $r(\ell)$ denotes

$$r(\ell) := -\sum_{j=2}^{K}(j-1)J_j(\min\{\ell,\gamma\}). \tag{3.189}$$

We prove the following equivalence result.

Proposition 3.39. *Let $J_1, \dots, J_K$ satisfy the hypotheses (LJ1)–(LJ7) and*

$$\lim_{z\to 0+} J_j(z) = +\infty \quad \textit{and} \quad J_j(z) = +\infty \textit{ if } z \leq 0, \tag{3.190}$$

for all $j \in \{1,\dots,K\}$. Let $\ell > 0$ and let $u_0^{(1)}, u_1^{(1)} \in \mathbb{R}_+^{K-1}$ given by $u_{0,s}^{(1)} = u_{1,s}^{(1)} = \min\{\ell,\gamma\}$ for $1 \leq s < K$. The sequences (H_n^ℓ) and (G_n^ℓ), defined in (3.4) and (3.186) are Γ-equivalent up to the first order with respect to $L^1(0,1)$-convergence.

Proof. Zero-order equivalence. By Theorem 3.7, we have to show that (G_n^ℓ) Γ-converges with respect to the $L^1(0,1)$-topology to the functional H^ℓ (see (3.26)), that is

$$G^\ell(u) := \Gamma\text{-}\lim_{n\to\infty} G_n^\ell(u) = H^\ell(u) = \begin{cases} \displaystyle\int_0^1 J_{CB}^{**}(u')dx & \text{if } u \in BV^\ell(0,1), \, D^s u \geq 0 \text{ in } [0,1], \\ +\infty & \text{else on } L^1(0,1). \end{cases}$$

Let $(u_n) \subset L^1(0,1)$ be such that $\sup_n G_n^\ell(u_n) < +\infty$. From the monotonicity of u_n and $u_n \in SBV^\ell(0,1)$, we deduce that $|Du_n|([0,1]) = Du_n([0,1]) = \ell$ and $\|u_n\|_{L^\infty(0,1)} \leq u_n(1+) = \ell$. Hence, $\|u_n\|_{BV(0,1)} \leq 2\ell$. This yields the existence of a subsequence $(u_{n_k})_k$ which weakly* converges in $BV(0,1)$ to some $u \in BV(0,1)$. Moreover, we obtain that $u \in BV^\ell(0,1)$, see Theorem 3.7.

Let $u_n \to u$ in $L^1(0,1)$ with $\sup_n G_n^\ell(u_n) < +\infty$. Since $B_{IJ} > 0$ and $r(\ell) \in \mathbb{R}$ independent of n, we have that

$$\liminf_{n\to\infty} G_n^\ell(u_n) \geq \liminf_{n\to\infty} H^\ell(u_n) \geq H^\ell(u).$$

Indeed, we have used for the first inequality that $W \geq J_{CB}^{**}$, $u_n \in SBV^\ell(0,1)$ and $D^s u_n \geq 0$ in $[0,1]$. The second inequality follows by the lower semicontinuity of H^ℓ.

Let us now show the limsup inequality. Fix $u \in L^1(0,1)$. The pointwise limit of $G_n^\ell(u)$ is given by

$$G_p^\ell(u) := \lim_{n\to\infty} G_n^\ell(u) = \begin{cases} \int_0^1 W(u'(x))dx & \text{if } u \in \mathcal{A}^\ell(0,1), \\ +\infty & \text{else.} \end{cases}$$

Note that we used here $\#S_u < +\infty$. Hence, $\Gamma\text{-}\limsup_n G_n^\ell(u) \le \overline{G_p^\ell}(u)$, where $\overline{G_p^\ell}$ denotes the lower semicontinuous envelope of G_p^ℓ with respect to the $L^1(0,1)$-topology. Indeed, the Γ-$\limsup$ is always smaller than the pointwise limit, see [24, Proposition 5.1], and is lower semicontinuous. Hence, it is left to show that $\overline{G_p^\ell} \le H^\ell$.

Fix $u \in \mathcal{A}^\ell(0,1)$ such that $H^\ell(u) < +\infty$. We can decompose u as $u = v + w$, where $v \in W^{1,1}(0,1)$ and w is a jump function. For given $N \in \mathbb{N}$, we set $t_i = \frac{i}{N}$. We define v_N such that $v_N(t_i) = v(t_i)$ and

$$v_N'(x) = \left(\fint_{t_i}^{t_{i+1}} v'(t)dt \right) \wedge \gamma$$

for $x \in (t_i, t_{i+1})$. Clearly, we have $v_N \to v$ in $L^1(0,1)$. Let us define $(u_N) \subset L^1(0,1)$ by $u_N := v_N + w$. Then we have $u_N \in \mathcal{A}^\ell(0,1)$ for all $N \in \mathbb{N}$ and $u_N \to v + w = u$ in $L^1(0,1)$. By the convexity of J_{CB}^{**}, $J_{CB}^{**}(z) = W(z)$ for $z \le \gamma$ and $J_{CB}^{**}(z) = W(\gamma)$ for $z \ge \gamma$, we have that

$$\begin{aligned} H^\ell(u) &= \int_0^1 J_{CB}^{**}(u'(x))dx = \sum_{i=1}^N \int_{t_{i-1}}^{t_i} J_{CB}^{**}(u'(x))dx \ge \sum_{i=1}^N \frac{1}{N} J_{CB}^{**} \left(\fint_{t_{i-1}}^{t_i} u'(t)dt \right) \\ &= \sum_{i=1}^N \frac{1}{N} W \left(\fint_{t_{i-1}}^{t_i} u'(t)dt \wedge \gamma \right) = \int_0^1 W(u_N'(x))dx = G_p^\ell(u_N). \end{aligned}$$

The limit $N \to \infty$ yields $\overline{G_p^\ell}(u) \le \liminf_{N\to\infty} G_p^\ell(u_N) \le H^\ell(u)$ and thus that $\overline{G_p^\ell}(u) \le H^\ell(u)$ for all $u \in \mathcal{A}^\ell(0,1)$. Let us now consider a general $u \in BV^\ell(0,1)$ satisfying $H^\ell(u) < +\infty$. We decompose the distributional derivative Du as $Du = u'\mathcal{L}^1 + D^s u$. As above, we set $t_i = \frac{i}{N}$ for given $N \in \mathbb{N}$. We define a jump function $w_N \in L^1(0,1)$ as

$$w_N(x) = \begin{cases} 0 & \text{if } x \in [0, t_1), \\ D^s u([0, t_{i-1}) & \text{if } x \in [t_{i-1}, t_i) \text{ for } i \in \{1, \dots, N\}, \\ D^s u([0,1]) & \text{if } x = 1. \end{cases}$$

We set $u_N = v + w_N$, with $v(x) = \int_0^x u'(t)dt$. The definition of u_N yields $u_N' \equiv u'$, $\#S_{u_N} \le N$ and $[u_N] \ge 0$ (using $D^s u \ge 0$). Hence, $u_N \in \mathcal{A}^\ell(0,1)$. Moreover, it holds that $w := u - v$ satisfies $w \in BV(0,1)$ and $w' \equiv 0$. Since, w_N is the piecewise constant interpolation of (a representative of) w, we have that $w_N \to w$ in $L^1(0,1)$ and thus

$u_N \to u$ in $L^1(0,1)$. Furthermore, it holds

$$H^\ell(u) = \int_0^1 J_{CB}^{**}(u')dx = \int_0^1 J_{CB}^{**}(u_N')dx \geq \overline{G_p^\ell}(u_N).$$

By letting $N \to \infty$, we obtain $\overline{G_p^\ell}(u) \leq \liminf_{N\to\infty} \overline{G_p^\ell}(u_N) \leq H^\ell(u)$. Altogether, we have $\overline{G_p^\ell}(u) \leq H^\ell(u)$ for all $u \in L^1(0,1)$, which proves the limsup inequality.

First-order equivalence. We define the functional $G_{1,n}^\ell : L^1(0,1) \to \mathbb{R} \cup \{+\infty\}$ as

$$\begin{aligned} G_{1,n}^\ell(u) :=& \frac{G_n^\ell(u) - J_{CB}^{**}(\ell)}{\lambda_n} \\ =& \begin{cases} \frac{1}{\lambda_n}\displaystyle\int_0^1 W(u'(x)) - J_{CB}^{**}(\ell)dx + B_{IJ}\#(S_u \cap [0,1]) + r(\ell) & \text{if } u \in \mathcal{A}^\ell(0,1), \\ +\infty & \text{else,} \end{cases} \end{aligned} \tag{3.191}$$

where $r(\ell)$ is defined in (3.189). For given $0 < \ell \leq \gamma$, we have to show that

$$G_1^\ell(u) := \Gamma\text{-}\lim_{n\to\infty} G_{1,n}^\ell(u) = H_1^\ell(u) = \begin{cases} r(\ell) & \text{if } u(x) = \ell x, \\ +\infty & \text{else,} \end{cases} \tag{3.192}$$

see Corollary 3.14 and (3.189). For $\ell > \gamma$, we have to prove that

$$G_1^\ell(u) := \Gamma\text{-}\lim_{n\to\infty} G_{1,n}^\ell(u) = H_1^\ell(u) = \begin{cases} B_{IJ}\#(S_u \cap [0,1]) + r(\gamma) & \text{if } u \in SBV_c^\ell(0,1), \\ +\infty & \text{else,} \end{cases} \tag{3.193}$$

where the set $SBV_c^\ell(0,1)$ is defined in (3.47), see Theorem 3.19 and Remark 3.25.

Compactness. Let $(u_n) \subset L^1(0,1)$ be such that $\sup_n G_{1,n}^\ell(u_n) < +\infty$. As in the proof of the zero-order equivalence, we deduce from the boundary conditions and the monotonicity of u_n that there exist $u \in BV^\ell(0,1)$ and a subsequence, not relabelled, such that $u_n \overset{*}{\rightharpoonup} u$ in $BV(0,1)$. Moreover, we have

$$\begin{aligned} G_{1,n}^\ell(u_n) =& \frac{1}{\lambda_n}\int_0^1 W(u_n'(x)) - J_{CB}^{**}(\ell) - (J_{CB}^{**})'(\ell)(u_n' - \ell)dx + B_{IJ}\#(S_u \cap [0,1]) + r(\ell) \\ &+ \frac{1}{\lambda_n}\int_0^1 (J_{CB}^{**})'(\ell)(u_n'(x) - \ell)dx. \end{aligned} \tag{3.194}$$

Next, we show that both integral terms in (3.194) are non-negative. Set

$$W_\ell(z) := W(z) - J_{CB}^{**}(\ell) - (J_{CB}^{**})'(\ell)(z - \ell). \tag{3.195}$$

Note that $W_\ell \geq 0$ and $W_\ell(z) = 0$ if and only if $z = \min\{\ell, \gamma\}$. Indeed, if $\ell \geq \gamma$ this follows by $(J_{CB}^{**})'(\ell) = 0$, $\{\gamma\} = \arg\min_z W(z)$ and $W(\gamma) = J_{CB}(\gamma)$, see (3.187). Let us consider $0 < \ell < \gamma$. From $W(z) = J_{CB}^{**}(z) = J_{CB}(z)$ for $z \leq \gamma$, we deduce that

$W_\ell(z) = W(z) - W(\ell) - W'(\ell)(z-\ell)$ and the claim follows by the strict convexity of W. Hence, the first integral in (3.194) is non-negative. Let us show that also the second integral is non-negative. For $\ell \geq \gamma$ this follows by $(J_{CB}^{**})'(\ell) = 0$. Consider $0 < \ell < \gamma$. Since $u_n \in \mathcal{A}^\ell(0,1)$, it holds

$$\ell = Du_n([0,1]) = \int_0^1 u_n' dx + D^s u_n([0,1]) \quad \text{and} \quad D^s u_n([0,1]) \geq 0.$$

Thus, using $(J_{CB}^{**})'(\ell) \leq 0$ yields

$$\frac{1}{\lambda_n}\int_0^1 (J_{CB}^{**})'(\ell)(u_n'(x)-\ell)dx = -\frac{1}{\lambda_n}(J_{CB}^{**})'(\ell) D^s u_n([0,1]) \geq 0. \tag{3.196}$$

From (3.194), $B_{IJ} > 0$ and (3.196), we obtain that

$$+\infty > \sup_n G_{1,n}^\ell(u_n) \geq G_{1,n}^\ell(u_n) \geq \frac{1}{\lambda_n}\int_0^1 W_\ell(u_n'(x))dx + r(\ell).$$

Since $W_\ell \geq 0$ and $W_\ell(z) = 0$ if and only if $z = \min\{\ell,\gamma\}$, we deduce that $u_n' \to \min\{\ell,\gamma\}$ in measure in $(0,1)$. Moreover, we deduce from (3.194), $B_{IJ} > 0$, and $\sup_n G_{1,n}^\ell(u_n) < +\infty$ that there exists a constant $C > 0$ such that

$$C \geq \frac{1}{\lambda_n}\int_0^1 W_\ell(u_n')dx + \#(S_u \cap [0,1]). \tag{3.197}$$

The definition of W yields $\lim_{z\to\pm\infty}|z|^{-1}W_\ell(z) = +\infty$. Hence, we deduce from $u_n \overset{*}{\rightharpoonup} u$ in $BV(0,1)$, (3.197) and Theorem 2.8 that $u \in SBV^\ell(0,1)$. Moreover, it holds $u_n' \rightharpoonup u'$ in $L^1(0,1)$, $D^j u_n \overset{*}{\rightharpoonup} D^j u$ weakly* in the sense of measures and $+\infty > \liminf_n \#S_{u_n} \geq \#S_u$. As in Proposition 3.9, we deduce $u' = \min\{\ell,\gamma\}$ a.e., $u_n' \to u'$ in $L^1(0,1)$ and $[u] \geq 0$. Altogether, we have in the case $0 < \ell \leq \gamma$ that $u(x) = \ell x$ a.e. in $(0,1)$ and for $\ell > \gamma$ that $u \in SBV_c^\ell(0,1)$, see (3.47).

Liminf inequality. Fix $0 < \ell \leq \gamma$. Let (u_n) be a sequence of functions such that $\sup_n G_{1,n}^\ell(u_n) < +\infty$ and $u_n \to u$ in $L^1(0,1)$. The above compactness considerations yield that $u(x) = \ell x$ a.e. in $(0,1)$. By using the convexity of W and $B_{IJ} > 0$, we obtain that

$$G_n^\ell(u_n) \geq \frac{1}{\lambda_n}\left(W\left(\int_0^1 u_n'(x)dx\right) - J_{CB}(\ell)\right) + r(\ell) \geq r(\ell) = H_1^\ell(u).$$

For the last inequality, we used that $J_{CB} \equiv W$ on $(0,\gamma]$ and W decreasing on $(0,\gamma]$, see (3.187). Furthermore, we used $\ell = \int_0^1 u_n' dx + D^j u_n([0,1])$ and $D^j u_n([0,1]) \geq 0$. By passing with n to $+\infty$, we obtain the liminf inequality in this case.

Let $\ell > \gamma$. Let $u \in L^1(0,1)$ and $(u_n) \subset SBV^\ell(0,1)$ be such that $\sup_n G_{1,n}^\ell(u_n) < +\infty$ and $u_n \to u$ in $L^1(0,1)$. By the compactness result it holds $u \in SBV_c^\ell(0,1)$ and $D^j u_n \overset{*}{\rightharpoonup} D^j u$ weakly* in the sense of measures. Set $S_u = \{s^1,\dots,s^k\} \subset [0,1]$. The weak* convergence of $D^j u_n$ to $D^j u$ yields that there exists for every s^i a sequence (s_n^i) with

$s_n^i \in S_{u_n}$ and $s_n^i \to s^i$. From $W(z) \geq J_{CB}(\gamma)$ for all $z \in \mathbb{R}$, $B_{IJ} > 0$ and the continuity of $r(z)$, we deduce that

$$\liminf_{n\to\infty} G_{1,n}^{\ell}(u_n) \geq r(\ell) + \liminf_{n\to\infty} B_{IJ}\#(S_{u_n} \cap [0,1]) \geq r(\gamma) + B_{IJ}\#(S_u \cap [0,1]),$$

which proves the assertion.

Limsup inequality. This follows for $0 < \ell$ by taking $u_n = u$ for all $n \in \mathbb{N}$. □

Let us now show that the continuum energy G_n^ℓ captures the behaviour of the discrete energy H_n^ℓ also in the vicinity of $\ell = \gamma$. For this, we consider the behaviour of $(G_n^{\ell_n})$ for some sequence $(\ell_n) \subset \mathbb{R}$ with $\ell_n \to \gamma$ as $n \to \infty$. More precisely, we assume that $\ell_n \geq \gamma$ for all $n \in \mathbb{N}$ and that the following limit exists

$$\delta_n := \frac{\ell_n - \gamma}{\sqrt{\lambda_n}} \to \delta \geq 0 \quad \text{as } n \to \infty. \tag{3.198}$$

For $u \in \mathcal{A}^{\ell_n}(0,1)$, we define $v := \frac{u-u_\gamma}{\sqrt{\lambda_n}}$, where $u_\gamma(x) := \gamma x$ for all $x \in [0,1]$. The definition of the function v implies that $v(0-) = 0$, $v(1+) = \frac{\ell_n - \gamma}{\sqrt{\lambda_n}} = \delta_n$, $S_v = S_u$ and $[v] \geq 0$ in $[0,1]$. Hence, $v \in \hat{\mathcal{A}}^{\delta_n}(0,1)$, where for $\delta \in \mathbb{R}$ the set $\hat{\mathcal{A}}^\delta(0,1)$ is defined by

$$\hat{\mathcal{A}}^\delta(0,1) := \{v \in SBV^\delta(0,1) : \ [v] \geq 0 \text{ in } [0,1], \#S_v < +\infty\}. \tag{3.199}$$

As in the discrete model, we can express the energy $G_{1,n}^{\ell_n}(u)$ (see (3.191)) with $u = u_\gamma + \sqrt{\lambda_n} v$ in terms of the displacement v by $F_n^{\delta_n}(v) = G_{1,n}^{\ell_n}(u)$, where the functional $F_n^{\delta_n} : L^1(0,1) \to (-\infty, +\infty]$ is given by

$$F_n^{\delta_n}(v) := \begin{cases} F_n(v) & \text{if } v \in \hat{\mathcal{A}}^{\delta_n}(0,1), \\ +\infty & \text{else,} \end{cases} \tag{3.200}$$

where F_n is defined by

$$F_n(v) := \frac{1}{\lambda_n} \int_0^1 W\left(\gamma + \sqrt{\lambda_n} v'\right) - J_{CB}(\gamma) dx + B_{IJ}\#(S_v \cap [0,1]) + r(\gamma).$$

Note that we used that $\ell_n \geq \gamma$ by assumption, which yields $J_{CB}^{**}(\ell_n) = J_{CB}(\gamma)$ and $r(\ell_n) = r(\gamma)$, see (3.18) and (3.189).

Proposition 3.40. *Let $J_1, \ldots, J_k$ and $u_0^{(1)}, u_1^{(1)} \in \mathbb{R}_+^{K-1}$ satisfy the same assumptions as in Proposition 3.39. Let $\delta_n \to \delta$ be such that* (3.198) *is satisfied. Then the sequences $(E_n^{\delta_n})$ and $(F_n^{\delta_n})$, defined in* (3.131) *and* (3.200) *are Γ-equivalent with respect to the $L^1(0,1)$-convergence.*

Proof. Thanks to Theorem 3.34 and the same considerations as in Remark 3.25, we have to show that

$$\Gamma\text{-}\lim_{n\to\infty} F_n^{\delta_n}(v) = E^\delta(v) = \begin{cases} \alpha \int_0^1 |v'|^2 dx + B_{IJ}\#(S_v \cap [0,1]) + r(\gamma) & \text{if } v \in SBV_e^\delta(0,1) \\ +\infty & \text{else,} \end{cases} \tag{3.201}$$

where $SBV_e^\delta(0,1)$ is defined in (3.150) and $\alpha := \frac{1}{2} J''_{CB}(\gamma)$.

Compactness. Let $(v_n) \subset L^1(0,1)$ be such that $\sup_n F_n^{\delta_n}(v_n) < +\infty$. From the definition of W, see (3.187), we obtain $\min W = W(\gamma) = J_{CB}(\gamma)$, $W'(\gamma) = 0$ and $W''(\gamma) > 0$. Using (3.190), we deduce that there exists a constant $c > 0$ such that $W(\gamma + z) - J_{CB}(\gamma) \geq cz^2$. Hence, we have

$$\begin{aligned} F_n^{\delta_n}(v_n) =& \frac{1}{\lambda_n} \int_0^1 W(\gamma + \sqrt{\lambda_n} v_n') - J_{CB}(\gamma) dx + B_{IJ}\#(S_v \cap [0,1]) + r(\gamma) \\ \geq& c \int_0^1 |v_n'|^2 dx + B_{IJ}\#(S_v \cap [0,1]) + r(\gamma). \end{aligned} \tag{3.202}$$

From $v_n \in \hat{\mathcal{A}}^{\delta_n}(0,1)$, we deduce

$$0 \leq |D^j v_n|([0,1]) = D^j v_n([0,1]) = \delta_n - \int_0^1 v_n'(x) dx \leq \delta_n + \|v_n'\|_{L^1(0,1)}.$$

From $\delta_n \to \delta$ and (3.202), we obtain that the right-hand side is bounded independently of n. Hence, $\sup_n |Dv_n|([0,1]) < +\infty$ and by the boundary conditions, we obtain that $\sup_n \|v_n\|_{L^\infty(0,1)} < +\infty$. Altogether, we have using $c, B_{IJ} > 0$ that there exists $C > 0$ such that

$$C \geq \int_0^1 |v_n'|^2 dx + \#S_{v_n} + \|v_n\|_{L^\infty(0,1)}$$

for all $n \in \mathbb{N}$. From this, we deduce, as in the discrete setting (see Lemma 3.33), that there exist a subsequence (v_{n_k}) and $v \in SBV_e^\delta(0,1)$ (see (3.150)) such that $v_{n_k} \to v$ in $L^1(0,1)$, $v_{n_k}' \rightharpoonup v'$ in $L^2(0,1)$ and $D^j v_{n_k} \overset{*}{\rightharpoonup} D^j v$ weakly* in the sense of measures.

Liminf inequality. Let $v_n \subset SBV(0,1)$, $v \in L^1(0,1)$ such that $v_n \to v$ in $L^1(0,1)$ and $\sup_n F_n^{\delta_n}(v_n) < +\infty$. By the above compactness result, we have $v \in SBV_e^\delta$ and we can assume that $v_n' \rightharpoonup v'$ in $L^2(0,1)$ and $D^j v_n \overset{*}{\rightharpoonup} D^j v$ weakly* in the sense of measures.
The estimate for the jumps can be done exactly as in the proof of Proposition 3.39. We only estimate the elastic part of the energy. This can be done in a similar fashion as for the discrete energy $E_n^{\delta_n}$, see Theorem 3.34. A Taylor expansion of W at γ yields $W(\gamma + z) - J_{CB}(\gamma) = \alpha z^2 + \eta(z)$ with $\lim_{z\to 0} \frac{\eta(z)}{|z|^2} = 0$. Defining $\omega(t) := \sup_{|z|\leq t} |\eta(z)|$, we have

$$W(\gamma + \sqrt{\lambda_n} z) - J_{CB}(\gamma) \geq \lambda_n \alpha z^2 - \omega(|\sqrt{\lambda_n} z|). \tag{3.203}$$

We define 'good' sets:

$$I_n = \left\{ x \in (0,1) : \ |v_n(x)| \leq \lambda_n^{-\frac{1}{4}} \right\}.$$

Since $\|v_n'\|_{L^2(0,1)}$ is equibounded, we have that the indicator functions $\chi_n := \chi_{I_n}$ satisfy $\chi_n \to 1$ strongly in $L^2(0,1)$. Hence, $\chi_n v_n' \rightharpoonup v'$ in $L^2(0,1)$. Moreover, we can Taylor expand W on the 'good' sets:

$$\forall x \in I_n : \quad \frac{1}{\lambda_n}\left(W(\gamma + \sqrt{\lambda_n} v_n'(x)) - J_{CB}(\gamma)\right) = \alpha v_n'(x)^2 + \frac{1}{\lambda_n}\eta(\sqrt{\lambda_n}|v_n'(x)|).$$

Hence, we obtain

$$\begin{aligned}
\liminf_{n\to\infty} F_n^{\delta_n}(v_n) \geq & \liminf_{n\to\infty}\left(\frac{1}{\lambda_n}\int_0^1 \chi_n(W(\gamma+\sqrt{\lambda_n}v_n') - J_{CB}(\gamma))dx\right) + B_{IJ}\#S_v + r(\gamma) \\
\geq & \liminf_{n\to\infty}\int_0^1 \chi_n\left(\alpha|v_n'|^2 - \frac{\omega(\sqrt{\lambda_n}v_n')}{\lambda_n}\right)dx + B_{IJ}\#S_v + r(\gamma) \\
\geq & \alpha\int_0^1 |v'|^2 dx + B_{IJ}\#S_v + r(\gamma) = E^\delta(v),
\end{aligned}$$

which completes the proof of the lim inf inequality. Note that we used in the last inequality that $\chi_n v_n' \rightharpoonup v'$ in $L^2(0,1)$ and that $\sqrt{\lambda_n}|v_n'| \leq \lambda_n^{\frac{1}{4}}$ if χ_n is non-zero and thus

$$\frac{\chi_n}{\lambda_n}\omega(\sqrt{\lambda_n}|v_n'|) = (v_n')^2 \cdot \chi_n \frac{\omega(\sqrt{\lambda_n}|v_n'|)}{\lambda_n|v_n'|^2} \to 0 \text{ in } L^1(0,1)$$

Indeed, the above quantify is a product of sequence which is equibounded in $L^1(0,1)$ and a sequence which converges to zero in $L^\infty(0,1)$ (using $\lim\limits_{z\to 0}\frac{\omega(z)}{z^2} = 0$ and $\sqrt{\lambda_n}|v_n'(x)| \leq \lambda_n^{\frac{1}{4}}$ if $\chi_n(x) \neq 0$).

Limsup inequality. To show the upper bound it is by density enough to consider functions $v \in SBV_e^\delta(0,1)$ such that $v \in C^2((0,1)\setminus S_v)$. Moreover, it is not restrictive to assume that there exists $\rho > 0$ such that $v' \equiv 0$ on $[0,\rho)\cup(1-\rho,1]$. We decompose v as $v = \tilde{v} + w$ where $\tilde{v} \in C^2(0,1)$ and w is a jump function, i.e. $\tilde{v}' \equiv v'$ and $w' \equiv 0$.

Let $(v_n) \subset L^1(0,1)$ be such that $v_n = v + z_n$, where $z_n(x) = (\delta_n - \delta)x$ for all $x \in \mathbb{R}$. From $v \in SBV_e^\delta$, we deduce that $v_n(1+) = v(1+) + \delta_n - \delta = \delta_n$ and $v_n \in \hat{A}^{\delta_n}$. By the definitions of v_n, we have $v_n = \tilde{v} + z_n + w$ where $\tilde{v}$ and w are as above. From $\tilde{v} \in C^2(0,1)$ and $v' \equiv 0$ on $[0,\rho)\cup(1-\rho,1]$, we deduce $\max\limits_{z\in[0,1]}|\tilde{v}'(z)| = c \in \mathbb{R}$. Taylor expansion yields

$$\begin{aligned}
&\limsup_{n\to\infty}\frac{1}{\lambda_n}\int_0^1 W(\gamma+\sqrt{\lambda_n}v_n') - J_{CB}(\gamma)dx \\
&= \limsup_{n\to\infty}\frac{1}{\lambda_n}\int_0^1 W\left(\gamma+\sqrt{\lambda_n}(\tilde{v}'+\delta_n-\delta)\right) - J_{CB}(\gamma)dx \\
&\leq \limsup_{n\to\infty}\frac{1}{\lambda_n}\int_0^1 \alpha\lambda_n(\tilde{v}'+\delta_n-\delta)^2 + \omega\left(|\sqrt{\lambda_n}(\tilde{v}'+\delta_n-\delta)|\right)dx \\
&\leq \alpha\int_0^1 \tilde{v}'(x)^2dx + \limsup_{n\to\infty}\left\{|\delta_n-\delta|\alpha\int_0^1(2|\tilde{v}'|+|\delta_n-\delta|)dx + \frac{\omega(\sqrt{\lambda_n}(c+|\delta_n-\delta|))}{\lambda_n}\right\} \\
&= \alpha\int_0^1 \tilde{v}'(x)^2dx,
\end{aligned}$$

where $\omega(z)$ is defined as in the proof of the lim inf inequality. Note that we used for the last equality that $\delta_n \to \delta$ and $\lim_{z\to 0} |z|^{-2}\omega(z) = 0$. Using $S_{v_n} = S_v$ for all $n \in \mathbb{N}$ and $\tilde{v}' = v'$, we obtain

$$\limsup_{n\to\infty} F_n^{\delta_n}(v_n) \leq \alpha \int_0^1 \tilde{v}'(x)^2 dx + B_{IJ}\#(S_v \cap [0,1]) + r(\gamma) = E^\delta(v),$$

see (3.201). This finishes the proof. □

Remark 3.41. We conclude this section with some general remarks on (G_n^ℓ) and possible generalisations.

(a) The map $\ell \mapsto \min_u G_n^\ell(u)$ is continuous in ℓ. For this, we show that

$$\min_u G_n^\ell(u) = \begin{cases} J_{CB}(\ell) + \lambda_n \sum_{j=2}^K (j-1)J_j(\ell) & \text{if } 0 < \ell \leq \gamma, \\ J_{CB}(\gamma) + \lambda_n \sum_{j=2}^K (j-1)J_j(\gamma) + \min\{\alpha(\ell-\gamma)^2, \lambda_n B_{IJ}\} & \text{if } \ell > \gamma, \end{cases}$$

where $\alpha = \frac{1}{2}J''_{CB}(\gamma)$. It is straightforward to see that this implies the continuity of $\ell \mapsto \min_u G_n^\ell(u)$.

Consider $u \in \mathcal{A}^\ell(0,1)$ such that $S_u = \emptyset$. By the convexity of W and $\int_0^1 u' dx = \ell$ (since $u \in SBV^\ell(0,1)$), we have

$$G_n^\ell(u) \geq W(\ell) + \lambda_n r(\ell),$$

and this lower bound is attained by $u(x) = \ell x$ for $x \in [0,1]$. For $u \in \mathcal{A}^\ell(0,1)$ such that $S_u \neq \emptyset$, we have that

$$G_n^\ell(u) \geq W(\ell - D^j u([0,1])) + \lambda_n B_{IJ} + \lambda_n r(\ell),$$

where we used the convexity of W, $\int_0^1 u' dx + D^j([0,1]) = \ell$ and $B_{IJ} > 0$. In the case $0 < \ell \leq \gamma$, we obtain, using $D^j u$ is a positive measure and W is decreasing on $(0,\gamma]$, that $\min_u G_n^\ell(u) = W(\ell) + \lambda_n r(\ell)$ which shows the assertion in this case. Since $W \geq W(\gamma)$, we have the following lower bound for functions $u \in \mathcal{A}^\ell(0,1)$ such that $S_u \neq \emptyset$:

$$G_n^\ell(u) \geq W(\gamma) + \lambda_n B_{IJ} + \lambda_n r(\ell),$$

and this lower bound is attained by $u(0) = 0$ and $u(x) = \gamma x + \ell - \gamma$ for $x \in (0,1]$ if $\ell > \gamma$. By the definition of W and r, this yields the assertion in the case $\ell > \gamma$.

(b) In [20], Braides and Truskinovsky introduced the notion of *uniform* Γ*-equivalence*, see [20, Definition 6.3]: Two sequences (H_n^ℓ) and (G_n^ℓ) are uniformly Γ-equivalent at order λ_n^q at $\ell_0 > 0$ if there exist translations m_n^ℓ such that for all $\ell_n \to \ell_0$ as $n \to \infty$ the following equation holds upon extraction of a subsequence

$$\Gamma\text{-}\lim_{n\to\infty} \frac{H_n^{\ell_n} - m_n^{\ell_n}}{\lambda_n^q} = \Gamma\text{-}\lim_{n\to\infty} \frac{G_n^{\ell_n} - m_n^{\ell_n}}{\lambda_n^q}$$

and these Γ-limit are non-trivial, see also [51]. Two sequences are *uniformly equivalent at order* λ_n^q if they are uniformly Γ-equivalent at order λ_n^q at ℓ_0 for all $\ell_0 > 0$. The uniform equivalence of (H_n^ℓ) and (G_n^ℓ) implies, under certain coercivity assumptions, that

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

see [20, Theorem 6.4]. A topic of future research is the question whether or not Proposition 3.39 can be generalised to uniform equivalence at order λ_n^q for $q \in \{0, 1\}$

(c) The $r(\ell)$-term in the energy G_n^ℓ is rather ad hoc and arises from the boundary layer energies $B(\theta, \ell)$ and $B_{BJ}(\theta)$ for the specific choice of $u_0^{(1)}$ and $u_1^{(1)}$ that we consider here. It is desirable to construct an equivalent continuum model with flexible boundary layer energies which depend on u' in a suitable sense; see [11, Theorem 6.2] for an example in an elastic setting. In particular this will be crucial if one includes external forces to the energy, see [35, Theorem 4.1].

Chapter 4

Analysis of a quasicontinuum method in one dimension

In this chapter, we present an analysis of a quasicontinuum method via Γ-convergence. We consider the discrete energy H_n^ℓ, see (3.4), as the fully atomistic model problem. From this, we derive a QC-approximation and perform a development by Γ-convergence. We study requirements on the QC-approximation which ensure that the minima and the minimiser of the first-order Γ-limits of the fully atomistic energy and the corresponding QC-approximation coincide.

4.1 Discrete model

Let us recall basic definitions and notations for the fully atomistic energy H_n^ℓ. For given $K \in \mathbb{N}$, the discrete energy $H_n : \mathcal{A}_n(0,1) \to \mathbb{R} \cup \{+\infty\}$, see (3.2), is defined by

$$H_n(u) = \sum_{j=1}^{K} \sum_{i=0}^{n-j} \lambda_n J_j \left(\frac{u^{i+j} - u^i}{j\lambda_n} \right),$$

where J_j, $j = 1, \dots, K$ are potentials of Lennard-Jones type and $\mathcal{A}_n(0,1)$ is defined in (3.1). Moreover, we impose boundary conditions: for given $\ell > 0$ and $u_0^{(1)},\ u_1^{(1)} \in \mathbb{R}_+^{K-1}$, we set

$$u^0 = 0,\ u^n = \ell,\ u^s - u^{s-1} = \lambda_n u_{0,s}^{(1)},\ u^{n+1-s} - u^{n-s} = \lambda_n u_{1,s}^{(1)}$$

for $1 \leq s < K$, see (3.3). The functional $H_n^\ell : L^1(0,1) \to (-\infty, +\infty]$ is defined by

$$H_n^\ell(u) = \begin{cases} H_n(u) & \text{if } u \in \mathcal{A}_n(0,1) \text{ satisfies (3.3)}, \\ +\infty & \text{else.} \end{cases}$$

The goal is to solve the minimisation problem

$$\min_{u \in \mathcal{A}_n(0,1)} H_n^\ell(u),$$

which we consider as our fully atomistic problem.

The idea of energy based quasicontinuum approximations is to replace the above minimisation problem by a simpler one of which minimisers and minimal energies are good approximations of the ones for H_n^ℓ. Typically this new problem is obtained in two steps:

(a) Define an energy where interactions beyond nearest neighbour interactions ('long range') are replaced by certain nearest neighbour interactions in some regions.

(b) Reduce the degree of freedom by choosing a smaller set of admissible functions.

