
Stochastic Homogenization in the Passage from Discrete to Continuous Systems – Fracture in Composite Materials



Dissertation zur Erlangung des naturwissenschaftlichen Doktorgrades
an der Fakultät für Mathematik und Informatik
der Julius-Maximilians-Universität Würzburg

vorgelegt

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Würzburg, August 2020



Abstract

The work in this thesis contains three main topics. These are the passage from discrete to continuous models by means of Γ -convergence, random as well as periodic homogenization and fracture enabled by non-convex Lennard-Jones type interaction potentials. Each of them is discussed in the following.

We consider a discrete model given by a one-dimensional chain of particles with randomly distributed interaction potentials. Our interest lies in the continuum limit, which yields the effective behaviour of the system. This limit is achieved as the number of atoms tends to infinity, which corresponds to a vanishing distance between the particles. The starting point of our analysis is an energy functional in a discrete system; its continuum limit is obtained by variational Γ -convergence.

The Γ -convergence methods are combined with a homogenization process in the framework of ergodic theory, which allows to focus on heterogeneous systems. On the one hand, composite materials or materials with impurities are modelled by a stochastic or periodic distribution of particles or interaction potentials. On the other hand, systems of one species of particles can be considered as random in cases when the orientation of particles matters. Nanomaterials, like chains of atoms, molecules or polymers, are an application of the heterogeneous chains in experimental sciences.

A special interest is in fracture in such heterogeneous systems. We consider interaction potentials of Lennard-Jones type. The non-standard growth conditions and the convex-concave structure of the Lennard-Jones type interactions yield mathematical difficulties, but allow for fracture. The interaction potentials are long-range in the sense that their modulus decays slower than exponential. Further, we allow for interactions beyond nearest neighbours, which is also referred to as long-range.

The main mathematical issue is to bring together the Lennard-Jones type interactions with ergodic theorems in the limiting process as the number of particles tends to infinity. The blow up at zero of the potentials prevents from using standard extensions of the Akcoglu-Krengel subadditive ergodic theorem. We overcome this difficulty by an approximation of the interaction potentials which shows suitable Lipschitz and Hölder regularity. Beyond that, allowing for continuous probability distributions instead of only finitely many different potentials leads to a further challenge.

The limiting integral functional of the energy by means of Γ -convergence involves a homogenized energy density and allows for fracture, but without a fracture contribution in the energy. In order to refine this result, we rescale our model and consider its Γ -limit, which is of Griffith's type consisting of an elastic part and a jump contribution.

In a further approach we study fracture at the level of the discrete energies. With an appropriate definition of fracture in the discrete setting, we define a fracture threshold separating the region of elasticity from that of fracture and consider the pointwise convergence of this threshold. This limit turns out to coincide with the one obtained in the variational Γ -convergence approach.

Zusammenfassung

Diese Arbeit vereinigt im Wesentlichen drei Themen: Den Übergang von diskreten zu kontinuierlichen Modellen mittels Γ -Konvergenz, stochastische sowie periodische Homogenisierung, sowie Bruchmechanik, die durch nicht-konvexe Wechselwirkungspotentiale vom Lennard-Jones-Typ ermöglicht wird. Jedes dieser drei Themen wird im Folgenden diskutiert.

Wir betrachten ein diskretes Modell, bestehend aus einer eindimensionalen Kette von Teilchen mit zufällig verteilten Wechselwirkungspotentialen. Wir sind am Kontinuumsgrenzwert interessiert, welcher das effektive Verhalten des Systems widerspiegelt. In diesem Grenzwert läuft die Anzahl der Atome gegen unendlich, was einem verschwindenden Abstand zwischen den Teilchen entspricht. Ausgehend von einer Energie eines diskreten Systems erhalten wir den Kontinuumsgrenzwert durch die variationelle Methode der Γ -Konvergenz, welche den Übergang zum kontinuierlichen System liefert.

Die Γ -Konvergenzmethoden werden im Rahmen der Ergodentheorie mit einem Homogenisierungsprozess kombiniert, wodurch die Betrachtung heterogener Systeme möglich wird. Einerseits werden Verbundwerkstoffe oder Materialien mit Verunreinigungen durch eine stochastische oder periodische Verteilung der Teilchen oder der Wechselwirkungspotentiale modelliert. Andererseits können Systeme einer Teilchenart als zufällig angesehen werden, wenn die Orientierung der Teilchen von Bedeutung ist. Nanomaterialien wie Ketten von Atomen, Molekülen oder Polymeren bieten eine Anwendung des Modells der heterogenen Ketten in den experimentellen Wissenschaften.

Von besonderem Interesse ist das Auftreten von Brüchen in diesen heterogenen Systemen. Wir betrachten Wechselwirkungspotentiale vom Lennard-Jones Typ. Die nicht-standardisierten Wachstumsbedingungen und die konvex-konkave Struktur der Lennard-Jones Potentiale werfen mathematische Schwierigkeiten auf, ermöglichen jedoch das Auftreten von Brüchen. Die Wechselwirkungen gelten als langreichweitig in dem Sinne, dass ihr Betrag langsamer als exponentiell abfällt. Darüber hinaus betrachten wir Wechselwirkungen jenseits der nächsten Nachbarn, was ebenfalls als langreichweitig bezeichnet wird.

Eine der größten mathematischen Schwierigkeiten besteht darin, die Wechselwirkungen vom Lennard-Jones Typ mit den Ergodensätzen zusammenzuführen. Die Singularität der Potentiale bei Null erlaubt keine Verwendung der Standardtechniken zur Erweiterung des subadditiven Ergodensatzes von Akcoglu-Krengel. Die Lösung dieses Problems ist eine Approximation der Wechselwirkungspotentiale, welche eine geeignete Lipschitz- und Hölder-Regularität besitzt. Darüber hinaus stellt die Verwendung von kontinuierlichen Wahrscheinlichkeitsverteilungen, anstelle von nur endlich vielen verschiedenen Potentialen, eine weitere Herausforderung dar.

Das Integralfunktional im Grenzwert besteht aus einer homogenisierten Energiedichte und ermöglicht Brüche, jedoch ohne einen Beitrag dieser Brüche zur Energie. Um dieses Ergebnis zu verfeinern, skalieren wir unser Modell neu und betrachten dessen Γ -Grenzwert, der in Form einer Energie vom Griffith-Typ gegeben ist und aus einem elastischen Teil und einem Sprungbeitrag besteht.

In einem weiteren Ansatz untersuchen wir Brüche auf Ebene der diskreten Energien. Mit einer geeigneten Definition des Bruchpunktes im diskreten System definieren wir eine Bruchschwelle, die den Elastizitätsbereich von dem Gebiet mit Brüchen trennt. Von diesem Schwellwert berechnen wir anschließend den punktweisen Grenzwert. Es stellt sich heraus, dass dieser Grenzwert mit dem durch die variationelle Γ -Konvergenz errechneten übereinstimmt.