To obtain (a), we follow Lin and Luskin [38, eq. (4.2)] and replace the jth ($j \geq 2$) nearest neighbour interactions by

$$J_j\left(\frac{u^{i+j}-u^i}{j\lambda_n}\right) = J_j\left(\frac{1}{j}\sum_{s=i}^{i+j-1}\frac{u^{s+1}-u^s}{\lambda_n}\right) \approx \frac{1}{j}\sum_{s=i}^{i+j-1} J_j\left(\frac{u^{s+1}-u^s}{\lambda_n}\right).$$

While this approximation turns out to be appropriate in the bulk, this is not the case close to surfaces, where boundary layers occur. This motivates us to construct a quasicontinuum model accordingly: for given $n \in \mathbb{N}$ let $k_n^1, k_n^2 \in \mathbb{N}$ with $0 < k_n^1 < k_n^2 < n-j$. For $k_n = (k_n^1, k_n^2)$, we define the energy $\hat{H}_n^{k_n}$ by using the above approximation of the jth interaction for $k_n^1 \leq i \leq k_n^2 - j$, (cf. Figure 4.1), and keeping the atomistic descriptions elsewhere,

$$\begin{aligned}\hat{H}_n^{k_n}(u) :=& \sum_{i=0}^{n-1}\lambda_n J_1\left(\frac{u^{i+1}-u^i}{\lambda_n}\right) + \sum_{j=2}^{K}\sum_{i=0}^{k_n^1-1}\lambda_n J_j\left(\frac{u^{i+j}-u^i}{j\lambda_n}\right) \\ &+ \sum_{j=2}^{K}\sum_{i=k_n^1}^{k_n^2-j}\frac{\lambda_n}{j}\sum_{s=i}^{i+j-1} J_j\left(\frac{u^{s+1}-u^s}{\lambda_n}\right) + \sum_{j=2}^{K}\sum_{i=k_n^2+1-j}^{n-j}\lambda_n J_j\left(\frac{u^{i+j}-u^i}{j\lambda_n}\right).\end{aligned}$$

Analogously to H_n^ℓ, we define the functional $\hat{H}_n^{\ell,k_n} : L^1(0,1) \to (-\infty, +\infty]$

$$\hat{H}_n^{\ell,k_n}(u) := \begin{cases}\hat{H}_n^{k_n}(u) & \text{if } u \in \mathcal{A}_n(0,1) \text{ satisfies (3.3)}, \\ +\infty & \text{else.}\end{cases}$$

For the following analysis it is useful to rewrite the energy $\hat{H}_n^{k_n}$ in various ways. For given $j \in \{1, \dots, K\}$, we define the sets

$$A(j) := \{0, \dots, k_n^1 - 1\} \cup \{k_n^2 - j + 1, \dots, n - j\}, \quad C(j) := \{k_n^1, \dots, k_n^2 - j\}. \tag{4.1}$$

The energy $\hat{H}_n^{k_n}(u)$ reads

$$\hat{H}_n^{k_n}(u) = \sum_{j=1}^{K}\lambda_n\left\{\sum_{i\in A(j)} J_j\left(\frac{u^{i+j}-u^i}{j\lambda_n}\right) + \frac{1}{j}\sum_{i\in C(j)}\sum_{s=i}^{i+j-1} J_j\left(\frac{u^{s+1}-u^s}{\lambda_n}\right)\right\}. \tag{4.2}$$

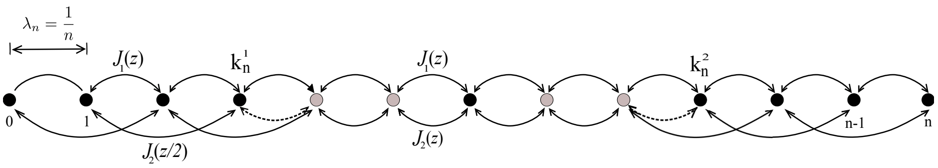

FIGURE 4.1: Illustration of the quasicontinuum approximation for $K = 2$. Here z denotes the scaled distance between the corresponding atoms in the deformed configuration and the two dotted lines stand for $\frac{1}{2}J_2(z)$. Moreover, the black balls symbolise the repatoms.

For $j \in \{2, \dots, K\}$, we can rewrite the terms in the sum over $i \in C(j)$ as follows:

$$\frac{1}{j}\sum_{i=k_n^1}^{k_n^2-j}\sum_{s=i}^{i+j-1} J_j\left(\frac{u^{s+1}-u^s}{\lambda_n}\right) = \sum_{i=k_n^1+j-1}^{k_n^2-j} J_j\left(\frac{u^{i+1}-u^i}{\lambda_n}\right)$$
$$+\sum_{i=1}^{j-1}\frac{i}{j}\left\{J_j\left(\frac{u^{k_n^1+i}-u^{k_n^1+i-1}}{\lambda_n}\right)+J_j\left(\frac{u^{k_n^2-i+1}-u^{k_n^2-i}}{\lambda_n}\right)\right\}.$$

Thus, we can rewrite the energy $\hat{H}_n^{k_n}(u)$ as

$$\hat{H}_n^{k_n}(u) = \sum_{i=k_n^1+K-1}^{k_n^2-K}\lambda_n J_{CB}\left(\frac{u^{i+1}-u^i}{\lambda_n}\right)+\sum_{j=1}^{K}\sum_{i\in A(j)}\lambda_n J_j\left(\frac{u^{i+j}-u^i}{j\lambda_n}\right)$$
$$+\sum_{j=1}^{K}\sum_{s=1}^{K-1}\lambda_n\left(\frac{s}{j}\wedge 1\right)\left\{J_j\left(\frac{u^{k_n^1+s}-u^{k_n^1+s-1}}{\lambda_n}\right)+J_j\left(\frac{u^{k_n^2-s+1}-u^{k_n^2-s}}{\lambda_n}\right)\right\}, \tag{4.3}$$

where $J_{CB} := \sum_{j=1}^{K} J_j$ is defined as in (3.17).

To obtain (b) we consider, instead of the deformation of all atoms, just the deformation of a possibly much smaller set of so-called representative atoms (repatoms). We denote the set of repatoms by $\mathcal{T}_n = \{t_n^0, \dots, t_n^{r_n}\} \subset \{0, \dots, n\}$ with $0 = t_n^0 < t_n^1 < \cdots < t_n^{r_n} = n$ and define

$$\mathcal{A}_{\mathcal{T}_n}(0,1) := \left\{u : [0,1] \to \mathbb{R} : u \text{ is affine on } (t_n^i, t_n^{i+1})\lambda_n \text{ for } t_n^i,\ t_n^{i+1} \in \mathcal{T}_n\right\}. \tag{4.4}$$

Since we are interested in the energy $\hat{H}_n^{\ell,k_n}(u)$ for deformations $u \in \mathcal{A}_{\mathcal{T}_n}(0,1)$, we define $\hat{H}_n^{\ell,k_n,\mathcal{T}_n} : L^1(0,1) \to \mathbb{R} \cup \{+\infty\}$ by

$$\hat{H}_n^{\ell,k_n,\mathcal{T}_n}(u) := \begin{cases} \hat{H}_n^{\ell,k_n}(u) & \text{if } u \in \mathcal{A}_{\mathcal{T}_n}(0,1), \\ +\infty & \text{else on } L^1(0,1). \end{cases} \tag{4.5}$$

In the following sections, we study $\hat{H}_n^{\ell,k_n,\mathcal{T}_n}$ as n tends to infinity. Therefore, we will assume that $k_n = (k_n^1, k_n^2)$ is such that

$$(i)\ \lim_{n\to\infty} k_n^1 = \lim_{n\to\infty} n - k_n^2 = +\infty, \text{ and } \quad (ii)\ \lim_{n\to\infty} \lambda_n k_n^1 = \lim_{n\to\infty} \lambda_n(n-k_n^2) = 0. \quad (4.6)$$

Hence, in particular $\lim_{n\to\infty} \lambda_n k_n^2 = 1$. The above assumption corresponds to the case that the size of the atomistic region becomes unbounded on a microscopic scale (i), but shrinks to a point on a macroscopic scale (ii). While assumption (i) is crucial (see also Remark 4.6), the assumption (ii) can be easily replaced by $\lim_{n\to\infty} \lambda_n k_n^1 = \xi_1$, $\lim_{n\to\infty} \lambda_n(n-k_n^2) = 1-\xi_2$ and $0 \leq \xi_1 < \xi_2 \leq 1$. In this case the analysis is essentially the same, but in the case of fracture, see Theorem 4.11, one has to distinguish more cases. We assume (4.6) (ii) here because it is the canonical case from a conceptual point of view. Otherwise the atomistic region and continuum region would be on the same macroscopic scale.

4.2 Γ-limit of zeroth order

In this section, we derive the Γ-limit of the sequence $(\hat{H}_n^{\ell,k_n,\mathcal{T}_n})$ defined in (4.5). We show that $(\hat{H}_n^{\ell,k_n,\mathcal{T}_n})$ Γ-converges to the same functional H^ℓ as the fully atomistic energy (H_n^ℓ), see Theorem 3.7.

Theorem 4.1. *Suppose that (LJ1)–(LJ5) are satisfied. Let $\ell > 0$ and $u_0^{(1)}, u_1^{(1)} \in \mathbb{R}_+^{K-1}$. Let $k_n = (k_n^1, k_n^2)$ satisfy (4.6) and let $\mathcal{T}_n = \{t_n^0, \dots, t_n^{r_n}\}$ with $0 = t_n^0 < t_n^1 < \dots < t_n^{r_n} = n$ and $\{0, \dots, K-1\} \cup \{n-K+1, \dots, n\} \subset \mathcal{T}_n$ be such that*

$$\exists (p_n) \subset \mathbb{N} \text{ such that } \lim_{n\to\infty} \lambda_n p_n = 0 \text{ and } \sup\{t_n^{i+1} - t_n^i : t_n^{i+1}, t_n^i \in \mathcal{T}_n\} \leq p_n. \quad (4.7)$$

Then $(\hat{H}_n^{\ell,k_n,\mathcal{T}_n})$ defined in (4.5) Γ-converges with respect to the $L^1(0,1)$-topology to the functional H^ℓ defined in (3.26) by

$$H^\ell(u) = \begin{cases} \int_0^1 J_{CB}^{**}(u')dx & \text{if } u \in BV^\ell(0,1),\ D^s u \geq 0 \text{ in } [0,1], \\ +\infty & \text{else on } L^1(0,1). \end{cases}$$

Proof. Let (u_n) be a sequence of functions such that $\sup_n \hat{H}_n^{\ell,k_n,\mathcal{T}_n}(u_n) < +\infty$. The same arguments as in the compactness part of the proof of Theorem 3.7 yield the existence of a subsequence (u_{n_k}) and $u \in BV^\ell(0,1)$ such that $u_{n_k} \overset{*}{\rightharpoonup} u$ weakly* in $BV(0,1)$.

Liminf inequality. Similar arguments as in the proof of Theorem 3.7 yield that it is sufficient to consider sequences of function (u_n) such that $u_n \overset{*}{\rightharpoonup} u$ weakly* in $BV(0,1)$ for some function $u \in BV^\ell(0,1)$ in order to prove the liminf inequality.

The definition of $A(j)$, see (4.1), and assumption (4.6) imply that

$$\lim_{n\to\infty}\lambda_n \# A(j) = \lim_{n\to\infty}\lambda_n(k_n^1+n-k_n^2)=0.$$

Hence, we obtain from (4.3) and $J_j \geq J_j(\delta_j)$ that

$$\begin{aligned}\hat{H}_n^{\ell,k_n,\mathcal{T}_n}(u_n) &\geq \sum_{i=k_n^1+K-1}^{k_n^2-K}\lambda_n J_{CB}\left(\frac{u_n^{i+1}-u_n^i}{\lambda_n}\right)+\sum_{j=1}^{K}\lambda_n J_j(\delta_j)\left\{\#A(j)+\sum_{s=1}^{K-1}2\left(\frac{s}{j}\wedge 1\right)\right\}\\ &= \sum_{i=k_n^1+K-1}^{k_n^2-K}\lambda_n J_{CB}\left(\frac{u_n^{i+1}-u_n^i}{\lambda_n}\right)+o(1),\end{aligned}$$

as $n\to\infty$. For every $\rho>0$ there exists an $N\in\mathbb{N}$ such that $(\rho,1-\rho)\subset\lambda_n(k_n^1+K,k_n^2-K)$ if $n\geq N$. Since $J_{CB}^{**}\geq J_{CB}(\gamma)$ and $J_{CB}(\gamma)<0$ it holds

$$\begin{aligned}\liminf_{n\to\infty}\hat{H}_n^{\ell,k_n,\mathcal{T}_n}(u_n) &\geq \liminf_{n\to\infty}\sum_{i=k_n^1+K}^{k_n^2-K}\lambda_n J_{CB}^{**}\left(\frac{u_n^{i+1}-u_n^i}{\lambda_n}\right)\\ &\geq \liminf_{n\to\infty}\int_\rho^{1-\rho}J_{CB}^{**}(u_n')dx+2\rho J_{CB}(\gamma).\end{aligned}$$

From $(u_n)\subset W^{1,\infty}(0,1)$, $u_n \overset{*}{\rightharpoonup} u$ in $BV(\rho,1-\rho)$ and Proposition 2.15, we deduce

$$\liminf_{n\to\infty}\hat{H}_n^{\ell,k_n,\mathcal{T}_n}(u_n)\geq\int_\rho^{1-\rho}J_{CB}^{**}(u')dx+2\rho J_{CB}(\gamma),$$

if $D^s u\geq 0$ in $(\rho,1-\rho)$, and $+\infty$ else. The required lower bound follows by taking $\rho\to 0$ and using the same arguments as in Theorem 3.7 to obtain $D^s u\geq 0$ in $[0,1]$.

Limsup inequality. The limsup inequality can be proven in a similar way as for the fully atomistic energy H_n^ℓ, see Theorem 3.7. We define the functional $\hat{H}_n^{k_n,\mathcal{T}_n}: L^1(0,1)\to\mathbb{R}\cup\{+\infty\}$ by

$$\hat{H}_n^{k_n,\mathcal{T}_n}(u):=\begin{cases}\hat{H}_n^{k_n}(u) & \text{if } u\in\mathcal{A}_{\mathcal{T}_n}(0,1),\\ +\infty & \text{else.}\end{cases}$$

We claim that for every $u\in BV(0,1)$ with $D^s u\geq 0$ in $(0,1)$, there exists a sequence $(u_n)\subset L^1(0,1)$ such that $u_n\to u$ in $L^1(0,1)$ and

$$\limsup_{n\to\infty}\hat{H}_n^{k_n,\mathcal{T}_n}(u_n)\leq\int_0^1 J_{CB}^{**}(u')dx. \tag{4.8}$$

We show this only for linear functions. This can be adapted to piecewise affine functions and the claim follows by density and relaxation arguments, see Theorem 3.7.

Let us first consider linear functions u such that $u(x)=zx$ with $z\leq\gamma$. Since $J_{CB}(z)=J_{CB}^{**}(z)$ for $z\leq\gamma$ it follows that the constant sequence $u_n=u$ satisfies (4.8). Indeed,

$u \in \mathcal{A}_{\mathcal{T}_n}(0,1)$ and (4.2) yields

$$\hat{H}_n^{k_n,\mathcal{T}_n}(u) = \sum_{j=1}^{K} J_j(z) - \lambda_n \sum_{j=2}^{K}(j-1)J_j(z) = J_{CB}^{**}(z) + \mathcal{O}(\lambda_n)$$

as $n \to \infty$. Note that we used $\#(A(j) \cup C(j)) = n - j + 1$. Let us now consider linear functions u such that $u(x) = zx$ with $z > \gamma$. For every (p_n) satisfying (4.7), we find a sequence (q_n) of natural numbers such that

$$\lim_{n\to\infty} \lambda_n q_n = 0, \quad \lim_{n\to\infty} \frac{p_n}{q_n} = 0,$$

e.g. $q_n = \lfloor \sqrt{np_n} \rfloor$. We define for every $n \in \mathbb{N}$ a set $\mathcal{T}_n' = \{t_n^{h_n^0}, \dots, t_n^{h_n^{N_n}}\} \subset \mathcal{T}_n$, where $0 = h_n^0 < h_n^1 < \dots < h_n^{N_n} = r_n$ such that there exists $C_1, C_2 > 0$ which satisfy

$$C_1 q_n \le t_n^{h_n^{k+1}} - t_n^{h_n^k} \le C_2 q_n \text{ for all } k \in \{0, \dots, N_n - 1\}.$$

From $n = \sum_{k=0}^{N_n-1}(t_n^{h_n^{k+1}} - t_n^{h_n^k})$, we deduce that $C_1 N_n q_n \le n \le C_2 N_n q_n$, and thus $N_n q_n = \mathcal{O}(n)$. Let us now define $u_n \in \mathcal{A}_{\mathcal{T}_n}(0,1)$ such that $u_n(1) = z$ and

$$u_n(x) = z\lambda_n t_n^{h_n^k} + \gamma(x - \lambda_n t_n^{h_n^k}) \text{ for } x \in [t_n^{h_n^k}, t_n^{h_n^{k+1}} - 1]\lambda_n \text{ and } k \in \{0, \dots, N_n - 1\}.$$

By using $t_n^{h_n^k} - t_n^{h_n^k - 1} \le p_n$ for all $k \in \{1, \dots, N_n\}$ and $|u(x) - u_n(x)| \le 2z$, we obtain

$$\begin{aligned}
\int_0^1 |u(x) - u_n(x)|dx &= \sum_{k=0}^{N_n-1} \int_{\lambda_n t_n^{h_n^k}}^{\lambda_n t_n^{h_n^{k+1}-1}} \left| zx - z\lambda_n t_n^{h_n^k} - \gamma\left(x - \lambda_n t_n^{h_n^k}\right) \right| dx \\
&\quad + \sum_{k=1}^{N_n} \int_{\lambda_n t_n^{h_n^k - 1}}^{\lambda_n t_n^{h_n^k}} |u(x) - u_n(x)|dx \\
&\le \sum_{k=0}^{N_n-1} \int_{\lambda_n t_n^{h_n^k}}^{\lambda_n t_n^{h_n^{k+1}-1}} (z-\gamma)(x - \lambda_n t_n^{h_n^k})dx + 2zN_n\lambda_n p_n \\
&= \sum_{k=0}^{N_n-1} \frac{1}{2}(z-\gamma)\lambda_n^2 \left(t_n^{h_n^{k+1}-1} - t_n^{h_n^k}\right)^2 + 2zN_n\lambda_n p_n \\
&\le \frac{1}{2}(z-\gamma)N_n C_2^2 q_n^2 \lambda_n^2 + 2z\lambda_n p_n N_n
\end{aligned}$$

and thus $u_n \to u$ in $L^1(0,1)$. Indeed, by $\lambda_n N_n q_n = \mathcal{O}(1)$, $\lambda_n q_n \to 0$ and $\mathcal{O}(\lambda_n p_n N_n) = \mathcal{O}\left(\frac{p_n}{q_n}\right)$, the terms in the last line above tend to zero as $n \to \infty$. Let us now show that (u_n) indeed satisfies (4.8). By definition, we have $u_n^{i+1} - u_n^i = \lambda_n \gamma$ for $0 \le i \le n-1$ and

$i \notin \left(\mathbb{N} \cap \cup_{k=1}^{N_n}[t_n^{h_n^k-1}, t_n^{h_n^k})\right)$ and by using $\#\left(\mathbb{N} \cap \cup_{k=1}^{N_n}[t_n^{h_n^k-1}, t_n^{h_n^k})\right) \le N_n p_n$, we have

$$\hat{H}_n^{k_n,\mathcal{T}_n}(u_n) = \sum_{k=0}^{N_n-1} \sum_{i=t_n^{h_n^k}}^{t_n^{h_n^{k+1}-1}-j} \lambda_n J_j(\gamma) + \mathcal{O}(\lambda_n p_n N_n) = J_{CB}(\gamma) + \mathcal{O}(\lambda_n p_n N_n).$$

Since $\lambda_n p_n N_n \to 0$ as $n \to \infty$, we deduce (4.8) in this case.

For every $u \in BV^\ell$ such that $H^\ell(u) < +\infty$, we can combine the above results with the same procedure as in Theorem 3.7 to construct sequence (u_n) such that $u_n \in \mathcal{A}_{\mathcal{T}_n}(0,1)$ satisfies (3.3) and

$$\limsup_{n\to\infty} \hat{H}_n^{\ell,k_n,\mathcal{T}_n}(u_n) \le H^\ell(u),$$

which proves the lim sup inequality. □

Remark 4.2. To underline that the zero-order Γ-limit is too coarse to measure the quality of the quasicontinuum method, we remark that one can show that the sequence of functionals defined as

$$H_n^{\ell,CB}(u) := \begin{cases} \displaystyle\sum_{i=0}^{n-1} \lambda_n J_{CB}\left(\frac{u^{i+1}-u^i}{\lambda_n}\right) & \text{if } u \in \mathcal{A}_{\mathcal{T}_n}(0,1) \text{ satisfies (3.3)}, \\ +\infty & \text{else}, \end{cases}$$

Γ-converges to H^ℓ with respect to the $L^1(0,1)$-convergence under the same assumptions on $(\mathcal{T}_n)$ as in Theorem 4.1. Note that the functional $H_n^{\ell,CB}$ can be understood as a continuum approximation of H_n^ℓ.

4.3 Γ-limit of first order

In this section, we derive the first-order Γ-limit of $(\hat{H}_n^{\ell,k_n,\mathcal{T}_n})$, i.e. the Γ-limit of the sequence of functionals $(\hat{H}_{1,n}^{\ell,k_n,\mathcal{T}_n})$ defined by

$$\hat{H}_{1,n}^{\ell,k_n,\mathcal{T}_n}(u) = \frac{\hat{H}_n^{\ell,k_n,\mathcal{T}_n}(u) - \min_v H^\ell(v)}{\lambda_n}. \tag{4.9}$$

It will be useful to rearrange the terms in the expression of the energy $\hat{H}_{1,n}^{\ell,k_n,\mathcal{T}_n}$. Let $u \in \mathcal{A}_{\mathcal{T}_n}(0,1)$ be such that the boundary conditions (3.3) are satisfied. For $j \in \{2, \dots, K\}$, we can rewrite the nearest neighbour interactions as

$$\sum_{i=0}^{n-1} J_1\left(\frac{u^{i+1}-u^i}{\lambda_n}\right) = \sum_{i=0}^{n-j} \frac{1}{j} \sum_{s=i}^{i+j-1} J_1\left(\frac{u^{s+1}-u^s}{\lambda_n}\right) + \sum_{s=1}^{j-1} \frac{j-s}{j}\left(J_1(u_{0,s}^{(1)}) + J_1(u_{1,s}^{(1)})\right),$$

see (3.5). Hence, using $A(j)\cup C(j)=\{0,\dots,n-j\}$, $A(j)\cap C(j)=\emptyset$ for all $j\in\{1,\dots,K\}$, $\sum_{j=2}^K c_j=1$, and $\min H^\ell = J_{CB}^{**}(\ell)=\sum_{j=2}^K \psi_j^{**}(\ell)$, see (3.14) and (3.18), we obtain that

$$\begin{aligned}
\hat{H}_{1,n}^{\ell,k_n,\mathcal{T}_n}(u) =&\sum_{j=1}^K \left\{ \sum_{i\in A(j)} J_j\left(\frac{u^{i+j}-u^i}{j\lambda_n}\right) + \sum_{i\in C(j)} \frac{1}{j}\sum_{s=i}^{i+j-1} J_j\left(\frac{u^{s+1}-u^s}{\lambda_n}\right)\right\} - nJ_{CB}^{**}(\ell)\\
=&\sum_{j=2}^K \sum_{i\in A(j)} \left\{ J_j\left(\frac{u^{i+j}-u^i}{j\lambda_n}\right) + \frac{c_j}{j}\sum_{s=i}^{i+j-1} J_1\left(\frac{u^{s+1}-u^s}{\lambda_n}\right) - \psi_j^{**}(\ell)\right\}\\
&+\sum_{j=2}^K \sum_{i\in C(j)} \frac{1}{j}\sum_{s=i}^{i+j-1} \left\{ J_j\left(\frac{u^{s+1}-u^s}{\lambda_n}\right) + c_jJ_1\left(\frac{u^{s+1}-u^s}{\lambda_n}\right) - \psi_j^{**}(\ell)\right\}\\
&+\sum_{j=2}^K c_j\sum_{s=1}^{j-1}\frac{j-s}{j}\left(J_1(u_{0,s}^{(1)})+J_1(u_{1,s}^{(1)})\right) - \sum_{j=2}^K (j-1)\psi_j^{**}(\ell).
\end{aligned}$$

Recall that for $j\in\{2,\dots,K\}$ it holds

$$\sum_{i=0}^{n-j}\left(\frac{u^{i+j}-u^i}{j\lambda_n}-\ell\right) = -\sum_{s=1}^{j-1}\frac{j-s}{j}\left(u_{0,s}^{(1)}+u_{1,s}^{(1)}-2\ell\right).$$

see (3.40). Adding and subtracting $\sum_{j=2}^K\sum_{i=0}^{n-j}(\psi_j^{**})'(\ell)(\frac{u_n^{i+j}-u_n^i}{j\lambda_n}-\ell)$ to $\hat{H}_{1,n}^{\ell,k_n,\mathcal{T}_n}(u)$ and (3.14) yield

$$\begin{aligned}
\hat{H}_{1,n}^{\ell,k_n,\mathcal{T}_n}(u) =&\sum_{j=2}^K \sum_{i\in A(j)} \left\{ J_j\left(\frac{u^{i+j}-u^i}{j\lambda_n}\right) + \frac{c_j}{j}\sum_{s=i}^{i+j-1} J_1\left(\frac{u^{s+1}-u^s}{\lambda_n}\right) - \psi_j^{**}(\ell)\right.\\
&\left.-(\psi_j^{**})'(\ell)\left(\frac{u^{i+j}-u^i}{j\lambda_n}-\ell\right)\right\} + \sum_{j=2}^K \sum_{i\in C(j)} \frac{1}{j}\sum_{s=i}^{i+j-1}\left\{\psi_j\left(\frac{u^{s+1}-u^s}{\lambda_n}\right)\right.\\
&\left.-\psi_j^{**}(\ell)-(\psi_j^{**})'(\ell)\left(\frac{u^{s+1}-u^s}{\lambda_n}-\ell\right)\right\} - \sum_{j=2}^K (j-1)\psi_j^{**}(\ell)\\
&+\sum_{j=2}^K c_j\sum_{s=1}^{j-1}\frac{j-s}{j}\left(J_1(u_{0,s}^{(1)})+J_1(u_{1,s}^{(1)})\right)\\
&-\sum_{j=2}^K (\psi_j^{**})'(\ell)\sum_{s=1}^{j-1}\frac{j-s}{j}\left(u_{0,s}^{(1)}+u_{1,s}^{(1)}-2\ell\right).
\end{aligned}\tag{4.10}$$

Let (u_n) be such that $u_n\in\mathcal{A}_n(0,1)$. For given $j\in\{2,\dots,K\}$, we recall that $\sigma_{j,n}^i(\ell)$ is defined by

$$\sigma_{j,n}^i(\ell) = J_j\left(\frac{u^{i+j}-u^i}{j\lambda_n}\right) + \frac{c_j}{j}\sum_{s=i}^{i+j-1} J_1\left(\frac{u^{s+1}-u^s}{\lambda_n}\right) - (\psi_j^{**})'(\ell)\left(\frac{u^{i+j}-u^i}{j\lambda_n}-\ell\right) - \psi_j^{**}(\ell)$$

see (3.42). Recall that $\sigma^i_{j,n}(\ell) \geq 0$, see (3.43). Moreover, we set

$$\mu^i_{j,n}(\ell) := \psi_j\left(\frac{u^{s+1}-u^s}{\lambda_n}\right) - (\psi_j^{**})'(\ell)\left(\frac{u^{s+1}-u^s}{\lambda_n} - \ell\right) - \psi_j^{**}(\ell). \tag{4.11}$$

By using $\psi_j \geq \psi_j(\gamma) = \psi_j^{**}(\gamma)$, we have $\mu^i_{j,n}(\ell) \geq 0$. In terms of $\sigma^i_{j,n}(\ell)$ and $\mu^i_{j,n}(\ell)$ the equation (4.10) reads

$$\begin{aligned}\hat{H}^{\ell,k_n,\mathcal{T}_n}_{1,n}(u) = &\sum_{j=2}^{K}\left\{\sum_{i\in A(j)}\sigma^i_{j,n}(\ell) + \sum_{i\in C(j)}\frac{1}{j}\sum_{s=i}^{i+j-1}\mu^i_{j,n}(\ell)\right\} - \sum_{j=2}^{K}(j-1)\psi_j^{**}(\ell)\\ &+\sum_{j=2}^{K}c_j\sum_{s=1}^{j-1}\frac{j-s}{j}\left(J_1(u^{(1)}_{0,s}) + J_1(u^{(1)}_{1,s})\right)\\ &-\sum_{j=2}^{K}(\psi_j^{**})'(\ell)\sum_{s=1}^{j-1}\frac{j-s}{j}\left(u^{(1)}_{0,s} + u^{(1)}_{1,s} - 2\ell\right).\end{aligned} \tag{4.12}$$

Applying similar arguments as in the proof of Proposition 3.9 for the fully atomistic energy $H^\ell_{1,n}$ to $\hat{H}^{\ell,k_n,\mathcal{T}_n}_{1,n}$ given as in (4.12) we obtain the following compactness result.

Proposition 4.3. *Let $\ell > 0$, $u^{(1)}_0, u^{(1)}_1 \in \mathbb{R}^{K-1}_+$ and suppose that assumptions (LJ1)–(LJ5) are satisfied. Let $(k_n) = (k^1_n, k^2_n)$ satisfy* (4.6) *and let (u_n) be a sequence of functions such that*

$$\sup_n \hat{H}^{\ell,k_n,\mathcal{T}_n}_{1,n}(u_n) < +\infty. \tag{4.13}$$

(1) If $\ell \leq \gamma$, then, up to subsequences, $u_n \to u$ in $L^\infty(0,1)$ with $u(x) = \ell x$, $x \in [0,1]$.
(2) In the case $\ell > \gamma$, then, up to subsequences, $u_n \to u$ in $L^1(0,1)$ where $u \in SBV^\ell_c(0,1)$; see (3.47)*.*

Proof. We can essentially copy the proof of Proposition 3.9. Let us only show how to adapt the argument for $u'_n \to \min\{\ell,\gamma\}$ in measure in $(0,1)$. For given $\varepsilon > 0$, we define the set I^ε_n as

$$I^\varepsilon_n := \left\{i \in \{0,\dots,n-1\} : \left|\frac{u^{i+1}_n - u^i_n}{\lambda_n} - \min\{\ell,\gamma\}\right| > \varepsilon\right\}.$$

By the definition of $\sigma^i_{2,n}(\ell)$, $\mu^i_{2,n}(\ell)$ (see (3.42), (4.11)) and Lemma 3.8, we deduce the existence of $\eta = \eta(\varepsilon) > 0$ such that $\sigma^i_{2,n}(\ell), \mu^i_{2,n} \geq \eta$ for $i \in I^\varepsilon_n$. From (4.4), (4.12), (4.13), $\sigma^i_{j,n}(\ell), \mu^i_{j,n}(\ell) \geq 0$ and J_j is bounded from below, we deduce that there exists a constant

$C > 0$ such that

$$C \geq \sum_{j=2}^{K} \left\{ \sum_{i \in A(j)} \sigma_{j,n}^{i}(\ell) + \sum_{i \in C(j)} \frac{1}{j} \sum_{s=i}^{i+j-1} \mu_{j,n}^{i}(\ell) \right\}$$
$$\geq \sum_{i=0}^{k_n^1 - 1} \sigma_{2,n}^{i}(\ell) + \sum_{i=k_n^1+1}^{k_n^2-2} \mu_{2,n}^{i}(\ell) + \sum_{i=k_n^2-1}^{n-2} \sigma_{2,n}^{i}(\ell) \geq \# I_n^{\varepsilon} \eta.$$

From this, we deduce exactly as in Proposition 3.9 that $u_n' \to \min\{\ell, \gamma\}$ in measure in $(0,1)$. We can now apply similar arguments as in the proof of Proposition 3.9 to show the assertions. □

Proposition 4.3 tells us that a sequence of deformations (u_n) with equibounded energy converges in $L^1(0,1)$ to a deformation u which has a constant gradient almost everywhere. In the following lemma, we prove that (u_n) yields a sequence of discrete gradients in the atomistic region converging to the same constant. This turns out to be crucial in the proofs of the first-order Γ-limits.

Lemma 4.4. *Let $\ell > 0$, $u_0^{(1)}, u_1^{(1)} \in \mathbb{R}_+^{K-1}$ and suppose that J_j, $j \in \{1, \dots, K\}$ satisfy (LJ1)–(LJ5). Let $(k_n) = (k_n^1, k_n^2)$ satisfy* (4.6) *and let (u_n) be a sequence of functions such that* (4.13) *is satisfied. Then there exist sequences $(T_n^1), (T_n^2) \subset \mathbb{N}$ with $T_n^1 \in \{0, \dots, k_n^1 - K - 1\}$ and $T_n^2 \in \{k_n^2, \dots, n-K\}$ such that, up to subsequences,*

$$\lim_{n \to \infty} \frac{u_n^{T_n^i+s+1} - u_n^{T_n^i+s}}{\lambda_n} = \min\{\ell, \gamma\}, \qquad \textit{for } s \in \{0, \dots, K-1\} \textit{ and } i = 1, 2. \tag{4.14}$$

Proof. The proof is an adaption of the proof of Lemma 3.11. Let us define $(\tilde{k}_n) \subset \mathbb{N}$ by $\tilde{k}_n = \min\{k_n^1, n - k_n^2\}$ and

$$I_n := \left\{ i \in \{0, \dots, k_n^1 - (K+1)\} \cup \{k_n^2, \dots, n-K\} : \sigma_{K,n}^{i}(\ell) > \frac{1}{\sqrt{\tilde{k}_n}} \right\}.$$

By (4.13), there exists $C > 0$ such that

$$C \geq \sup_n \left(\sum_{i=0}^{k_n^1 - K - 1} \sigma_{K,n}^{i}(\ell) + \sum_{i=k_n^2}^{n-K} \sigma_{K,n}^{i}(\ell) \right) \geq \sup_n \sum_{i \in I_n} \frac{1}{\sqrt{\tilde{k}_n}} = \sup_n \frac{\# I_n}{\sqrt{\tilde{k}_n}}.$$

Hence, we have $\# I_n = \mathcal{O}(\sqrt{\tilde{k}_n})$.

Now let $i \notin I_n$. By using the definition of $J_{0,K}$ and $J_{0,K}(z) \geq \psi_K^{**}(z) \geq (\psi_K^{**})'(\ell)(z - \ell) + \psi_K^{**}(\ell)$, we deduce from $0 \leq \sigma_{K,n}^i(\ell) \leq \frac{1}{\sqrt{\tilde{k}_n}}$ that

$$0 \leq J_K\left(\frac{u_n^{i+K} - u_n^i}{K\lambda_n}\right) + \sum_{s=i}^{i+K-1} \frac{c_K}{K} J_1\left(\frac{u_n^{s+1} - u_n^s}{\lambda_n}\right) - J_{0,K}\left(\frac{u_n^{i+K} - u_n^i}{j\lambda_n}\right) \leq \frac{1}{\sqrt{\tilde{k}_n}}, \quad (4.15)$$

$$0 \leq J_{0,K}\left(\frac{u_n^{i+K} - u_n^i}{K\lambda_n}\right) - \psi_K^{**}(\ell) - (\psi_K^{**})'(\ell)\left(\frac{u_n^{i+K} - u_n^i}{K\lambda_n} - \ell\right) \leq \frac{1}{\sqrt{\tilde{k}_n}}. \quad (4.16)$$

Let $(h_n) \subset \mathbb{N}$ be such that $h_n \in \{0, \dots, k_n^1 - K - 1\} \cup \{k_n^2, \dots, n - K\}$ and $h_n \notin I_n$. By using the fact that $J_{0,K}(z) = \psi_K^{**}(\ell) + (\psi_K^{**})'(\ell)(z - \ell)$ if and only if $z = \min\{\ell, \gamma\}$, we conclude from (4.6) and (4.16) that

$$\frac{u_n^{h_n+K} - u_n^{h_n}}{K\lambda_n} \to \min\{\ell, \gamma\} \quad \text{as } n \to \infty.$$

Combining this with (4.15) and assumption (LJ4) (see (3.13)), we deduce

$$\lim_{n\to\infty} \frac{u_n^{h_n+s+1} - u_n^{h_n+s}}{\lambda_n} = \min\{\ell, \gamma\} \qquad \text{for } s \in \{0, \dots, K-1\}.$$

Hence, for sequences $(h_n^1), (h_n^2) \subset \mathbb{N}$ with $h_n^1 \in \{0, \dots, k_n^1 - K - 1\} =: K_n^1$ and $h_n^2 \in \{k_n^2, \dots, n - K\} =: K_n^2$ and $h_n^i \notin I_n$, for n big enough and $i = 1, 2$, we deduce

$$\lim_{n\to\infty} \frac{u_n^{h_n^i+1} - u_n^{h_n^i}}{\lambda_n} = \min\{\ell, \gamma\}.$$

It is left to prove existence of such sequences. Since $\#I_n = \mathcal{O}(\sqrt{\tilde{k}_n})$, we conclude by the assumption (4.6) that $K_n^i \setminus \left(I_n \cap K_n^i\right) \neq \emptyset$ for n sufficiently large and $i = 1, 2$ which shows the existence. $\square$

4.3.1 The case $0 < \ell \leq \gamma$

As for the fully atomistic model studied in Chapter 3, we distinguish between the cases $0 < \ell \leq \gamma$ and $\ell > \gamma$, where ℓ denotes the boundary condition on the last atom in the chain and γ denotes the unique minimum point of $J_{0,j}$ for $j \in \{2, \dots, K\}$. In the case $0 < \ell \leq \gamma$ no fracture occurs by Proposition 4.3. In this section, we show that the first-order Γ-limit of $(\hat{H}_n^{\ell,k_n,\mathcal{T}_n})$ coincides with the first-order Γ-limit H_1^ℓ of the fully atomistic model (H_n^ℓ), cf. Theorem 3.19.

Theorem 4.5. *Let $0 < \ell \leq \gamma$ and $u_0^{(1)}, u_1^{(1)} \in \mathbb{R}_+^{K-1}$. Let k_n^1, k_n^2 satisfy (4.6) and let $\mathcal{T}_n \subset \{0, 1, \dots, n\}$ be such that*

$$\{0, \dots, k_n^1\} \cup \{k_n^2, \dots, n\} \subset \mathcal{T}_n = \{t_n^0, \dots, t_n^{r_n}\}. \quad (4.17)$$

Then the sequence $(\hat{H}_{1,n}^{\ell,k_n,\mathcal{T}_n})$ *defined in* (4.9) Γ*-converges with respect to the* $L^\infty(0,1)$*-topology to the functional* H_1^ℓ *defined in* (3.51)*.*

Proof. Liminf inequality. Let $(u_n) \subset L^1(0,1)$ and $u \in L^1(0,1)$ with $u_n \to u$ in $L^1(0,1)$ and $\liminf_{n\to\infty} \hat{H}_{1,n}^{\ell,k_n,\mathcal{T}_n}(u_n) < +\infty$. By Proposition 4.3, we deduce that $u(x) = \ell x$ a.e. in $(0,1)$ and $u_n \to u$ in $L^\infty(0,1)$. We have to show that

$$\begin{aligned}\liminf_{n\to\infty} \hat{H}_{1,n}^{\ell,k_n,\mathcal{T}_n}(u_n) \geq & B(u_0^{(1)},\ell) + B(u_1^{(1)},\ell) - \sum_{j=2}^{K}(j-1)\psi_j(\ell) \\ & - \sum_{j=2}^{K}\psi_j'(\ell)\sum_{s=1}^{j-1}\frac{j-s}{j}\left(u_{0,s}^{(1)} + u_{1,s}^{(1)} - 2\ell\right), \end{aligned} \tag{4.18}$$

see (3.51). By Lemma 4.4, there exist sequences $(T_n^1), (T_n^2) \subset \mathbb{N}$ such that $T_n^1 < k_n^1 - K$, $T_n^2 > k_n^2$ and

$$\lim_{n\to\infty} \frac{u_n^{T_n^i+s+1} - u_n^{T_n^i+s}}{\lambda_n} = \ell \quad \text{for } i \in \{1,2\} \text{ and } s \in \{1,\dots,K-1\}. \tag{4.19}$$

Using $\sigma_{j,n}^i(\ell), \mu_{j,n}^i(\ell) \geq 0$, we obtain from (4.1), $T_n^1 < k_n^1$, $T_n^2 > k_n^2$ and (4.12) that

$$\begin{aligned}\hat{H}_{1,n}^{\ell,k_n,\mathcal{T}_n}(u_n) \geq & \sum_{j=2}^{K}\left\{\sum_{i=0}^{T_n^1}\sigma_{j,n}^i(\ell) + \sum_{i=T_n^2+1}^{n-j}\sigma_{j,n}^i(\ell) + c_j\sum_{s=1}^{j-1}\frac{j-s}{j}\left(J_1(u_{0,s}^{(1)}) + J_1(u_{1,s}^{(1)})\right)\right\} \\ & - \sum_{j=2}^{K}(j-1)\psi_j(\ell) - \sum_{j=2}^{K}\psi_j'(\ell)\sum_{s=1}^{j-1}\frac{j-s}{j}\left(u_{0,s}^{(1)} + u_{1,s}^{(1)} - 2\ell\right). \end{aligned} \tag{4.20}$$

We can now use the same estimates as in the fully atomistic case, see Theorem 3.12. By using (4.19) and the estimates (3.55) and (3.57), we obtain

$$\liminf_{n\to\infty}\sum_{j=2}^{K}\left\{c_j\sum_{s=1}^{j-1}\frac{j-s}{j}J_1(u_{0,s}^{(1)}) + \sum_{i=0}^{T_n^1}\sigma_{j,n}^i(\ell)\right\} \geq B(u_0^{(1)},\ell), \tag{4.21}$$

$$\liminf_{n\to\infty}\sum_{j=2}^{K}\left\{c_j\sum_{s=1}^{j-1}\frac{j-s}{j}J_1(u_{1,s}^{(1)}) + \sum_{i=T_n^2+1}^{n-j}\sigma_{j,n}^i(\ell)\right\} \geq B(u_1^{(1)},\ell). \tag{4.22}$$

The estimates (4.20)–(4.22) yield (4.18).

Limsup inequality. Since $H_1^\ell(u)$ (see (3.51)) is finite if and only if $u(x) = \ell x$ it is sufficient to construct a recovery sequence for $u(x) = \ell x$. As for the liminf inequality, we can follow the proof for the fully atomistic system. In fact, we can even use the same recovery sequence. Fix $\eta > 0$. By the definition of $B(\theta,\ell)$, see (3.50), we can find $v : \mathbb{N}_0 \to \mathbb{R}$ and $N_1 \in \mathbb{N}$ with $v^0 = 0$, $v^s - v^{s-1} = u_{0,s}^{(1)}$ for $s \in \{1,\dots,K-1\}$ and $v^{i+1} - v^i = \ell$ for $i \geq N_1$ satisfying (3.58). Furthermore, there exists $w : \mathbb{N}_0 \to \mathbb{R}$ and $N_2 \in \mathbb{N}$ with $w^0 = 0$, $w^s - w^{s-1} = u_{1,s}^{(1)}$ for $s = 1,\dots,K-1$ and $w^{i+1} - w^i = \ell$ for $i \geq N_2$ satisfying (3.59). By means of the functions v and w we can construct a recovery sequence (u_n) for u,

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

As we mentioned above this is exactly the same recovery sequence that we have used in Theorem 3.12. We have shown that $u_n \to u$ in $L^\infty(0,1)$ and that u_n satisfies the boundary conditions (3.3) for n large enough. Moreover, since $k_n^1 \to +\infty$ and $n - k_n^2 \to +\infty$, we can assume $N_1 + K \leq k_n^1$ and $n - N_2 - K \geq k_n^2$ for n sufficiently large. Thus u_n is affine on $\lambda_n(k_n^1, k_n^2)$ which implies $u_n \in \mathcal{A}_{\mathcal{T}_n}(0,1)$ for arbitrary $\mathcal{T}_n$ satisfying $\{0, \ldots, k_n^1\} \cup \{k_n^2, ..n\} \subset \mathcal{T}_n$. Using (3.58) and (3.59), we obtain

$$\sum_{j=2}^{K} \left\{ c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(u_{0,s}^{(1)}) + \sum_{i=0}^{N_1} \sigma_{j,n}^i(\ell) \right\} \leq B(u_0^{(1)}, \ell) + \eta,$$

$$\sum_{j=2}^{K} \left\{ c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(u_{1,s}^{(1)}) + \sum_{i=n-N_2-K}^{n-j} \sigma_{j,n}^i(\ell) \right\} \leq B(u_1^{(1)}, \ell) + \eta.$$

By (3.51) and (4.12), it remains to show that

$$\Sigma_n := \sum_{j=2}^{K} \left\{ \sum_{i=N_1+1}^{k_n^1 - 1} \sigma_{j,n}^i(\ell) + \sum_{i=k_n^1}^{k_n^2 - j} \frac{1}{j} \sum_{s=i}^{i+j-1} \mu_{j,n}^s(\ell) + \sum_{i=k_n^2 - j + 1}^{n - N_2 - K - 1} \sigma_{j,n}^i(\ell) \right\}$$

is infinitesimal as $n \to \infty$. This follows directly from the proof of Theorem 3.12. Indeed, in Theorem 3.12 we have shown that for u_n it holds that

$$\lim_{n \to \infty} \sum_{j=2}^{K} \sum_{i=N_1+1}^{n-N_2-K-1} \sigma_{j,n}^i(\ell) = 0.$$

By using the fact that u_n is affine on $\lambda_n(N_1, \ldots, n - N_2)$, we have that $\sigma_{j,n}^i(\ell) = \mu_{j,n}^i(\ell)$ for $j \in \{2, \ldots, K\}$ and $i \in \{N_1 + K, \ldots, n - N_2 - K - 1\}$, and thus the statement follows. □

Remark 4.6. In the proof of Theorem 3.12, the assumption (4.6) (i) is crucial. If one drops this assumption, for example to let k_n^1 and $n - k_n^2$ be independent of n, the first-order Γ-limits of $H_n^{\ell, k_n, \mathcal{T}_n}$ and $\hat{H}_n^\ell$ do not coincide in general. In this case the boundary layer energies $B(\theta, \ell)$ would be replaced by some "truncated" boundary layer energies $B_T(\theta, \ell)$ in the first-order Γ-limit of $\hat{H}_n^{\ell, k_n \mathcal{T}_n}$. To quantify the difference between $B(\theta, \ell)$ and $B_T(\theta, \ell)$ one has to perform a deeper analysis, as in the spirit of Section 3.4.3, on the decay of the boundary layers.

4.3.2 The case $\ell > \gamma$

According to Proposition 4.3, the case $\ell > \gamma$ leads to fracture. In the fully atomistic model, $H^{\ell}_{1,n}$, each crack costs a certain amount of fracture energy, see Theorem 3.19. Moreover, the fracture energy depends on whether the crack is located in $(0,1)$ or $\{0,1\}$. In this section, we aim for an analogous result for the quasicontinuum model $\hat{H}^{\ell,k_n,\mathcal{T}_n}_{1,n}$. Here the specific structure of $\mathcal{T} = (\mathcal{T}_n)$ turns out to be important. We will show that every jump corresponds to the debonding of a pair of representative atoms and this induces the debonding of all atoms in between. Thus the distance between two neighbouring repatoms quantifies the jump energy.

Let (u_n) be a sequence such that $u_n \in \mathcal{A}_{\mathcal{T}_n}(0,1)$ and u_n satisfies (3.3). Then, we deduce from (4.12) that

$$\begin{aligned}\hat{H}^{\ell,k_n,\mathcal{T}_n}_{1,n}(u_n) = &\sum_{j=2}^{K}\Bigg\{c_j\sum_{s=1}^{j-1}\frac{j-s}{j}J_1(u^{(1)}_{0,s}) + \sum_{i=0}^{k^1_n-1}\sigma^i_{j,n} + \sum_{s=1}^{j-1}\frac{s}{j}\mu^{k^1_n+s-1}_{j,n} + \sum_{i=k^1_n+j-1}^{k^2_n-j}\mu^i_{j,n}\\ &+\sum_{s=1}^{j-1}\frac{s}{j}\mu^{k^2_n-s}_{j,n} + \sum_{i=k^2_n-j+1}^{n-j}\sigma^i_{j,n} + c_j\sum_{s=1}^{j-1}\frac{j-s}{j}J_1(u^{(1)}_{1,s}) - (j-1)\psi_j(\gamma)\Bigg\},\end{aligned} \tag{4.23}$$

with $\sigma^i_{j,n} := \sigma^i_{j,n}(\gamma)$ and $\mu^i_{j,n} := \mu^i_{j,n}(\gamma)$, see (3.42) and (4.11). Note that we used $\psi^{**}_j \equiv \psi_j(\gamma)$ on $[\gamma,+\infty)$. Let us now introduce some notations and state assumptions on the set of representative atoms $\mathcal{T} = (\mathcal{T}_n)$ under which the Γ-limit of $(\hat{H}^{\ell,k_n,\mathcal{T}_n}_{1,n})$ will be derived. In particular the repatoms at the interface between the local and nonlocal region have to be treated with extra care.

(T1) The set of representative atoms $\mathcal{T} = (\mathcal{T}_n)$ satisfy (4.7) and (4.17).

(T2) The following limits exist in $\mathbb{N}\cup\{+\infty\}$

$$\begin{aligned}\hat{r}(\mathcal{T}) &:= \lim_{n\to\infty}\left(r(\mathcal{T}_n) - k^1_n\right), \text{ with } r(\mathcal{T}_n) := \min\{r \in \mathcal{T}_n : k^1_n + K - 1 \le r\},\\ \hat{l}(\mathcal{T}) &:= \lim_{n\to\infty}\left(k^2_n - l(\mathcal{T}_n)\right), \text{ with } l(\mathcal{T}_n) := \max\{l \in \mathcal{T}_n : k^2_n - K + 1 \ge l\}.\end{aligned} \tag{4.24}$$

(T3) There exist $M \in \mathbb{N}$ and $k^{\mathcal{T}}_r, k^{\mathcal{T}}_l \in \{1,\dots,K\}$ such that the sets $\mathcal{I}^r(\mathcal{T}_n)$ and $\mathcal{I}^l(\mathcal{T}_n)$ defined by

$$\begin{aligned}\mathcal{I}^r(\mathcal{T}_n) &:= \{i \in \mathcal{T}_n, i \in \{k^1_n,\dots,r(\mathcal{T}_n)\}\},\\ \mathcal{I}^l(\mathcal{T}_n) &:= \{i \in \mathcal{T}_n, i \in \{l(\mathcal{T}_n),\dots,k^2_n\}\},\end{aligned} \tag{4.25}$$

satisfy $\#(\mathcal{I}^r(\mathcal{T}_n)) = k_r^{\mathcal{T}}$ and $\#(\mathcal{I}^l(\mathcal{T}_n)) = k_l^{\mathcal{T}}$ for all $n \geq M$. For $n \geq M$, we define $\hat{r}_n^{\mathcal{T}} = (\hat{r}_{1,n}^{\mathcal{T}}, \dots, \hat{r}_{k_r^{\mathcal{T}},n}^{\mathcal{T}})$ and $\hat{l}_n^{\mathcal{T}} = (\hat{l}_{1,n}^{\mathcal{T}}, \dots, \hat{l}_{k_l^{\mathcal{T}},n}^{\mathcal{T}})$ as

$$\begin{aligned} \hat{r}_{1,n}^{\mathcal{T}} &:= k_n^1, \quad \hat{r}_{s,n}^{\mathcal{T}} := \min\{r \in \mathcal{T}_n : \hat{r}_{s-1,n}^{\mathcal{T}} < r \leq r(\mathcal{T}_n)\} \quad \text{for } s \in \{2, \dots, k_r^{\mathcal{T}}\}, \\ \hat{l}_{1,n}^{\mathcal{T}} &:= k_n^2, \quad \hat{l}_{s,n}^{\mathcal{T}} := \max\{l \in \mathcal{T}_n : \hat{l}_{s-1,n}^{\mathcal{T}} > l \geq l(\mathcal{T}_n)\} \quad \text{for } s \in \{2, \dots, k_l^{\mathcal{T}}\}. \end{aligned} \tag{4.26}$$

Moreover, we assume that the following limits exist in $\mathbb{N}_0$:

$$\begin{aligned} \hat{r}_i^{\mathcal{T}} &:= \lim_{n\to\infty} \left(\hat{r}_{i,n}^{\mathcal{T}} - k_n^1\right) \quad \text{for } i \in \{1, \dots, k_r^{\mathcal{T}} - 1\}, \\ \hat{l}_i^{\mathcal{T}} &:= \lim_{n\to\infty} \left(k_n^2 - \hat{l}_{i,n}^{\mathcal{T}}\right) \quad \text{for } i \in \{1, \dots, k_l^{\mathcal{T}} - 1\}. \end{aligned} \tag{4.27}$$

We define $\hat{r}^{\mathcal{T}} \in (\mathbb{N}_0 \cup \{+\infty\})^{k_r^{\mathcal{T}}}$ and $\hat{l}^{\mathcal{T}} \in (\mathbb{N}_0 \cup \{+\infty\})^{k_l^{\mathcal{T}}}$ as

$$\hat{r}^{\mathcal{T}} = (\hat{r}_1^{\mathcal{T}}, \dots, \hat{r}_{k_r^{\mathcal{T}}}^{\mathcal{T}}),\ \hat{l}^{\mathcal{T}} = (\hat{l}_1^{\mathcal{T}}, \dots, \hat{l}_{k_l^{\mathcal{T}}}^{\mathcal{T}}),\ \text{with } \hat{r}_{k_r^{\mathcal{T}}}^{\mathcal{T}} := \hat{r}(\mathcal{T}) \text{ and } \hat{l}_{k_l^{\mathcal{T}}}^{\mathcal{T}} := \hat{l}(\mathcal{T}). \tag{4.28}$$

(T4) For given $x \in [0, 1]$, the following limit exists in $\mathbb{N} \cup \{+\infty\}$

$$\begin{aligned} b(x, \mathcal{T}) := \lim_{n\to\infty} \min\big\{q_n^2 - q_n^1 \ :\ (q_n^1), (q_n^2) \subset \mathbb{N}, r(\mathcal{T}_n) \leq q_n^1 < q_n^2 \leq l(\mathcal{T}_n), \\ q_n^1,\ q_n^2 \in \mathcal{T}_n, \lim_{n\to\infty} \lambda_n q_n^1 = \lim_{n\to\infty} \lambda_n q_n^2 = x\big\}. \end{aligned} \tag{4.29}$$

Remark 4.7. (a) Assume that $\mathcal{T} = (\mathcal{T}_n)$ satisfies (T1)–(T4). By (4.26) and (4.27) it holds $\hat{r}_1^{\mathcal{T}} = \hat{l}_1^{\mathcal{T}} = 0$. For given $k \in \{2, \dots, K\}$, we define the set $\mathcal{I}(k) \subset (\mathbb{N}_0 \cup \{+\infty\})^k$ as

$$\mathcal{I}(k) := \big\{(r_1, \dots, r_k) \in (\mathbb{N}_0 \cup \{+\infty\})^k : 0 = r_1 < r_2 < \dots < r_{k-1} < K - 1 \leq r_k\big\}. \tag{4.30}$$

Clearly, we have that $\hat{r}^{\mathcal{T}} \in \mathcal{I}(k_r^{\mathcal{T}})$ and $\hat{l}^{\mathcal{T}} \in \mathcal{I}(k_l^{\mathcal{T}})$. Since $\hat{r}_{s,n}^{\mathcal{T}}, \hat{l}_{s,n}^{\mathcal{T}} \in \mathbb{N}$, it follows from (4.27) that there exists $\tilde{M} \in \mathbb{N}$ such that

$$\begin{aligned} \hat{r}_i^{\mathcal{T}} &= \hat{r}_{i,n}^{\mathcal{T}} - k_n^1 \quad \text{for } i \in \{1, \dots, k_r^{\mathcal{T}} - 1\}, \\ \hat{l}_i^{\mathcal{T}} &= k_n^2 - \hat{l}_{i,n}^{\mathcal{T}} \quad \text{for } i \in \{1, \dots, k_l^{\mathcal{T}} - 1\}, \end{aligned} \tag{4.31}$$

for $n \geq \tilde{M}$. Moreover, if $\hat{r}(\mathcal{T}) < +\infty$ (or $\hat{l}(\mathcal{T}) < +\infty$) it is not restrictive to assume that $\hat{r}(\mathcal{T}) = r(\mathcal{T}_n) - k_n^1$ (or $\hat{l}(\mathcal{T}) = k_n^2 - l(\mathcal{T}_n)$) for $n \geq \tilde{M}$.
(b) In the case of nearest and next-to-nearest neighbour interactions only, we deduce from the definitions of $r(\mathcal{T}_n)$ and $l(\mathcal{T}_n)$, see (4.24), and (T3) that

$$\hat{r}_n^{\mathcal{T}} = (k_n^1, r(\mathcal{T}_n)),\ \hat{l}_n^{\mathcal{T}} = (k_n^2, l(\mathcal{T}_n)) \quad \text{and} \quad \hat{r}^{\mathcal{T}} = (0, \hat{r}(\mathcal{T})),\ \hat{l}^{\mathcal{T}} = (0, \hat{l}(\mathcal{T})). \tag{4.32}$$

Let us now introduce boundary layer energies which correspond to a jump close respectively at the interface between the atomistic and continuum region. Firstly, we introduce further abbreviations. For a given function $v : \mathbb{N}_0 \to \mathbb{R}$, an $i \in \mathbb{N}_0$ and a $j \in \{2, \dots, K\}$, we define $\sigma_j^i(v)$ and $\mu_j^i(v)$ by

$$\sigma_j^i(v) = J_j\left(\frac{v^{i+j}-v^i}{j}\right) + \frac{c_j}{j}\sum_{s=i}^{i+j-1} J_1(v^{s+1}-v^s) - \psi_j(\gamma) \tag{4.33}$$

$$\mu_j^i(v) = \psi_j(v^{i+1}-v^i) - \psi_j(\gamma). \tag{4.34}$$

For a given $r = (r_1, \dots, r_k) \in \mathcal{I}(k)$, we define the following minimum problem

$$\begin{aligned} B_{IF}^{(1)}(r) := \inf_{q\in\mathbb{N}} \min \Bigg\{ \sum_{j=2}^{K} \Bigg\{ c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(v^s - v^{s-1}) + \sum_{i=0}^{q-1} \sigma_j^i(v) + \sum_{s=1}^{j-1} \frac{s}{j} \mu_j^{q+s-1}(v) \\ + \sum_{i=q+j-1}^{q+r_k-1} \mu_j^i(v) \Bigg\} : v : \mathbb{N}_0 \to \mathbb{R}, v^0 = 0, v^{q+i+1} - v^{q+i} = v^{q+r_s+1} - v^{q+r_s}, \\ \text{if } 1 \le s < k \text{ and } r_s \le i < r_{s+1} \Bigg\}. \end{aligned} \tag{4.35}$$

The boundary layer energy $B_{IF}^{(1)}(r)$ yields the optimal position of a fracture that occurs in the atomistic region but close to the atomistic/continuum interface. Note that the reduced degree of freedom in the quasicontinuum energy yields an additional constraint compared to the previous defined boundary layer energies.

Remark 4.8. Let $J_1, \dots, J_k$ satisfy (LJ1)–(LJ5).

(i) Let $r \in \mathcal{I}(k)$ be such that $r_k = +\infty$. In this case the constraints in (4.35) imply that $v^{i+1} - v^i = v^{q+r_{k-1}+1} - v^{q+r_{k-1}}$ for $i \ge q + r_{k-1}$. Moreover, the last sum from $i = q+j-1$ to $q + r_k - 1$ reads

$$\sum_{i=q+j-1}^{\infty} \mu_j^i(v) = \sum_{i=q+j-1}^{q+r_{k-1}-1} \mu_j^i(v) + \sum_{i=q+r_{k-1}}^{\infty} \left(\psi_j(v^{q+r_{k-1}+1} - v^{q+r_{k-1}}) - \psi_j(\gamma)\right).$$

Since γ is the unique minimiser of ψ_j, the above quantity is finite only if $v^{q+r_{k-1}+1} - v^{q+r_{k-1}} = \gamma$. Hence, for $r \in \mathcal{I}(k)$ with $r_k = +\infty$ the boundary layer energy $B_{IF}^{(1)}(r)$ reads

$$\begin{aligned} B_{IF}^{(1)}(r) = \inf_{q\in\mathbb{N}} \min \Bigg\{ \sum_{j=2}^{K} \Bigg\{ c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(v^s - v^{s-1}) + \sum_{i=0}^{q-1} \sigma_j^i(v) \\ + \sum_{i=q}^{q+r_{k-1}-1} \left(\frac{i-q+1}{j} \wedge 1\right) \mu_j^i(v) \Bigg\} : v : \mathbb{N}_0 \to \mathbb{R}, v^0 = 0,\ v^{i+1} - v^i = \gamma \\ \text{if } i \ge q + r_{k-1},\ v^{q+i+1} - v^{q+i} = v^{q+r_s+1} - v^{q+r_s} \text{ if } 1 \le s \le k-2 \text{ and} \\ r_s \le i < r_{s+1} \Bigg\}. \end{aligned} \tag{4.36}$$

(ii) Consider the special case $k = 2$. Note that if we consider nearest and next-to-nearest neighbour interactions only this is the sole case of interest. Indeed this follows by

$2 \le k \le K$, see Remark 4.7. Fix $r \in \mathcal{I}(2)$. Then $r = (r_1, r_2) = (0, r_2)$, see (4.30), and the constraint on v in (4.35) reads $v^0 = 0$ and $v^{q+i+1} - v^{q+i} = v^{q+1} - v^q$ for $i \in \{0, \dots, r_2 - 1\}$. This yields $\mu_j^{q+i}(v) = \mu_j^q(v)$ for $0 \le i < r_2$. Hence, we have

$$\begin{aligned} B_{IF}^{(1)}((r_1, r_2)) = \inf_{q \in \mathbb{N}} \min \Bigg\{ \sum_{j=2}^{K} \Bigg\{ c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(v^s - v^{s-1}) + \sum_{i=0}^{q-1} \sigma_j^i(v) \\ + \left(r_2 - \frac{1}{2}(j-1) \right) \mu_j^q(v) \Bigg\} : v : \mathbb{N}_0 \to \mathbb{R}, v^0 = 0, \\ v^{q+i+1} - v^{q+i} = v^{q+1} - v^q \text{ if } 0 \le i \le r_2 - 1 \Bigg\} =: B_{IF}(r_2). \end{aligned} \tag{4.37}$$

Let $r_2 = +\infty$. As above, we have the constraint $v^{i+1} - v^i = \gamma$ for $i \ge q$ in (4.37). This implies $\mu_j^q(v) = 0$ and we obtain that $B_{IF}(\infty) = B(\gamma)$, see (3.71).

Next, we introduce two further boundary layer energies corresponding to a jump exactly at the interface between the atomistic and continuum region. Before we state the precise definitions let us first give some heuristic explanations. Consider the debonding of two atoms labelled by i and $i+1$ with $k_n^1 \le i < r(\mathcal{T}_n)$. Then there exists $m \in \{1, \dots, k_r^{\mathcal{T}} - 1\}$ such that $\hat{r}_{m,n}^{\mathcal{T}} \le i < i+1 \le \hat{r}_{m+1,n}^{\mathcal{T}}$. This causes two boundary layers. One of them 'starts' at $\hat{r}_{m,n}^{\mathcal{T}}$ and 'moves into' the atomistic region, $B_{IF}^{(2)}$, and the other one 'starts' at $\hat{r}_{m+1,n}^{\mathcal{T}}$ and 'moves into' the continuum region, $B_{IF}^{(3)}$.

For a given $r = (r_1, \dots, r_k) \in \mathcal{I}(k)$ and $m \in \{1, \dots, k-1\}$, we define

$$\begin{aligned} B_{IF}^{(2)}(r, m, \gamma) := \inf_{N \in \mathbb{N}} \min \Bigg\{ \sum_{j=2+r_m}^{K} c_j \sum_{s=1}^{j-1} \frac{j - (s \vee (r_m + 1))}{j} J_1(v^s - v^{s-1}) \\ + \sum_{j=2}^{K} \sum_{i \ge (r_m + 1 - j) \vee 0} \sigma_j^i(v) + \sum_{j=2}^{K} \sum_{i=0}^{r_m - 1} \left(\frac{r_m - i}{j} \wedge 1 \right) \mu_j^i(v) : v : \mathbb{N}_0 \to \mathbb{R}, \\ v^0 = 0,\ v^{i+1} - v^i = \gamma \text{ if } i \ge N,\ v^{i+1} - v^i = v^{r_m - r_s + 1} - v^{r_m - r_s} \\ \text{if } 2 \le s \le m \text{ and } r_m - r_s \le i < r_m - r_{s-1} \Bigg\} \end{aligned} \tag{4.38}$$

Furthermore, we define for $r = (r_1, \dots, r_k) \in \mathcal{I}(k)$ and $m \in \{1, \dots, k\}$

$$\begin{aligned} B_{IF}^{(3)}(r, m) := \min \Bigg\{ \sum_{j=2+r_m}^{K} c_j \sum_{s=1}^{j-r_m-1} \frac{j - r_m - s}{j} J_1(v^s - v^{s-1}) \\ + \sum_{j=2}^{K} \sum_{i=1}^{r_k - r_m} \left(\frac{i + r_m}{j} \wedge 1 \right) \mu_j^{i-1}(v) : v : \mathbb{N}_0 \to \mathbb{R}, v^0 = 0, \\ v^{i+1} - v^i = v^{r_s - r_m + 1} - v^{r_s - r_m} \text{ if } m \le s \le k-1 \text{ and} \\ r_s - r_m \le i < r_{s+1} - r_m \Bigg\}. \end{aligned} \tag{4.39}$$

Remark 4.9. Fix $k \in \{2, \dots, K\}$ and let $r \in \mathcal{I}(k)$. Using $r_1 = 0$, we deduce from (4.38) that

$$B_{IF}^{(2)}(r, 1, \gamma) = \inf_{N \in \mathbb{N}} \min \Bigg\{ \sum_{j=2}^{K} c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(v^s - v^{s-1}) + \sum_{j=2}^{K} \sum_{i \geq 0} \sigma_j^i(v) : \\ v : \mathbb{N}_0 \to \mathbb{R},\ v^0 = 0,\ v^{i+1} - v^i = \gamma \text{ if } i \geq N \Bigg\} = B(\gamma), \tag{4.40}$$

see (3.71). Moreover, using $r_k \geq K - 1$, we obtain from (4.39) that $B_{IF}^{(3)}(r, k) = 0$. Assume that $J_1, \dots, J_K$ satisfy the assumptions (LJ1)–(LJ5). Let $r \in \mathcal{I}(k)$ be such that $r_k = +\infty$. In the same way as in Remark 4.8, we obtain

$$B_{IF}^{(3)}(r, m) = \min \Bigg\{ \sum_{j=2+r_m}^{K} c_j \sum_{s=1}^{j-r_m-1} \frac{j - r_m - s}{j} J_1(v^s - v^{s-1}) \\ + \sum_{j=2}^{K} \sum_{i=1}^{r_{k-1}-r_m} \left(\frac{i + r_m}{j} \wedge 1 \right) \mu_j^{i-1}(v) : v : \mathbb{N}_0 \to \mathbb{R}, v^0 = 0, \\ v^{i+1} - v^i = \gamma \text{ if } i \geq r_{k-1} - r_m,\ v^{i+1} - v^i = v^{r_s - r_m + 1} - v^{r_s - r_m} \\ \text{if } m \leq s \leq k-2 \text{ and } r_s - r_m \leq i < r_{s+1} - r_m \Bigg\}. \tag{4.41}$$

Lemma 4.10. *Let $J_1, \dots, J_K$ satisfy (LJ1)–(LJ5). Let $\mathcal{T}_n = \{t_n^0, t_n^1, \dots, t_n^{r_n}\}$ with $0 = t_n^0 < t_n^1 < \dots < t_n^{r_n} = n$ for all $n \in \mathbb{N}$. Let (u_n) be a sequence of functions satisfying (4.13). Furthermore, let $(h_n) \subset \mathbb{N}$ be such that $k_n^1 \leq t_n^{h_n} < t_n^{h_n+1} \leq k_n^2$ and $\liminf_{n\to\infty} \left(t_n^{h_n+1} - t_n^{h_n}\right) = +\infty$. Then, we have*

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

Proof. From $\sup_n \hat{H}_{1,n}^{\ell, k_n, \mathcal{T}_n}(u_n) < +\infty$, $\sigma_{j,n}^i, \mu_{j,n}^i \geq 0$ and (4.23), we deduce the existence of a constant $C > 0$ such that

$$C \geq \sup_n \frac{1}{2} \sum_{i=t_n^{h_n}}^{t_n^{h_n+1}-1} \mu_{2,n}^i = \frac{1}{2} \sup_n (t_n^{h_n+1} - t_n^{h_n}) \mu_n^{t_n^{h_n}},$$

where we used that $u_n'(x) = \lambda_n^{-1}(t_n^{h_n+1} - t_n^{h_n})^{-1}(u_n^{t_n^{h_n+1}} - u_n^{t_n^{h_n}})$ for all $x \in \lambda_n(t_n^{h_n}, t_n^{h_n+1})$. This implies $\mu_n^{t^{h_n}} = \mathcal{O}((t_n^{h_n+1} - t_n^{h_n})^{-1})$ and thus $\mu_n^{t^{h_n}} \to 0$ as $n \to \infty$. Similar steps as in Lemma 4.4 yield

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

□

Next, we will state the main theorem of this section concerning the Γ-limit of the functionals $\hat{H}_{1,n}^{\ell,k_n,\mathcal{T}_n}$ for $\ell > \gamma$. The Γ-limit is different to the one obtained for the fully atomistic energy $H_{1,n}^{\ell}$, see Theorem 3.19. We will come back to this in Section 4.4.

Theorem 4.11. *Suppose that hypotheses (LJ1)–(LJ5) hold. Let $\ell > \gamma$ and $u_0^{(1)}, u_1^{(1)} \in \mathbb{R}_+^{K-1}$. Let $(k_n^1), (k_n^2)$ satisfy (4.6) and let $\mathcal{T} = (\mathcal{T}_n)$ satisfy (T1)–(T4). Then $(\hat{H}_{1,n}^{\ell,k_n,\mathcal{T}_n})$ Γ-converges with respect to the $L^1(0,1)$-topology to the functional $\hat{H}_1^{\ell,\mathcal{T}}$ defined by*

$$\begin{aligned}\hat{H}_1^{\ell,\mathcal{T}}(u) =& B(u_0^{(1)},\gamma)(1-\#(S_u\cap\{0\})) + B(u_1^{(1)},\gamma)(1-\#(S_u\cap\{1\}))\\ &+ B_{IFJ}\left(\hat{r}^{\mathcal{T}}, b(0,\mathcal{T}), u_0^{(1)}\right)\#(S_u\cap\{0\}) - \sum_{x:x\in S_u\cap(0,1)} b(x,\mathcal{T})J_{CB}(\gamma)\\ &+ B_{IFJ}\left(\hat{l}^{\mathcal{T}}, b(1,\mathcal{T}), u_1^{(1)}\right)\#(S_u\cap\{1\}) - \sum_{j=2}^{K}(j-1)\psi_j(\gamma)\end{aligned} \tag{4.42}$$

if $u \in SBV_c^{\ell}(0,1)$, and $+\infty$ else on $L^1(0,1)$, where $B_{IFJ}(r,s,\theta)$ is defined for $r = (r_1,\dots,r_k) \in \mathcal{I}(k)$, $s \in \mathbb{N}\cup\{+\infty\}$ and $\theta \in \mathbb{R}_+^{K-1}$ as

$$B_{IFJ}(r,s,\theta) = \min\left\{\min\{B_{AIF}(r), B_{BIF}(r), -sJ_{CB}(\gamma)\} + B(\theta,\gamma), B_{BJ}(\theta)\right\} \tag{4.43}$$

with

$$B_{AIF}(r) := B_{IF}^{(1)}(r) + B(\gamma) - \sum_{j=2}^{K} j\psi_j(\gamma), \tag{4.44}$$

and

$$\begin{aligned}B_{BIF}(r) := \min\Bigg\{&B_{IF}^{(2)}(r,m,\gamma) + B_{IF}^{(3)}(r,m+1) - \sum_{j=2+r_m}^{K}\psi_j(\gamma)(j-r_m-1)\\ &-\sum_{j=2}^{K}\sum_{s=r_m+1}^{r_{m+1}}\left(\frac{s}{j}\wedge 1\right)\psi_j(\gamma):\ m\in\{1,\dots,k-1\}\Bigg\},\end{aligned} \tag{4.45}$$

where B_{BJ}, $B_{IF}^{(1)}$, $B_{IF}^{(2)}$ and $B_{IF}^{(3)}$ are given in (3.74), (4.35), (4.38) *and* (4.39), *respectively.*

Remark 4.12. The definition of the jump energies for a jump at the interface are somewhat cumbersome. Note that in the case of nearest and next-to-nearest neighbour interactions ($K = 2$) the situation is much simpler. We have already noted that in this case $\hat{r}^{\mathcal{T}}$ and $\hat{l}^{\mathcal{T}}$ are completely described by the scalars $\hat{r}(\mathcal{T}), \hat{l}(\mathcal{T}) \in \mathbb{N}\cup\{\infty\}$. In particular, we have that the minimisation over m in (4.45) is trivial since $1 \leq m \leq k-1 \leq 1$. Hence, we have by Remark 4.9 that $B_{BIF}(r) = B(\gamma) - \left(r + \frac{1}{2}\right)J_{CB}(\gamma)$. See Proposition 4.14 below for the precise statement in this case.