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List of symbols

Discrete chain of atoms

$\mathbb{N}, \mathbb{Z}, \mathbb{R}$	positive integers, integers, real numbers	
$n \in \mathbb{N}$	system size, chain of $n + 1$ particles	
λ_n	lattice spacing of reference configuration, $\lambda_n = \frac{1}{n}$, $n \in \mathbb{N}$	page 27
x_n^i	reference configuration	page 27
$u^i := u(x_n^i)$	deformed configuration, deformation	page 27
v^i	rescaled displacement	page 86
$\mathcal{A}_n(0, 1)$	set of piecewise affine, continuous functions	page 27
$\hat{\mathcal{A}}_n^{\gamma_n}(0, 1)$	space of functions $v \in \mathcal{A}_n(0, 1)$ with boundary values	page 87
i_{\min}^A, i_{\max}^A	$\min/\max\{i : i \in NA \cap \mathbb{Z}\}$	page 42
ℓ	boundary value of Dirichlet boundary conditions	page 34
(ℓ_n)	sequence of boundary values near fracture threshold	page 86
(γ_n)	rescaled boundary values	page 86

The space BV and SBV

$BV(0, 1)$	space of functions of bounded variation in $(0, 1)$	page 16
$SBV(0, 1)$	space of special functions of bounded variation in $(0, 1)$	page 19
$(S)BV^\ell(0, 1)$	$(S)BV(0, 1)$ -functions with boundary values	page 19
$SBV_c^\gamma(0, 1)$	SBV -functions with boundary values and additional conditions	page 96
$D^a u$	absolutely continuous part of the measure Du	page 17
$D^s u$	singular part of the measure Du	page 17
$D^j u$	jump part of the measure Du	page 17
$D^c u$	Cantor part of the measure Du	page 17
$u(x^+)$	right-hand side limit of u at x	page 17
$u(x^-)$	left-hand side limit of u at x	page 17
$[u](x)$	$[u](x) := u(x^+) - u(x^-)$	page 18
S_u	jump set of $u \in BV(0, 1)$	page 18

Stochastic and periodic modelling

$(\Omega, \mathcal{F}, \mathbb{P})$	probability space	page 29
$\mathbb{E}[X]$	expectation value of random variable X	
$(\tau_i)_{i \in \mathbb{Z}}$	additive group action, that is stationary and ergodic	page 19
$\underline{\alpha}$	elastic constant, $(\mathbb{E}[\alpha^{-1}])^{-1}$	page 97
β	jump constant, $\inf \{-J(\omega, \delta(\omega)) : \omega \in \Omega\}$	page 97
$\bar{\delta}$	average of δ_i over periodicity cell	page 119
$\overline{J_{\min}}$	average of $J_i(\delta_i)$ over periodicity cell	page 119
z_{dom}	lower boundary of the domain of J in periodic setting	page 120
χ_A	indicator function of a set A	

Lennard-Jones type potentials

$\mathcal{J}(\alpha, b, d, \Psi)$	Lennard-Jones type class satisfying (LJ1)–(LJ3)	page 27
$\mathcal{J}_{\text{reg}}(\alpha, b, c, d, \Psi, \eta)$	Lennard-Jones type class satisfying (LJ1)–(LJ5)	page 87
$\mathcal{J}_{\text{curv}}(\alpha, b, c, d, \Psi, \eta)$	Lennard-Jones type class satisfying (LJ1)–(LJ9)	page 132
Ψ	convex function, deterministic bound from (LJ2)	page 27
δ	minimizer of Lennard-Jones type potential	page 27
$J(\delta)$	minimum value of Lennard-Jones type potential	page 27
J_j^L	approximation of function J_j	page 38
J^{**}	convex, lower semicontinuous envelope of J	
α	$\frac{1}{2} \frac{\partial^2 J(z)}{\partial z^2} \Big _{z=\delta}$	page 38
$[f]_{C^{0,\alpha}(A)}$	Hölder semi-norm of $f \in C^{0,\alpha}(A)$	
$C_j^H(\omega)$	random variable of Hölder semi-norm	page 31
$C^\kappa(\omega)$	random variable of bound on third derivative of J	page 88
κ^*	bound used in the assumption (H2)	page 89

Discrete fracture threshold

z_{frac}	fracture point	page 127
m_{frac}	minimum value of J on $[z_{\text{frac}}, +\infty)$	page 132
M_n	minimal energy	page 130
$M_n^{\text{el}}, M_n^{\text{frac}}$	minimal elastic/fracture energy	page 130
ℓ_n^*	fracture threshold	page 130
γ_n^*	rescaled fracture threshold	page 139

1 Introduction

Calculus of variations is a branch in the field of mathematical analysis. Its main subject is finding minima and maxima of functionals. Thereby, a variation is a small change in the argument near an extremal point of the functional under consideration. A basic example is the problem of finding a connection of two points with shortest length, while fulfilling given constraints like boundary conditions. Solutions to that problem are known as geodesics. Another prominent example is Fermat's principle from 1662, according to which light takes the path that needs the least time.

A first mathematical theory of the calculus of variations was written in 1756 and published in 1766 in Leonhard Euler's *Elementa Calculi Variationum*, cf. [51], inspired by the work of Lagrange. The first problems in this field are even older. Probably the oldest one is the previously mentioned Fermat's principle from 1662 in *Analysis ad refractiones*, followed by Newton's minimal resistance problem from 1687, published in *Philosophiae Naturalis Principia Mathematica*, see [95], and the brachistochrone curve problem of Johann Bernoulli in 1696, cf. [13]. For a historical overview, we refer to [67].

Continuum mechanics and variational models date back at least to the 19th century and the work in elasticity by Augustin-Louis Cauchy, see [43]. In this framework, models are often based on minimization problems. This is the starting point of this thesis. We consider a minimum problem of a discrete energy functional of n particles and are interested in its continuous counterpart in the limit when the number n of particles tends to infinity. In the continuous limiting functional fracture can be studied by means of discontinuity points of the deformation.

Energy minimization, as already mentioned, is one of the key elements in variational models. Since the minimum problem increases the number of variables with the size n of the system, it is difficult to handle for large particle numbers n , even numerically. On the other hand, the limiting system involves just a few continuous variables and is therefore easier to handle. One variational approach in the passage from discrete to continuum is Γ -convergence, since it focusses on minimizers of the energy and thus fits well to the energy minimization problems. This technique of deriving a macroscopic limit out of a microscopic energy functional yields the main property, i.e. that it preserves minimizers, as explained in Chapter 2 in detail.

In particular, we consider discrete one-dimensional chains of particles and minimum problems like

$$\min_{\substack{u \in \mathcal{A}_n(0,1) \\ (bc)}} \sum_{j=1}^K \sum_{i=0}^{n-j} \lambda_n J_j \left(\frac{u^{i+j} - u^i}{j\lambda_n} \right),$$

and their asymptotic behaviour in the passage from discrete to continuous systems. Here, u is the deformation of the chain and $\mathcal{A}_n(0,1)$ is the space of piecewise affine functions interpolating the discrete values of the deformation. The reference configuration of the chain is equidistributed in the interval $[0,1]$ with lattice spacing λ_n and subjected to given boundary conditions (bc). The interaction potentials J_j take into account neighbour interactions up to order K . Especially the case $K \geq 2$ is captured in this thesis. In comparison to the case of only nearest neighbour interactions, referring to $K = 1$, higher order interactions are more involved, see [34, 103].

The main focus of this thesis lies on fracture in heterogeneous media. We consider the question under which conditions the minimizers of the given minimum problem show discontinuities of the deformation which are interpreted as fracture of the material. Fracture in heterogeneous media or composite materials is a topic of ongoing interest and importance for mechanical and technological applications and has resulted in several mathematical contributions, e.g., [10, 11, 48, 54, 77]. Fracture models can be derived inter alia by considering Lennard-Jones type interaction potentials J . Due to their asymptotic decay to zero for large positive values, they allow for fracture. Further, their blow-up at zero, i.e. $J(z) \rightarrow +\infty$ as $z \rightarrow 0^+$, serves as a non-interpenetration assumption. There is a wide range of applications of Lennard-Jones type potentials in physics and chemistry, see, e.g., the Gay-Berne potential in [116] or the Girifalco interaction of fullerene molecules in [64].

The Lennard-Jones type structure can be considered as long-range interactions in a twofold way. First, the potentials $J(z)$ shows a decay to zero for large values of z slower than exponential. Secondly, the notion of long-range interaction refers to interactions beyond nearest neighbours, i.e. up to order $K \geq 2$. Both notions are referred to as long-range character, cf. [57].

A further feature of our model is its heterogeneous structure and the related homogenization problem. Heterogeneities of the considered material can arise in different ways, for instance due to fault atoms or different bonds between the same kind of elements, e.g. carbon chains as $\dots \text{C} \equiv \text{C} = \text{C} \equiv \text{C} = \text{C} \equiv \text{C} \dots$ in [80]. The heterogeneous structure is included in our model by a stochastic or periodic distribution of the interaction potentials. The process of deriving a homogeneous limit of the heterogeneous system is called homogenization. The distribution of the potentials is assumed to be stationary and ergodic. Roughly speaking, ergodicity ensures that the limit of a sample average converges to the expectation value and therefore that the limit of the discrete heterogeneous system is given as a continuous homogeneous formula. Ergodicity allows to use results from ergodic theory, e.g., Birkhoff's ergodic theorem and the subadditive ergodic theorem of Akcoglu and Krengel.