Proof. Liminf inequality. Without loss of generality, we can assume that there is only one jump point. By symmetry, we only need to distinguish between a jump in 0 and in $(0,1)$.

Jump in 0. Let (u_n) be a sequence of functions converging to u with $S_u = \{0\}$ such that $\sup_n \hat{H}^{\ell,k_n,\mathcal{T}_n}_{1,n}(u_n) < +\infty$. Then Proposition 4.3 implies that $u_n \to u$ in $L^1(0,1)$ with

$$u(x) = \begin{cases} 0 & \text{if } x = 0, \\ (\ell-\gamma)+\gamma x & \text{if } 0 < x \leq 1. \end{cases} \tag{4.46}$$

By Lemma 4.4 there exist sequences $(T_n^1), (T_n^2) \subset \mathbb{N}$ with $0 < T_n^1 < k_n^1 - K < k_n^2 + 1 < T_n^2 < n - K$ such that

$$\lim_{n\to\infty} \frac{u_n^{T_n^i+1+s} - u_n^{T_n^i+s}}{\lambda_n} = \gamma, \quad \text{for } i \in \{1,2\} \text{ and } 0 \leq s \leq K-1. \tag{4.47}$$

We can write the energy in (4.23) as

$$\begin{aligned} \hat{H}^{\ell,k_n,\mathcal{T}_n}_{1,n}(u_n) = \sum_{j=2}^{K} \Bigg\{ & c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(u_{0,s}^{(1)}) + \sum_{i=0}^{T_n^1} \sigma_{j,n}^i + \sum_{i=T_n^1+1}^{k_n^1-1} \sigma_{j,n}^i + \sum_{s=1}^{j-1} \frac{s}{j} \mu_{j,n}^{k_n^1+s-1} \\ & + \sum_{i=k_n^1+j-1}^{k_n^2-j} \mu_{j,n}^i + \sum_{s=1}^{j-1} \frac{s}{j} \mu_{j,n}^{k_n^2-s} + \sum_{i=k_n^2-1}^{T_n^2} \sigma_{j,n}^i + \sum_{T_n^2+1}^{n-j} \sigma_{j,n}^i \\ & + c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(u_{1,s}^{(1)}) - (j-1)\psi_j(\gamma) \Bigg\} \end{aligned} \tag{4.48}$$

The estimate for the elastic boundary layer energy at 1 is exactly the same as in the case $\ell \leq \gamma$, see (4.22), and is given by

$$\liminf_{n\to\infty} \sum_{j=2}^{K} \left(\sum_{i=T_n^2+1}^{n-j} \sigma_{j,n}^i + c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(u_{1,s}^{(1)}) \right) \geq B(u_1^{(1)}, \gamma). \tag{4.49}$$

To estimate the remaining terms, we note that there exists $(h_n) \subset \mathbb{N}$ with $\lambda_n h_n \to 0$ such that

$$\lim_{n\to\infty} \frac{u_n^{h_n+1} - u_n^{h_n}}{\lambda_n} = +\infty. \tag{4.50}$$

We have to consider the following cases:

$$(1)\ h_n < T_n^1, \quad (2)\ T_n^1 + K \leq h_n < k_n^1, \quad (3)\ k_n^1 \leq h_n < r(\mathcal{T}_n), \quad (4)\ r(\mathcal{T}_n) \leq h_n. \tag{4.51}$$

Indeed, by extracting a subsequence, we can assume that $\liminf_{n\to\infty} \hat{H}^{\ell,k_n,\mathcal{T}_n}_{1,n}(u_n) = \lim_{n\to\infty} \hat{H}^{\ell,k_n,\mathcal{T}_n}_{1,n}(u_n)$. Note that by (4.47), we deduce $h_n \notin \{T_n^1, \dots, T_n^1 + K - 1\}$ for n sufficiently large. Let (h_n) be such that it oscillates between at least two of the cases (1)–(4), then we can extract a further subsequence which satisfies only one of the cases, which does not change the limit.

The first two cases correspond to a jump in the atomistic region. In the first case, the jump is sufficiently far from the atomistic/continuum interface and leads to the same jump energy as a jump in 0 in the fully atomistic model. The jump in the second case is closer to the continuum region and leads to a jump energy of the form $B_{AIF}(\hat{r}^{\mathcal{T}})$, see (4.44). In the third case, the jump is exactly at the interface between the atomistic region and the continuum region. This yields a jump energy of the form $B_{BIF}(\hat{r}^{\mathcal{T}})$, see (4.45). The last case corresponds to a jump within the continuum region.

Case (1). Consider (u_n) as above with (h_n) satisfying (4.50) and (4.51, (1)). We show

$$\liminf_{n\to\infty} \hat{H}_{1,n}^{\ell,k_n,\mathcal{T}_n}(u_n) \geq B_{BJ}(u_0^{(1)}) + B(u_1^{(1)},\gamma) - \sum_{j=2}^{K}(j-1)\psi_j(\gamma). \tag{4.52}$$

With the same arguments as in Theorem 3.19, we obtain

$$\liminf_{n\to\infty} \sum_{j=2}^{K}\sum_{i=0}^{T_n^1} \sigma_{j,n}^i \geq B_b(u_0^{(1)}) + B(\gamma) - \sum_{j=2}^{K} j\psi_j(\gamma). \tag{4.53}$$

Combining (3.74), (4.48), (4.49), (4.53) and $\sigma_{j,n}^i, \mu_{j,n}^i \geq 0$ implies (4.52).

Case (2). Assume that (u_n) satisfies (4.50) with (h_n) such that (4.51, (2)) holds true. We show that

$$\liminf_{n\to\infty} \hat{H}_{1,n}^{\ell,k_n,\mathcal{T}_n}(u_n) \geq B(u_0^{(1)},\gamma)+B(u_1^{(1)},\gamma)+B(\gamma)+B_{IF}^{(1)}(\hat{r}^{\mathcal{T}})-\sum_{j=2}^{K}(2j-1)\psi_j(\gamma), \tag{4.54}$$

where $\hat{r}^{\mathcal{T}} = (\hat{r}_1^{\mathcal{T}},\dots,\hat{r}_{k_r^{\mathcal{T}}}^{\mathcal{T}})$ is given in (4.28). First, we estimate the elastic boundary layer energy at 0. This can be done in a similar way as in the case $\ell \leq \gamma$, see (4.21), and we obtain

$$\liminf_{n\to\infty} \sum_{j=2}^{K}\left(c_j\sum_{s=1}^{j-1}\frac{j-s}{j}J_1(u_{0,s}^{(1)}) + \sum_{i=0}^{T_n^1}\sigma_{j,n}^i\right) \geq B(u_0^{(1)},\gamma). \tag{4.55}$$

We will now estimate

$$\Omega_n := \sum_{j=2}^{K}\left\{\sum_{i=T_n^1+1}^{k_n^1-1}\sigma_{j,n}^i + \sum_{s=1}^{j-1}\frac{s}{j}\mu_{j,n}^{k_n^1+s-1} + \sum_{i=k_n^1+j-1}^{r(\mathcal{T}_n)-1}\mu_{j,n}^i\right\}. \tag{4.56}$$

As in the proof of Theorem 3.19, we deduce from (4.50) that

$$\begin{aligned}\sum_{j=2}^{K}\sum_{h_n-j+1}^{h_n}\sigma_{j,n}^i =& \sum_{j=2}^{K}c_j\sum_{s=1}^{j-1}\frac{j-s}{j}\left\{J_1\left(\frac{u_n^{h_n-s+1}-u_n^{h_n-s}}{\lambda_n}\right) + J_1\left(\frac{u_n^{h_n+s+1}-u_n^{h_n+s}}{\lambda_n}\right)\right\}\\ &-\sum_{j=2}^{K}j\psi_j(\gamma) + r(n)\end{aligned} \tag{4.57}$$

where

$$r(n)=\sum_{j=1}^{K}\sum_{s=-j+1}^{0}J_j\left(\frac{u_n^{h_n+j+s}-u_n^{h_n+s}}{j\lambda_n}\right)\to 0\quad\text{as } n\to\infty.$$

Thus it remains to prove that for n sufficiently large it holds

$$\sum_{j=2}^{K}\left\{\sum_{i=T_n^1+1}^{h_n-j}\sigma_{j,n}^i+c_j\sum_{s=1}^{j-1}\frac{j-s}{j}J_1\left(\frac{u_n^{h_n-s+1}-u_n^{h_n-s}}{\lambda_n}\right)\right\}\geq B(\gamma)-\omega_1(n) \tag{4.58}$$

$$\sum_{j=2}^{K}\left\{c_j\sum_{s=1}^{j-1}\frac{j-s}{j}J_1\left(\frac{u_n^{h_n+s+1}-u_n^{h_n+s}}{\lambda_n}\right)+\sum_{i=h_n+1}^{k_n^1-1}\sigma_{j,n}^i+\sum_{s=1}^{j-1}\frac{s}{j}\mu_{j,n}^{k_n^1+s-1}+\sum_{i=k_n^1+j-1}^{r(\mathcal{T}_n)-1}\mu_{j,n}^i\right\}$$
$$\geq B_{IF}^{(1)}(\hat r^{\mathcal{T}})-\omega_2(n), \tag{4.59}$$

where $\omega_1(n)$, $\omega_2(n)\to 0$ as $n\to\infty$. The estimate (4.58) can be proven in the same way as inequality (3.93) and thus we show (4.59) only.

Let us first assume that $\hat r(\mathcal{T})<+\infty$, where $\hat r(\mathcal{T})$ is defined in (4.24). Since we are interested in the behaviour as $n\to\infty$, it is not restrictive to assume that

$$\hat r_{s,n}^{\mathcal{T}}-k_n^1=\hat r_s^{\mathcal{T}}\quad\text{for all } s\in\{1,\dots,k_r^{\mathcal{T}}\}, \tag{4.60}$$

see Remark 4.7. We define for $0\leq i\leq r(\mathcal{T}_n)-h_n-1$,

$$\hat u_n^i=\frac{u_n^{i+h_n+1}-u_n^{h_n+1}}{\lambda_n}.$$

The definition of $\hat u_n$ and $\sigma_j^i(\hat u_n)$, see (4.33), imply that

$$\sigma_j^{i-h_n-1}(\hat u_n)=J_j\left(\frac{u_n^{i+j}-u_n^i}{j\lambda_n}\right)+\frac{c_j}{j}\sum_{s=i}^{i+j-1}J_1\left(\frac{u_n^{s+1}-u_n^s}{\lambda_n}\right)-\psi_j(\gamma)=\sigma_{j,n}^i,$$

for $h_n+1\leq i\leq k_n^1-1$. Moreover, we have that $\mu_j^{i-h_n-1}(\hat u)=\mu_{j,n}^i$ for $k_n^1\leq i\leq r(\mathcal{T}_n)-1$, see (4.34). Let us set $q_n=k_n^1-h_n-1$ and let us recall that $\hat r^{\mathcal{T}}=(\hat r_1^{\mathcal{T}},\dots,\hat r_{k_r^{\mathcal{T}}}^{\mathcal{T}})$ is such that $\hat r_{k_r^{\mathcal{T}}}^{\mathcal{T}}=\hat r(\mathcal{T})$, see assumption (T3). The left-hand side of (4.59) reads in terms of $\hat u_n$ as

$$\sum_{j=2}^{K}\left\{c_j\sum_{s=1}^{j-1}\frac{j-s}{j}J_1\left(\frac{u_n^{h_n+s+1}-u_n^{h_n+s}}{\lambda_n}\right)+\sum_{i=h_n+1}^{k_n^1-1}\sigma_{j,n}^i+\sum_{s=1}^{j-1}\frac{s}{j}\mu_{j,n}^{k_n^1-1+s}+\sum_{i=k_n^1+j-1}^{r(\mathcal{T}_n)-1}\mu_{j,n}^i\right\}$$
$$=\sum_{j=2}^{K}\left\{c_j\sum_{s=1}^{j-1}\frac{j-s}{j}J_1\left(\hat u_n^s-\hat u_n^{s-1}\right)+\sum_{i=0}^{q_n-1}\sigma_j^i(\hat u_n)+\sum_{s=1}^{j-1}\frac{s}{j}\mu_j^{q_n-1+s}(\hat u_n)\right.$$
$$\left.+\sum_{i=q_n-1+j}^{\hat r(\mathcal{T})+q_n-1}\mu_j^i(\hat u_n)\right\}\geq B_{IF}^{(1)}(\hat r^{\mathcal{T}}).$$

Note that we used $r(\mathcal{T}_n) = k_n^1 + \hat{r}(\mathcal{T})$, see (4.60). The last inequality follows from the fact that $\hat{u}_n$ is a competitor for the infimum problem in the definition of $B_{IF}^{(1)}(\hat{r}^{\mathcal{T}})$, see (4.35), for n sufficiently large. Clearly, we have $\hat{u}_n^0 = 0$ for all $n \in \mathbb{N}$. Consider $s \in \{1, \ldots, k_r^{\mathcal{T}} - 1\}$ and $i \in \{\hat{r}_s^{\mathcal{T}}, \ldots, \hat{r}_{s+1}^{\mathcal{T}} - 1\}$. The assumptions (T3), (4.60) and $u_n \in \mathcal{A}_{\mathcal{T}_n}(0,1)$ imply that u_n' is constant on $\lambda_n(k_n^1 + \hat{r}_s^{\mathcal{T}}, k_n^1 + \hat{r}_{s+1}^{\mathcal{T}})$. Hence, we have for $\hat{u}_n$ and $q_n = k_n^1 - h_n - 1$ that

$$\hat{u}_n^{q_n+i+1} - \hat{u}_n^{q_n+i} = \frac{u_n^{k_n^1+i+1} - u_n^{k_n^1+i}}{\lambda_n} = \frac{u_n^{k_n^1+\hat{r}_s^{\mathcal{T}}+1} - u_n^{k_n^1+\hat{r}_s^{\mathcal{T}}}}{\lambda_n} = \hat{u}_n^{\hat{r}_s^{\mathcal{T}}+q_n+1} - \hat{u}_n^{\hat{r}_s^{\mathcal{T}}+q_n}.$$

Hence, $\hat{u}_n$ is an admissible test function for $B_{IF}^{(1)}(\hat{r}^{\mathcal{T}})$, with $q = k_n^1 - h_n - 1$, and (4.59) holds true in the case $\hat{r}(\mathcal{T}) < +\infty$.

Let us now consider $\hat{r}(\mathcal{T}) = \infty$. By (4.27), it is not restrictive to assume that

$$\hat{r}_{s,n}^{\mathcal{T}} - k_n^1 = \hat{r}_s^{\mathcal{T}} \quad \text{for all } s \in \{1, \ldots, k_r^{\mathcal{T}} - 1\}. \tag{4.61}$$

Moreover, we deduce from Lemma 4.10 and $(r(\mathcal{T}_n) - \hat{r}_{k_r^{\mathcal{T}}-1,n}^{\mathcal{T}}) \to +\infty$ that

$$\lim_{n\to\infty} \frac{u_n^{\hat{r}_{k_r^{\mathcal{T}}-1,n}^{\mathcal{T}}+i+1} - u_n^{\hat{r}_{k_r^{\mathcal{T}}-1,n}^{\mathcal{T}}+i}}{\lambda_n} = \gamma, \tag{4.62}$$

for $0 \leq i \leq K - 1$. We define the function $v_n : \mathbb{N}_0 \to \mathbb{R}$ by

$$v_n^i = \begin{cases} \frac{u_n^{i+h_n+1} - u_n^{h_n+1}}{\lambda_n} & \text{if } 0 \leq i \leq \hat{r}_{k_r^{\mathcal{T}}-1,n}^{\mathcal{T}} - h_n - 1, \\ \gamma(i - \hat{r}_{k_r^{\mathcal{T}}-1,n}^{\mathcal{T}} + h_n + 1) + \frac{u_n^{\hat{r}_{k_r^{\mathcal{T}}-1,n}^{\mathcal{T}}} - u_n^{h_n+1}}{\lambda_n} & \text{if } \hat{r}_{k_r^{\mathcal{T}}-1,n}^{\mathcal{T}} - h_n - 1 \leq i. \end{cases}$$

We show that the definition of v_n implies that v_n is a competitor for the infimum problem in the definition of $B_{IF}^{(1)}(\hat{r}^{\mathcal{T}})$ with $q_n = k_n^1 - h_n - 1$, see (4.36). Clearly, it holds $v_n^0 = 0$. Consider $s \in \{1, \ldots, k_r^{\mathcal{T}} - 2\}$ and $i \in \{\hat{r}_s^{\mathcal{T}}, \ldots, \hat{r}_{s+1}^{\mathcal{T}} - 1\}$. As in the case $\hat{r}(\mathcal{T}) < +\infty$, we deduce from $u_n \in \mathcal{A}_{\mathcal{T}_n}(0,1)$, (4.61) and $q_n = k_n^1 - h_n - 1$ that

$$v_n^{q_n+i+1} - v_n^{q_n+i} = v_n^{q_n+\hat{r}_s^{\mathcal{T}}+1} - v_n^{q_n+\hat{r}_s^{\mathcal{T}}}.$$

Moreover, the definition of v_n yields $v_n^{i+1} - v_n^i = \gamma$ for $i \geq q_n + \hat{r}_{k_r^{\mathcal{T}}-1}^{\mathcal{T}}$. Hence, v_n is a test function for $B_{IF}^{(1)}(\hat{r}^{\mathcal{T}})$, see (4.36). Note that the definition of v_n and (4.62) imply that

$$\begin{aligned} \frac{u_n^{i+1} - u_n^i}{\lambda_n} &= v_n^{i-h_n} - v_n^{i-h_n-1} \quad \text{for } h_n + 1 \leq i \leq \hat{r}_{k_r^{\mathcal{T}}-1,n}^{\mathcal{T}} - 1, \\ \lim_{n\to\infty} \frac{u_n^{i+1} - u_n^i}{\lambda_n} &= \gamma = v_n^{i-h_n} - v_n^{i-h_n-1} \quad \text{for } \hat{r}_{k_r^{\mathcal{T}}-1,n}^{\mathcal{T}} \leq i \leq \hat{r}_{k_r^{\mathcal{T}}-1,n}^{\mathcal{T}} + K - 1. \end{aligned} \tag{4.63}$$

As in the case $\hat{r}(\mathcal{T}) < +\infty$, we deduce that

$$\begin{aligned}\sigma_{j,n}^i =& \sigma_j^{i-h_n-1}(v_n) \quad \text{for } h_n+1 \le i \le \hat{r}^{\mathcal{T}}_{k_r^{\mathcal{T}}-1,n} - j \\ \mu_{j,n}^i =& \mu_j^{i-h_n-1}(v_n) \quad \text{for } k_n^1 \le i \le \hat{r}^{\mathcal{T}}_{k_r^{\mathcal{T}}-1,n} - 1.\end{aligned} \tag{4.64}$$

From (4.64), $\hat{r}^{\mathcal{T}}_{k_r^{\mathcal{T}}-1,n} = \hat{r}^{\mathcal{T}}_{k_r^{\mathcal{T}}-1} + k_n^1 < r(\mathcal{T}_n)$ and $\mu_{j,n}^i \ge 0$, we obtain that

$$\begin{aligned}&\sum_{j=2}^K \Bigg\{ \sum_{i=h_n+1}^{k_n^1-1} \sigma_{j,n}^i + \sum_{s=1}^{j-1} \frac{s}{j} \mu_{j,n}^{s+k_n^1-1} + \sum_{i=k_n^1+j-1}^{r(\mathcal{T}_n)-1} \mu_{j,n}^i \Bigg\} \\ &\ge \sum_{j=2}^K \Bigg\{ \sum_{i=h_n+1}^{(k_n^1-1)\wedge(\hat{r}^{\mathcal{T}}_{k_r^{\mathcal{T}}-1,n}-j)} \sigma_{j,n}^i + \sum_{i=\hat{r}^{\mathcal{T}}_{k_r^{\mathcal{T}}-1,n}-j+1}^{k_n^1-1} \sigma_{j,n}^i + \sum_{i=k_n^1}^{\hat{r}^{\mathcal{T}}_{k_r^{\mathcal{T}}-1,n}-1} \left(\frac{i-k_n^1+1}{j} \wedge 1 \right) \mu_{j,n}^i \Bigg\} \\ &\ge \sum_{j=2}^K \Bigg\{ \sum_{i=0}^{k_n^1-h_n-2} \sigma_j^i(v_n) + \sum_{i=k_n^1-h_n-1}^{\hat{r}^{\mathcal{T}}_{k_r^{\mathcal{T}}-1}+k_n^1-h_n-2} \left(\frac{i-k_n^1+h_n+2}{j} \wedge 1 \right) \mu_j^i(v_n) \Bigg\} - \hat{\omega}(n),\end{aligned}$$

where

$$\hat{\omega}(n) = \sum_{j=2}^K \sum_{i=k_n^1+\hat{r}^{\mathcal{T}}_{k_r^{\mathcal{T}}-1}-j+1}^{k_n^1-1} |\sigma_{j,n}^i - \sigma_j^{i-h_n-1}(v_n)| \to 0 \quad \text{as } n \to \infty. \tag{4.65}$$

Indeed, (4.65) follows from (4.63) and the continuity of $J_1, \dots, J_K$ on its domain. Altogether, using the previous calculations and $q_n = k_n^1 - h_n - 1$, we can rewrite the left-hand side of (4.59) as

$$\begin{aligned}&\sum_{j=2}^K \Bigg\{ c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1\left(\frac{u_n^{h_n+s+1} - u_n^{h_n+s}}{\lambda_n} \right) + \sum_{i=h_n+1}^{k_n^1-1} \sigma_{j,n}^i + \sum_{s=1}^{j-1} \frac{s}{j} \mu_{j,n}^{k_n^1-1+s} + \sum_{i=k_n^1+j-1}^{r(\mathcal{T}_n)-1} \mu_{j,n}^i \Bigg\} \\ &\ge \sum_{j=2}^K \Bigg\{ c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1\left(v_n^s - v_n^{s-1} \right) + \sum_{i=0}^{q_n-1} \sigma_j^i(v_n) + \sum_{i=q_n}^{\hat{r}^{\mathcal{T}}_{k_r^{\mathcal{T}}-1}+q_n-1} \left(\frac{i-q_n+1}{j} \wedge 1 \right) \mu_j^i(v_n) \Bigg\} \\ &\quad - \hat{\omega}(n) - \tilde{\omega}(n) \ge B_{IF}^{(1)}(\hat{r}^{\mathcal{T}}) - \hat{\omega}(n) - \tilde{\omega}(n).\end{aligned}$$

where

$$\tilde{\omega}(n) = \sum_{j=2}^K \sum_{i=k_n^1+\hat{r}^{\mathcal{T}}_{k_r^{\mathcal{T}}-1}}^{h_n+j-1} \frac{j-(i-h_n)}{j} \left| J_1\left(\frac{u_n^{i+1}-u_n^i}{\lambda_n} \right) - J_1(\gamma) \right|,$$

and $\tilde{\omega}(n) \to 0$ as $n \to \infty$, see (4.63). The last inequality follows by the fact that v_n is an admissible test function for the infimum problem in the definition of $B_{IF}^{(1)}(\hat{r}^{\mathcal{T}})$. Combining this with (4.65) proves the inequality (4.59) in the remaining case $\hat{r}(\mathcal{T}) = +\infty$.

By using (4.48), (4.49), (4.55), (4.57)–(4.59) and the fact that $\sigma^i_{j,n}, \mu^i_{j,n} \geq 0$, we obtain (4.54).

Case (3). Let (u_n) satisfy (4.50) with (h_n) such that ((4.51), (3)) holds true. We show that

$$\liminf_{n\to\infty} \hat{H}^{\ell,k_n,\mathcal{T}_n}_{1,n}(u_n) \geq B(u_0^{(1)},\gamma) + B(u_1^{(1)},\gamma) + B_{BIF}(\hat{r}^{\mathcal{T}}) - \sum_{j=2}^{K}(j-1)\psi_j(\gamma). \tag{4.66}$$

It is not restrictive to assume that

$$\hat{r}^{\mathcal{T}}_{m,n} \leq h_n < \hat{r}^{\mathcal{T}}_{m+1,n}, \tag{4.67}$$

for some $1 \leq m \leq k_r^{\mathcal{T}} - 1$. Indeed, since $k_n^1 = \hat{r}^{\mathcal{T}}_{1,n} \leq h_n < r(\mathcal{T}_n) = \hat{r}^{\mathcal{T}}_{k_r^{\mathcal{T}},n}$ we obtain by passing to a subsequence (4.67) for some $m \in \{1,\dots,k_r^{\mathcal{T}}-1\}$. Assuming (4.67), we show that

$$\begin{aligned}\liminf_{n\to\infty} \Omega_n \geq B^{(2)}_{IF}(\hat{r}^{\mathcal{T}},m,\gamma) + B^{(3)}_{IF}(\hat{r}^{\mathcal{T}},m+1) - \sum_{j=2+\hat{r}^{\mathcal{T}}_m}^{K} \left(j - \hat{r}^{\mathcal{T}}_m - 1\right)\psi_j(\gamma)\\ - \sum_{j=2}^{K} \sum_{i=\hat{r}^{\mathcal{T}}_m+1}^{\hat{r}^{\mathcal{T}}_{m+1}} \left(\frac{i}{j} \wedge 1\right)\psi_j(\gamma),\end{aligned} \tag{4.68}$$

where Ω_n is defined in (4.56). Combining (4.68) with the definition of $B_{BIF}(\hat{r}^{\mathcal{T}})$, see (4.45), and (4.48), (4.49), (4.55), we obtain (4.66).

If $m = k_r^{\mathcal{T}} - 1$, we can assume that $\hat{r}(\mathcal{T}) < +\infty$. Otherwise, we have by the definition of $\hat{r}^{\mathcal{T}}$ that $\lim_{n\to\infty}(\hat{r}^{\mathcal{T}}_{m+1,n} - \hat{r}^{\mathcal{T}}_{m,n}) = +\infty$ and Lemma 4.10 combined with $u_n \in \mathcal{A}_{\mathcal{T}_n}(0,1)$ yields

$$\lim_{n\to\infty} \frac{u_n^{h_n+1} - u_n^{h_n}}{\lambda_n} = \lim_{n\to\infty} \frac{u_n^{\hat{r}^{\mathcal{T}}_{m,n}+1} - u_n^{\hat{r}^{\mathcal{T}}_{m,n}}}{\lambda_n} = \gamma,$$

which contradicts (4.50). Let us assume that n is sufficiently large such that it holds

$$\hat{r}^{\mathcal{T}}_{s,n} - k_n^1 = \hat{r}^{\mathcal{T}}_s \quad \text{for } s \in \{1,\dots,k_r^{\mathcal{T}}-1\}. \tag{4.69}$$

From (4.50), (4.67) and $u_n \in \mathcal{A}_{\mathcal{T}_n}(0,1)$, we deduce that

$$\lim_{n\to\infty} \frac{u_n^{s+k_n^1+1} - u_n^{s+k_n^1}}{\lambda_n} = \lim_{n\to\infty} \frac{u_n^{h_n+1} - u_n^{h_n}}{\lambda_n} = +\infty, \text{ for } s \in \{\hat{r}^{\mathcal{T}}_m,\dots,\hat{r}^{\mathcal{T}}_{m+1}-1\}. \tag{4.70}$$

For n sufficiently large, such that (4.69) holds, the term Ω_n, see (4.56), reads

$$\begin{aligned}\Omega_n =& \sum_{j=2}^{K}\left\{\sum_{i=T_n^1+1}^{(k_n^1-1)\wedge(\hat r_{m,n}^{\mathcal T}-j)}\sigma_{j,n}^i + \sum_{s=1}^{\hat r_m^{\mathcal T}}\left(\frac{s}{j}\wedge 1\right)\mu_{j,n}^{k_n^1+s-1} + \sum_{s=\hat r_{m+1}^{\mathcal T}+1}^{r(\mathcal T_n)-k_n^1}\left(\frac{s}{j}\wedge 1\right)\mu_{j,n}^{k_n^1+s-1}\right\}\\ &+\sum_{j=2+\hat r_m^{\mathcal T}}^{K}\frac{c_j}{j}\sum_{i=\hat r_{m,n}^{\mathcal T}-j+1}^{k_n^1-1}\sum_{s=i}^{\hat r_{m,n}^{\mathcal T}-1}J_1\left(\frac{u_n^{s+1}-u_n^s}{\lambda_n}\right)-\sum_{j=2+\hat r_m^{\mathcal T}}^{K}(j-1-\hat r_m^{\mathcal T})\psi_j(\gamma)\\ &+\sum_{j=2+\hat r_{m+1}^{\mathcal T}}^{K}\frac{c_j}{j}\sum_{i=\hat r_{m,n}^{\mathcal T}-j+1}^{k_n^1-1}\sum_{s=\hat r_{m+1,n}^{\mathcal T}}^{i+j-1}J_1\left(\frac{u_n^{s+1}-u_n^s}{\lambda_n}\right)-\sum_{j=2}^{K}\sum_{s=\hat r_m^{\mathcal T}+1}^{\hat r_{m+1}^{\mathcal T}}\left(\frac{s}{j}\wedge 1\right)\psi_j(\gamma)\\ &+r(n),\end{aligned}\tag{4.71}$$

where $r(n)$ is defined by

$$r(n)=\sum_{j=2+\hat r_m^{\mathcal T}}^{K}\sum_{i=\hat r_{m,n}^{\mathcal T}-j+1}^{k_n^1-1}J_j\left(\frac{u_n^{i+j}-u_n^i}{\lambda_n}\right)+\sum_{j=1}^{K}\sum_{s=\hat r_m^{\mathcal T}+1}^{\hat r_{m+1}^{\mathcal T}}\left(\frac{s}{j}\wedge 1\right)J_j\left(\frac{u_n^{s+k_n^1}-u_n^{s+k_n^1-1}}{\lambda_n}\right).$$

From (4.70) and $\lim_{z\to+\infty}J_j(z)=0$ for $j\in\{1,\dots,K\}$, we deduce that $r(n)\to 0$ as $n\to\infty$. To prove (4.68), it remains to show the following inequalities

$$\begin{aligned}&\sum_{j=2+\hat r_m^{\mathcal T}}^{K}\frac{c_j}{j}\sum_{i=\hat r_{m,n}^{\mathcal T}-j+1}^{k_n^1-1}\sum_{s=i}^{\hat r_{m,n}^{\mathcal T}-1}J_1\left(\frac{u_n^{s+1}-u_n^s}{\lambda_n}\right)\\ &+\sum_{j=2}^{K}\left\{\sum_{i=T_n^1+1}^{(k_n^1-1)\wedge(\hat r_{m,n}^{\mathcal T}-j)}\sigma_{j,n}^i+\sum_{s=1}^{\hat r_m^{\mathcal T}}\left(\frac{s}{j}\wedge 1\right)\mu_{j,n}^{k_n^1+s-1}\right\}\ge B_{IF}^{(2)}(\hat r^{\mathcal T},m,\gamma)-r_1(n)\end{aligned}\tag{4.72}$$

$$\begin{aligned}&\sum_{j=2+\hat r_{m+1}^{\mathcal T}}^{K}\frac{c_j}{j}\sum_{i=\hat r_{m,n}^{\mathcal T}-j+1}^{k_n^1-1}\sum_{s=\hat r_{m+1,n}^{\mathcal T}}^{i+j-1}J_1\left(\frac{u_n^{s+1}-u_n^s}{\lambda_n}\right)+\sum_{j=2}^{K}\sum_{s=\hat r_{m+1}^{\mathcal T}+1}^{r(\mathcal T_n)-k_n^1}\left(\frac{s}{j}\wedge 1\right)\mu_{j,n}^{k_n^1+s-1}\\ &\quad\ge B_{IF}^{(3)}(\hat r^{\mathcal T},m+1)-r_2(n),\end{aligned}\tag{4.73}$$

where $r_1(n),r_2(n)\to 0$ as $n\to\infty$. In order to prove (4.72), we define suitable test functions for the boundary layer energy $B_{IF}^{(2)}(\hat r^{\mathcal T},m,\gamma)$. Let us define for $i\ge 0$

$$\tilde u_n^i=\begin{cases}\frac{u_n^{\hat r_{m,n}^{\mathcal T}}-u_n^{\hat r_{m,n}^{\mathcal T}-i}}{\lambda_n} & \text{if } 0\le i\le \hat r_{m,n}^{\mathcal T}-T_n^1-1,\\ \gamma(i-\hat r_{m,n}^{\mathcal T}+T_n^1+1)+\frac{u_n^{\hat r_{m,n}^{\mathcal T}}-u_n^{T_n^1+1}}{\lambda_n} & \text{if } i\ge \hat r_{m,n}^{\mathcal T}-T_n^1-1.\end{cases}\tag{4.74}$$

We claim that $\tilde u_n$ is a competitor for the infimum problem defining $B_{IF}^{(2)}(\hat r^{\mathcal T},m,\gamma)$, see (4.38), if n is sufficiently large. The above construction implies $\tilde u_n^0=0$ and $\tilde u_n^{i+1}-\tilde u_n^i=\gamma$ for $i\ge\hat r_{m,n}^{\mathcal T}-T_n^1-1$. Fix $s\in\{2,\dots,m\}$ and $i\in\{\hat r_m^{\mathcal T}-\hat r_s^{\mathcal T},\dots,\hat r_m^{\mathcal T}-\hat r_{s-1}^{\mathcal T}-1\}$. From

$u_n \in \mathcal{A}_{\mathcal{T}_n}(0,1)$ and (4.69), we deduce that u_n' is constant on $\lambda_n(k_n^1+\hat{r}_{s-1}^{\mathcal{T}}, k_n^1+\hat{r}_s^{\mathcal{T}})$. Hence,

$$\tilde{u}_n^{i+1} - \tilde{u}_n^i = \frac{u_n^{k_n^1+\hat{r}_m^{\mathcal{T}}-i} - u_n^{k_n^1+\hat{r}_m^{\mathcal{T}}-i-1}}{\lambda_n} = \frac{u_n^{k_n^1+\hat{r}_s^{\mathcal{T}}} - u_n^{k_n^1+\hat{r}_s^{\mathcal{T}}-1}}{\lambda_n} = \tilde{u}_n^{\hat{r}_m^{\mathcal{T}}-\hat{r}_s^{\mathcal{T}}+1} - \tilde{u}_n^{\hat{r}_m^{\mathcal{T}}-\hat{r}_s^{\mathcal{T}}}.$$

This matches the constraint in (4.38). Let us rewrite the left-hand side of (4.72) in terms of $\tilde{u}_n$. By the definition of $\tilde{u}$ and σ_j^i, we have

$$\begin{aligned}\sigma_j^i(\tilde{u}) =& J_j\left(\frac{u_n^{\hat{r}_{m,n}^{\mathcal{T}}-i} - u_n^{\hat{r}_{m,n}^{\mathcal{T}}-i-j}}{j\lambda_n}\right) + \frac{c_j}{j}\sum_{s=i}^{i+j-1} J_1\left(\frac{u_n^{\hat{r}_{m,n}^{\mathcal{T}}-s} - u_n^{\hat{r}_{m,n}^{\mathcal{T}}-s-1}}{\lambda_n}\right) - \psi_j(\gamma)\\ =&\sigma_{j,n}^{\hat{r}_{m,n}^{\mathcal{T}}-j-i}\end{aligned}$$

for $i \in \{0, \ldots, \hat{r}_{m,n}^{\mathcal{T}} - j - T_n^1 - 1\}$. Hence, we obtain, using (4.69), that

$$\begin{aligned}\sum_{j=2}^{K}\sum_{i=T_n^1+1}^{(k_n^1-1)\wedge(\hat{r}_{m,n}^{\mathcal{T}}-j)} \sigma_{j,n}^i =& \sum_{j=2}^{K}\sum_{i=(\hat{r}_{m,n}^{\mathcal{T}}-j-(k_n^1-1))\vee 0}^{\hat{r}_{m,n}^{\mathcal{T}}-j-T_n^1-1} \sigma_{j,n}^{\hat{r}_{m,n}^{\mathcal{T}}-j-i} = \sum_{j=2}^{K}\sum_{i=(\hat{r}_m^{\mathcal{T}}+1-j)\vee 0}^{\hat{r}_{m,n}^{\mathcal{T}}-j-T_n^1-1} \sigma_j^i(\tilde{u}_n)\\ =& \sum_{j=2}^{K}\sum_{i\geq(\hat{r}_m^{\mathcal{T}}+1-j)\vee 0} \sigma_j^i(\tilde{u}_n) - r_1(n)\end{aligned} \tag{4.75}$$

with

$$r_1(n) = \sum_{j=2}^{K}\sum_{i=\hat{r}_{m,n}^{\mathcal{T}}-j-T_n^1}^{\hat{r}_{m,n}^{\mathcal{T}}-T_n^1-2}\left\{J_j\left(\frac{\tilde{u}_n^{i+j}-\tilde{u}_n^i}{j}\right) + \frac{c_j}{j}\sum_{s=i}^{i+j-1} J_1\left(\tilde{u}_n^{s+1}-\tilde{u}_n^s\right) - \psi_j(\gamma)\right\} \to 0$$

as $n \to \infty$. Indeed, the definition of $\tilde{u}_n$ implies $\tilde{u}_n^{i+1} - \tilde{u}_n^i = \gamma$ for $i \geq \hat{r}_{m,n}^{\mathcal{T}} - T_n^1 - 1$. Hence, $\sigma_j^i(\tilde{u}_n) = J_j(\gamma) + c_j J_1(\gamma) - \psi_j(\gamma) = 0$ for $i \geq \hat{r}_{m,n}^{\mathcal{T}} - T_n^1 - 1$. Furthermore, by the choice of T_n^1, see (4.47), we have

$$\lim_{n\to\infty}(\tilde{u}_n^{\hat{r}_{m,n}^{\mathcal{T}}-T_n^1-K+s} - \tilde{u}_n^{\hat{r}_{m,n}^{\mathcal{T}}-T_n^1-K+s-1}) = \lim_{n\to\infty}\frac{u_n^{T_n^1+K-s+1} - u_n^{T_n^1-K-s}}{\lambda_n} = \gamma$$

for $s \in \{1, \ldots, K-1\}$. Hence, $r_1(n) \to 0$ as $n \to \infty$. Moreover, we can rewrite the terms involving $\mu_{j,n}^i$ in (4.72) by

$$\begin{aligned}\sum_{j=2}^{K}\sum_{s=1}^{\hat{r}_m^{\mathcal{T}}}\left(\frac{s}{j}\wedge 1\right)\mu_{j,n}^{s+k_n^1-1} =& \sum_{j=2}^{K}\sum_{s=1}^{\hat{r}_m^{\mathcal{T}}}\left(\frac{\hat{r}_m^{\mathcal{T}}-s+1}{j}\wedge 1\right)\mu_{j,n}^{\hat{r}_m^{\mathcal{T}}+k_n^1-s}\\ =& \sum_{j=2}^{K}\sum_{s=0}^{\hat{r}_m^{\mathcal{T}}-1}\left(\frac{\hat{r}_m^{\mathcal{T}}-s}{j}\wedge 1\right)\mu_j^s(\tilde{u}_n).\end{aligned} \tag{4.76}$$

Note that we used $\mu_j^i(\tilde{u}) = \mu_j^{\hat{r}_m^{\mathcal{T}}+k_n^1-i-1}$ for $i \in \{0, \ldots, \hat{r}_m^{\mathcal{T}} - 1\}$. It is left to rewrite the terms involving only J_1 on the left-hand side in (4.72) in terms of $\tilde{u}_n$. For given $j \in \{2+\hat{r}^{\mathcal{T}}_m, \dots, K\}$ and n sufficiently large such that (4.69) holds true, we have that

$$\begin{aligned}
&\sum_{i=\hat{r}^{\mathcal{T}}_{m,n}-j+1}^{k^1_n-1} \sum_{s=i}^{\hat{r}^{\mathcal{T}}_{m,n}-1} J_1\left(\frac{u^{s+1}_n - u^s_n}{\lambda_n}\right) = \sum_{i=\hat{r}^{\mathcal{T}}_{m,n}-j+1}^{k^1_n-1} \sum_{s=0}^{\hat{r}^{\mathcal{T}}_{m,n}-i-1} J_1\left(\frac{u_n^{\hat{r}^{\mathcal{T}}_{m,n}-s} - u_n^{\hat{r}^{\mathcal{T}}_{m,n}-s-1}}{\lambda_n}\right)\\
&= \sum_{i=\hat{r}^{\mathcal{T}}_{m,n}-j+1}^{k^1_n-1} \sum_{s=0}^{\hat{r}^{\mathcal{T}}_{m,n}-i-1} J_1\left(\tilde{u}^{s+1}_n - \tilde{u}^s_n\right) = \sum_{i=0}^{j-\hat{r}^{\mathcal{T}}_m-2} \sum_{s=0}^{j-i-2} J_1\left(\tilde{u}^{s+1}_n - \tilde{u}^s_n\right)\\
&= \sum_{s=0}^{j-2} \sum_{i=0}^{j-2-s\vee \hat{r}^{\mathcal{T}}_m} J_1\left(\tilde{u}^{s+1}_n - \tilde{u}^s_n\right) = \sum_{s=1}^{j-1} (j - s \vee (\hat{r}^{\mathcal{T}}_m+1)) J_1\left(\tilde{u}^{s}_n - \tilde{u}^{s-1}_n\right). \qquad (4.77)
\end{aligned}$$

Since $\tilde{u}_n$ is a competitor for the infimum problem in the definition of $B^{(2)}_{IF}(\hat{r}^{\mathcal{T}}, m, \gamma)$, we deduce from (4.75)–(4.77) that the estimate (4.72) holds true.

Let us now show (4.73). Firstly, we consider the case $\hat{r}(\mathcal{T}) < +\infty$. As in case (2) it is not restrictive to assume (4.60). We define $\tilde{v}^i_n$ for $i \geq 0$ by

$$\tilde{v}^i_n = \frac{u_n^{\hat{r}^{\mathcal{T}}_{m+1,n}+i} - u_n^{\hat{r}^{\mathcal{T}}_{m+1,n}}}{\lambda_n}. \qquad (4.78)$$

Let us check that $\tilde{v}_n$ is a competitor for the infimum problem of $B^{(3)}_{IF}(\hat{r}^{\mathcal{T}}, m+1)$, see (4.39). Clearly, $\tilde{v}^0_n = 0$. Fix $s \in \{m+1, \dots, k^{\mathcal{T}}_r - 1\}$ and $i \in \{\hat{r}^{\mathcal{T}}_s - \hat{r}^{\mathcal{T}}_{m+1}, \dots, \hat{r}^{\mathcal{T}}_{s+1} - \hat{r}^{\mathcal{T}}_{m+1} - 1\}$. From $u_n \in \mathcal{A}_{\mathcal{T}_n}(0,1)$ and (4.60), we obtain that

$$\tilde{v}^{i+1}_n - \tilde{v}^i_n = \frac{u_n^{\hat{r}^{\mathcal{T}}_{m+1,n}+i+1} - u_n^{\hat{r}^{\mathcal{T}}_{m+1,n}+i}}{\lambda_n} = \frac{u_n^{k^1_n+\hat{r}^{\mathcal{T}}_s+1} - u_n^{k^1_n+\hat{r}^{\mathcal{T}}_s}}{\lambda_n} = \tilde{v}_n^{\hat{r}^{\mathcal{T}}_s - \hat{r}^{\mathcal{T}}_{m+1}+1} - \tilde{v}_n^{\hat{r}^{\mathcal{T}}_s - \hat{r}^{\mathcal{T}}_{m+1}}.$$

Hence, $\tilde{v}_n$ satisfies the constraints in the definition of $B^{(3)}_{IF}(\hat{r}^{\mathcal{T}}, m+1)$, see (4.39). Let us now rewrite the left-hand side of (4.73) in terms of $\tilde{v}_n$. Firstly, we consider the terms involving only J_1. For given $j \in \{2+\hat{r}^{\mathcal{T}}_{m+1}, \dots, K\}$ and n sufficiently large such that (4.60) holds true, we have that

$$\begin{aligned}
&\sum_{i=\hat{r}^{\mathcal{T}}_{m+1,n}-j+1}^{k^1_n-1} \sum_{s=\hat{r}^{\mathcal{T}}_{m+1,n}}^{i+j-1} J_1\left(\frac{u^{s+1}_n - u^s_n}{\lambda_n}\right) = \sum_{i=\hat{r}^{\mathcal{T}}_{m+1,n}-j+1}^{k^1_n-1} \sum_{s=1}^{i+j-\hat{r}^{\mathcal{T}}_{m+1,n}} J_1\left(\tilde{v}^s_n - \tilde{v}^{s-1}_n\right)\\
&= \sum_{i=0}^{j-\hat{r}^{\mathcal{T}}_{m+1}-2} \sum_{s=1}^{i+1} J_1\left(\tilde{v}^s_n - \tilde{v}^{s-1}_n\right) = \sum_{s=1}^{j-\hat{r}^{\mathcal{T}}_{m+1}-1} \sum_{i=s-1}^{j-\hat{r}^{\mathcal{T}}_{m+1}-2} J_1\left(\tilde{v}^s_n - \tilde{v}^{s-1}_n\right)\\
&= \sum_{s=1}^{j-\hat{r}^{\mathcal{T}}_{m+1}-1} (j - \hat{r}^{\mathcal{T}}_{m+1} - s) J_1\left(\tilde{v}^s_n - \tilde{v}^{s-1}_n\right). \qquad (4.79)
\end{aligned}$$

Moreover, we have for the terms involving only $\mu^i_{j,n}$, using (4.60), that

$$\begin{aligned}\sum_{s=\hat{r}^{\mathcal{T}}_{m+1}+1}^{r(\mathcal{T}_n)-k^1_n}\left(\frac{s}{j}\wedge 1\right)\mu^{k^1_n+s-1}_{j,n} &= \sum_{s=1}^{\hat{r}^{\mathcal{T}}_{k^{\mathcal{T}}_r}-\hat{r}^{\mathcal{T}}_{m+1}}\left(\frac{s+\hat{r}^{\mathcal{T}}_{m+1}}{j}\wedge 1\right)\mu^{k^1_n+\hat{r}^{\mathcal{T}}_{m+1}+s-1}_{j,n}\\ &= \sum_{s=1}^{\hat{r}^{\mathcal{T}}_{k^{\mathcal{T}}_r}-\hat{r}^{\mathcal{T}}_{m+1}}\left(\frac{s+\hat{r}^{\mathcal{T}}_{m+1}}{j}\wedge 1\right)\mu^{s-1}_j(\tilde{v}_n). \qquad (4.80)\end{aligned}$$

Combining (4.79), (4.80) and the fact that v_n is a competitor for the infimum problem in the definition of $B^{(3)}_{IF}(\hat{r}^{\mathcal{T}}, m+1)$ yields (4.73) in the case $\hat{r}(\mathcal{T}) < +\infty$.

It is left to consider the case $\hat{r}(\mathcal{T}) = +\infty$. Clearly, we have $r(\mathcal{T}_n) - \hat{r}^{\mathcal{T}}_{k^{\mathcal{T}}_r-1,n} \to +\infty$ as $n \to \infty$. Lemma 4.10 and the definition of $\tilde{v}_n$, see (4.78), yields

$$\lim_{n\to\infty}\frac{u_n^{k^1_n+\hat{r}^{\mathcal{T}}_{m+1}+1+s} - u_n^{k^1_n+\hat{r}^{\mathcal{T}}_{m+1}+s}}{\lambda_n} = \lim_{n\to\infty}\left(\tilde{v}^{s+1}_n - \tilde{v}^s_n\right) = \gamma, \qquad (4.81)$$

for $s \in \{\hat{r}^{\mathcal{T}}_{k^{\mathcal{T}}_r-1} - \hat{r}^{\mathcal{T}}_{m+1}, \dots, K - \hat{r}^{\mathcal{T}}_{m+1} - 2\}$. We define $\hat{v}_n : \mathbb{N}_0 \to \mathbb{R}$, by

$$\hat{v}^i_n = \begin{cases}\tilde{v}^i_n & \text{if } i \in \{0,\dots,\hat{r}^{\mathcal{T}}_{k^{\mathcal{T}}_r-1} - \hat{r}^{\mathcal{T}}_{m+1}\},\\ \gamma(i - \hat{r}^{\mathcal{T}}_{k^{\mathcal{T}}_r-1} + \hat{r}^{\mathcal{T}}_{m+1}) + \tilde{v}_n^{\hat{r}^{\mathcal{T}}_{k^{\mathcal{T}}_r-1}-\hat{r}^{\mathcal{T}}_{m+1}} & \text{if } i \geq \hat{r}^{\mathcal{T}}_{k^{\mathcal{T}}_r-1} - \hat{r}^{\mathcal{T}}_{m+1}.\end{cases} \qquad (4.82)$$

The definition of $\hat{v}_n$ and the previous considerations about $\tilde{v}$ imply that $\hat{v}$ is a competitor for the infimum problem in the definition of $B^{(3)}_{IF}(\hat{r}^{\mathcal{T}}, m+1)$ with $\hat{r}^{\mathcal{T}}_{k^{\mathcal{T}}_r} = +\infty$, see (4.41). Hence, we obtain

$$\begin{aligned}&\sum_{j=2+\hat{r}^{\mathcal{T}}_{m+1}}^{K}\frac{c_j}{j}\sum_{i=\hat{r}^{\mathcal{T}}_{m,n}-j+1}^{k^1_n-1}\sum_{s=\hat{r}^{\mathcal{T}}_{m+1,n}}^{i+j-1} J_1\left(\frac{u^{s+1}_n - u^s_n}{\lambda_n}\right) + \sum_{j=2}^{K}\sum_{s=\hat{r}^{\mathcal{T}}_{m+1}+1}^{r(\mathcal{T}_n)-k^1_n}\left(\frac{s}{j}\wedge 1\right)\mu^{k^1_n+s-1}_{j,n}\\ &\geq \sum_{j=2+\hat{r}^{\mathcal{T}}_{m+1}}^{K}\frac{c_j}{j}\sum_{s=1}^{j-\hat{r}^{\mathcal{T}}_{m+1}-1}(j-\hat{r}^{\mathcal{T}}_{m+1}-s)J_1\left(\hat{v}^s_n - \hat{v}^{s-1}_n\right)\\ &\quad + \sum_{j=2}^{K}\sum_{s=1}^{\hat{r}^{\mathcal{T}}_{k^{\mathcal{T}}_r-1}-\hat{r}^{\mathcal{T}}_{m+1}}\left(\frac{s+\hat{r}^{\mathcal{T}}_{m+1}}{j}\wedge 1\right)\mu^{s-1}_j(\hat{v}_n) - r_2(n)\\ &\geq B^{(3)}_{IF}(\hat{r}^{\mathcal{T}}, m+1) - r_2(n),\end{aligned}$$

with

$$r_2(n) = \sum_{j=2}^{K}\frac{c_j}{j}\sum_{s=\hat{r}^{\mathcal{T}}_{k^{\mathcal{T}}_r-1}-\hat{r}^{\mathcal{T}}_{m+1}+1}^{j-\hat{r}^{\mathcal{T}}_{m+1}-1}(j-\hat{r}^{\mathcal{T}}_{m+1}-s)\left(J_1(\gamma) - J_1(\tilde{v}^s_n - \tilde{v}^{s-1}_n)\right).$$

By (4.81), we obtain that $\lim_{n\to\infty} r_2(n) = 0$ and thus (4.73) is proven.

Case (4). Finally, let (u_n) satisfy (4.50) with (h_n) such that ((4.51), (4)) holds. We show

$$\liminf_{n\to\infty} \hat{H}_{1,n}^{\ell,k_n,\mathcal{T}_n}(u_n) \geq B(u_0^{(1)},\gamma) + B(u_1^{(1)},\gamma) - b(0,\mathcal{T})J_{CB}(\gamma) - \sum_{j=2}^{K}(j-1)\psi_j(\gamma). \quad (4.83)$$

With a similar argument as in case (3), we deduce from Lemma 4.10 that $b(0,\mathcal{T})$ has to be finite. Let us define sequences $(h_n^1),(h_n^2) \subset \mathbb{N}$ by

$$h_n^1 := \max\{q \in \mathcal{T}_n,\ q \leq h_n\}, \quad h_n^2 := \min\{q \in \mathcal{T}_n,\ q > h_n\}.$$

From $u_n \in \mathcal{A}_{\mathcal{T}_n}(0,1)$, we have $\mu_{j,n}^i = \mu_{j,n}^{h_n}$ for $h_n^1 \leq i \leq h_n^2 - 1$. The assumption ((4.51), (4)) and the definition of h_n^1, imply $k_n^1 + K - 1 \leq r(\mathcal{T}_n) \leq h_n^1$. Hence, using $\sigma_{j,n}^i, \mu_{j,n}^i \geq 0$, we obtain

$$\begin{aligned}&\sum_{j=2}^{K}\left\{\sum_{i=T_n^1+1}^{k_n^1-1}\sigma_{j,n}^i + \sum_{i=1}^{j-1}\frac{i}{j}\mu_{j,n}^{k_n^1+i-1} + \sum_{i=k_n^1+j-1}^{h_n^1-1}\mu_{j,n}^i + \sum_{i=h_n^1}^{h_n^2-1}\mu_{j,n}^i + \sum_{i=h_n^2}^{k_n^2-j}\mu_{j,n}^i\right\}\\ &\quad\geq (h_n^2 - h_n^1)\sum_{j=2}^{K}\mu_{j,n}^{h_n}.\end{aligned}$$

By the definition of h_n^1, h_n^2 and (4.7), we obtain from $\lim_{n\to\infty}\lambda_n h_n = 0$ that $\lim_{n\to\infty}\lambda_n h_n^1 = \lim_{n\to\infty}\lambda_n h_n^2 = 0$. Hence, there exists a constant $N \in \mathbb{N}$ such that $(h_n^2 - h_n^1) \geq b(0,\mathcal{T})$ for all $n \geq N$. From $\mu_{j,n}^{h_n} \geq 0$ and $\lim_{n\to\infty}\mu_{j,n}^{h_n} = -\psi_j(\gamma)$, we deduce

$$\liminf_{n\to\infty}(h_n^2 - h_n^1)\sum_{j=2}^{K}\mu_{j,n}^{h_n} \geq -b(0,\mathcal{T})\sum_{j=2}^{K}\psi_j(\gamma) = -b(0,\mathcal{T})J_{CB}(\gamma),$$

where we used $\sum_{j=2}^{K}\psi_j(\gamma) = J_{CB}(\gamma)$. Combining the above considerations with (4.48), (4.49), (4.55) and $\sigma_{j,n}^i, \mu_{j,n}^i \geq 0$, we obtain inequality (4.83).

In summary, for the jump in 0, we have the estimate

$$\begin{aligned}&\liminf_{n\to\infty}\hat{H}_{1,n}^{\ell,k_n,\mathcal{T}_n}(u_n)\\ &\geq B(u_1^{(1)},\gamma) - \sum_{j=2}^{K}(j-1)\psi_j(\gamma)\\ &\quad + \min\left\{\min\left\{B_{AIF}(\hat{r}(\mathcal{T})), B_{BIF}(\hat{r}^{\mathcal{T}}), -b(0,\mathcal{T})J_{CB}(\gamma)\right\} + B(u_0^{(1)},\gamma), B_{BJ}(u_0^{(1)})\right\},\end{aligned}$$

which meets (4.42) for a jump in 0.

Jump in $(0,1)$. Assume that $S_u = \{t\}$, with $t \in (0,1)$. Let (u_n) be a sequence converging to u such that $\sup_n \hat{H}_{1,n}^{\ell,k_n,\mathcal{T}_n}(u_n) < \infty$. Then Proposition 4.3 implies that $u_n \to u$ in

$L^1(0,1)$ with

$$u(x) = \begin{cases} \gamma x & \text{if } 0 \le x < t, \\ (\ell - \gamma) + \gamma x & \text{if } t < x \le 1. \end{cases} \tag{4.84}$$

Combining (4.55), (4.49) and the arguments of case (4) above, we can prove

$$\liminf_{n\to\infty} \hat{H}_{1,n}^{\ell,k_n,\mathcal{T}_n}(u_n) \ge B(u_0^{(1)},\gamma) + B(u_1^{(1)},\gamma) - b(x,\mathcal{T})J_{CB}(\gamma) - \sum_{j=2}^{K}(j-1)\psi_j(\gamma), \tag{4.85}$$

which is the asserted estimate.

Limsup inequality. As for the lower bound it is sufficient to consider a single jump either in 0 or in $(0,1)$.
Jump in 0. Corresponding to the cases (1)–(4), see (4.51), we construct sequences $(u_n^{(i)})$ with $u_n^{(i)} \to u$ for $i = 1,\dots,4$, where u is given by (4.46) such that

$$\limsup_{n\to\infty} \hat{H}_{1,n}^{\ell,k_n,\mathcal{T}_n}(u_n^{(1)}) \le B(u_1^{(1)},\gamma) + B_{BJ}(u_0^{(1)}) - \sum_{j=2}^{K}(j-1)\psi_j(\gamma), \tag{4.86}$$

$$\limsup_{n\to\infty} \hat{H}_{1,n}^{\ell,k_n,\mathcal{T}_n}(u_n^{(2)}) \le B(u_0^{(1)},\gamma) + B(u_1^{(1)},\gamma) + B_{AIF}(\hat{r}^{\mathcal{T}}) - \sum_{j=2}^{K}(j-1)\psi_j(\gamma), \tag{4.87}$$

$$\limsup_{n\to\infty} \hat{H}_{1,n}^{\ell,k_n,\mathcal{T}_n}(u_n^{(3)}) \le B(u_0^{(1)},\gamma) + B(u_1^{(1)},\gamma) + B_{BIF}(\hat{r}^{\mathcal{T}}) - \sum_{j=2}^{K}(j-1)\psi_j(\gamma), \tag{4.88}$$

$$\limsup_{n\to\infty} \hat{H}_{1,n}^{\ell,k_n,\mathcal{T}_n}(u_n^{(4)}) \le B(u_0^{(1)},\gamma) + B(u_1^{(1)},\gamma) - \sum_{j=2}^{K}(b(0,\mathcal{T}) + j - 1)\psi_j(\gamma). \tag{4.89}$$

To show these inequalities, we recall some definitions of sequences from Chapter 3. Let $\eta > 0$. By the definition of $B(\theta,\gamma)$, see (3.72), we find a function $v : \mathbb{N}_0 \to \mathbb{R}$ and an $N_1 \in \mathbb{N}$ such that $v^0 = 0$, $v^s - v^{s-1} = u_{0,s}^{(1)}$, for $1 \le s < K$ and $v^{i+1} - v^i = \gamma$ if $i \ge N_1$, satisfying

$$\sum_{j=2}^{K} c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(u_{0,s}^{(1)}) + \sum_{j=2}^{K}\sum_{i\ge 0} \sigma_j^i(v) \le B(u_0^{(1)},\gamma) + \eta. \tag{4.90}$$

Moreover, we find $w : \mathbb{N}_0 \to \mathbb{R}$ and an $N_2 \in \mathbb{N}$ with $w^0 = 0$, $w^s - w^{s-1} = u_{1,s}^{(1)}$ for $1 \le s < K$ and $w^{i+1} - w^i = \gamma$ if $i \ge N_2$, such that

$$\sum_{j=2}^{K} c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(u_{1,s}^{(1)}) + \sum_{j=2}^{K}\sum_{i\ge 0} \sigma_j^i(w) \le B(u_1^{(1)},\gamma) + \eta. \tag{4.91}$$

By the definition of $B(\gamma)$, see (3.71), we find a function $\tilde{u} : \mathbb{N}_0 \to \mathbb{R}$ and an $\tilde{N} \in \mathbb{N}$ such that $\tilde{u}^0 = 0, \tilde{u}^{i+1} - \tilde{u}^i = \gamma$ if $i \geq \tilde{N}$ and

$$\sum_{j=2}^{K} c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1\left(\tilde{u}^s - \tilde{u}^{s-1}\right) + \sum_{j=2}^{K} \sum_{i \geq 0} \sigma_j^i(\tilde{u}) \leq B(\gamma) + \eta. \tag{4.92}$$

Let us recall that the infinite sums in (4.90)–(4.92) can be replaced by the sum from $i = 0$ to $i = N_1 - 1$ respectively $N_2 - 1$, $\tilde{N} - 1$.

Case (1). We construct a sequence (u_n) converging to u in $L^1(0,1)$, given in (4.46), satisfying (4.86). For this, we can use the same recovery sequence which was constructed for a jump in 0 in Theorem 3.19. Let $\eta > 0$. By the definition of $B_b(\theta)$ given in (3.70), there exist $\hat{w} : \mathbb{N}_0 \to \mathbb{R}$ and $\hat{k}_0 \in \mathbb{N}$, $\hat{k}_0 \geq K-1$ such that $\hat{w}^{k_0} = 0$, $\hat{w}^{k_0+1-s} - \hat{w}^{k_0-s} = u_{0,s}^{(1)}$ for $s = 1, \ldots, K-1$ and (3.98) is satisfied. The recovery sequence (u_n) is defined means of the sequences $\tilde{u}$, $\hat{w}$ and w, as

$$u_n^i = \begin{cases} -\lambda_n \hat{w}^{i-\hat{k}_0} & \text{if } 0 \leq i \leq \hat{k}_0, \\ \ell + \lambda_n(\tilde{u}^{i-(\hat{k}_0+1)} - \tilde{u}^{k_n^2+1-(\hat{k}_0+1)} - w^{n-(k_n^2+1)}) & \text{if } \hat{k}_0 + 1 \leq i \leq k_n^2 + 1, \\ \ell - \lambda_n w^{n-i} & \text{if } k_n^2 + 1 \leq i \leq n. \end{cases}$$

By the definition of $\hat{w}$ and w the function u_n satisfies the boundary conditions (3.3). Moreover, since k_n^1, k_n^2 are such that $\lim_{n\to\infty} k_n^1 = \lim_{n\to\infty}(n - k_n^2) = +\infty$ we have for n large enough that

$$k_n^1 - (\hat{k}_0 + K) > \tilde{N} \quad \text{and} \quad k_n^2 + N_2 + K \leq n.$$

This implies that $u_n^{i+1} - u_n^i = \lambda_n \gamma$ for $i \in \{k_n^1, \ldots, k_n^2\}$ for n sufficiently large and thus $u_n \in \mathcal{A}_{\mathcal{T}_n}(0,1)$. In a similar way as in the proof of Theorem 3.19, we can show that $\lim_{n\to\infty} u_n = u$ in $L^1(0,1)$ and, by using the above inequalities and (3.74), that

$$\limsup_{n\to\infty} \hat{H}_{1,n}^{\ell,k_n,\mathcal{T}_n}(u_n) \leq B(u_1^{(1)}, \gamma) + B_{BJ}(u_0^{(1)}) - \sum_{j=2}^{K}(j-1)\psi_j(\gamma) + 3\eta.$$

The assertion follows from the arbitrariness of $\eta > 0$.

Case (2). Next, we construct a sequence (u_n) which converges in $L^1(0,1)$ to u, given in (4.46), and satisfies (4.87).

Let us first assume that $\hat{r}(\mathcal{T}) < +\infty$. Fix $\eta > 0$. By the definition of $B_{IF}^{(1)}(r)$, see (4.35), we find a function $z : \mathbb{N}_0 \to \mathbb{R}$ and a $q \in \mathbb{N}$ such that $z^0 = 0$ and $z^{q+i+1} - z^{q+i} =$

$z^{q+\hat{r}_s^{\mathcal{T}}+1} - z^{q+\hat{r}_s^{\mathcal{T}}}$ if $s \in \{1, \dots, k_r^{\mathcal{T}} - 1\}$ and $i \in \{\hat{r}_s^{\mathcal{T}}, \dots, \hat{r}_{s+1}^{\mathcal{T}} - 1\}$, satisfying

$$\sum_{j=2}^{K} \left\{ c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(z^s - z^{s-1}) + \sum_{i=0}^{q-1} \sigma_j^i(z) + \sum_{s=1}^{j-1} \frac{s}{j} \mu_j^{q-1+s}(z) + \sum_{i=q+j-1}^{\hat{r}(\mathcal{T})-1} \mu_j^i(z) \right\} \\ \leq B_{IF}(\hat{r}^{\mathcal{T}}) + \eta. \tag{4.93}$$

Set $h_n := k_n^1 - q - 1$; then we have $\lambda_n h_n \to 0$. Set $k_n^0 = \lfloor \sqrt{k_n^1} \rfloor$. Clearly, we have $\lim_n \lambda_n k_n^0 = 0$ and $\lim_n (k_n^1 - k_n^0) = +\infty$. For n sufficiently large, we can assume that the following relations hold true:

$$\begin{aligned} &k_n^0 \geq N_1 + K, \quad \tilde{N} \leq h_n - k_n^0 - K, \quad n - k_n^2 - K \geq N_2, \\ &\hat{r}_{s,n}^{\mathcal{T}} - k_n^1 = \hat{r}_s^{\mathcal{T}} \quad \text{for} \quad s \in \{1, \dots, k_r^{\mathcal{T}}\}. \end{aligned} \tag{4.94}$$

We are now able to construct a recovery sequence (u_n) by means of the functions z, v, w and $\tilde{u}$:

$$u_n^i = \begin{cases} \lambda_n v^i & \text{if } 0 \leq i \leq k_n^0, \\ \lambda_n \left(v^{k_n^0} - \tilde{u}^{h_n - i} + \tilde{u}^{h_n - k_n^0} \right) & \text{if } k_n^0 \leq i \leq h_n, \\ \ell + \lambda_n \left(z^{i-h_n-1} - z^{r(\mathcal{T}_n)-h_n-1} - w^{n-r(\mathcal{T}_n)} \right) & \text{if } h_n + 1 \leq i \leq r(\mathcal{T}_n), \\ \ell - \lambda_n w^{n-i} & \text{if } r(\mathcal{T}_n) \leq i \leq n. \end{cases} \tag{4.95}$$

By definition of v and w the functions u_n satisfy the boundary conditions (3.3). Let us now check that $u_n \in \mathcal{A}_{\mathcal{T}_n}(0,1)$ for n sufficiently large. The definition of w and (4.94) yields $u_n^{i+1} - u_n^i = \lambda_n \gamma$ for $r(\mathcal{T}_n) \leq i \leq k_n^2$. Thus it is left to show that for given $s \in \{1, \dots, k_r^{\mathcal{T}} - 1\}$ and n sufficiently large it holds u_n' is constant on $\lambda_n(\hat{r}_{s,n}^{\mathcal{T}}, \hat{r}_{s+1,n}^{\mathcal{T}})$. Fix $s \in \{1, \dots, k_r^{\mathcal{T}} - 1\}$ and let $i \in \{\hat{r}_s^{\mathcal{T}}, \dots, \hat{r}_{s+1}^{\mathcal{T}}\}$. By the definition of u_n, z, (4.94) and $h_n = k_n^1 - q - 1$, we obtain that

$$\frac{u_n^{k_n^1+i+1} - u_n^{k_n^1+i}}{\lambda_n} = z^{q+i+1} - z^{q+i} = z^{q+\hat{r}_s^{\mathcal{T}}+1} - z^{q+\hat{r}_s^{\mathcal{T}}} = \frac{u_n^{k_n^1+\hat{r}_s^{\mathcal{T}}+1} - u_n^{k_n^1+\hat{r}_s^{\mathcal{T}}}}{\lambda_n}.$$

This implies that $u_n' = \lambda_n^{-1}(u_n^{\hat{r}_{s,n}^{\mathcal{T}}+1} - u_n^{\hat{r}_{s,n}^{\mathcal{T}}})$ on $\lambda_n(\hat{r}_{s,n}^{\mathcal{T}}, \hat{r}_{s+1,n}^{\mathcal{T}})$. Hence, $u_n \in \mathcal{A}_{\mathcal{T}_n}(0,1)$. Next, we show that

$$\lim_{n\to\infty} \left(u_n^{h_n+1} - u_n^{h_n} \right) = \ell - \gamma. \tag{4.96}$$

Since we have $h_n = k_n^1 - q - 1$, $r(\mathcal{T}_n) - k_n^1 = \hat{r}(\mathcal{T})$ and $k_n^2 > r(\mathcal{T}_n)$ for n sufficiently large, we obtain

$$
\begin{aligned}
u_n^{h_n+1} - u_n^{h_n} &= \ell + \lambda_n \left(z^0 - z^{r(\mathcal{T}_n)-h_n-1} - w^{n-r(\mathcal{T}_n)} - v^{k_n^0} + \tilde{u}^0 - \tilde{u}^{h_n-k_n^0} \right) \\
&= \ell + \lambda_n \big(w^{N_2} - w^{n-r(\mathcal{T}_n)} - w^{N_2} - z^{q+\hat{r}(\mathcal{T})} - v^{k_n^0} + v^{N_1} - v^{N_1} - \tilde{u}^{h_n-k_n^0} + \tilde{u}^{\tilde{N}} - \tilde{u}^{\tilde{N}} \big) \\
&= \ell + \lambda_n \big(\gamma(N_2 + r(\mathcal{T}_n) - n - k_n^0 + N_1 - h_n + k_n^0 + \tilde{N}) - w^{N_2} - z^{q+\hat{r}(\mathcal{T})} - v^{N_1} - \tilde{u}^{\tilde{N}} \big) \\
&= \ell - \gamma + \lambda_n \big(\gamma(q + 1 + \hat{r}(\mathcal{T}) + N_2 + N_1 + \tilde{N}) - w^{N_2} - z^{q+\hat{r}(\mathcal{T})} - v^{N_1} - \tilde{u}^{\tilde{N}} \big). \qquad (4.97)
\end{aligned}
$$

Since the terms which are multiplied by λ_n are independent of n, we have (4.96) and similar arguments as in the proof of Theorem 3.19 yield $u_n \to u$ in $L^1(0,1)$. From (4.96), we deduce $\frac{u_n^{h_n+1} - u_n^{h_n}}{\lambda_n} \to +\infty$ as $n \to \infty$. Thus, for fixed $j \in \{2, \dots, K\}$ it holds

$$
\begin{aligned}
\sum_{i=h_n-j+1}^{h_n} \sigma_{j,n}^i =& c_j \sum_{s=1}^{j-1} \frac{j-s}{j} \left(J_1 \left(\frac{u_n^{h_n+1-s} - u_n^{h_n-s}}{\lambda_n} \right) + J_1 \left(\frac{u_n^{h_n+s+1} - u_n^{h_n+s}}{\lambda_n} \right) \right) \\
& - j\psi_j(\gamma) + r_j(n) \\
=& c_j \sum_{s=1}^{j-1} \frac{j-s}{j} \left(J_1 \left(\tilde{u}^s - \tilde{u}^{s-1} \right) + J_1 \left(z^s - z^{s-1} \right) \right) - j\psi_j(\gamma) + r_j(n), \qquad (4.98)
\end{aligned}
$$

where $r_j(n) \to 0$ as $n \to \infty$. By the definition of $v, w, \tilde{u}$ and u_n and (4.94), we obtain that $u_n^{i+1} - u_n^i = \gamma$ for $i \in \{N_1, \dots, h_n - \tilde{N} - 1\} \cup \{r(\mathcal{T}_n), \dots, n - N_2 - 1\}$. Hence

$$
\sum_{j=2}^{K} \left\{ \sum_{i=N_1}^{h_n-\tilde{N}-1-K} \sigma_{j,n}^i + \sum_{i=r(\mathcal{T}_n)}^{k_n^2-j} \mu_{j,n}^i + \sum_{s=1}^{j-1} \frac{s}{j} \mu_{j,n}^{k_n^2-s} + \sum_{i=k_n^2-1}^{n-N_2-1-K} \sigma_{j,n}^i \right\} = 0. \qquad (4.99)
$$

Moreover, we observer by the definition of u_n, the function v and w and (3.108), (3.99) that

$$
\begin{aligned}
&\sum_{j=2}^{K} \sum_{i=0}^{N_1-1} \sigma_{j,n}^i = \sum_{j=2}^{K} \sum_{i \geq 0} \sigma_j^i(v) \leq B(u_0^{(1)}, \gamma) - \sum_{j=2}^{K} c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(u_{0,s}^{(1)}) + \eta, \\
&\sum_{j=2}^{K} \sum_{i=n-N_2-K}^{n-j} \sigma_{j,n}^i = \sum_{j=2}^{K} \sum_{i \geq 0} \sigma_j^i(w) \leq B(u_1^{(1)}, \gamma) - \sum_{j=2}^{K} c_j \sum_{s=1}^{j-1} \frac{j-s}{j} J_1(u_{1,s}^{(1)}) + \eta.
\end{aligned} \qquad (4.100)
$$

Combining the definition of u_n, the functions $\tilde{u}$ and z with (4.92), (4.93), (4.98) and (4.99), we get

$$\begin{aligned}
&\sum_{j=2}^{K}\left\{\sum_{i=h_n-\tilde{N}-K}^{k_n^1-1}\sigma_{j,n}^i+\sum_{s=1}^{j-1}\frac{s}{j}\mu_{j,n}^{k_n^1-1+s}+\sum_{i=k_n^1+j-1}^{r(\mathcal{T}_n)-1}\mu_{j,n}^i\right\}\\
=&\sum_{j=2}^{K}\left\{\sum_{i=h_n-\tilde{N}-K}^{h_n-j}\sigma_{j,n}^i+c_j\sum_{s=1}^{j-1}\frac{j-s}{j}\left(J_1(\tilde{u}^s-\tilde{u}^{s-1})+J_1(z^s-z^{s-1})\right)+\sum_{i=h_n+1}^{k_n^1-1}\sigma_{j,n}^i\right.\\
&\left.+\sum_{s=1}^{j-1}\frac{s}{j}\mu_{j,n}^{k_n^1-1+s}+\sum_{i=k_n^1+j-1}^{r(\mathcal{T}_n)-1}\mu_{j,n}^i-j\psi_j(\gamma)+r_j(n)\right\}\\
=&\sum_{j=2}^{K}\left\{\sum_{i=0}^{\tilde{N}+K-j}\sigma_j^i(\tilde{u})+c_j\sum_{s=1}^{j-1}\frac{j-s}{j}\left(J_1(\tilde{u}^s-\tilde{u}^{s-1})+J_1(z^s-z^{s-1})\right)+\sum_{i=0}^{q-1}\sigma_j^i(z)\right.\\
&\left.+\sum_{s=1}^{j-1}\frac{s}{j}\mu_j^{q-1+s}(z)+\sum_{i=q-1+j}^{\hat{r}(\mathcal{T})-1}\mu_j^i(z)-j\psi_j(\gamma)+r_j(n)\right\}\\
\leq& B(\gamma)+B_{IF}^{(1)}(\hat{r}^{\mathcal{T}})-\sum_{j=2}^{K}j\psi_j(\gamma)+2\eta+\sum_{j=2}^{K}r_j(n).
\end{aligned}\tag{4.101}$$

Altogether, we have by (4.23) and (4.99)–(4.101) that

$$\limsup_{n\to\infty}\hat{H}_{1,n}^{\ell,k_n,\mathcal{T}_n}(u_n)\leq B(u_0^{(1)},\gamma)+B(u_1^{(1)},\gamma)+B(\gamma)+B_{IF}^{(1)}(\hat{r}^{\mathcal{T}})-\sum_{j=2}^{K}(2j-1)\psi_j(\gamma)+4\eta.$$

The assertion (4.87) in the cases $\hat{r}(\mathcal{T})<+\infty$ follows by the arbitrariness of $\eta>0$ and the definition of $B_{AIF}(\hat{r}^{\mathcal{T}})$, see (4.44).