Stochastic and periodic homogenization in the discrete to continuum analysis can be found, e.g., in [3, 4, 94], where the authors consider interaction potentials with polynomial growth. These conditions rule out fracture, i.e. jump discontinuities in the limit. An approach allowing for fracture was published in [30, 73], closely related to our setting; we compare our results to those ones in detail in Section 1.2.3. A main difference to our setting is that neither of those works includes the Lennard-Jones potential and a continuous probability distribution of this potentials. The differences in the setting of this thesis compared to the those ones are also discussed in detail in Section 1.2.3. The extension to potentials of fully non-convex Lennard-Jones type, allowing for cracks, is the main contribution of this thesis. We combine the passage from discrete to continuous systems with homogenization of heterogeneous systems in the framework of fracture mechanics involving non-convex interaction potentials.

We give here some motivation for the one-dimensional setting of our problem. There are two perspectives. First, one-dimensional chains of particles serve as a toy model, see [44, 74], and pave the path to higher dimensions. One of the main mathematical advantages is the monotone ordering of particles and thus a simpler mathematical modelling, see [28, 35]. Secondly, there are indeed one-dimensional real world nanomaterials as applications, like carbon atom wires, cf. [41, 93, 117], silicon, cf. [85], chains of gold atoms on the surface of semiconductors, cf. [112], fullerene nanochain lattices, cf. [114] and fullerenes in carbon nanotubes, cf. [113].

In the following we outline the results of this thesis and give an overview of existing related literature.

1.1 Discussion of the main results

In the following, we outline the main results of this thesis. The contents of Chapter 4 and Chapter 6, as well as the underlying model in Chapter 3 are already published by myself together with S. Neukamm, M. Schäffner and A. Schlömerkemper in [81, 82]. In this thesis, the proofs and discussions are presented in more detail, compared to the published papers.

The outline of this section is as follows: We start with describing the model which we consider throughout this thesis, together with its energy. A main focus lies on the interaction potentials that are of Lennard-Jones type. This modelling is the content of Chapter 3. Moreover, we summarize the results of the variational limit (Chapter 4), the rescaled model (Chapter 5), the special case of a periodic setting (Chapter 6) and the ansatz of fracture in the discrete scale (Chapter 7).

Modelling.

The model under consideration is a one-dimensional chain of $n + 1$ particles, which is illustrated in Figure 3.1. In the reference configuration they occupy the continuous interval $[0, 1]$ and are equidistributed with lattice spacing $\lambda_n := \frac{1}{n}$. The particles interact via random potentials of Lennard-Jones type and the distribution of these non-convex potentials is assumed to be stationary and ergodic. We consider interactions up to K nearest-neighbours, i.e. two particles with reference positions i and j interact if $|i - j| \leq K$, with $K \in \mathbb{N}$. Thus for K large, the interaction potentials show a long-range character, as described above.

The energy of the chain depends on the deformed configuration, i.e. on the deformation of the particles, which we call $u : \lambda_n \mathbb{Z} \cap [0, 1] \rightarrow \mathbb{R}$. This corresponds to the actual/current position of the particles. Even if some of the theorems are proven below for arbitrary K , we give here the simplified version of some of the result for $K = 1$ for illustration purpose. The energy of the chain of particles is given by the sum of all interaction potentials and reads

$$H_n(\omega, u) = \lambda_n \sum_{i=0}^{n-1} J \left(\omega, i, \frac{u^{i+1} - u^i}{\lambda_n} \right). \quad (1.1)$$

The extension to K interacting neighbours is given in (3.13). The parameter $\omega \in \Omega$ represents the random distribution according to a probability space $(\Omega, \mathcal{F}, \mathbb{P})$. The assumptions of stationarity and ergodicity are formulated by means of a stationary and ergodic group action $(\tau_i)_{i \in \mathbb{Z}}$ of measurable mappings $\tau_i : \Omega \rightarrow \Omega$ that couple the random and the space variables by

$$J(\omega, i, z) := \tilde{J}(\tau_i \omega, z),$$

with \tilde{J} being a Lennard-Jones type potential.

We impose Dirichlet boundary conditions on the deformation $u(0) = 0$ and $u(1) = \ell$ with $\ell > 0$. Typically the reference configuration does not minimize the energy with the boundary constraints. In the homogeneous case the minimizing state is given by equidistributed particles. In heterogeneous systems, minimizers of the energy are typically non-trivial in the sense that they are neither given by the reference configuration nor equidistributed. For an illustration, see Figures 1.1 and 1.2.

Variational limit.

The first main result is Γ -convergence of the energy of the discrete chain to a continuous integral functional as the number n of particles tends to ∞ , which is asserted in Theorem 4.14. The limiting

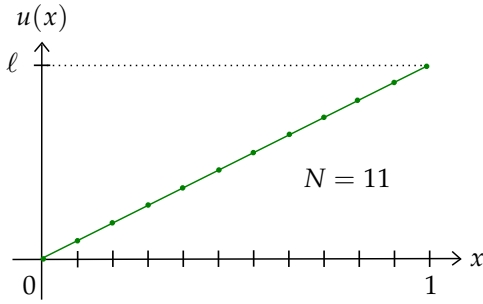


Figure 1.1 | Minimizer in the homogeneous case.

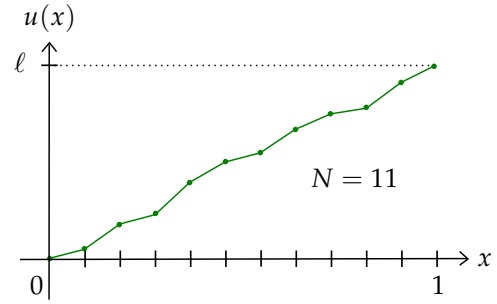


Figure 1.2 | Minimizer in the heterogeneous case.

energy consists of a deterministic, spatially homogeneous and convex integrand, given by an asymptotic homogenization formula. The limit is the result of a passage from the discrete to the continuous system combined with a homogenization procedure. In what follows, we give a brief and simplified overview of the setting and the main results, starting with the interactions potentials that we use.

Again, we consider here only nearest neighbour interactions leaving the more general case for the sections to follow. Additionally, instead of giving the general assumptions of the class of Lennard-Jones type, we focus on the classical Lennard-Jones potential. This is defined by the two-parameter family $J_{LJ}(z) := A/z^{12} - B/z^6$ with $A, B > 0$ and can be given in the equivalent form

$$J_{LJ}(z) = \epsilon \left(\frac{\delta}{z} \right)^6 \left[\left(\frac{\delta}{z} \right)^6 - 2 \right]$$

where $\delta > 0$ is the minimizer and $-\epsilon < 0$ is the minimum of the potential, cf. Figure 2.1. The stochastic setting can be interpreted as a random choice of the parameters. Let the set Ω be defined as $\Omega = \{(\delta, \epsilon), \delta \in [1, 2], \epsilon \in [3, 4]\}$. That is, all potentials that are available in this example have a minimizer in the interval $[1, 2]$ and a minimum in the interval $[-4, -3]$, randomly chosen by the random variable $\tilde{J}(\omega, \cdot)$ for every particle of the chain.