Let us now consider the case $\hat{r}(\mathcal{T})=+\infty$. In this case we have to change the definition of z in the recovery sequence. By the definition of $B_{IF}^{(1)}(\hat{r}^{\mathcal{T}})$, see also (4.36), there exist a function $\hat{z}:\mathbb{N}_0\to\mathbb{R}$ and a $q\in\mathbb{N}$ such that $\hat{z}^0=0$, $\hat{z}^{q+i+1}-\hat{z}^{q+i}=\hat{z}^{q+\hat{r}_s^{\mathcal{T}}+1}-\hat{z}^{q+\hat{r}_s^{\mathcal{T}}}$ if $s\in\{1,\dots,k_r^{\mathcal{T}}-2\}$ and $i\in\{\hat{r}_s^{\mathcal{T}},\dots,\hat{r}_{s+1}^{\mathcal{T}}-1\}$ satisfying $\hat{z}^{q+i+1}-\hat{z}^{q+i}=\gamma$ for $i\geq\hat{r}_{k_r^{\mathcal{T}}-1}^{\mathcal{T}}$ and

$$\begin{aligned}
&\sum_{j=2}^{K}\left\{c_j\sum_{s=1}^{j-1}\frac{j-s}{j}J_1(\hat{z}^s-\hat{z}^{s-1})+\sum_{i=0}^{q-1}\sigma_j^i(\hat{z})+\sum_{s=1}^{j-1}\frac{s}{j}\mu_j^{q-1+s}(\hat{z})+\sum_{i\geq q+j-1}\mu_j^i(\hat{z})\right\}\\
&\quad\leq B_{IF}(\hat{r}^{\mathcal{T}})+\eta.
\end{aligned}\tag{4.102}$$

Note that $\mu_j^i(\hat{z})=0$ for $i\geq q+\hat{r}_{k_r^{\mathcal{T}}-1}^{\mathcal{T}}$. Define u_n as in (4.95) with z replaced by $\hat{z}$. Then the sequence (u_n) is a recovery sequence for u. Note that u_n satisfies (3.3). Moreover, similar arguments as for the case $\hat{r}(\mathcal{T})<+\infty$ combined with $\hat{z}^{i+1}-\hat{z}^i=\gamma$ for $i\geq q+\hat{r}_{k_r^{\mathcal{T}}-1}^{\mathcal{T}}$ yields $u_n\in\mathcal{A}_{\mathcal{T}_n}(0,1)$ for n sufficiently large. Let us show (4.96). For n sufficiently large such that it holds $\hat{r}_{k_r^{\mathcal{T}}-1,n}^{\mathcal{T}}=k_n^1+\hat{r}_{k_r^{\mathcal{T}}-1}^{\mathcal{T}}$, we deduce from the calculations in (4.97) and

$\hat{z}^{i+1} - \hat{z}^i = \gamma$ for $i \geq q + r^{\mathcal{T}}_{k^{\mathcal{T}}_r - 1}$ that

$$\begin{aligned} u_n^{h_n+1} - u_n^{h_n} =& \ell - \gamma + \lambda_n \big(\gamma (r(\mathcal{T}_n) - k_n^1) - \hat{z}^{q + r(\mathcal{T}_n) - k_n^1} + \hat{z}^{q + \hat{r}^{\mathcal{T}}_{k^{\mathcal{T}}_r - 1}} - \hat{z}^{q + \hat{r}^{\mathcal{T}}_{k^{\mathcal{T}}_r - 1}} \big) + \mathcal{O}(\lambda_n) \\ =& \ell - \gamma + \lambda_n \big(\gamma (r(\mathcal{T}_n) - k_n^1 - (q + r(\mathcal{T}_n) - k_n^1) - \hat{r}^{\mathcal{T}}_{k^{\mathcal{T}}_r - 1}) - \hat{z}^{q + \hat{r}^{\mathcal{T}}_{k-1}} \big) + \mathcal{O}(\lambda_n) \\ =& \ell - \gamma + \mathcal{O}(\lambda_n), \end{aligned}$$

which yields (4.96). Similar arguments as in the case $\hat{r}(\mathcal{T}) < +\infty$ yields (4.87), which finishes the proof in this case.

Case (3). We have to prove that there exists a sequence (u_n) converging in $L^1(0,1)$ to u, given in (4.46), satisfying (4.88).

Let us first assume that $\hat{r}(\mathcal{T}) < +\infty$. Let $m \in \{1, \dots, k^{\mathcal{T}}_r - 1\}$ be such that

$$\begin{aligned} B_{BIF}\left(\hat{r}^{\mathcal{T}}\right) =& B^{(2)}_{IF}(\hat{r}^{\mathcal{T}}, m, \gamma) + B^{(3)}_{IF}(\hat{r}^{\mathcal{T}}, m+1) - \sum_{j=2+\hat{r}^{\mathcal{T}}_m}^{K} \left(j - \hat{r}^{\mathcal{T}}_m - 1 \right) \psi_j(\gamma) \\ & - \sum_{j=2}^{K} \sum_{i=\hat{r}^{\mathcal{T}}_m + 1}^{\hat{r}^{\mathcal{T}}_{m+1}} \left(\frac{i}{j} \wedge 1 \right) \psi_j(\gamma). \end{aligned} \tag{4.103}$$

Fix $\eta > 0$. By the definition of $B^{(2)}_{IF}(r, m, \gamma)$, see (4.38), there exist a function $\bar{u} : \mathbb{N}_0 \to \mathbb{R}$ and an $\bar{N} \in \mathbb{N}$ such that $\bar{u}^0 = 0$, $\bar{u}^{i+1} - \bar{u}^i = \gamma$ for $i \geq \bar{N}$ and $\bar{u}^{i+1} - \bar{u}^i = \bar{u}^{\hat{r}^{\mathcal{T}}_m - \hat{r}^{\mathcal{T}}_s + 1} - \bar{u}^{\hat{r}^{\mathcal{T}}_m - \hat{r}^{\mathcal{T}}_s}$ if $s \in \{2, \dots, m\}$ and $\hat{r}^{\mathcal{T}}_m - \hat{r}^{\mathcal{T}}_s \leq i < \hat{r}^{\mathcal{T}}_m - \hat{r}^{\mathcal{T}}_{s-1}$, such that the following inequality holds

$$\begin{aligned} & \sum_{j=2+\hat{r}^{\mathcal{T}}_m}^{K} c_j \sum_{s=1}^{j-1} \frac{j - (s \vee (\hat{r}^{\mathcal{T}}_m + 1))}{j} J_1(\bar{u}^s - \bar{u}^{s-1}) + \sum_{j=2}^{K} \sum_{i \geq (\hat{r}^{\mathcal{T}}_m + 1 - j) \vee 0} \sigma^i_j(\bar{u}) \\ & + \sum_{j=2}^{K} \sum_{i=0}^{\hat{r}^{\mathcal{T}}_m - 1} \left(\frac{\hat{r}^{\mathcal{T}}_m - i}{j} \wedge 1 \right) \mu^i_j(\bar{u}) \leq B^{(2)}_{IF}(\hat{r}^{\mathcal{T}}, m, \gamma) + \eta. \end{aligned}$$

Furthermore, by the definition of $B(\hat{r}^{\mathcal{T}}, m+1)$, see (4.39), there exists a function $\bar{v} : \mathbb{N}_0 \to \mathbb{R}$ with $\bar{v}^0 = 0$ and $\bar{v}^{i+1} - \bar{v}^i = \bar{v}^{\hat{r}^{\mathcal{T}}_s - \hat{r}^{\mathcal{T}}_{m+1} + 1} - \bar{v}^{\hat{r}^{\mathcal{T}}_s - \hat{r}^{\mathcal{T}}_{m+1}}$ if $s \in \{m+1, \dots, k^{\mathcal{T}}_r - 1\}$ and $\hat{r}^{\mathcal{T}}_s - \hat{r}^{\mathcal{T}}_{m+1} \leq i < \hat{r}^{\mathcal{T}}_{s+1} - \hat{r}^{\mathcal{T}}_{m+1}$ such that

$$\begin{aligned} & \sum_{j=2+\hat{r}^{\mathcal{T}}_{m+1}}^{K} c_j \sum_{s=1}^{j - \hat{r}^{\mathcal{T}}_{m+1} - 1} \frac{j - s - \hat{r}^{\mathcal{T}}_{m+1}}{j} J_1(\bar{v}^s - \bar{v}^{s-1}) \\ & + \sum_{j=2}^{K} \sum_{i=1}^{\hat{r}(\mathcal{T}) - \hat{r}^{\mathcal{T}}_{m+1} - 1} \left(\frac{i + \hat{r}^{\mathcal{T}}_{m+1}}{j} \wedge 1 \right) \mu^{i-1}_j(\bar{v}) \leq B^{(3)}_{IF}(\hat{r}^{\mathcal{T}}, m+1) + \eta. \end{aligned}$$

Set $k_n^0 := \lfloor\sqrt{k_n^1}\rfloor$. Clearly, we have $\lim_n \lambda_n k_n^0 = 0$ and $\lim_n(k_n^1 - k_n^0) = +\infty$. For n sufficiently large, we can assume that the following relations hold true:

$$\begin{aligned} &k_n^0 \geq N_1 + 1, \quad \bar{N} \leq k_n^1 - k_n^0 - 2, \quad n - k_n^2 - 1 \geq N_2, \\ &\hat{r}_{s,n}^{\mathcal{T}} - k_n^1 = \hat{r}_s^{\mathcal{T}} \quad \text{for} \quad s \in \{1, \ldots, k_r^{\mathcal{T}}\}. \end{aligned} \tag{4.104}$$

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

$$u_n^i = \begin{cases} \lambda_n v^i & \text{if } 0 \leq i \leq k_n^0, \\ \lambda_n(v^{k_n^0} - \bar{u}^{\hat{r}_{m,n}^{\mathcal{T}}-i} + \bar{u}^{\hat{r}_{m,n}^{\mathcal{T}}-k_n^0}) & \text{if } k_n^0 \leq i \leq \hat{r}_{m,n}^{\mathcal{T}}, \\ u_n^{\hat{r}_{m,n}^{\mathcal{T}}} + \frac{i-\hat{r}_{m,n}^{\mathcal{T}}}{\hat{r}_{m+1,n}^{\mathcal{T}}-\hat{r}_{m,n}^{\mathcal{T}}} u_n^{\hat{r}_{m+1,n}^{\mathcal{T}}} & \text{if } \hat{r}_{m,n}^{\mathcal{T}} < i < \hat{r}_{m+1,n}^{\mathcal{T}}, \\ \ell + \lambda_n\left(\bar{v}^{i-\hat{r}_{m+1,n}^{\mathcal{T}}} - \bar{v}^{r(\mathcal{T}_n)-\hat{r}_{m+1,n}^{\mathcal{T}}} - w^{n-r(\mathcal{T}_n)}\right) & \text{if } \hat{r}_{m+1,n}^{\mathcal{T}} \leq i \leq r(\mathcal{T}_n), \\ \ell - \lambda_n w^{n-i} & \text{if } r(\mathcal{T}_n) \leq i \leq n. \end{cases} \tag{4.105}$$

Note that $u_n^{\hat{r}_{m,n}^{\mathcal{T}}} = \lambda_n(v^{k_n^0} + \bar{u}^{\hat{r}_{m,n}^{\mathcal{T}}-k_n^0})$ and $u_n^{\hat{r}_{m+1,n}^{\mathcal{T}}} = \ell - \lambda_n(\bar{v}^{r(\mathcal{T}_n)+\hat{r}_{m+1,n}^{\mathcal{T}}} + w^{n-r(\mathcal{T}_n)})$ in the definition of u_n. By definition of the function v and w the sequence u_n satisfies the boundary conditions (3.3). Moreover, we have that $u_n^{i+1} - u_n^i = \lambda_n\gamma$ for $N_1 \leq i \leq \hat{r}_{m,n}^{\mathcal{T}} - \bar{N} - 1$ and $r(\mathcal{T}_n) \leq i \leq n - N_2 - 1$ for n large enough. Let us show that u_n' is constant on $\lambda_n(\hat{r}_{s,n}^{\mathcal{T}}, \hat{r}_{s+1,n}^{\mathcal{T}})$ for $s \in \{1, \ldots, k_r^{\mathcal{T}} - 1\}$ and n sufficiently large. Fix $s \in \{2, \ldots, m\}$ and $\hat{r}_{s-1,n}^{\mathcal{T}} \leq i \leq \hat{r}_{s,n}^{\mathcal{T}} - 1$. Note that this implies $\hat{r}_m^{\mathcal{T}} - \hat{r}_s^{\mathcal{T}} \leq \hat{r}_m^{\mathcal{T}} - (i - k_n^1) - 1 < \hat{r}_m^{\mathcal{T}} - \hat{r}_{s-1}^{\mathcal{T}}$ for n such that (4.104) holds. By the definition of u_n, $\bar{u}$ and (4.104), we obtain

$$\frac{u_n^{i+1} - u_n^i}{\lambda_n} = \bar{u}^{\hat{r}_m^{\mathcal{T}}-i} - \bar{u}^{\hat{r}_m^{\mathcal{T}}-i-1} = \bar{u}^{\hat{r}_m^{\mathcal{T}}-\hat{r}_s^{\mathcal{T}}+1} - \bar{u}^{\hat{r}_m^{\mathcal{T}}-\hat{r}_s^{\mathcal{T}}} = \frac{u_n^{k_n^1+\hat{r}_s^{\mathcal{T}}} - u_n^{k_n^1+\hat{r}_s^{\mathcal{T}}-1}}{\lambda_n}.$$

This implies that $u_n' = \lambda_n^{-1}(u_n^{\hat{r}_{s,n}^{\mathcal{T}}} - u_n^{\hat{r}_{s,n}^{\mathcal{T}}-1})$ on $\lambda_n(\hat{r}_{s-1,n}^{\mathcal{T}}, \hat{r}_{s,n}^{\mathcal{T}})$ for $s \in \{2, \ldots, m\}$. Let us now show that u_n' is constant on $\lambda_n(\hat{r}_{s,n}^{\mathcal{T}}, \hat{r}_{s+1,n}^{\mathcal{T}})$ for $s \in \{m, \ldots, k_r^{\mathcal{T}} - 1\}$. The case $s = m$ follows directly from the definition of u_n. Fix $s \in \{m+1, \ldots, k_r^{\mathcal{T}} - 1\}$ and $r_{s,n}^{\mathcal{T}} \leq i \leq r_{s+1,n}^{\mathcal{T}} - 1$. From (4.104) and the definition of u_n and $\bar{v}$, we obtain

$$\frac{u_n^{i+1} - u_n^i}{\lambda_n} = \bar{v}^{i-\hat{r}_{m+1,n}^{\mathcal{T}}+1} - \bar{v}^{i-\hat{r}_{m+1,n}^{\mathcal{T}}} = \bar{v}^{\hat{r}_s^{\mathcal{T}}-\hat{r}_{m+1}^{\mathcal{T}}+1} - \bar{v}^{\hat{r}_s^{\mathcal{T}}-\hat{r}_{m+1}^{\mathcal{T}}} = \frac{u_n^{k_n^1+\hat{r}_s^{\mathcal{T}}+1} - u_n^{k_n^1+\hat{r}_s^{\mathcal{T}}}}{\lambda_n}.$$

Hence, $u_n' = \lambda_n^{-1}(u_n^{\hat{r}_{s,n}^{\mathcal{T}}+1} - u_n^{\hat{r}_{s,n}^{\mathcal{T}}})$ on $\lambda_n(\hat{r}_{s,n}^{\mathcal{T}}, \hat{r}_{s+1,n}^{\mathcal{T}})$ for $s \in \{m+1, \ldots, k_r^{\mathcal{T}} - 1\}$. Altogether, we have that $u_n \in \mathcal{A}_{\mathcal{T}_n}(0,1)$. Let us show

$$\lim_{n\to\infty}\left(u_n^{\hat{r}_{m+1,n}^{\mathcal{T}}} - u_n^{\hat{r}_{m,n}^{\mathcal{T}}}\right) = \ell - \gamma. \tag{4.106}$$

We have

$$
\begin{aligned}
u_n^{\hat{r}^{\mathcal{T}}_{m+1,n}} - u_n^{\hat{r}^{\mathcal{T}}_{m,n}} =& \ell + \lambda_n \left(\bar{v}^0 - \bar{v}^{r(\mathcal{T}_n) - \hat{r}^{\mathcal{T}}_{m+1,n}} - w^{n-r(\mathcal{T}_n)} - v^{k_n^0} + \bar{u}^0 - \bar{u}^{\hat{r}^{\mathcal{T}}_{m,n} - k_n^0} \right) \\
=& \ell + \lambda_n \big(w^{N_2} - w^{n-r(\mathcal{T}_n)} - w^{N_2} - \bar{v}^{r(\mathcal{T}_n) - \hat{r}^{\mathcal{T}}_{m+1,n}} + v^{N_1} - v^{k_n^0} - v^{N_1} \\
&+ \bar{u}^{\bar{N}} - \bar{u}^{\hat{r}^{\mathcal{T}}_{m,n} - k_n^0} - \bar{u}^{\bar{N}} \big) \\
=& \ell + \lambda_n \big(\gamma \left(N_2 - n + r(\mathcal{T}_n) + N_1 - k_n^0 + \bar{N} - \hat{r}^{\mathcal{T}}_{m,n} + k_n^0 \right) - w^{N_2} - v^{N_1} \\
&- \bar{u}^{\bar{N}} - \bar{v}^{r(\mathcal{T}_n) - k_n^1 - \hat{r}^{\mathcal{T}}_{m+1}} \big) \\
=& \ell - \gamma + \lambda_n \big(\gamma \left(N_2 + N_1 + \bar{N} + r(\mathcal{T}_n) - k_n^1 - \hat{r}^{\mathcal{T}}_m \right) - \bar{v}^{r(\mathcal{T}_n) - k_n^1 - \hat{r}^{\mathcal{T}}_{m+1}} \\
&- w^{N_2} - v^{N_1} - \bar{u}^{\bar{N}} \big). \qquad (4.107)
\end{aligned}
$$

Since $r(\mathcal{T}_n) - k_n^1 = \hat{r}(\mathcal{T}) < +\infty$, the terms which are multiplied by λ_n are independent of n. This yields (4.106). Similar arguments as in the proof of Theorem 3.19 imply that $u_n \to u$ in $L^1(0,1)$. For $s \in \{\hat{r}^{\mathcal{T}}_m, \ldots, \hat{r}^{\mathcal{T}}_{m+1} - 1\}$, we deduce from the definition of u_n and (4.106) that

$$
\frac{u_n^{k_n^1+s+1} - u_n^{k_n^1+s}}{\lambda_n} = \frac{u_n^{\hat{r}^{\mathcal{T}}_{m+1,n}} - u_n^{\hat{r}^{\mathcal{T}}_{m,n}}}{\lambda_n (\hat{r}^{\mathcal{T}}_{m+1} - \hat{r}^{\mathcal{T}}_m)} \to \infty \quad \text{as } n \to \infty. \qquad (4.108)
$$

Let us assume that n is sufficiently large such that $\hat{r}^{\mathcal{T}}_{s,n} = k_n^1 + \hat{r}^{\mathcal{T}}_s$ for $s \in \{1, \ldots, m\}$. Then similar calculations as for the liminf inequality (e.g. (4.77), (4.79)) yield

$$
\begin{aligned}
&\sum_{j=2+\hat{r}^{\mathcal{T}}_m}^{K} \sum_{i=\hat{r}^{\mathcal{T}}_{m,n}-j+1}^{k_n^1-1} \sigma^i_{j,n} \\
=& \sum_{j=2+\hat{r}^{\mathcal{T}}_m}^{K} \frac{c_j}{j} \sum_{i=\hat{r}^{\mathcal{T}}_{m,n}-j+1}^{k_n^1-1} \sum_{s=i}^{\hat{r}^{\mathcal{T}}_{m,n}-1} J_1\left(\frac{u_n^{s+1} - u_n^s}{\lambda_n} \right) - \sum_{j=2+\hat{r}^{\mathcal{T}}_m}^{K} (k_n^1 - 1 - \hat{r}^{\mathcal{T}}_{m,n} + j) \psi_j(\gamma) \\
&+ \sum_{j=2+\hat{r}^{\mathcal{T}}_{m+1}}^{K} \frac{c_j}{j} \sum_{i=\hat{r}^{\mathcal{T}}_{m,n}-j+1}^{k_n^1-1} \sum_{s=\hat{r}^{\mathcal{T}}_{m+1,n}}^{i+j-1} J_1\left(\frac{u_n^{s+1} - u_n^s}{\lambda_n} \right) + r_1(n) \\
=& \sum_{j=2+\hat{r}^{\mathcal{T}}_m}^{K} \frac{c_j}{j} \sum_{i=\hat{r}^{\mathcal{T}}_{m,n}-j+1}^{k_n^1-1} \sum_{s=0}^{\hat{r}^{\mathcal{T}}_{m,n}-i-1} J_1\left(\bar{u}^{s+1} - \bar{u}^s \right) - \sum_{j=2+\hat{r}^{\mathcal{T}}_m}^{K} (j - 1 - \hat{r}^{\mathcal{T}}_m) \psi_j(\gamma) \\
&+ \sum_{j=2+\hat{r}^{\mathcal{T}}_{m+1}}^{K} \frac{c_j}{j} \sum_{i=\hat{r}^{\mathcal{T}}_{m,n}-j+1}^{k_n^1-1} \sum_{s=1}^{i+j-\hat{r}^{\mathcal{T}}_{m+1,n}} J_1\left(\bar{v}^s - \bar{v}^{s-1} \right) + r_1(n) \\
=& \sum_{j=2+\hat{r}^{\mathcal{T}}_m}^{K} \frac{c_j}{j} \sum_{s=1}^{j-1} (j - (s \vee (\hat{r}^{\mathcal{T}}_m + 1))) J_1\left(\bar{u}^s - \bar{u}^{s-1} \right) - \sum_{j=2+\hat{r}^{\mathcal{T}}_m}^{K} (j - 1 - \hat{r}^{\mathcal{T}}_m) \psi_j(\gamma) \\
&+ \sum_{j=2+\hat{r}^{\mathcal{T}}_{m+1}}^{K} \frac{c_j}{j} \sum_{s=1}^{j-\hat{r}^{\mathcal{T}}_{m+1}-1} (j - \hat{r}^{\mathcal{T}}_{m+1} - s) J_1\left(\bar{v}^s - \bar{v}^{s-1} \right) + r_1(n) \qquad (4.109)
\end{aligned}
$$

with

$$r_1(n) = \sum_{j=2+\hat{r}_m^{\mathcal{T}}}^{K} \left\{ \sum_{i=\hat{r}_{m,n}^{\mathcal{T}}-j+1}^{k_n^1-1} J_j\left(\frac{u_n^{i+j}-u_n^i}{j\lambda_n}\right) + \frac{c_j}{j} \sum_{s=\hat{r}_{m,n}^{\mathcal{T}}}^{(\hat{r}_{m+1,n}^{\mathcal{T}}\wedge(i+j))-1} J_1\left(\frac{u_n^{s+1}-u_n^s}{\lambda_n}\right) \right\} \to 0$$

as $n \to \infty$, which follows from (4.108). Moreover, we have

$$\sum_{j=2}^{K} \sum_{i=\hat{r}_{m,n}^{\mathcal{T}}}^{\hat{r}_{m+1,n}^{\mathcal{T}}-1} \left(\frac{i-k_n^1+1}{j} \wedge 1\right) \mu_{j,n}^i = -\sum_{j=2}^{K} \sum_{s=\hat{r}_m^{\mathcal{T}}+1}^{\hat{r}_{m+1}^{\mathcal{T}}} \left(\frac{s}{j}\wedge 1\right)\psi_j(\gamma) + r_2(n), \tag{4.110}$$

with

$$r_2(n) = \sum_{j=2}^{K} \sum_{s=\hat{r}_m^{\mathcal{T}}+1}^{\hat{r}_{m+1}^{\mathcal{T}}} \left(\frac{s}{j}\wedge 1\right)\psi_j\left(\frac{u_n^{\hat{r}_{m+1,n}^{\mathcal{T}}} - u_n^{\hat{r}_{m,n}^{\mathcal{T}}}}{(\hat{r}_{m+1,n}^{\mathcal{T}} - \hat{r}_{m,n}^{\mathcal{T}})\lambda_n}\right) \to 0 \quad \text{as } n \to \infty.$$

Hence, using (4.109) and (4.110), we obtain

$$\begin{aligned}
&\sum_{j=2}^{K} \left\{ \sum_{i=k_n^0}^{k_n^1-1} \sigma_{j,n}^i + \sum_{s=1}^{j-1} \frac{s}{j}\mu_{j,n}^{k_n^1+s-1} + \sum_{i=k_n^1+j-1}^{r(\mathcal{T}_n)} \mu_{j,n}^i \right\} \\
=&\sum_{j=\hat{r}_m^{\mathcal{T}}+2}^{K} c_j \sum_{s=1}^{j-1} \frac{j-(s\vee\hat{r}_m^{\mathcal{T}})}{j} J_1\left(\bar{u}^s - \bar{u}^{s-1}\right) + \sum_{j=2}^{K} \sum_{i=(\hat{r}_m^{\mathcal{T}}-j+1)\vee 0}^{k_n^1+\hat{r}_m^{\mathcal{T}}-j-k_n^0} \sigma_j^i(\bar{u}) \\
&+\sum_{j=2}^{K} \sum_{i=0}^{\hat{r}_m^{\mathcal{T}}-1} \left(\frac{\hat{r}_m^{\mathcal{T}}-i}{j}\wedge 1\right)\mu_j^i(\bar{u}) + \sum_{j=2+\hat{r}_{m+1}^{\mathcal{T}}}^{K} c_j \sum_{s=1}^{j-\hat{r}_{m+1}^{\mathcal{T}}-1} \frac{j-\hat{r}_{m+1}^{\mathcal{T}}-s}{j} J_1\left(\bar{v}^s - \bar{v}^{s-1}\right) \\
&-\sum_{j=2}^{K} \sum_{s=\hat{r}_m^{\mathcal{T}}+1}^{\hat{r}_{m+1}^{\mathcal{T}}} \left(\frac{s}{j}\wedge 1\right)\psi_j(\gamma) + \sum_{j=2}^{K} \sum_{i=1}^{r(\mathcal{T}_n)-\hat{r}_{m+1,n}^{\mathcal{T}}} \left(\frac{i+\hat{r}_{m+1}^{\mathcal{T}}}{j}\wedge 1\right)\mu_j^{i-1}(\bar{v}) \\
&-\sum_{j=2+\hat{r}_m^{\mathcal{T}}}^{K} (j-1-\hat{r}_m^{\mathcal{T}})\psi_j(\gamma) + r(n) \\
\leq& B_{IF}^{(2)}(\hat{r}^{\mathcal{T}}, m, \gamma) + B_{IF}^{(3)}(\hat{r}^{\mathcal{T}}, m+1) + 2\eta - \sum_{j=\hat{r}_m^{\mathcal{T}}+2}^{K} (j-1-\hat{r}_m^{\mathcal{T}})\psi_j(\gamma) \\
&-\sum_{j=2}^{K} \sum_{s=\hat{r}_m^{\mathcal{T}}+1}^{\hat{r}_{m+1}^{\mathcal{T}}} \left(\frac{s}{j}\wedge 1\right)\psi_j(\gamma) + r(n),
\end{aligned}$$

with $r(n) := r_1(n) + r_2(n)$. Now similar calculations as before lead, by using (3.108) and (3.99), to

$$\begin{aligned}\limsup_{n\to\infty} \hat{H}_{1,n}^{\ell,k_n,\mathcal{T}_n}(u_n) \leq& B(u_0^{(1)},\gamma) + B(u_1^{(1)},\gamma) + B_{IF}^{(2)}(\hat{r}^{\mathcal{T}},m,\gamma) + B_{IF}^{(3)}(\hat{r}^{\mathcal{T}},m+1)\\ &+ 4\eta - \sum_{j=\hat{r}_m^{\mathcal{T}}+2}^{K} (j-1-\hat{r}_m^{\mathcal{T}})\psi_j(\gamma) - \sum_{j=2}^{K} \sum_{s=\hat{r}_m^{\mathcal{T}}+1}^{\hat{r}_{m+1}^{\mathcal{T}}} \left(\frac{s}{j}\wedge 1\right)\psi_j(\gamma)\\ &- \sum_{j=2}^{K}(j-1)\psi_j(\gamma),\end{aligned}$$

which proves (4.88) by the arbitrariness of $\eta > 0$ and the definition of m.

Let us now consider $\hat{r}(\mathcal{T}) = +\infty$. By the definition of $B_{IF}^{(3)}$, there exists a function $\hat{v} : \mathbb{N}_0 \to \mathbb{R}$ with $\hat{v}^0 = 0$ and $\hat{v}^{i+1} - \hat{v}^i = \hat{v}^{\hat{r}_s^{\mathcal{T}} - \hat{r}_{m+1}^{\mathcal{T}}+1} - \hat{v}^{\hat{r}_s^{\mathcal{T}} - \hat{r}_{m+1}^{\mathcal{T}}}$ for $\hat{r}_s^{\mathcal{T}} - \hat{r}_{m+1}^{\mathcal{T}} \leq i < \hat{r}_{s+1}^{\mathcal{T}} - \hat{r}_{m+1}^{\mathcal{T}}$ with $s \in \{m+1,\dots,k_r^{\mathcal{T}}-2\}$ and $\hat{v}^{i+1} - \hat{v}^i = \gamma$ for $i \geq \hat{r}_{k_r^{\mathcal{T}}-1}^{\mathcal{T}} - \hat{r}_{m+1}^{\mathcal{T}}$ such that

$$\begin{aligned}&\sum_{j=2+\hat{r}_{m+1}^{\mathcal{T}}}^{K} c_j \sum_{s=1}^{j-\hat{r}_{m+1}^{\mathcal{T}}-1} \frac{j-s-\hat{r}_{m+1}^{\mathcal{T}}}{j} J_1(\hat{v}^s - \hat{v}^{s-1})\\ &\quad+ \sum_{j=2}^{K}\sum_{i\geq 1} \left(\frac{i+\hat{r}_{m+1}^{\mathcal{T}}}{j}\wedge 1\right)\mu_j^{i-1}(\hat{v}) \leq B_{IF}^{(3)}(\hat{r}^{\mathcal{T}},m+1) + \eta.\end{aligned}$$

Note that $\mu_j^i(\hat{v}) = 0$ for $i \geq \hat{r}_{k_r^{\mathcal{T}}-1}^{\mathcal{T}} - \hat{r}_{m+1}^{\mathcal{T}}$. Define u_n as in (4.105) with $\bar{v}$ replaced by $\hat{v}$. Similar calculations as above yield that (u_n) is a recovery sequence for u. We only show that (u_n) satisfies (4.106). By (4.107) and $\hat{v}^{i+1} - \hat{v}^i = \gamma$ for $i \geq \hat{r}_{k_r^{\mathcal{T}}-1}^{\mathcal{T}} - r_{m+1}^{\mathcal{T}}$, we obtain that there exists $C \in \mathbb{R}$ independent of n such that

$$\begin{aligned}u_n^{\hat{r}_{m+1,n}^{\mathcal{T}}} - u_n^{\hat{r}_{m,n}^{\mathcal{T}}} =& \ell - \gamma + \lambda_n\left(\gamma(r(\mathcal{T}_n) - k_n^1) - \hat{v}^{r(\mathcal{T}_n)-k_n^1-\hat{r}_{m+1}^{\mathcal{T}}} + C\right)\\ =& \ell - \gamma + \lambda_n\left(\gamma\hat{r}_{k_r^{\mathcal{T}}-1}^{\mathcal{T}} - \hat{v}^{\hat{r}_{k_r^{\mathcal{T}}-1}^{\mathcal{T}} - r_{m+1}^{\mathcal{T}}} + C\right) \to \ell - \gamma \quad \text{as } n\to\infty.\end{aligned}$$

We can now use similar arguments as in the case $\hat{r}(\mathcal{T}) < +\infty$ to prove (4.88).

Case (4): Here, we prove that there exists a sequence (u_n) converging in $L^1(0,1)$ to u, given by (4.46), which satisfies (4.89).

Without loss of generality we can assume $b(0,\mathcal{T}) < +\infty$. By the definition of $b(0,\mathcal{T})$, we can find a sequence $(h_n) \subset \mathbb{N}$ with $t_n^{h_n}, t_n^{h_n+1} \in \mathcal{T}_n$, $r(\mathcal{T}_n) \leq t^{h_n} < t_n^{h_n+1}$ and $\lim_{n\to\infty} \lambda_n t_n^{h_n} = \lim_{n\to\infty}\lambda_n t_n^{h_n+1} = 0$ such that

$$\lim_{n\to\infty}(t_n^{h_n+1} - t_n^{h_n}) = b(0,\mathcal{T}).$$

We construct now the sequence (u_n) by means of the functions v and w:

$$u_n^i = \begin{cases} \lambda_n v^i & \text{if } 0 \leq i \leq t_n^{h_n}, \\ \frac{t_n^{h_n+1}-i}{t_n^{h_n+1}-t_n^{h_n}}\lambda_n v^{t_n^{h_n}} + \frac{i-t_n^{h_n}}{t_n^{h_n+1}-t_n^{h_n}}(\ell - \lambda_n w^{n-t_n^{h_n+1}}) & \text{if } t_n^{h_n} < i < t_n^{h_n+1}, \\ \ell - \lambda_n w^{n-i} & \text{if } t_n^{h_n+1} \leq i \leq n. \end{cases}$$

This sequence satisfies the boundary conditions (3.3) and $u_n^{i+1} - u_n^i = \lambda_n\gamma$ for $N_1 \leq i \leq t_n^{h_n}$ and for $t_n^{h_n+1} \leq i \leq n - N_2$ and we have

$$\begin{aligned} u_n^{t_n^{h_n+1}} - u_n^{t_n^{h_n}} =& \ell + \lambda_n(w^{t_n^{h_n+1}-n} - v^{t_n^{h_n}}) \\ =& \ell + \lambda_n(w^{t_n^{h_n+1}-n} - w^{-N_2} + w^{-N_2} - v^{t_n^{h_n}} + v^{N_1} - v^{N_1}) \\ =& \ell + \lambda_n(\gamma(t_n^{h_n+1} - t_n^{h_n} - n + N_2 + N_1) + w^{-N_2} - v^{N_1}) \to \ell - \gamma \end{aligned}$$

as $n \to \infty$. Thus, $u_n \to u$ in $L^1(0,1)$. Furthermore, we obtain for $t_n^{h_n} \leq i \leq t_n^{h_n+1} - 1$,

$$\mu_{j,n}^i = \psi_j\left(\frac{u_n^{t_n^{h_n+1}} - u_n^{t_n^{h_n}}}{\lambda_n(t_n^{h_n+1} - t_n^{h_n})}\right) - \psi_j(\gamma) \to -\psi_j(\gamma)$$

as $n \to \infty$. This implies

$$\sum_{j=2}^{K} \sum_{i=t_n^{h_n}}^{t_n^{h_n+1}-1} \mu_{j,n}^i = -b(0,\mathcal{T})\sum_{j=2}^{K}\psi_j(\gamma) = -b(0,\mathcal{T})J_{CB}(\gamma),$$

and together with (3.108) and (3.99) the desired inequality (4.89) follows.