In Theorem 4.14 it is shown that the Γ -limit of the discrete energy (1.1), subjected to the Dirichlet boundary conditions from above, is finite in the space $BV(0, 1)$ of functions of bounded variation with the additional constraint on the singular part of the measure $D^s u \geq 0$ and is given by

$$H_{\text{hom}}(u) = \int_0^1 J_{\text{hom}}(u'(x)) \, dx \quad (1.2)$$

with the homogenized energy density

$$J_{\text{hom}}(z) = \lim_{N \rightarrow \infty} \frac{1}{N} \inf \left\{ \sum_{i=0}^{N-1} J(\omega, i, z + \phi^{i+1} - \phi^i) : \phi^i \in \mathbb{R}, \phi^0 = \phi^N = 0 \right\}, \quad z \in \mathbb{R}.$$

We highlight that J_{hom} is deterministic, convex and spatially homogeneous as shown in Proposition 4.12. Since the energy is finite on the space BV , the system can show cracks, i.e. jump discontinuities of the deformation u . The additional condition $D^s u \geq 0$ ensures non-interpenetration of the chain. In contrast to the non-trivial and non-affine minimizers of the discrete problem, minimizers

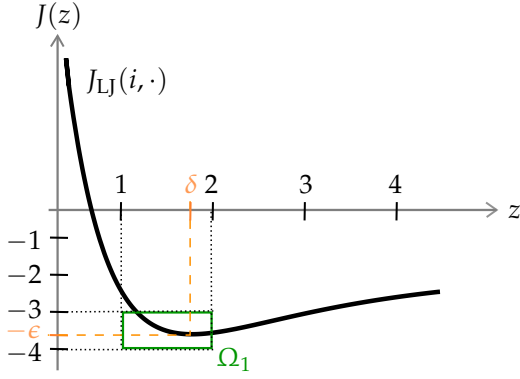


Figure 1.3 | A prototypical potential $J_{LJ}(i, \cdot)$ in the setting $(\Omega_1, \mathcal{F}_1, \mathbb{P}_1)$.

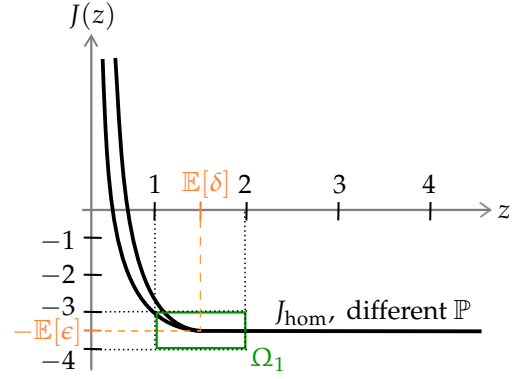


Figure 1.4 | Two different functions J_{hom} related to different probability distributions with identical expectation values $\mathbb{E}[\delta]$ and $\mathbb{E}[\epsilon]$.

of the limiting energy are affine under compressive boundary constraints. In detail, it holds true that

$$J_{\text{hom}}(z) \begin{cases} > -\mathbb{E}[\epsilon] & \text{for } z < \mathbb{E}[\delta] & \text{(compressive case),} \\ = -\mathbb{E}[\epsilon] & \text{for } z \geq \mathbb{E}[\delta] & \text{(tensile case),} \end{cases} \quad (1.3)$$

with the expectation value \mathbb{E} , according to Propositions 4.12 and 4.13. For an illustration, see Figure 1.4. The structure of the limit (1.2), together with the convexity of J_{hom} , shows that for $\ell \leq \mathbb{E}[\delta]$ the affine function $x \mapsto \ell x$ is the unique global minimizer for the Γ -limit in (1.2). No jumps are possible in this regime. On the other hand, the result (1.3) shows that for $\ell > \mathbb{E}[\delta]$ the minimizer of the limiting energy is not unique, allows for jumps and gives no information about the number or location of possible cracks. In particular, this justifies the value $\mathbb{E}[\delta]$ as the threshold of the boundary constraint ℓ separating the elastic from the fracture regime.

The exact shape of the energy density J_{hom} for $z < \mathbb{E}[\delta]$ depends on the given distribution of the parameters (δ, ϵ) . We clarify this by two examples. The first one, see Figure 1.3, assumes (δ, ϵ) to be uniformly distributed in $\Omega_1 := [1, 2] \times [3, 4]$. The second one supposes that δ_i and ϵ_i are independent and two-valued with $\mathbb{P}(\delta_i = 1) = 0.9$, $\mathbb{P}(\delta_i = 6) = 0.1$, $\mathbb{P}(\epsilon_i = 3) = 0.9$, and $\mathbb{P}(\epsilon_i = 8) = 0.1$. In both examples it holds true that $\mathbb{E}[\delta] = 1.5$ and $\mathbb{E}[\epsilon] = 3.5$. Therefore, while J_{hom} coincides for $z \geq \mathbb{E}[\delta]$ in both cases, they differ for $z < \mathbb{E}[\delta]$, see Figure 1.4.

The homogenized energy density J_{hom} is given as an asymptotic cell formula, which is typical in homogenization problems. This is also related to homogenization problems for non-convex integral functionals, see [22, 92]. The limit is in general not obtained for finite N . However, in the periodic case, we prove the existence of a cell problem formula for the homogenized energy density. This essentially relies on the fact that we restricted our analysis to only nearest neighbour interactions in the periodic case. The energy density reduces to a minimization problem on the periodicity cell.

The proof of Theorem 4.14 brings together the passage from the discrete to the continuous system and homogenization methods by ergodic theory. It requires extensions of known Γ -convergence methods and homogenization results since the Lennard-Jones potentials blow up at zero, are non-convex and do not satisfy polynomial growth conditions neither from below nor from above.

The basic feature of stochastic homogenization in an ergodic setting are ergodic theorems, in our case mainly the subadditive ergodic theorem by Akcoglu and Krengel as well as Birkhoff's ergodic theorem. Applied to a function not only depending on the probability parameter $\omega \in \Omega$ but also on another variable $z \in \mathbb{R}$, the existence of the limit in the ergodic theorems has to be extended to an uncountable set of functions in order to get existence for all $z \in \mathbb{R}$. In the case of Lipschitz continuity, this can be easily done. The demonstration of this fact for Lennard-Jones potentials is one of the main challenges in the proofs.

The non-convex Lennard-Jones potentials do not fulfil any polynomial growth condition due to the blow up at zero. We circumvent this issue by a linear approximation of the interaction potentials, indexed by L . In the setting with the approximating potentials, we can apply the subadditive ergodic theorem by Akcoglu and Krengel [2] and prove the existence of a corresponding infinite cell-formula J_{hom}^L . Afterwards, we remove the approximation by showing that J_{hom} is given as the monotone limit of J_{hom}^L as $L \rightarrow \infty$ and hence exists. Then, the assumption of uncountability on the set of interaction potentials is difficult to handle in the limit $L \rightarrow \infty$ and therefore needs some technical lemmas preparing the result.

In the proof of the Γ -convergence result, an intermediate scale η is introduced, complementing the macroscopic scale $[0, 1]$ and the microscopic scale λ_n . The stochastic setting has no natural intrinsic coarser scale, unlike the periodic case where the periodicity length serves as the coarser scale. Therefore, this intermediate scale has to be introduced artificially. To remove this scale afterwards in the limit, the Attouch-Lemma 2.23 provides the necessary results.

Rescaled model.

The continuum limit in (1.2) is finite on the space of BV and therefore allows for cracks. However, there is no contribution in the energy accounting for these jumps. This is not reasonable from a physical perspective, since the creation of new surfaces is supposed to cost energy. Mathematically speaking, the limit shows a separation of scales between bulk and jump part. In order to overcome this problem, we introduce a suitable rescaling of the energy, since jumps are obtained for rescaled energies in the limit, cf. [34, 101, 103]. This rescaling yields a bulk and a surface contribution of the same order, which both are present in the limiting energy. More precisely, we use the $\sqrt{\lambda_n}$ -scaling, i.e.

$$v^i := \frac{u^i - \sum_{k=0}^{i-1} \lambda_n \delta(\tau_k \omega)}{\sqrt{\lambda_n}} \quad \text{for all } i \in \{0, \dots, n\},$$

and obtain the rescaled energy

$$E_n(\omega, v) := \sum_{i=0}^{n-1} \left(J \left(\tau_i \omega, \frac{v^{i+1} - v^i}{\sqrt{\lambda_n}} + \delta(\tau_i \omega) \right) - J(\tau_i \omega, \delta(\tau_i \omega)) \right). \quad (1.4)$$

We also need to rescale the boundary condition $u(1) = \ell$. Moreover, we consider values ℓ of the boundary condition $u(1) = \ell$ close to the threshold between the elastic and the fracture regime. Due to (1.3), this threshold is given by $\ell = \mathbb{E}[\delta]$. Following the ideas of [101], adjusted to our stochastic setting, we focus on some sequence $(\ell_n) \subset \mathbb{R}$ with $\ell_n \rightarrow \mathbb{E}[\delta]$, satisfying $\ell_n > \mathbb{E}[\delta]$ for every $n \in \mathbb{N}$ and

$$\gamma_n := \frac{\ell_n - \sum_{k=0}^{n-1} \lambda_n \delta(\tau_k \omega)}{\sqrt{\lambda_n}} \rightarrow \gamma,$$

for some $\gamma \in \mathbb{R}$. This new boundary value yields the new Dirichlet boundary condition $v(0) = 0$ and $v(1) = \gamma_n$.

In Theorem 5.8 it is shown that the rescaled energy (1.4) Γ -converges to a deterministic energy that is finite on the space $SBV(0, 1)$ of special functions of bounded variation, with certain additional constraints, and reads

$$E(v) = \underline{\alpha} \int_0^1 |v'(x)|^2 dx + \beta \#S_v, \quad (1.5)$$

where $\underline{\alpha} := \left(\mathbb{E}\left[\frac{1}{\alpha}\right]\right)^{-1}$ and $\beta := \inf\{-J(\omega, \delta(\omega)) : \omega \in \Omega\}$ with $\alpha(\omega) := \frac{1}{2} \frac{\partial^2 J(\omega, z)}{\partial z^2} \Big|_{z=\delta(\omega)}$. The jump set of $v \in SBV(0, 1)$ is denoted by S_v . This limiting energy is an energy of Griffith type and consists of a bulk contribution due to elastic deformations and a surface term due to cracks. While the elastic constant is an expectation value, the parameter in the jump part is the minimal height that has to be overcome for a jump and can be interpreted as a jump at the weakest bond. Compared to the Γ -limit of the original energy, where jumps occur without any contribution to the energy, in the rescaled setting each jump costs energy.

The proof of the rescaled case, Theorem 5.8, also uses ergodic theory, in particular the Birkhoff ergodic theorem. This results in a homogenized elastic constant $\underline{\alpha}$ in front of the integral of the elastic part of the energy. The underlying idea is a harmonic approximation of the potentials at their minimum. This leads to a quadratic energy with well known solutions for minimum problems due to the method of Lagrange multipliers.

The structure of the energy (1.5) is similar to that of the limiting energy in [30], where truncated parabolas are considered instead of Lennard-Jones potentials. Due to the periodicity in that setting, the elastic constant $\underline{\alpha}$ is given as a harmonic mean instead of the expectation value and the infimum in the constant β becomes a minimum. Having the stochastic results at hand as well as the limiting energy for the truncated parabolas, we continue with the periodic case and the question to which extent the constants in the limit of the energy are comparable or even a simplification of the stochastic setting. This is outlined in the following.

Periodic setting.

The Γ -limit of zeroth order as well as the rescaled limit are additionally considered in a periodic setting in Theorem 6.3 and 6.4. More precisely, we assume a fixed periodicity length $M \in \mathbb{N}$ and interaction potentials J_i of Lennard-Jones type satisfying the periodicity assumption $J_i = J_{i+M}$, $i \in \mathbb{Z}$. As mentioned above, the main difference to the stochastic setting is the representation formula of the homogenized energy density, considered in Lemma 6.2. In the periodic case, the asymptotic homogenization formula J_{hom} reduces to a cell problem formula $f_{\text{hom}} : \mathbb{R} \rightarrow (-\infty, \infty]$ given by

$$f_{\text{hom}}(z) := \min \left\{ \frac{1}{M} \sum_{i=0}^{M-1} J_i^{**}(z_i) : \sum_{i=0}^{M-1} z_i = Mz \right\}.$$

The threshold $\mathbb{E}[\delta]$ of the stochastic setting is replaced by the arithmetic mean $\bar{\delta}$ of the global minimizer for J_i over a periodicity cell. In the rescaled setting, the expectation value of the elastic modulus $\underline{\alpha}$ is represented by a harmonic mean over the periodicity cell and the infimum in the jump constant β becomes a minimum.

Fracture on the discrete scale.

The third main part of the thesis is devoted to a completely different approach to the topic of fracture. So far, fracture occurs in the limit functionals in the sense that the admissible functions are in the space $BV(0, 1)$. In this space, a jump is well-defined by means of the measure. Phrased differently, discontinuities of the deformation are interpreted as cracks of the material. In the discrete system, the functions are piecewise affine and therefore continuous by definition. Hence, the definition of a fracture point cannot be kept.

The idea is to define a jump, or fracture, respectively, of a discrete function by the steepness of the slope of the affine interpolation. In particular, we say that the chain has a jump at position i if and only if the discrete gradient $\frac{u^{i+1}-u^i}{\lambda_n}$ at this position is larger than the jump point z_{frac} . The value z_{frac} is given as the inflection point of the Lennard-Jones potential, generalized to an appropriate definition in the case of Lennard-Jones type potentials.

With the definition of this jump point z_{frac} , we define the jump threshold ℓ_n^* separating the regimes where the energy is minimized with and without a jump. The analogue of this value ℓ_n^* in the previous approach is the threshold $\mathbb{E}[\delta]$. The asymptotics of the jump threshold ℓ_n^* are considered by means of a pointwise convergence in Theorem 7.12. Further, a rescaled version of ℓ_n^* in the $\sqrt{\lambda_n}$ rescaling is considered regarding its convergence in Theorem 7.11. The results of both methods are in well accordance with those of the Γ -limits. In detail, the limiting thresholds separating the elastic and the fracture regime are identical in both cases.

The analysis is mainly based on a subtle choice of properties of the Lennard-Jones type potentials and well chosen definitions for the jump point and the jump threshold together with the minimal energies in the elastic and fracture case.

1.2 Overview of related literature

The work in this thesis contains three main concepts. The first one is the passage from a discrete model problem to the continuum picture by means of Γ -convergence. The discrete aspect is incorporated in the description of the main model as a discrete chain of particles. The second main topic is fracture, which enters the system through the choice of the interaction potentials being of Lennard-Jones type. The convex-concave structure allows for jumps of the deformation, referring to cracks of the chain, in the limiting energies. The third essential concept is the heterogeneous structure. Different species of atoms as well as impurities or oriented ellipsoidal particles are covered by the choice of a periodic or stochastic setting of the model. The following sections provide an overview of the literature related to this work.

1.2.1 Γ -convergence in the passage from discrete to continuous systems

Naturally, there are two different ways of describing a model problem, the continuous and the discrete one. Continuum theories have the great advantage of involving just a few continuous variables, while discrete systems increase the number of variables with the size of the system. Thus, continuous equations are easier to handle. Especially in fracture mechanics, the continuous system has the further advantage that discontinuities of the deformation can be interpreted as cracks in the material, while in the discrete system there is at first no intuitive analogue. On the other side, the discrete system is the natural representation of an atomic or molecular system within classical mechanics. Therefore, it is of interest to connect both theories and combine the advantages of each

description, which can be done by passing to a suitable limit. Thus, a question that is addressed by discrete to continuum analysis is the derivation of a continuum model starting from the discrete system by keeping its main features. This passage from discrete to continuous systems is well established in literature, see e.g. [16, 37]. Seen from another point of view, the passage from discrete to continuous systems justifies and establishes the macroscopic model as a good description of the system, since it is derived by an underlying microscopic one.

The feature that is of interest is energy minimization. Since it focusses on minimizers of the energy, Γ -convergence is a suitable tool for deriving a continuous model from a discrete one. This notion of convergence preserves minimizers of the energy, as explained in Chapter 2 in detail. For an introduction, see e.g. [30] and [46], and for an overview [15].