Jump in $(0,1)$ We have to prove that there exists a sequence (u_n) converging in $L^1(0,1)$ to u, given in (4.84), satisfying

$$\lim_n \hat{H}_{1,n}^{\ell,k_n,\mathcal{T}_n}(u_n) \leq B(u_0^{(1)},\gamma) + B(u_1^{(1)},\gamma) - b(x,\mathcal{T})J_{CB}(\gamma) - \sum_{j=2}^{K}(j-1)\psi_j(\gamma).$$

This can be shown analogously to case (4) for a jump in 0, by using sequence $(h_n) \subset \mathbb{N}$ with $t_n^{h_n}, t_n^{h_n+1} \in \mathcal{T}_n$ for all $n \in \mathbb{N}$ such that $\lim_n \lambda_n t_n^{h_n} = \lim_n \lambda_n t_n^{h_n+1} = x$ and

$$\lim_{n\to\infty}(t_n^{h_n+1} - t_n^{h_n}) = b(x,\mathcal{T}).$$

□

4.4 Minimum Problems

According to Theorem 3.19 and Theorem 4.11, the sequences $(H_{1,n}^{\ell})$ and $(\hat{H}_{1,n}^{\ell,k_n,\mathcal{T}_n})$ do not have the same Γ-limit for $\ell > \gamma$, while they coincide in the case $0 < \ell \leq \gamma$. In order to analyse the validity of the QC-approximation also for $\ell > \gamma$, we study the minimum of $\hat{H}_1^{\ell,\mathcal{T}}$ in dependence of the choice of the representative atoms described by $\mathcal{T} = (\mathcal{T}_n)$.

Here, we consider the case of nearest and next-to-nearest neighbour interactions only; for a short comment on the general case, see Remark 4.24 at the end of this section. We give sufficient conditions on $\mathcal{T}$ such that $\min_u H_1^\ell(u) = \min_u \hat{H}_1^{\ell,\mathcal{T}}(u)$. Moreover, we provide examples in which the minimal energies and minimisers of H_1^ℓ and $\hat{H}_1^{\ell,\mathcal{T}}$ do not coincide. To this end, certain relations between different boundary layer and jump energies are needed, which we provide in several lemmas in this section. Some of these relations are proven under additional assumptions on the potentials J_1 and J_2. In Proposition 3.2, we show that all these assumptions are satisfied for the classical Lennard-Jones potentials and Morse-potentials; see (3.22) and (3.24). The following results are contained in [55, Section 5].

Throughout this section, we assume that J_1 and J_2 satisfy the assumptions (LJ1)–(LJ5) (for $K = 2$). Recall that in this case, we have

$$J_0(z) := J_{0,2}(z) = J_2(z) + \frac{1}{2} \inf \{J_1(z_1) + J_1(z_2) : \; z_1 + z_2 = 2z\}$$

and $\psi_2(z) = J_{CB}(z) = J_1(z) + J_2(z)$ for all $z \in \mathbb{R}$. Let us recast the boundary layer energies derived in Section 3.3 for the case $K = 2$. For a function $v : \mathbb{N}_0 \to \mathbb{R}$ and $i \in \mathbb{N}_0$ we define $\sigma^i(v)$ as

$$\sigma^i(v) = J_2\left(\frac{v^{i+2} - v^i}{2}\right) + \frac{1}{2}\left(J_1(v^{i+2} - v^{i+1}) + J_1(v^{i+1} - v^i)\right) - J_0(\gamma). \tag{4.111}$$

The boundary layer energies $B(\theta, \gamma)$, $B_b(\theta)$, defined in (3.72), (3.70) for $\theta \in \mathbb{R}_+^{K-1}$ and $B(\gamma)$ defined in (3.71) reads in the case $K = 2$ and $\theta > 0$ as

$$\begin{aligned} B(\theta, \gamma) = \inf_{N \in \mathbb{N}} \min \Bigg\{ & \frac{1}{2} J_1(v^1 - v^0) + \sum_{i \geq 0} \sigma^i(v) : \\ & v : \mathbb{N}_0 \to \mathbb{R}, v^0 = 0, v^1 = \theta, v^{i+1} - v^i = \gamma \text{ for } i \geq N \Bigg\}, \end{aligned} \tag{4.112}$$

$$\begin{aligned} B_b(\theta) = \inf_{q \in \mathbb{N}} \min \Bigg\{ & \frac{1}{2} J_1(v^1 - v^0) + \sum_{i=0}^{q-2} \sigma^i(v) : \\ & v : \mathbb{N}_0 \to \mathbb{R}, v^q = 0, v^{q-1} = -\theta \Bigg\}, \end{aligned} \tag{4.113}$$

$$\begin{aligned} B(\gamma) = \inf_{N \in \mathbb{N}_0} \min \Bigg\{ & \frac{1}{2} J_1(v^1 - v^0) + \sum_{i \geq 0} \sigma^i(v) : \\ & v : \mathbb{N}_0 \to \mathbb{R}, v^0 = 0, v^{i+1} - v^i = \gamma \text{ for } i \geq N \Bigg\}. \end{aligned} \tag{4.114}$$

Next, we restate Theorem 3.19 in the case $K = 2$. Note that in this case the result was already proven in [50, Theorem 4.2].

Proposition 4.13. *Let $K = 2$ and suppose that J_1 and J_2 satisfy the assumptions (LJ1)–(LJ5). Let $\ell > \gamma$ and $u_0^{(1)}, u_1^{(1)} > 0$. Then $(H_{1,n}^\ell)$ Γ-converges with respect to the $L^1(0,1)$-topology to the functional H_1^ℓ defined by*

$$\begin{aligned} H_1^\ell(u) =& B(u_0^{(1)},\gamma)(1-\#(S_u\cap\{0\})) + B_{BJ}(u_0^{(1)})\#(S_u\cap\{0\}) + B_{IJ}\#(S_u\cap(0,1)) \\ &+ B(u_1^{(1)},\gamma)(1-\#(S_u\cap\{1\})) + B_{BJ}(u_1^{(1)})\#(S_u\cap\{1\}) - J_0(\gamma) \end{aligned} \tag{4.115}$$

if $u \in SBV_c^\ell(0,1)$, and $+\infty$ else on $L^1(0,1)$, where, for $\theta > 0$,

$$B_{BJ}(\theta) = \frac{1}{2}J_1(\theta) + B_b(\theta) + B(\gamma) - 2J_0(\gamma) \tag{4.116}$$

is the boundary layer energy due to a jump at the boundary and

$$B_{IJ} = 2B(\gamma) - 2J_0(\gamma) \tag{4.117}$$

is the boundary layer energy due to a jump at an internal point of $(0,1)$, where $B(\theta,\gamma)$, $B_b(\theta)$ and $B(\gamma)$ are defined in (4.112)–(4.114).

Let us now rewrite the results for $H_{1,n}^{\ell,k_n,\mathcal{T}_n}$ in the case of nearest and next-to-nearest neighbour interactions. In this case, the definitions of the boundary layer energies for a jump at the interface between the atomistic and continuum region simplifies significantly. Let $r(\mathcal{T}_n), \hat{r}(\mathcal{T}), l(\mathcal{T}_n)$ and $\hat{l}(\mathcal{T})$ be defined as in (4.24). In the case $K = 2$, we have $\hat{r}^{\mathcal{T}} = (0, \hat{r}(\mathcal{T})) \in \mathcal{I}(2)$ and $\hat{l}^{\mathcal{T}} = (0, \hat{l}(\mathcal{T})) \in \mathcal{I}(2)$, see (4.28). Moreover, the boundary layer energy $B_{IF}(n)$ for $n \in \mathbb{N}$, defined in (4.37), reads

$$B_{IF}(n) := \inf_{q\in\mathbb{N}} \min\left\{ J_1(v^1 - v^0) + \sum_{i=0}^{q-1} \sigma^i(v) + \left(n - \frac{1}{2}\right)\mu^q(v) : \ v : \mathbb{N}_0 \to \mathbb{R}, v^0 = 0 \right\}, \tag{4.118}$$

where $\mu^i(v)$ is defined for functions $v : \mathbb{N}_0 \to \mathbb{R}$ and $i \in \mathbb{N}_0$ as

$$\mu^i(v) = J_{CB}\left(v^{i+1} - v^i\right) - J_{CB}(\gamma). \tag{4.119}$$

Note that the additional constraint $v^{q+i+1} - v^{q+i} = v^{q+1} - v^q$ for $0 \le i \le n-1$ in (4.37), vanishes in (4.118). This follows from the fact that, for given $q \in \mathbb{N}$, the minimum problem in the definition of (4.118) is independent of $v^{i+1} - v^i$ for $i \ge q+1$, see (4.111). The following result follows directly from Theorem 4.11; see also [55, Theorem 4.8] for a direct proof.

Proposition 4.14. *Let $K = 2$ and suppose that J_1 and J_2 satisfy the assumptions (LJ1)–(LJ5). Let $\ell > \gamma$, and $u_0^{(1)}, u_1^{(1)} > 0$. Let $(k_n^1), (k_n^2)$ satisfy (4.6), and let $\mathcal{T} = (\mathcal{T}_n)$ satisfies* *the assumptions of Theorem 4.11. Then* $\hat{H}_1^{\ell,\mathcal{T}}$*, given in* (4.42)*, reads*

$$\begin{aligned}\hat{H}_1^{\ell,\mathcal{T}}(u) =& B(u_0^{(1)},\gamma)(1-\#(S_u\cap\{0\}))+B(u_1^{(1)},\gamma)(1-\#(S_u\cap\{1\}))\\ &+B_{IFJ}\left(\hat{r}(\mathcal{T}),b(0,\mathcal{T}),u_0^{(1)}\right)\#\left(S_u\cap\{0\}\right)-\sum_{x:x\in S_u\cap(0,1)}b(x,\mathcal{T})J_{CB}(\gamma)\\ &+B_{IFJ}\left(\hat{l}(\mathcal{T}),b(1,\mathcal{T}),u_1^{(1)}\right)\#\left(S_u\cap\{1\}\right)-J_0(\gamma)\end{aligned} \tag{4.120}$$

if $u\in SBV_c^\ell(0,1)$*, and* $+\infty$ *else on* $L^1(0,1)$*, where* $b(x,\mathcal{T})$ *is defined in* (4.29) *and* $B_{IFJ}(n,k,\theta)$ *is defined for* $n,k\in\mathbb{N}\cup\{+\infty\}$*,* $\theta>0$ *as*

$$B_{IFJ}(n,k,\theta)=\min\left\{\min\left\{B_{AIF}(n),B_{BIF}(n),-kJ_{CB}(\gamma)\right\}+B(\theta,\gamma),B_{BJ}(\theta)\right\} \tag{4.121}$$

with

$$B_{AIF}(n):=B_{IF}(n)+B(\gamma)-2J_0(\gamma), \tag{4.122}$$

and

$$B_{BIF}(n):=B(\gamma)-\left(\frac{1}{2}+n\right)J_0(\gamma), \tag{4.123}$$

where $B_{BJ}(\theta)$ *and* $B_{IF}(n)$ *are given in* (4.116) *and* (4.118)*.*

Proof. We only have to show that for all $r=(r_1,r_2)\in\mathcal{I}(2)$ (see (4.30)) it holds $B_{BIF}(r)=B_{BIF}(r_2)$, see (4.45), (4.123). Fix $r\in\mathcal{I}(2)$. Using $B_{IF}^{(2)}(r,1,\gamma)=B(\gamma)$ and $B_{IF}^{(3)}(r,2)=0$ (see Remark 4.9) and $\psi_2(\gamma)=J_{CB}(\gamma)$, we obtain from (4.45) that

$$\begin{aligned}B_{BIF}(r)=&B_{IF}(r,1,\gamma)+B_{IF}^{(3)}(r,2)-J_{CB}(\gamma)-\sum_{s=1}^{r_2}\left(\frac{s}{2}\wedge 1\right)J_{CB}(\gamma)\\ =&B(\gamma)-J_{CB}(\gamma)\left(r_2+\frac{1}{2}\right)=B_{BIF}(r_2).\end{aligned}$$

We used that the constraint in (4.45) reads $m=1$ and that $r_1=0$. □

Let us now give some estimates for the boundary layer energies in the case $K=2$.

Lemma 4.15. *Let (LJ1)–(LJ5) for* $K=2$ *be satisfied. Then*

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

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

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

(4) $B_b(\delta_1)=\frac{1}{2}J_1(\delta_1)$*;*

(5) $\frac{1}{2}J_1(\delta_1)\le B_{IF}(m)\le\frac{1}{2}J_1(\gamma)$ *for every* $m\in\mathbb{N}\cup\{+\infty\}$*.*

Proof. (1)–(3) follows directly from Lemma 3.22 and (3) implies (4); see also [50, Lemma 5.1] for direct proves. Let us show (5). Since γ is the minimum point of J_0 and J_{CB} the terms involving $\sigma^i(v)$ and $\mu^i(v)$ in the definition of $B_{IF}(m)$, see (4.118), are non-negative. Hence, we have

$$B_{IF}(m) \geq \min \frac{1}{2}J_1(z) = \frac{1}{2}J_1(\delta_1).$$

To show the upper bound, we can use the function $u : \mathbb{N}_0 \to \mathbb{R}$ with $u^i = i\gamma$ as a competitor for $B_{IF}(m)$ for every $m \in \mathbb{N}$ and deduce the upper bound. □

To compare $\min_u H_1^\ell(u)$ and $\min_u \hat{H}_1^{\ell,\mathcal{T}}(u)$, we need to estimate $B_{IFJ}(n,k,\theta)$, defined in (4.121). This will be done, under additional assumptions on J_1, J_2, in the following lemmas.

Lemma 4.16. *Let J_1, J_2 be such that (LJ1)–(LJ5) are satisfied and $J_1(\gamma)$, $J_2(\gamma)$, $J_2(\delta_1) < 0$. Define the quantity*

$$\tilde{B}_{IFJ}(n,k) := \min\left\{B_{AIF}(n), B_{BIF}(n), -kJ_0(\gamma)\right\}, \tag{4.124}$$

where B_{AIF} and B_{BIF} are defined in (4.122) *and* (4.123)*. Then*

(i) $\tilde{B}_{IFJ}(n,1) = -J_0(\gamma)$ *for all $n \in \mathbb{N} \cup \{+\infty\}$, $n \geq 1$,*

(ii) $\tilde{B}_{IFJ}(1,k) = B_{BIF}(1) = B(\gamma) - \frac{3}{2}J_0(\gamma)$ *for all $k \in \mathbb{N} \cup \{+\infty\}, k \geq 2$,*

(iii) $\tilde{B}_{IFJ}(n,k) = B_{AIF}(n)$ *for all $n,k \in \mathbb{N} \cup \{+\infty\}$ with $n \geq 2, k \geq 2$.*

Proof. (i) From $J_2(\delta_1) < 0$, we deduce $J_0(\gamma) \leq J_0(\delta_1) \leq J_1(\delta_1) + J_2(\delta_1) < J_1(\delta_1)$. Hence, we obtain by $B(\gamma), B_{IF}(n) \geq \frac{1}{2}J_1(\delta_1)$, see Lemma 4.15 (1) and (5), and the definitions of $B_{AIF}(n)$ and $B_{BIF}(n)$, see (4.122) and (4.123), that

$$\begin{aligned}
B_{AIF}(n) \geq& J_1(\delta_1) - 2J_0(\gamma) > -J_0(\gamma),\\
B_{BIF}(n) \geq& B(\gamma) - \frac{3}{2}J_0(\gamma) \geq \frac{1}{2}J_1(\delta_1) - \frac{3}{2}J_0(\gamma) > -J_0(\gamma).
\end{aligned}$$

(ii) From $B_{IF}(m) \geq \frac{1}{2}J_1(\delta_1)$, $0 > J_1(\delta_1) > J_0(\gamma)$ and $B(\gamma) \leq \frac{1}{2}J_1(\gamma) < 0$, $J_0(\gamma) < J_1(\gamma)$, we deduce

$$\begin{aligned}
B_{AIF}(1) \geq& \frac{1}{2}J_1(\delta_1) + B(\gamma) - 2J_0(\gamma) > B(\gamma) - \frac{3}{2}J_0(\gamma) = B_{BIF}(1),\\
-kJ_0(\gamma) \geq& -2J_0(\gamma) > \frac{1}{2}J_1(\gamma) - \frac{3}{2}J_0(\gamma) \geq B(\gamma) - \frac{3}{2}J_0(\gamma) = B_{BIF}(1).
\end{aligned}$$

(iii) Again by $B_{IF}(m), B(\gamma) \leq \frac{1}{2}J_1(\gamma) < 0$ and $J_0(\gamma) < 0$, we conclude

$$\begin{aligned}
B_{AIF}(n) \leq& \frac{1}{2}J_1(\gamma) + B(\gamma) - 2J_0(\gamma) < B(\gamma) - \frac{5}{2}J_0(\gamma) \leq B_{BIF}(n)\\
B_{AIF}(n) \leq& J_1(\gamma) - 2J_0(\gamma) < -kJ_0(\gamma),
\end{aligned}$$

for $n, k \geq 2$, which proves the statement. □

In order to compute the value of $B_{IFJ}(n,k,\theta)$, see (4.121), we provide an estimate for $B_{AIF}(n)$.

Lemma 4.17. *Let J_1, J_2 satisfy assumptions (LJ1)–(LJ5) and additionally*

$$R(t) := J_2\left(\frac{\gamma+t}{2}\right) + \frac{1}{2}\left(J_1(\gamma)+J_1(t)\right) - J_0(\gamma) - \frac{3}{2}\left(J_{CB}(t) - J_0(\gamma)\right) \le 0 \qquad (4.125)$$

for all $t \in \operatorname{dom} J_1$. Then $B_{IF}(m) = B(\gamma)$ for any $m \ge 2$ and $B_{AIF}(n) = B_{IJ}$ for $n \ge 2$, where $B_{IF}(m)$, $B(\gamma)$, $B_{AIF}(n)$ and B_{IJ} are defined in (4.118), (4.113), (4.122) *and* (4.117).

Proof. Let us first show that $B_{IF}(m) \le B(\gamma)$ for all $m \in \mathbb{N}$. For every $\eta > 0$ there exists, by the definition of $B(\gamma)$, in (4.114), a function $\tilde{u} : \mathbb{N} \to \mathbb{R}$ and an $\tilde{N} \in \mathbb{N}$ such that $\tilde{u}^0 = 0$, $\tilde{u}^{i+1} - \tilde{u}^i = \gamma$ if $i \ge \tilde{N}$, satisfying (4.92) in the case $K = 2$, i.e.

$$\frac{1}{2}J_1(\tilde{u}^1 - \tilde{u}^0) + \sum_{i\ge 0}\sigma^i(\tilde{u}) \le B(\gamma) + \eta.$$

The function $\tilde{u}$ is also a competitor for the minimum problem for $B_{IF}(m)$, see (4.118). For $q > \tilde{N}+1$, we have that $\mu^q(\tilde{u}) = 0$, $\sigma^i(\tilde{u}) = 0$ for $i \ge q$ and thus

$$B_{IF}(m) \le \frac{1}{2}J_1(\tilde{u}^1 - \tilde{u}^0) + \sum_{i=0}^{q-1}\sigma^i(\tilde{u}) + \left(m - \frac{1}{2}\right)\mu^q(\tilde{u}) \le B(\gamma) + \eta$$

and the assertion follows by the arbitrariness of $\eta > 0$.

Let us now show $B_{IF}(m) \ge B(\gamma)$ for $m \ge 2$. The definition of $B_{IF}(m)$, see (4.118), implies $B_{IF}(m) \ge B_{IF}(2)$ for all $m \ge 2$. Let $\eta > 0$. By the definition of $B_{IF}(2)$ in (4.118) there exist a function $u : \mathbb{N}_0 \to \mathbb{R}$ and a $q \in \mathbb{N}$ such that $u^0 = 0$ and

$$\frac{1}{2}J_1(u^1 - u^0) + \sum_{i=0}^{q-1}\sigma^i(u) + \frac{3}{2}\mu^q(u) \le B_{IF}(2) + \eta.$$

Next, we define the function $\bar{u} : \mathbb{N}_0 \to \mathbb{R}$ by $\bar{u}^i = u^i$ if $i \le q+1$ and $\bar{u}^{i+1} - \bar{u}^i = \gamma$ if $i \ge q+1$. The function $\bar{u}$ is a competitor for $B(\gamma)$, see (4.114). Thus

$$\begin{aligned} B(\gamma) \le& \frac{1}{2}J_1(\bar{u}^1 - \bar{u}^0) + \sum_{i\ge 0}\sigma^i(\bar{u}) \\ =& \frac{1}{2}J_1(u^1 - u^0) + \sum_{i=0}^{q-1}\sigma^i(u) + J_2\left(\frac{\gamma + u^{q+1} - u^q}{2}\right) + \frac{1}{2}J_1(u^{q+1} - u^q) \\ &+ \frac{1}{2}J_1(\gamma) - J_0(\gamma) \le B_{IF}(2) + \eta + R(u^{q+1} - u^q). \end{aligned}$$

By assumption (4.125), we have $R(u^{q+1} - u^q) \le 0$. Hence, by the arbitrariness of $\eta > 0$, we have $B_{IF}(m) \ge B_{IF}(2) \ge B(\gamma)$ for all $m \ge 2$.

Altogether, we have $B_{IF}(m) = B(\gamma)$ for $m \geq 2$. Hence, we have by the definition of $B_{AIF}(n)$ and B_{IJ}, see (4.122) and (4.117), that $B_{AIF}(n) = B_{IJ}$ for $n \geq 2$. □

Before we state our main result of this section, we recall some estimates for the boundary layer energies in H_1^ℓ given in Lemma 3.23 and Proposition 3.24, and refine them under additional assumptions on J_1 and J_2.

Lemma 4.18. *Let J_1, J_2 satisfy (LJ1)–(LJ5). Then*

$$B(\theta,\gamma) \leq B_{BJ}(\theta) \leq B(\theta,\gamma) + B_{IJ} \qquad \forall \theta > 0, \tag{4.126}$$

$$\min_u H_1^\ell(u) = \min\left\{B_{BJ}(u_0^{(1)}) + B(u_1^{(1)},\gamma), B_{BJ}(u_1^{(1)}) + B(u_0^{(1)},\gamma)\right\} - J_0(\gamma). \tag{4.127}$$

and $B_{IJ} > 0$, where $B(\theta,\gamma)$, $B_{BJ}(\theta)$ and B_{IJ} are defined in (4.112), (4.116) *and* (4.117). *If, for $\theta > 0$, there exists a constant $\eta_\theta > 0$ such that $\frac{1}{2}J_1(\gamma) + J_2\left(\frac{t+\gamma}{2}\right) \leq 0$ for all $t \in \mathbb{R}$ with $J_1(t) < J_1(\theta) + 2\eta_\theta$, it holds that $B(\theta,\gamma) < B_{BJ}(\theta)$.*

Proof. The inequalities (4.126), $B_{IJ} > 0$ and (4.127) follow from Lemma 3.23 and Proposition 3.24, where the case of arbitrary $K \geq 2$ is considered.

We prove $B(\theta,\gamma) < B_{BJ}(\theta)$ under the additional assumption. Let $\eta > 0$ be such that $\eta < \eta_\theta$ and $\frac{1}{2}B_{IJ} - \eta > 0$. We show $B_{BJ}(\theta) - (\frac{1}{2}B_{IJ} - \eta) \geq B(\theta,\gamma)$, which clearly proves $B(\theta,\gamma) < B_{BJ}(\theta)$. By the definition of $B_b(\theta)$, see (4.113), there exist $q \in \mathbb{N}$ and $v : \mathbb{N}_0 \to \mathbb{R}$ such that $v^q = 0$ and $v^{q-1} = -\theta$ with

$$B_b(\theta) + \eta \geq \frac{1}{2}J_1(v^1 - v^0) + \sum_{i=0}^{q-2}\sigma^i(v).$$

By the upper bound $B_b(\theta) \leq \frac{1}{2}J_1(\theta)$ (see Lemma 4.15 (3)) and the fact that the terms in the above sum are non-negative, we deduce $J_1(v^1 - v^0) \leq J_1(\theta) + 2\eta$. Let us define the function $u : \mathbb{N}_0 \to \mathbb{R}$ by $u^i = -v^{q-i}$ for $i \in \{0,\dots,q\}$ and $u^{i+1} - u^i = \gamma$ for $i \geq q$. Note that $u^1 - u^0 = v^q - v^{q-1} = \theta$ and thus that u is a competitor for the minimum problem which defines $B(\theta,\gamma)$, see (4.112). Hence,

$$\begin{aligned}
B(\theta,\gamma) &\leq \frac{1}{2}J_1(u^1 - u^0) + \sum_{i\geq 0}\sigma^i(u) \\
&= \frac{1}{2}J_1(\theta) + \sum_{i=0}^{q-2}\sigma^i(v) + J_2\left(\frac{\gamma + v^1 - v^0}{2}\right) + \frac{1}{2}J_1(v^1 - v^0) + \frac{1}{2}J_1(\gamma) - J_0(\gamma) \\
&\leq \frac{1}{2}J_1(\theta) + B_b(\theta) + \eta - J_0(\gamma) = B_{BJ}(\theta) + \eta - (B(\gamma) - J_0(\gamma)) \\
&= B_{BJ}(\theta) - \left(\frac{1}{2}B_{IJ} - \eta\right),
\end{aligned}$$

where we used $\frac{1}{2}J_1(\gamma) + J_2\left(\frac{v^1 - v^0 + \gamma}{2}\right) \leq 0$. □

Combining the previous results, we are able to give sufficient conditions on the representative atoms $\mathcal{T} = (\mathcal{T}_n)$ in order to ensure $\min_u H_1^\ell(u) = \min_u \hat{H}_1^{\ell,\mathcal{T}}(u)$. In plain terms, it is enough to make sure that the representative atoms $\mathcal{T}_n$ are such that $k_n^1+1, k_n^2-1 \notin \mathcal{T}_n$ and for all $i, j \in \{k_n^1 + 2, \ldots, k_n^2 - 2\} \cap \mathcal{T}_n$ it holds $|i - j| \geq 2$.

Theorem 4.19. *Let $u_0^{(1)}, u_1^{(1)} > 0$ and $\ell > \gamma$. Let J_1, J_2 satisfy (LJ1)–(LJ5), $J_1(\gamma)$, $J_2(\gamma)$, $J_2(\delta_1) < 0$ and (4.125). If $\mathcal{T} = (\mathcal{T}_n)$ satisfies (4.17) and $\hat{l}(\mathcal{T})$, $\hat{r}(\mathcal{T})$, $b(x, \mathcal{T}) \geq 2$, for all $x \in (0, 1)$, see (4.24), (4.29). Then $\hat{H}_1^{\ell,\mathcal{T}}$ defined in (4.120) reads*

$$\hat{H}_1^{\ell,\mathcal{T}}(u) = H_1^\ell(u) - \sum_{x:x\in S_u\cap(0,1)} (b(x, \mathcal{T})J_0(\gamma) + B_{IJ}) \tag{4.128}$$

for $u \in SBV_c^\ell(0, 1)$, and $+\infty$ else on $L^1(0, 1)$. Moreover, for given $u_0^{(1)}, u_1^{(1)} > 0$

$$\min_u \hat{H}_1^{\ell,\mathcal{T}}(u) = \min_u H_1^\ell(u). \tag{4.129}$$

For $u \in \operatorname{argmin} \hat{H}_1^{\ell,\mathcal{T}}$, the jump set satisfies $S_u \subset \{0, 1\}$. If furthermore J_1 and J_2 satisfy all assumptions of Lemma 4.18, it holds $\#S_u = 1$.

Proof. Let us first prove (4.128). By the definition of H_1^ℓ and $\hat{H}_1^{\ell,\mathcal{T}}$ (see (4.115), (4.120)), we have to show $B_{IFJ}(\hat{r}(\mathcal{T}), b(0, \mathcal{T}), u_0^{(1)}) = B_{BJ}(u_0^{(1)})$ and $B_{IFJ}(\hat{l}(\mathcal{T}), b(1, \mathcal{T}), u_1^{(1)}) = B_{BJ}(u_1^{(1)})$. By Lemma 4.17, we have $B_{AIF}(n) = B_{IJ}$, for $n \geq 2$. Hence, we have for $B_{IFJ}(n, k, \theta)$, defined in (4.121), with $n, k \geq 2$ and $\theta > 0$ by Lemma 4.16 (iii) and inequality (4.126) that

$$B_{IFJ}(n, k, \theta) = \min\{B_{AIF}(n) + B(\theta, \gamma), B_{BJ}(\theta)\} = B_{BJ}(\theta).$$

Hence, by $b(x, \mathcal{T}), \hat{l}(\mathcal{T}), \hat{r}(\mathcal{T}) \geq 2$, for all $x \in (0, 1)$ the assertion (4.128) is proven.

From $J_0(\gamma) < 0$, Lemma 4.16 (iii), Lemma 4.17 and Lemma 4.18, we deduce that

$$-b(x, \mathcal{T})J_0(\gamma) \geq -2J_0(\gamma) > \tilde{B}_{IFJ}(2, 2) = B_{AIF}(2) = B_{IJ} > 0 \tag{4.130}$$

for all $x \in (0, 1)$. Combining (4.130) with (4.126), we obtain that $B_{BJ}(\theta) < B(\theta, \gamma) - 2J_0(\gamma)$ for all $\theta > 0$. Hence, the jump set S_u of minimisers u of $\hat{H}_1^{\ell,\mathcal{T}}$ satisfies $S_u \subset \{0, 1\}$ and by (4.126)–(4.128)

$$\begin{aligned}\min_u \hat{H}_1^{\ell,\mathcal{T}}(u) &= \min\left\{B_{BJ}(u_0^{(1)}) + B(u_1^{(1)}, \gamma), B_{BJ}(u_1^{(1)}) + B(u_0^{(1)}, \gamma)\right\} - J_0(\gamma)\\ &= \min_u H_1^\ell(u).\end{aligned}$$

If J_1 and J_2 are such that $B(\theta, \gamma) < B_{BJ}(\theta)$ for all $\theta > 0$, see Lemma 4.18, we obtain from the above equation that every minimiser u of $\hat{H}_1^{\ell,\mathcal{T}}$ satisfies $\#S_u = 1$. □

In the next theorem which is based on the previous Γ-convergence statements, we deduce a convergence result for the difference between the minimal energies of the fully atomistic model and the quasicontinuum model.

Theorem 4.20. *Let $u_0^{(1)}, u_1^{(1)} > 0$, $\ell > 0$ and let k_n^1, k_n^2 satisfy* (4.6)*. Let J_1, J_2 and $(\mathcal{T}_n)$ satisfy the assumptions of Theorem 4.5 and, if $\ell > \gamma$, also the additional assumptions of Theorem 4.11 and Theorem 4.19 such that* (4.129) *is valid. Then it holds*

$$\inf_u H_n^\ell(u) - \inf_u \hat{H}_n^{\ell,k_n,\mathcal{T}_n}(u) = o(\lambda_n), \tag{4.131}$$

as $n \to \infty$.

Proof. Let us first note that the functionals H_n^ℓ, $\hat{H}_n^{\ell,k_n,\mathcal{T}_n}$ are equi-coercive in $L^1(0,1)$, which follows by the compactness argument in the proofs of Theorem 3.7 and Theorem 4.1. Moreover, by Proposition 3.9 and Proposition 4.3 the functionals $H_{1,n}^\ell$, $\hat{H}_{1,n}^{\ell,k_n,\mathcal{T}_n}$ are equi-coercive. In the case $0 < \ell \leq \gamma$, Theorem 3.12 and Theorem 4.5 ensure that H_n^ℓ and $\hat{H}_n^{\ell,k_n,\mathcal{T}_n}$ are Γ-equivalent at order λ_n, see [20, Definition 4.2], and (4.131) follows from [20, Theorem 4.4]. Similarly, if $\gamma < \ell$, we deduce from Theorem 4.1 and Theorem 4.11

$$\inf_u \hat{H}_n^{\ell,k_n,\mathcal{T}_n}(u) = \min_u H^\ell(u) + \lambda_n \min_u \hat{H}_1^{\ell,\mathcal{T}}(u) + o(\lambda_n),$$

see [9, Theorem 1.47]. Further, by (4.129), we obtain

$$\inf_u \hat{H}_n^{\ell,k_n,\mathcal{T}_n}(u) = \inf_u H^\ell(u) + \lambda_n \inf_u H_1^\ell(u) + o(\lambda_n) = \inf_u H_n^\ell(u) + o(\lambda_n).$$

□

Remark 4.21. In the case $0 < \ell \leq \gamma$, the estimate (4.131) holds under the assumptions of Theorem 4.5 for arbitrary $K \geq 2$. Indeed, Theorem 3.12 and Theorem 4.5 ensure that H_n^ℓ and $\hat{H}_n^{\ell,k_n,\mathcal{T}_n}$ are Γ-equivalent at order λ_n for all $K \geq 2$. Hence, the QNL-method is valid for general finite range interactions of Lennard-Jones type in an elastic regime.

In the next proposition, we show that the sufficient conditions of Theorem 4.19 are sharp in the case $\ell > \gamma$. To this end, we show for a particular choice of $u_0^{(1)}, u_1^{(1)} > 0$ that if the representative atoms are not chosen as in the above theorem, neither the minima nor the minimisers of H_1^ℓ and $\hat{H}_1^{\ell,\mathcal{T}}$ coincide.

Proposition 4.22. *Let $\ell > \gamma$, $u_0^{(1)} = \delta_1$ and $u_1^{(1)} = \gamma$. Let J_1, J_2 satisfy (LJ1)–(LJ5). Then it holds for H_1^ℓ*

$$\min_u H_1^\ell(u) = B_{BJ}(\delta_1) + B(\gamma,\gamma) - J_0(\gamma), \tag{4.132}$$

and the unique minimiser u satisfies $S_u = \{0\}$. Let J_1, J_2 satisfy the assumptions of Theorem 4.19 and $J_2(\gamma) > 2J_2\left(\frac{\delta_1+\gamma}{2}\right)$. Then the following assertions hold true:

(a) *Let* $\mathcal{T}^1 = (\mathcal{T}^1_n)$ *be such that there exists* $z \in [0,1]$ *with* $b(z, \mathcal{T}^1) = 1$. *Then* $\min_u \hat{H}_1^{\ell,\mathcal{T}^1} = B(\delta_1, \gamma) + B(\gamma, \gamma) - 2J_0(\gamma) < \min_u H_1^\ell$ *and the jump appears indifferently in* $z \in [0,1]$ *with* $b(z, \mathcal{T}^1) = 1$.

(b) *Let* $\mathcal{T}^2 = (\mathcal{T}^2_n)$ *be such that* $\hat{l}(\mathcal{T}^2) = 1$ *and* $\hat{r}(\mathcal{T}^2), b(z, \mathcal{T}^2) \geq 2$ *for all* $z \in [0,1]$. *Then* $\min_u \hat{H}_1^{\ell,\mathcal{T}^2} = B(\delta_1, \gamma) + B(\gamma, \gamma) + B(\gamma) - \frac{3}{2}J_0(\gamma) < \min_u H_1^\ell$ *and the jump appears in* 1.

Proof. Let us first prove the part regarding the energy H_1^ℓ. Proposition 3.24 yields that $B_{BJ}(\delta_1) < B(\delta_1, \gamma) + B_{IJ}$ and $B_{BJ}(\gamma) = B(\gamma, \gamma) + B_{IJ}$ (see also [50, Theorem 5.1]). This implies

$$B_{BJ}(\delta_1) + B(\gamma, \gamma) < B(\delta_1, \gamma) + B(\gamma, \gamma) + B_{IJ} = B(\delta_1, \gamma) + B_{BJ}(\gamma),$$

which proves (4.132) and that the unique minimiser u of H_1^ℓ satisfies $S_u = \{0\}$. Let us now show the assertions concerning the minimal energies of $\hat{H}_1^{\ell,\mathcal{T}}$. We test the minimum problem for $B(\delta_1, \gamma)$, see (4.112), with $v : \mathbb{N}_0 \to \mathbb{R}$ such that $v^{i+1} - v^i = \gamma$ for all $i \geq 1$. By using $J_2(\gamma) > 2J_2\left(\frac{\delta_1+\gamma}{2}\right)$ and $J_0(\gamma) = J_1(\gamma) + J_2(\gamma)$, we obtain

$$B(\delta_1, \gamma) \leq J_1(\delta_1) + \frac{1}{2}J_1(\gamma) + J_2\left(\frac{\delta_1 + \gamma}{2}\right) - J_0(\gamma) < J_1(\delta_1) - \frac{1}{2}J_0(\gamma). \tag{4.133}$$

From (4.43) and Lemma 4.16, we deduce $B_{IFJ}(n, k, \theta) \geq \min\{-J_0(\gamma) + B(\theta, \gamma), B_{BJ}(\theta)\}$.