A fundamental step towards elasticity theory was made in [29–32], where the authors consider discrete problems and their limits by Γ -convergence under varying conditions on the interaction potentials. In [3], the authors prove a general integral representation result for continuum limits of discrete energies. This work was extended in [38] for more general interaction potentials and full finite-range multi-body interactions. Further, [36] provides a continuous linear elasticity energy from a discrete energy functional for a specific class of pair interactions. In [104], the author extends the latter work by considering full next-to-nearest neighbour interactions, more general cell energies and more general non-affine boundary conditions.

Especially in the one-dimensional case, there exists ample literature dealing with the passage from discrete to continuum via Γ -convergence. In [26], the authors derived, to the best of our knowledge, for the first time fracture by Γ -convergence techniques in the passage from discrete to continuous systems. Their discrete chain of atoms was subjected to nearest neighbour interactions. Further models allowing for fracture are considered in [24, 29, 35] beyond nearest neighbours. In [33], the polynomial growth conditions prevent the limiting energy from showing fracture and a homogenization formula for the limiting energy density can be shown, as it was done in [24] in the fracture model. Further, in [71] second neighbour interactions and point defects also allowing for fracture are considered. Finally in [29, 32], the authors deal with a setting similar to that in this thesis, but in the homogeneous case. Our heterogeneous model in the periodic setting and its homogenization results are considered in [30]. Both works, the homogeneous one and the periodic heterogeneous one do not include random heterogeneous systems as in this thesis. One of the main challenges of our model is to combine the methods from the stochastic and ergodic homogenization with the passage from discrete to continuous systems by methods of Γ -convergence.

Another widely explored related research area is that of crystallization, see, e.g., [19] for an overview. It is investigated from the viewpoint of molecular mechanics and includes two- and three-body interactions. In particular when considering graphene models, new and interesting structural features can occur, e.g., so-called armchair and zigzag topologies, cf. [49, 87–89]. Also finite one-dimensional models are considered, cf. [14, 61], where the first one features Lennard-Jones type interactions. In [58, 59], the authors extend the crystallization problem by different species of particles and two-body short-range interaction in order to model ionic dimers, which is connected to the work in this thesis by the one-dimensional discrete ansatz and Lennard-Jones type interactions.

Γ -convergence methods are not only used for the passage from discrete to continuous systems. They are also a well established tool when small parameters are involved in the modelling of integral energy functionals. These parameters may arise, e.g., due to periodic structures, see [50, 75], or a dimension reduction, cf., e.g., [8, 83]. Besides Γ -convergence, there are also other approaches for passages from discrete to continuum systems. Thermodynamic limits are considered in [16, 42]

and the asymptotics of gradient flows in [110]. Further, [74] deals with the zero-temperature limit in atomistic models of elasticity involving non-zero pressure.

1.2.2 Fracture and Lennard-Jones type potentials

A main feature of our model is the occurrence of fracture. In continuum models allowing for fracture the energy often involves two terms, a bulk contribution due to elastic deformations and a surface contribution due to crack growth, see e.g. [56]. In the framework of Γ -convergence, fracture is obtained in the continuum limit when using interaction potentials in the discrete model satisfying suitable growth conditions, cf. [26, 29, 32], for nearest neighbour interactions and beyond nearest neighbours, respectively. These conditions are fulfilled by the class of Lennard-Jones type potentials. Among others, this is a class of potentials allowing for fracture in the limiting energy. Lennard-Jones type potentials are widely used in physical literature (cf. Section 2.1); moreover, they are of interest in mathematics. The authors in [62, 111], e.g., consider finite chains of particles in one dimension with Lennard-Jones interaction potentials. Also in the discrete to continuum setting, many authors implemented the Lennard-Jones potential, see [24, 29, 32, 35, 71] which are already discussed above, and additionally [100, 101, 103] including extended boundary conditions and boundary layer energies.

In the last two decades, many authors worked on fracture models by deriving continuous theories starting from an underlying discrete model. One of the first contributions to fracture derived from a discrete to continuum analysis can be found in [109], where nonlinear elasticity containing fracture was discussed by methods of asymptotic analysis. Further, the method of Γ -convergence was used, starting with [26, 29–32], to derive fracture in the passage from discrete to continuum systems.

In [109], the author discussed the importance of keeping the microscopic lattice parameter in the macroscopic limit. This property is not fulfilled in [26, 29, 32]. Therefore, further methods on dealing with fracture were carried out. One is deriving the Γ -limit of first order instead of the zero order limit, see [24, 37, 100]. The other one uses a rescaled version of the functional, e.g. [34, 37, 101, 103]. In this thesis both approaches are considered. There are also different ways of dealing with fracture. We name here the method of minimal movements. For the Lennard-Jones case, this can be found in [27]. Another ansatz uses discrete differential geometry, cf. [49].

The Γ -convergence result in our case of the rescaled functional is a Griffith type energy. Models using other growth conditions, instead of the Lennard-Jones type, achieve comparable results, e.g. [30, 35], which is consistent with our findings. In [30], truncated parabolas are used with the same structure of the limit. Therefore, the Lennard-Jones case also gives a justification for using a model with linearised Lennard-Jones potentials.

Even in the research on crystallization Lennard-Jones type potentials are used. In [60], the authors consider the Γ -convergence of a two-dimensional triangular lattice model with nearest neighbour interactions of Lennard-Jones type. The limit then is a continuum Griffith energy functional in the small displacement regime. Further, the contribution [115] uses short-range pair potentials similar to Lennard-Jones type again in the Γ -convergence framework. Short-range in their work means that the potentials $J(z)$ are set to zero for all $z > \beta$ and a given constant $\beta > 0$. Fracture in higher dimensions in the discrete to continuum approach can be found, e.g., in [78]. Further approaches to fracture models and surface energies in the passage from discrete to continuum can be found in [71, 73, 74]. The first one focusses on point defects in a one-dimensional homogeneous Lennard-Jones systems with next-to-nearest neighbour interactions by means of

Γ -convergence. The work in [74] deals with the zero-temperature limit and the thermodynamic limit instead of variational methods. In their model, pressure and positive temperature are allowed. The model and the methods in [73] are closer related to this thesis and will be discussed in detail in Section 1.2.3. Further, [44, 45] considers linear elasticity without the use of Γ -convergence. That work is not directly related to this thesis, since it uses harmonic interactions and, especially the second one, deals with quasicontinuum methods. It is mentioned here because it is also settled in the one-dimensional discrete setting and can be seen as a harmonic approximation of the Lennard-Jones case.

1.2.3 Periodic and stochastic homogenization

The last feature of our model is homogenization. This automatically enters the model when composite materials are under consideration, whether in a periodic or stochastic setting. An overview of homogenization results in the calculus of variations can be found in [90]. Homogenization of integral functions, with growth conditions not allowing for jumps, are considered in [22, 75, 92] in the periodic case and in [1, 47] in the stochastic case. Fracture in heterogeneous media is discussed in [54] by means of periodically perforated domains, in [11, 48] dealing with materials reinforced by periodic elastic fibers and in [10] considering a brittle composite with soft periodic inclusions. Those works all fall in the framework of continuum theories. In the discrete to continuum setting, homogenization results are, e.g., derived in [3, 4] where superlinear growth conditions in a periodic or, respectively, stochastic setting are considered. Further, [52, 53, 94] deal with degenerate growth conditions in the stochastic setting and [25] with ferromagnetic spin systems. Moreover, related results can be found in [4, 38]. There, the authors work in higher dimensions and in the framework of stochastic homogenization of discrete energies. They however involve different growth and coercivity conditions, that rule out the Lennard-Jones type potentials. In all of these models, jumps do not occur because the growth conditions do not allow for them. Instead of stochastically distributed potentials, some authors work with stochastic lattices, see [4, 99], or stochastic diffeomorphisms, e.g. [17, 66]. Finally, different approaches without the use of Γ -convergence techniques can be found in literature. In [72], stochastic homogenization is considered using two-scale convergence as introduced in [20]. The authors of [18] derive limiting energies for stochastic lattices by application of a thermodynamic limit process. Last, also energies defined by integral functionals are considered in the framework of homogenization, see, e.g., [40].

Homogenization in the passage from microscopic to macroscopic scales allowing for jumps, that we are interested in here, can be found in [73]. There, the authors consider a similar discrete energy density as in our model, with random interaction potentials. The limiting energy is obtained by means of Γ -convergence and has a structure similar to our rescaled case, consisting of an integral term with a homogenized energy density and a jump part. The homogenized energy is given by an infinite cell formula, as usual in non-convex homogenization and in accordance with our results. The main difference of our work compared to their contribution is given threefold. First, the interaction potentials in [73] are convex and satisfy a linear growth condition from below, which rules out the Lennard-Jones potentials. Second, we additionally include finite-range interactions up to order K in the Γ -limit of zeroth order, whereas [73] considers nearest-neighbour interactions. Third, in [73] a discrete probability density is considered, while in this thesis, we allow for an infinite set of interaction potentials, which actually can be uncountable. Although some arguments of the proofs in this work and in [73] are similar, we have to introduce several new ideas in order to deal with the differences in the setting described before. One of these are the approximation

of the interaction potentials by Lipschitz-continuous functions in order to use the subadditive ergodic theorem, a refined treatment of the competitors for the minimization problem and a proper adaption to the case of K interacting neighbours.

Another setting allowing for jumps is considered in [30], where a periodic homogenization of truncated quadratic interaction potentials is discussed. In this case, the Γ -limit, cf. [30, Theorem 18], coincides with the Γ -limit of the rescaled fully nonlinear Lennard-Jones setting, in consideration of suitably chosen constants. A periodic setting with superlinear growth of the potentials can be found, e.g., in [3]. For an introduction to that topic, we refer to [21].

2 Mathematical background

In this chapter, we give a brief introduction to some topics which of this thesis is based on. In particular, we consider Lennard-Jones type potentials, define functions of bounded variation, state some ergodic theorems and recall the concept of Γ -convergence. In every section, we give the basic definitions which are needed to understand the main ideas and results used in this thesis.

2.1 Lennard-Jones type potentials

The interaction potentials of our model are called Lennard-Jones type. Here, we want to give an idea of that class of potentials as well as some examples that fall into this setting and are used in the physics literature. There is plenty of literature in mathematics referring to the class of Lennard-Jones type potentials, which is discussed in Chapter 1.

In view of the upcoming mathematical analysis, we emphasize that the potentials of Lennard-Jones type are neither convex nor do they fulfil a standard polynomial growth condition. Therefore, the analysis becomes more advanced and a lot of preliminary results one usually refers to are ruled out because they assume standard growth conditions or convexity. Further, the potentials are long-range interactions. As discussed in the introduction, this is due to their decay of the modulus being slower than exponential.

The classical Lennard-Jones potential is a prototypical example of a function in this class and therefore was chosen for giving its name. In the subsequent chapters, the basic assumptions (LJ1)–(LJ3), see Section 3.1, are extended by (LJ4) and (LJ5) in Section 5.2 and by (LJ6)–(LJ9) in Section 7.2, in a way that is necessary for the proofs. A summation of the assumptions on the Lennard-Jones type potentials can be found on page 153 and onwards.

A function is called a Lennard-Jones type potential if it fulfils the following properties:

- Suitable regularity conditions, e.g. continuity.
- Asymptotic decay:

$$\lim_{z \rightarrow +\infty} J(z) = 0.$$

- Convex lower and upper bound: There exists a convex function $\Psi : \mathbb{R} \rightarrow [0, +\infty]$ and constants $d_1, d_2 > 0$ with

$$\lim_{z \rightarrow -\infty} \frac{\Psi(z)}{|z|} = +\infty$$

such that

$$d_1(\Psi(z) - 1) \leq J(z) \leq d_2 \max\{\Psi(z), |z|\} \quad \text{for all } z \in \mathbb{R}.$$

- Minimum and minimizer: J has a unique minimum point δ with $J(\delta) < 0$ and it is strictly convex in $(-\infty, \delta)$ on its domain.

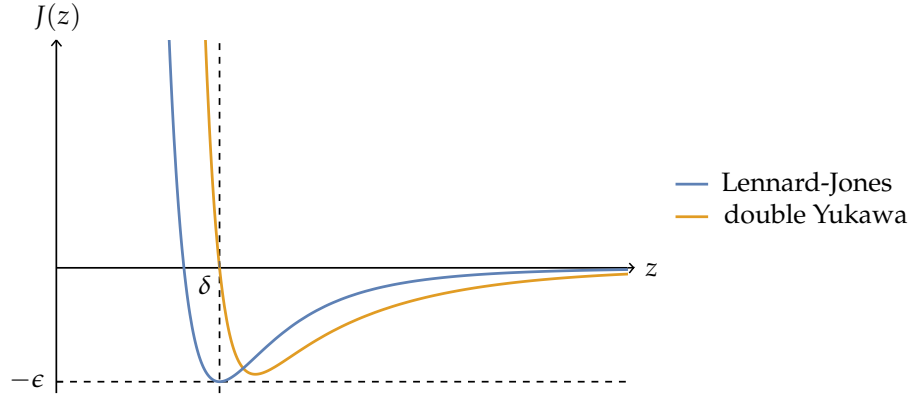


Figure 2.1 | Lennard-Jones and double Yukawa potential.

The decay to zero as $z \rightarrow \infty$ does not admit the potential to have a polynomial bound from below and the superlinear growth at $z \rightarrow -\infty$ rules out a polynomial growth from above. These conditions are designed to cover a wide range of potentials with convex-concave structure. Some examples are discussed below.

It is of interest to keep the assumptions as general as possible instead of giving a precise formula for the potential, because the special choice of the potential depends on the field of application. Atomistic and molecular interactions, e.g., are treated differently. Further, even the classical Lennard-Jones potential is just an approximation and not an exact measured or mathematically derived formula, therefore it is useful to have assumptions keeping the main features of the potential without fixing it in detail.

The following formulas show two examples of functionals fulfilling the properties of the class of Lennard-Jones type potentials. Let $\epsilon, \delta, \alpha, \beta, C_{DY} > 0$, then the classical Lennard-Jones potentials and double Yukawa potentials for $z > 0$ are given by

$$J_{LJ}(z) = \epsilon \left(\left(\frac{\delta}{z} \right)^{12} - 2 \left(\frac{\delta}{z} \right)^6 \right),$$

$$J_{DY}(z) = \frac{C_{DY}}{z} (\exp(-\alpha(z - \delta)) - \exp(-\beta(z - \delta))),$$

respectively, cf. [55, 84, 86]. Fig. 2.1 shows the two mentioned potentials for a suitable choice of parameters. It can be easily proven that these potentials fulfil the properties of the Lennard-Jones type setting. Another way of representing the classical Lennard-Jones potential is given by

$$J_{LJ}(z) := \frac{A}{z^{12}} - \frac{B}{z^6} \quad \text{with } A, B > 0.$$

This classical Lennard-Jones type potential, especially in the first representation, is a special case, referring to $n = 12$ and $m = 6$, of the Mie- (n, m) -potential

$$J_{MIE}(z) := \left(\frac{n}{n-m} \right) \left(\frac{n}{m} \right)^{m/(n-m)} \epsilon \left[\left(\frac{\sigma}{z} \right)^n - \left(\frac{\sigma}{z} \right)^m \right],$$

with $\sigma = \delta \sqrt[n-m]{m/n}$ being the value of z for which the potential is zero, i.e. $J_{MIE}(\sigma) = 0$. Those potentials consist of a repulsive short-range and an attractive long-range term, which is a standard

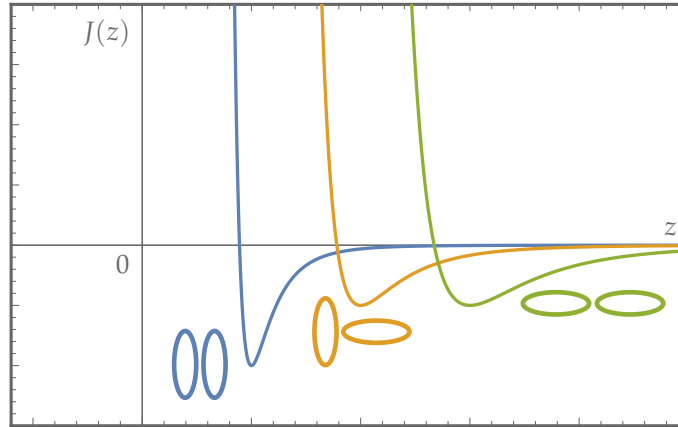


Figure 2.2 | Gay-Berne potential for three different orientations.

way of modelling particle interactions in physics and chemistry, see, e.g., [65, 69, 108].