(a) Combining the above considerations with (4.120) it is enough to show that $B(\delta_1, \gamma) - J_0(\gamma) < B_{BJ}(\delta_1)$. This follows by using (4.133), Lemma 4.15 (1), (4) and $J_0(\gamma) = J_{CB}(\gamma) < J_1(\delta_1)$:

$$B(\delta_1, \gamma) - J_0(\gamma) < J_1(\delta_1) - \frac{3}{2}J_0(\gamma) \leq \frac{1}{2}J_1(\delta_1) + B_b(\delta_1) + B(\gamma) - 2J_0(\gamma) = B_{BJ}(\delta_1).$$

(b) From (4.120), Theorem 4.19 and $\hat{r}(\mathcal{T}^2), b(z, \mathcal{T}^2) \geq 2$ for all $z \in [0,1]$, we deduce $\hat{H}_1^{\ell,\mathcal{T}^2}(u) \geq \min H_1^\ell$ for $u \in SBV_c^\ell(0,1)$ with $S_u \cap [0,1) \neq \emptyset$. Let us compute the energy for a jump at 1: For $k \geq 2$, we have by Lemma 4.16 (ii) that $\tilde{B}_{IFJ}(1,k) = B(\gamma) - \frac{3}{2}J_0(\gamma)$. As in Lemma 4.16 (ii), we have, by using $B(\gamma) \geq \frac{1}{2}J_1(\delta_1) > \frac{1}{2}J_0(\gamma)$ if $J_2(\gamma) < 0$, that $B_{IJ} \geq B(\gamma) - \frac{3}{2}J_0(\gamma)$. Hence, by applying $B_{BJ}(\gamma) = B(\gamma, \gamma) + B_{IJ}$ and the definition of $B_{IFJ}(n, k, \theta)$, see (4.43), we deduce

$$B_{IFJ}(1, k, \gamma) = \min\left\{B(\gamma) - \frac{3}{2}J_0(\gamma), B_{IJ}\right\} + B(\gamma, \gamma) = B(\gamma) - \frac{3}{2}J_0(\gamma) + B(\gamma, \gamma).$$

Thus, we deduce from $\hat{l}(\mathcal{T}^2) = 1$ and $b(1, \mathcal{T}^2) = 2$ that $B_{IFJ}(\hat{l}(\mathcal{T}^2), b(1, \mathcal{T}^2), \gamma) = B(\gamma) - \frac{3}{2}J_0(\gamma) + B(\gamma, \gamma)$. Hence, by the definition of $\hat{H}_1^{\ell,\mathcal{T}}$, see (4.120), and by (4.132) it remains to show that $B(\delta_1, \gamma) + B(\gamma) - \frac{3}{2}J_0(\gamma) < B_{BJ}(\delta_1)$, which follows by using (4.133) and

Lemma 4.15 (1), (4)

$$\begin{aligned} B(\delta_1,\gamma)+B(\gamma)-\frac{3}{2}J_0(\gamma) <& J_1(\delta_1)+B(\gamma)-2J_0(\gamma) \\ =& \frac{1}{2}J_1(\delta_1)+B_b(\delta_1)+B(\gamma)-2J_0(\gamma)=B_{BJ}(\delta_1). \end{aligned}$$

□

Next, we show that all additional assumptions on J_1, J_2 in this chapter are satisfied by the classical Lennard-Jones potentials and Morse potentials, defined in (3.22) and (3.24) respectively.

Proposition 4.23. *Let J_1, J_2 be as in (3.22) or (3.24) respectively. Then J_1 and J_2 satisfy $J_1(\gamma)$, $J_2(\gamma), J_2(\delta_1) < 0$, $J_2(\gamma) > 2J_2\left(\frac{\delta_1+\gamma}{2}\right)$ and inequality (4.125) holds on $\operatorname{dom} J_1$. Furthermore, there exists for all $\theta > 0$ a constant $\eta_\theta > 0$ such that $J_2\left(\frac{t+\gamma}{2}\right) < 0$ for $t \in \operatorname{dom} J_1$ such that $J_1(t) < J_1(\theta) + 2\eta_\theta$.*

Proof. Let J_1, J_2 satisfy (3.22), i.e., there exist $k_1, k_2 > 0$ such that $J_1(z) = \frac{k_1}{z^{12}} - \frac{k_2}{z^6}$ and $J_2(z) = J_1(2z)$. Straightforward calculations lead to

$$\delta_1 = \left(\frac{2k_1}{k_2}\right)^{1/6}, \quad \gamma = \left(\frac{1+2^{-12}}{1+2^{-6}}\right)^{1/6}\delta_1, \quad z_0 = \left(\frac{k_1}{k_2}\right)^{1/6} = \left(\frac{1}{2}\right)^{1/6}\delta_1, \tag{4.134}$$

where δ_1 is the unique minimiser of J_1, γ the unique minimiser of J_0 (and J_{CB}) and z_0 is the unique zero of J_1 with $J_1 < 0$ on $(z_0, +\infty)$. Note that $z_0 < \gamma < \delta_1$. Moreover, we have that J_1 is strictly decreasing on $(0, \delta_1)$ and strictly increasing on $(\delta_1, +\infty)$. A simple calculation yield $J_1(z) < 0$ for $z > \left(\frac{k_1}{k_2}\right)^{1/6} := z_0$. From $\gamma > z_0$, we deduce $J_1(\gamma) < 0$ and thus $J_2\left(\frac{\gamma+t}{2}\right) = J_1(\gamma+t) < 0$ on $\{t : t > 0\} = \operatorname{dom} J_1$. Since $\gamma < 2\gamma < 2\delta_1$, we have $J_2(\gamma), J_2(\delta_1) < 0$. Moreover, by $\delta_1/2 < \gamma < \delta_1$ and the definition of J_2, it is sufficient to show $J_2(\gamma) > 2J_2(\delta_1)$ to obtain $J_2(\gamma) > 2J_2\left(\frac{\delta_1+\gamma}{2}\right)$:

$$\begin{aligned} J_2(\gamma)-2J_2(\delta_1) =& \frac{k_1}{2^{12}\delta_1^{12}}\left(\frac{(1+2^{-6})^2}{(1+2^{-12})^2}-2\right)-\frac{k_2}{2^6\delta_1^6}\left(\frac{1+2^{-6}}{1+2^{-12}}-2\right) \\ =& \frac{k_2^2}{4k_1 2^{12}}\left(\frac{(1+2^{-6})^2}{(1+2^{-12})^2}-2-2^7\left(\frac{1+2^{-6}}{1+2^{-12}}-2\right)\right) > 0. \end{aligned}$$

Let us now show inequality (4.125). Since $J_0(\gamma) = J_{CB}(\gamma) = J_1(\gamma) + J_2(\gamma)$ and $J_0'(\gamma) = J_{CB}'(\gamma) = 0$ one directly has $R(\gamma) = 0$ and $R'(\gamma) = 0$. Consider the function $J_1 + 2J_2$ given by

$$J_1(z)+2J_2(z) = \frac{k_1}{z^{12}} - \frac{k_2}{z^6} + \frac{k_1}{2^{11}z^{12}} - \frac{k_2}{2^5 z^6} = \frac{k_1(1+2^{-11})}{z^{12}} - \frac{k_2(1+2^{-5})}{z^6}.$$

This is again a Lennard-Jones potential and there exists a constant $z_c > 0$ such that $J_1''(z) + 2J_2''(z) > 0$ for all $z \in (0, z_c)$. To compute z_c we set the second derivative of

$J_1 + 2J_2$ equal to zero:

$$0 = \frac{156k_1(1+2^{-11})}{z_c^{14}} - \frac{42k_2(1+2^{-5})}{z_c^8}, \quad z_c > 0 \quad \Leftrightarrow \quad z_c = \delta_1 \left(\frac{13}{7}\frac{1+2^{-11}}{1+2^{-5}}\right)^{1/6}.$$

From an analogous calculation we obtain that $J''_{CB}(z) > 0$ for $z \in (0, z_*)$ with $z_* = \delta_1 \left(\frac{13}{7}\frac{1+2^{-12}}{1+2^{-6}}\right)^{1/6} > z_c$. Now we estimate R on $[z_c, +\infty)$. Since $z_c > \delta_1 > \gamma$, we have $\frac{1}{2}J_1 - \frac{3}{2}J_{CB} = -\frac{1}{2}J_2 - J_{CB}$ is decreasing on $(z_c, +\infty)$. Since $J_2\left(\frac{t+\gamma}{2}\right) = J_1(t+\gamma) < 0$ for $t \geq 0$, we have

$$R(t) \leq -\frac{1}{2}J_2(z_c) - J_{CB}(z_c) + \frac{1}{2}(J_1(\gamma) + J_0(\gamma)) \approx -0.0469\frac{k_2^2}{k_1} < 0,$$

for $t \geq z_c$. We now show that $R'(t) \geq 0$ for $t \leq \gamma$ and $R'(t) \leq 0$ for $\gamma \leq t \leq z_c$, which proves the statement. For $0 < t \leq \gamma < z_c < z_*$, we have

$$\begin{aligned} R'(t) =& \frac{1}{2}J'_2\left(\frac{t+\gamma}{2}\right) + \frac{1}{2}J'_1(t) - \frac{3}{2}J'_{CB}(t) = \frac{1}{2}\left(J'_2\left(\frac{t+\gamma}{2}\right) - J'_2(t)\right) - J'_{CB}(t) \\ =& \frac{1}{2}\int_t^{\frac{t+\gamma}{2}} J''_2(z)dz + \int_t^{\gamma} J''_{CB}(z)dz \geq \frac{1}{2}\int_t^{\frac{t+\gamma}{2}} J''_2(z) + J''_{CB}(z)dz > 0. \end{aligned}$$

Analogously we get for $\gamma \leq t \leq z_c$

$$R'(t) = -\frac{1}{2}\int_{\frac{t+\gamma}{2}}^{t} J''_2(z)dz - \int_{\gamma}^{t} J''_{CB}(z)dz \leq -\frac{1}{2}\int_{\frac{t+\gamma}{2}}^{t} J''_2(z) + J''_{CB}(z)dz < 0.$$

Hence, Lennard-Jones potentials satisfy all the properties asserted.

Let now J_1 and J_2 be Morse potentials as in (3.24), i.e., there exist $k_1, k_2, \delta_1 > 0$ such that $J_1(z) = k_1\left(1 - e^{-k_2(z-\delta_1)}\right)^2 - k_1$ and $J_2(z) = J_1(2z)$. In this case, we do not have such an explicit expression for γ as in the Lennard-Jones case and therefore derive bounds on γ. Since $J'_1(z) < 0$ if and only if $z < \delta_1$ and $J'_1(z) > 0$ if and only if $z > \delta_1$, we deduce from $0 = J'_{CB}(\gamma) = J'_1(\gamma) + 2J'_1(2\gamma)$ that $\delta_1/2 < \gamma < \delta_1$. A straightforward calculation yields $J_1(z) < 0$ if and only if $z > \frac{k_2\delta_1 - \ln(2)}{k_2} =: z_0$. In order to prove $J_1(\gamma) < 0$, we show $J'_{CB}(z_0) < 0$, which implies $z_0 < \gamma$. Indeed, we have

$$J'_{CB}(z_0) = -4k_1k_2(16e^{-2k_2\delta_1} - 4e^{-k_2\delta_1} + 1) = -4k_1k_2\left((1 - 2e^{-k_2\delta_1})^2 + 12e^{-2k_2\delta_1}\right) < 0.$$

As in the Lennard-Jones case, we deduce from $J_1(\gamma) < 0$, $\gamma < \delta_1$ and the definition of J_2 that $J_2(\gamma), J_2(\delta_1) < 0$ and $J_2\left(\frac{\gamma+t}{2}\right) < 0$ for all $t > 0$. Define for $\theta > 0$ the constant $\eta_\theta := \frac{1}{2}(J_1(0) - J_1(\theta)) > 0$, then we deduce $J_2\left(\frac{t+\gamma}{2}\right) < 0$ for $t \in \{t : J_1(t) < J_1(\theta) + 2\eta_\theta\} \subset \{t : t > 0\}$.

Let us show $J_2(\gamma) - 2J_2\left(\frac{\delta_1+\gamma}{2}\right) = J_1(2\gamma) - 2J_1(\delta_1+\gamma) > 0$. From $\{\gamma\} = \operatorname{argmin} J_{CB}$, we deduce

$$\begin{aligned}
0 = J'_{CB}(\gamma) =& -k_1k_2\left(-2e^{k_2\delta_1}(e^{-k_2\gamma}+2e^{-2k_2\gamma}) + e^{2k_2\delta_1}(2e^{-2k_2\gamma}+4e^{-4k_2\gamma})\right)\\
=&2k_1k_2e^{k_2\delta_1}e^{-4k_2\gamma}\left(e^{3k_2\gamma}+2e^{2k_2\gamma}-e^{k_2\delta_1}(2+e^{2k_2\gamma})\right)\\
=&2k_1k_2q_{\delta_1}q_\gamma^{-4}\left(q_\gamma^3+2q_\gamma^2-q_{\delta_1}(2+q_\gamma^2)\right)
\end{aligned}$$

with $q_\gamma := e^{k_2\gamma} > 1$ and $q_{\delta_1} := e^{k_2\delta_1} > 1$. This yields $q_{\delta_1} = \frac{q_\gamma^3+2q_\gamma^2}{2+q_\gamma^2}$ and allows us to show

$$\begin{aligned}
&J_2(\gamma) - 2J_2\left(\frac{\delta_1+\gamma}{2}\right) = k_1\left(-2e^{-k_2(2\gamma-\delta_1)} + e^{-2k_2(2\gamma-\delta_1)} + 4e^{-k_2\gamma} - 2e^{-2k_2\gamma}\right)\\
&= k_1e^{-4k_2\gamma}\left(-2e^{k_2\delta_1}e^{2k_2\gamma} + e^{2k_2\delta_1} + 4e^{3k_2\gamma} - 2e^{2k_2\gamma}\right)\\
&= k_1q_\gamma^{-4}\left(4q_\gamma^3 - 2(1+q_{\delta_1})q_\gamma^2 + q_{\delta_1}^2\right)\\
&= \frac{k_1}{q_\gamma^2(q_\gamma^2+2)^2}\left(2q_\gamma^5 - 5q_\gamma^4 + 16q_\gamma^3 - 12q_\gamma^2 + 16q_\gamma - 8\right)\\
&> \frac{k_1}{q_\gamma^2(q_\gamma^2+2)^2}\left(q_\gamma^3\left(\sqrt{2}q_\gamma - \tfrac{5}{2\sqrt{2}}\right)^2 + 12q_\gamma^2(q_\gamma-1) + 16q_\gamma - 8\right) > 0
\end{aligned}$$

since $q_\gamma > 1$.

It is left to show that $R = R(t) \leq 0$ for all $t \in \mathbb{R}$. We prove the inequality in a different way than in the Lennard-Jones case. We have $\lim_{t\to+\infty} R(t) = \frac{1}{2}J_1(\gamma) + \frac{1}{2}J_0(\gamma) < 0$ and by using $J_1(t+\gamma) < J_1(2t)$ for $t < 0$ we obtain that

$$\lim_{t\to-\infty} R(t) \leq \lim_{t\to-\infty}\left(-J_1(t) - \frac{1}{2}J_2(t) + \frac{1}{2}J_1(\gamma) + \frac{1}{2}J_0(\gamma)\right) = -\infty.$$

Moreover, by the definition of $R = R(t)$ and γ, we have that $R(\gamma) = R'(\gamma) = 0$. To show that $R(t) \leq 0$ it is sufficient to show that R has no critical point except γ. Indeed, if $R(t) > 0$ for some $t \in \mathbb{R}$, then in order to satisfy the conditions at infinity there has to exist a maximum point $\hat{t}$ with $R(\hat{t}) > 0$ and $R'(\hat{t}) = 0$. By the definition of J_1, J_2 and $R = R(t)$, we have

$$\begin{aligned}
R'(t) =&J'_1(t+\gamma) - J'_1(t) - 3J'_1(2t)\\
=&2k_1k_2e^{k_2\delta_1}\Bigg(e^{-k_2(t+\gamma)}(1-e^{-k_2(t+\gamma-\delta_1)}) - e^{-k_2t}(1-e^{-k_2(t-\delta_1)})\\
&-3e^{-2k_2t}(1-e^{-k_2(2t-\delta_1)})\Bigg)\\
=&2k_1k_2e^{k_2\delta_1}e^{-4k_2t}\left((e^{-k_2\gamma}-1)e^{3k_2t} + (e^{k_2\delta_1}(1-e^{-2k_2\gamma})-3)e^{2k_2t} + 3e^{k_2\delta_1}\right)\\
=&2k_1k_2e^{k_2\delta_1}q_t^{-4}\left((e^{-k_2\gamma}-1)q_t^3 + (e^{k_2\delta_1}(1-e^{-2k_2\gamma})-3)q_t^2 + 3e^{k_2\delta_1}\right)\\
=&2k_1k_2e^{k_2\delta_1}q_t^{-4}f(q_t)
\end{aligned}$$

with $q_t = e^{k_2 t}$. From $R'(\gamma) = 0$ it follows $f(q_\gamma) = 0$. Let us show that q_γ is the unique zero of f. We have $f(0) = 3e^{k_2\delta_1} > 0$ and from $k_2, \gamma > 0$, we deduce $e^{-k_2\gamma} - 1 < 0$ and thus $\lim_{q\to\infty} f(q) = -\infty$. This implies that if f has a second zero, it would have a local minimum and a local maximum in $(0, +\infty)$. But

$$f'(q) = q\left(3(e^{-k_2\gamma} - 1)q + 2(e^{k_2\delta_1}(1 - e^{-2k_2\gamma}) - 3)\right)$$

and thus f has at most one local extremum in $(0, +\infty)$. Hence, q_γ is the unique zero of f and γ the unique zero of $R'(t)$. □

Remark 4.24. In Theorem 4.19 and Proposition 4.22, we provide necessary and sufficient conditions on the repatoms $\mathcal{T} = (\mathcal{T}_n)$ to ensure $\min_u H_1^\ell(u) = \min_u \hat{H}_1^{\ell,\mathcal{T}}(u)$ for $\ell > \gamma$ and nearest and next-to-nearest neighbour interactions. An extension of these results to general finite range Lennard-Jones type interactions requires refined estimates on the different boundary layer energies for $K > 2$ which we will not present here. Let us illustrate that in general a sufficiently coarse mesh at the interface and in the continuum region ensure $\min_u H_1^\ell(u) = \min_u \hat{H}_1^{\ell,\mathcal{T}}(u)$.

Let us assume that the hypotheses (LJ1)–(LJ5) hold true. Let $\ell > \gamma$ and $u_0^{(1)}, u_1^{(1)} \in \mathbb{R}_+^{K-1}$. From (3.73), (3.117), (3.118) and (4.42), we deduce that it is sufficient to ensure that

$$\begin{aligned} &B_{BJ}(u_0^{(1)}) = B_{IFJ}(u_0^{(1)}, \hat{r}^{\mathcal{T}}, b(0,\mathcal{T})),\ B_{BJ}(u_1^{(1)}) = B_{IFJ}(u_1^{(1)}, \hat{l}^{\mathcal{T}}, b(1,\mathcal{T})) \\ &B_{BJ}(u_i^{(1)}) \le B(u_i^{(1)}, \gamma) - b(x,\mathcal{T})J_{CB}(\gamma) \quad \text{for all } x \in [0,1] \text{ and } i \in \{0,1\} \end{aligned} \tag{4.135}$$

to obtain $\min_u H_1^\ell(u) = \min_u \hat{H}_1^{\ell,\mathcal{T}}(u)$. The relations (4.135) can be achieved by choosing the repatoms $\mathcal{T} = (\mathcal{T}_n)$ such that it holds

$$\hat{r}^{\mathcal{T}} = \hat{l}^{\mathcal{T}} = (0, +\infty) \in (\mathbb{N}_0 \cup \{+\infty\})^2 \quad \text{and} \quad b(x,\mathcal{T}) = +\infty \quad \text{for all } x \in [0,1], \tag{4.136}$$

where $\hat{r}^{\mathcal{T}}, \hat{l}^{\mathcal{T}}$ and $b(x,\mathcal{T})$ are defined in (4.28) and (4.29). Indeed, since $\psi_j(\gamma) < 0$ (see (3.19)) for $j \in \{2, \dots, K\}$, we have that $B_{BIF}((0, +\infty)) = +\infty$ (see (4.45)) and $-b(x,\mathcal{T})J_{CB}(\gamma) = +\infty$ for all $x \in [0,1]$. Thus, the definition of B_{IJ} and B_{IFJ} (see (3.75), (4.43)), the equality $B_{IF}^{(1)}((0,+\infty)) = B(\gamma)$ (see Remark 4.8 (ii)) and (3.117) imply that

$$\begin{aligned} B_{IFJ}((0,+\infty), +\infty, \theta) &= \min\{B_{AIF}((0,+\infty)) + B(\theta,\gamma), B_{BJ}(\theta)\} \\ &= \min\left\{B_{IF}^{(1)}((0,+\infty)) + B(\gamma) - \sum_{j=2}^{K} j\psi_j(\gamma) + B(\theta,\gamma), B_{BJ}(\theta)\right\} \\ &= \min\{B_{IJ} + B(\theta,\gamma), B_{BJ}(\theta)\} = B_{BJ}(\theta), \end{aligned}$$

for all $\theta \in \mathbb{R}_+^{K-1}$. Hence, we have that $\hat{H}_1^{\ell,\mathcal{T}}(u) = H_1^\ell(u)$ if $S_u \subset \{0,1\}$, and $+\infty$ otherwise. Note that (4.136) is satisfied for $\mathcal{T} = (\mathcal{T}_n)$ such that the assumptions of

Theorem 4.11 hold true and that there exists $(q_n) \subset \mathbb{N}$ such that $\lim_{n\to\infty} q_n = +\infty$ and $\min\{s - t : k_n^1 \le t < s \le k_n^2, t, s \in \mathcal{T}_n\} \ge q_n$.

We close this remark by showing that for Lennard-Jones potentials, see (3.22), and arbitrary $K \ge 2$ it is sufficient to ensure $b(x, \mathcal{T}) \ge 2$ to obtain $B_{BJ}(\theta) \le B(\theta, \gamma) - b(x, \mathcal{T})J_{CB}(\gamma)$. Therefore, we define the function $f : (0, +\infty) \to \mathbb{R}$ by

$$f(z) := J_1(z) - \sum_{j=3}^{K} (j-2)J_j(z) = k_1 \left(1 - \sum_{j=3}^{K} \frac{j-2}{j^{12}}\right) z^{-12} - k_2 \left(1 - \sum_{j=3}^{K} \frac{j-2}{j^6}\right) z^{-6}$$

It is easy to see that f has a unique root $z_0 > 0$ given by

$$z_0 = \left(\frac{k_1}{k_2}\right)^{\frac{1}{6}} \left(\frac{1 - \sum_{j=3}^{K} \frac{j-2}{j^{12}}}{1 - \sum_{j=3}^{K} \frac{j-2}{j^6}}\right)^{\frac{1}{6}},$$

and that $f(z) < 0$ for $z > z_0$. Using (3.23), we obtain

$$z_0 < \left(\frac{k_1}{k_2}\right)^{\frac{1}{6}} \left(\frac{1}{2 - \zeta(5)}\right)^{\frac{1}{6}} < \left(\frac{k_1}{k_2}\right)^{\frac{1}{6}} \left(\frac{2}{\zeta(6)}\right)^{\frac{1}{6}} < \left(\frac{2k_1}{k_2}\right)^{\frac{1}{6}} \left(\frac{\sum_{j=1}^{K} j^{-12}}{\sum_{j=1}^{K} j^{-6}}\right)^{\frac{1}{6}} = \gamma,$$

where $\zeta(n) = \sum_{j\ge1} n^{-j}$ denotes the Riemann Zeta function. Hence, $f(\gamma) < 0$. Using the definition of B_{IJ} (see (3.75)), (3.117), Lemma 3.22 (1) and $\sum_{j=2}^{K} c_j = 1$, we obtain for $b(x, \mathcal{T}) \ge 2$ that

$$\begin{aligned} B_{BJ}(\theta) - (B(\theta, \gamma) - b(x, \mathcal{T})J_{CB}(\gamma)) &\le B_{IJ} + 2J_{CB}(\gamma) \\ &\le J_1(\gamma) \sum_{j=2}^{K} (j-1)c_j - \sum_{j=2}^{K} j\psi_j(\gamma) + 2J_{CB}(\gamma) \\ &= -\sum_{j=1}^{K} jJ_j(\gamma) + 2\sum_{j=1}^{K} J_j(\gamma) = f(\gamma) < 0. \end{aligned}$$

This shows $B_{BJ}(\theta) < B(\theta, \gamma) - b(x, \mathcal{T})J_{CB}(\gamma)$ if $b(x, \mathcal{T}) \ge 2$ for Lennard-Jones interactions of finite range.

Bibliography

[1] G. Anzellotti and S. Baldo, Asymptotic development by Γ-convergence, *Appl. Math. Optim.* **27** (1993), 105–123.

[2] R. Alicandro and M. Cicalese, A general integral representation result for continuum limits of discrete energies with superlinear growth, *SIAM J. Math. Anal.* **36** (2004), 1–37.

[3] L. Ambrosio, N. Fusco and D. Pallara, *Functions of bounded variation and free discontinuity problems*, Oxford Univ. Press, 2000.

[4] J. M. Ball, Some open problems in elasticity. In *Geometry, mechanics and dynamics*, Springer, New York, 2002, 3–59.

[5] X. Blanc, C. Le Bris and F. Legoll, Analysis of a prototypical multiscale method coupling atomistic and continuum mechanics, *M2AN Math. Model. Numer. Anal.* **39** (2005), 797–826.

[6] X. Blanc, C. Le Bris and P.-L. Lions, From molecular models to continuum mechanics, *Arch. Ration. Mech. Anal.* **164** (2002), 341–381.

[7] X. Blanc, C. Le Bris and P.-L. Lions, Atomistic to Continuum limits for computational materials science, *M2AN Math. Model. Numer. Anal.* **41** (2007), 391–426.

[8] A. Braides, *Approximation of Free-Discontinuity problems*, Lecture Notes In Mathematics, **1694** Springer Verlag, Berlin, 1998.

[9] A. Braides, Γ-*Convergence for Beginners*, Oxford Univ. Press, 2002.

[10] A. Braides, A. Defranceschi and E. Vitali, Variational evolution of one-dimensional Lennard-Jones systems, *Netw. Heterog. Media* **9** (2014), 217-238.

[11] A. Braides and M. Cicalese, Surface energies in nonconvex discrete systems, *Math. Models Methods Appl. Sci.* **17** (2007), 985–1037.

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

[13] A. Braides and M. S. Gelli, Continuum limits of discrete systems without convexity hypotheses, *Math. Mech. Solids* **7** (2002), 41–66.

[14] A. Braides and M. S. Gelli, The passage from discrete to continuous variational problems: a nonlinear homogenization process, in *Nonlinear Homogenization and its Applications to Composites, Polycrystals and Smart Materials* NATO Sci. Ser. II Math. Phys. Chem., 170, Kluwer Acad. Publ., Dordrecht, 2004.

[15] A. Braides and M. S. Gelli, From discrete systems to continuous variational problems: An introduction, *Lect. Notes Unione Mat. Ital.* **2** (2006), 3–77.

[16] A. Braides, M. S. Gelli and M. Sigalotti, The passage from non-convex discrete systems to variational problem in Sobolev spaces: The one-dimensional case, *Proc. Steklov Inst.* **236** (2002), 395–414.

[17] A. Braides, A. Lew and M. Ortiz, Effective cohesive behavior of Layers of interatomic planes, *Arch. Ration. Mech. Anal.* **180** (2006), 151–182.

[18] A. Braides and M. Solci, Asymptotic analysis of Lennard-Jones systems beyond the nearest-neighbour setting: A one-dimensional prototypical case, *Math. Mech. Solids*, published online August 13, 2014, doi: 10.1177/1081286514544780.

[19] A. Braides, M. Solci and E. Vitali, A derivation of linear elastic energies from pair-interaction atomistic systems, *Netw. Heterog. Media* **2** (2007), 551–567.

[20] A. Braides and L. Truskinovsky, Asymptotic expansions by Γ-convergence, *Cont. Mech. Thermodyn.* **20** (2008), 21–62.

[21] J. Braun and B. Schmidt, On the passage from atomistic systems to nonlinear elasticity theory for general multi-body potentials with p-growth, *Netw. Heterog. Media* **8** (2013), 879–912.

[22] M. Charlotte and L. Truskinovsky, Linear elastic chain with a hyper-pre-stress, *J. Mech. Phys. Solids* **50** (2002), 217–251.

[23] S. Conti, G. Dolzmann, B. Kirchheim and S. Müller, Sufficient conditions for the validity of the Cauchy-Born rule close to $SO(n)$, *J. Eur. Math. Soc.* **8** (2006), 515–530.

[24] G. Dal Maso, *An Introduction to Γ–Convergence,* Birkhäuser, 1993.

[25] M. Dobson and M. Luskin, An optimal order error analysis of the one-dimensional quasicontinuum approximation, *SIAM J. Numer. Anal.* **47** (2009), 2455–2475.

[26] W. E, J. Lu and J. Yang, Uniform Accuracy of the Quasicontinuum Method, *Phys. Rev. B* **74** (2006), 214115.

[27] W. E and P. Ming, Cauchy-Born rule and the stability of crystalline solids: Static problems, *Arch. Ration. Mech. Anal.* **183** (2007), 241–297.

[28] J. L. Ericksen, On the Cauchy-Born rule, *Math. Mech. Solids* **13** (2008), 199–220.

[29] M. Español, D. Kochmann, S. Conti and M. Ortiz, A Γ-convergence analysis of the quasicontinuum method, *Multiscale Model. Simul.* **11** (2013), 766–794.

[30] M. Friedrich and B. Schmidt, An atomistic-to-continuum analysis of crystal cleavage in a two-dimensional model problem. *J. Nonlinear Sci.* **24** (2014), 145–183.

[31] M. Friedrich and B. Schmidt, An analysis of crystal cleavage in the passage from atomistic models to continuum theory, *Arch. Ration. Mech. Anal.* **217** (2015), 263–308.

[32] G. Friesecke and F. Theil, Validity and failure of the Cauchy-Born hypothesis in a two-dimensional mass-spring lattice, *J. Nonlinear Sci.* **12** (2002), 445–478.

[33] M. G. D. Geers, R. H. J. Peerlings, M. A. Peletier and L. Scardia, Asymptotic behaviour of a pile-up of infinite walls of edge dislocations, *Arch. Ration. Mech. Anal.* **209** (2013), 495–539.

[34] M. S. Gelli, Variational limits of discrete systems, Ph.D. thesis, Scuola Internazionale Superiore di Studi Avanzati, Triesete, 1999.

[35] T. Hudson, Gamma-expansion for a 1D Confined Lennard-Jones model with point defect, *Netw. Heterog. Media* **8** (2013), 501–527.

[36] K. Jayawardana, C. Mordacq, C. Ortner and H. Park, An analysis of the boundary layer in the 1D surface Cauchy-Born model, *ESAIM Math. Model. Numer. Anal.* **47** (2013), 109–123.

[37] J. E. Lennard-Jones, Cohesion, *Proc. Phys. Soc.* **43** (1931), 461–482.

[38] X. H. Li and M. Luskin, A generalized quasinonlocal atomistic-to-continuum coupling method with finite-range interaction, *IMA J. Numer. Anal.* **32** (2012), 373-393.

[39] X. Li and P. Ming, A study on the quasicontinuum approximations of a one-dimensional fracture model, *Multiscale Model. Simul.* **12** (2014), 1379–1400.

[40] P. Lin, Theoretical and numerical analysis for the approximation of a material particle model, *Math. Comp.* **72** (2003), 657–675.

[41] M. Luskin and C. Ortner, Atomistic-to-continuum coupling, *Acta Numer.* **22** (2013), 397–508.

[42] R. E. Miller and E. Tadmor, The Quasicontinuum Method: Overview, applications and current directions, *Journal of Computer-Aided Materials Design* **9** (2002), 203–239.

[43] P. Ming and J. Z. Yang, Analysis of a one-dimensional nonlocal quasi-continuum method, *Multiscale Model. Simul.* **7** (2009), 1838–1875.

[44] P. M. Morse, Diatomic molecules according to the wave mechanics. II. Vibrational levels, *Phys. Rev.* **34** (1929), 57–64.

[45] C. Ortner, A priori and a posteriori analysis of the quasinonlocal quasicontinuum method in 1D, *Math. Comp.* **80** (2011), 1265–1285.

[46] C. Ortner and E. Süli, Analysis of the quasicontinuum method in one dimension, *M2AN Math. Model. Numer. Anal.* **42** (2008), 57–91.

[47] C. Ortner and F. Theil, Justification of the Cauchy-Born approximation of elastodynamics, *Arch. Ration. Mech. Anal.* **207** (2013), 1025–1073.

[48] C. Ortner and H. Wang, A priori estimates for energy-based quasicontinuum approximations of a periodic chain, *Math. Models Methods Appl. Sci.* **21** (2011), 2491–2521.

[49] R. T. Rockafellar and R. Wets, *Variational Analysis*, Grundlehren Math. Wiss., vol. 317, Springer, 1998.

[50] L. Scardia, A. Schlömerkemper and C. Zanini, Boundary layer energies for nonconvex discrete systems, *Math. Models Methods Appl. Sci.* **21** (2011), 777–817.

[51] L. Scardia, A. Schlömerkemper and C. Zanini, Towards uniformly Γ-equivalent theories for nonconvex discrete systems, *Discrete Contin. Dyn. Syst. Ser. B* **17** (2012), 661–686.

[52] B. Schmidt, On the derivation of linear elasticity from atomistic models, *Netw. Heterog. Media* **4** (2009), 789–812.

[53] M. Schäffner and A. Schlömerkemper, About an analytical verification of quasicontinuum methods with Γ-convergence techniques, *MRS Proceedings*, 1535 (2013).

[54] M. Schäffner und A. Schlömerkemper, About an analytical approach to a quasicontinuum method via Γ-convergence, *PAMM* **14** (2014), 759–760.

[55] M. Schäffner and A. Schlömerkemper, On a Γ-convergence analysis of a quasicontinuum method, *Multiscale Model. Simul.* **13** (2015), 132–172.

[56] M. Schäffner and A. Schlömerkemper, On Lennard-Jones systems with finite range interactions and their asymptotic analysis, arXiv:1501.06423.

[57] A. Shapeev, Consistent energy-based atomistic/continuum coupling for two-body potentials in one and two dimensions. *Multiscale Model. Simul.* **9** (2011), 905–932.

[58] T. Shimokawa, J.J. Mortensen, J. Schiotz and K.W. Jacobsen, Matching conditions in the quasicontinuum method: Removel of the error introduced at the interface between coarse grained and fully atomistic region, *Phys. Rev. B* **69** (2004), 214104.

[59] E. Tadmor, M. Ortiz and R. Phillips, Quasicontinuum analysis of defects in solids, *Phil. Mag. A* **73** (1996), 1529–1563.

[60] L. Truskinovsky, Fracture as a phase transition, in *Contemporary Research in the Mechanics and Mathematics of Materials* (1996), 322–332.

Acknowledgements

First and foremost, I would like to express my sincere gratitude to my supervisor Anja Schlömerkemper for all her valuable advice and support during my doctorate studies. She introduced me to a, for me, very interesting field of research and generously shared her time for many stimulating discussions.

I thank Maria Stella Gelli and Giuliano Lazzaroni for several valuable discussions on the subject of this thesis. Further, I would like to thank Marta Lewicka for a fruitful collaboration which is not a direct part of this thesis but has been a precious source of inspiration. Furthermore, my thanks belong to Barbora Benešová and Johannes Forster for proofreading parts of the thesis.

I gratefully acknowledge the financial support by a grant of the Deutsche Forschungsgemeinschaft (DFG) SCHL 1706/2-1.