A further example is the so called hard-core potential. Here, the potential $J(z)$ is set to $+\infty$ for $z \leq z_{\text{hc}}$, with $z_{\text{hc}} > 0$. As long as the potential satisfies

$$\lim_{z \rightarrow z_{\text{hc}}^+} J(z) = \infty,$$

our class of Lennard-Jones type potentials includes hard-core potentials.

It is also possible to truncate and shift the potential such that $J(z) = 0$ for $z \geq z_{\text{tr}}$, with $z_{\text{tr}} > 0$. These potentials are also captured by our general assumptions on the interaction potentials, and are used, e.g., in [9, 105, 107].

Further, we mention the Gay-Berne potentials, see, e.g., [12], which is a generalization of a Lennard-Jones potential between two particles. Those particles are assumed to be, e.g., of ellipsoidal shape. Therefore, the orientation of the axis relative to each other affects the interaction potential. Even in a one-dimensional chain of particles, there are uncountably many possible interaction potentials that have to be taken into account, represented by the continuous variable angle of the orientation. An illustration can be found in Figure 2.2. Applications of the Gay-Berne potential are shown, e.g., in [91, 96–98, 116], dealing with fullerenes, and nanoparticles in liquid crystals. Another application of Lennard-Jones type potentials is the Girifalco potential [64], which is used to model interaction of fullerene molecules.

2.2 Functions of bounded variation

We give here a short introduction to the functions of bounded variation, following the overview of [5], where further details and proofs can be found. Generally speaking, the space BV of functions of bounded variation is a potential candidate to work with when one considers problems in fracture mechanics. As it will be derived in the following, functions in the space BV allow for jumps. When considering deformations of a certain material, the jumps are interpreted as cracks in the material.

In the following, let $I = (a, b) \subset \mathbb{R}$ be an open and bounded interval and let $C_c(I)$ denote the space of continuous functions with compact support on I . We start with the definition of the total variation and of functions of bounded variation

Definition 2.1 ([5, Def. 1.4]). Let (X, \mathcal{E}) be a measure space and let μ be a signed measure with respect to (X, \mathcal{E}) . We define the total variation $|\mu|$ for every $E \in \mathcal{E}$ as follows:

$$|\mu|(E) := \sup \left\{ \sum_{h=0}^{\infty} |\mu(E_h)| : E_h \in \mathcal{E} \text{ pairwise disjoint, } E = \bigcup_{h=0}^{\infty} E_h \right\}.$$

Definition 2.2 ([5, Def. 3.1]). Let $u \in L^1(I)$. We say that u is a function of bounded variation in I if the distributional derivative of u is representable by a finite Radon measure in I , i.e. if

$$\int_I u \phi' \, dx = - \int_I \phi \, dDu \quad \forall \phi \in C_c^\infty(I),$$

for some \mathbb{R} -valued measure Du in I . The vector space of all functions of bounded variation in I is denoted by $BV(I)$.

The Sobolev space $W^{1,1}(I)$ is contained in $BV(I)$, since for any $u \in W^{1,1}(I)$ the distributional derivative is given by $\nabla u \mathcal{L}$. This inclusion is strict, which can be seen by considering the function $\chi_{(c,b)} \in BV(I) \setminus W^{1,1}(I)$, with $c \in I$ and $a < c < b$.

The space $BV(I)$, equipped with the norm

$$\|u\|_{BV(I)} := \int_I |u| \, dx + |Du|(I),$$

is a Banach space. This norm-topology is too narrow for many applications. Continuously differentiable functions, e.g., are not dense in $BV(I)$. However, $BV(I)$ functions can be approximated, in the $L^1(I)$ topology, by smooth functions whose gradients are bounded in $L^1(I)$.

In comparison to the strong convergence, a different notion turns out to be useful, the so called weak* convergence. It is useful for compactness properties of the space BV , which we will see later on.

Definition 2.3 ([5, Def. 3.11]). Let $u, u_h \in BV(I)$. We say that (u_h) weakly* converges in $BV(I)$ to u if (u_h) converges to u in $L^1(I)$ and (Du_h) weakly* converges to Du in I , i.e.

$$\lim_{h \rightarrow \infty} \int_I \phi \, dDu_h = \int_I \phi \, dDu \quad \forall \phi \in C_0(I),$$

where $C_0(I)$ is the space of continuous functions $I \rightarrow \mathbb{R}$ vanishing at the boundary.

The next proposition gives a simple criterion for weak* convergence.

Proposition 2.4 ([5, Prop. 3.13]). Let $(u_h) \subset BV(I)$. Then (u_h) weakly* converges to u in $BV(I)$ if and only if (u_h) is bounded in $BV(I)$ and converges to u in $L^1(I)$.

This leads to the compactness result in BV .

Theorem 2.5 ([5, Thm. 3.23]). Every sequence $(u_h) \subset BV_{\text{loc}}(I)$ satisfying

$$\sup \left\{ \int_A |u_h| \, dx + |Du_h|(A) : h \in \mathbb{N} \right\} < \infty \quad \forall A \subset\subset I \text{ open}$$

admits a subsequence $(u_{h(k)})$ converging in $L^1_{\text{loc}}(I)$ to some $u \in BV_{\text{loc}}(I)$. If the sequence is bounded in $BV(I)$ we can say that $u \in BV(I)$ and that the subsequence weakly* converges to u .

2.2.1 BV functions of one variable

The previous definitions and results were all stated in one dimension, even though they are also valid in higher dimensions. It follows a characterisation of functions of bounded variation that holds only true in the one-dimensional case. Again, let $I = (a, b) \subset \mathbb{R}$ be an interval. We highlight some statements which are used in the proofs of this thesis. Further details can be found in [5].

First, we fix some notation. The right-hand side and left-hand side limits

$$u(x^+) := \lim_{h \rightarrow 0^+} \frac{1}{h} \int_x^{x+h} u(s) ds, \quad u(x^-) := \lim_{h \rightarrow 0^+} \frac{1}{h} \int_{x-h}^x u(s) ds$$

exist for all $x \in [0, 1)$ and for all $x \in (0, 1]$, respectively. In the following theorem, a definition of a good representative is given. We denote by $A = \{t \in I : Du(\{t\}) \neq 0\}$ the set of atoms of the measure Du .

Theorem 2.6 ([5, Thm. 3.28]). *Let $u \in BV(I)$. Then, the following statements hold:*

a) *There exists a unique $c \in \mathbb{R}$ such that*

$$u^l(t) := c + Du((a, t)), \quad u^r(t) := c + Du((a, t]) \quad t \in I$$

are good representatives of u , the left continuous one and the right continuous one. Any other function $\bar{u} : I \rightarrow \mathbb{R}$ is called a good representative of u if and only if

$$\bar{u}(t) \in \left\{ \theta u^l(t) + (1 - \theta) u^r(t) : \theta \in [0, 1] \right\} \quad \forall t \in I.$$

b) *Any good representative \bar{u} is continuous in $I \setminus A$ and has a jump discontinuity at any point of A :*

$$\bar{u}(t^-) = u^l(t) = u^r(t^-), \quad \bar{u}(t^+) = u^l(t^+) = u^r(t) \quad \forall t \in A.$$

c) *Any good representative \bar{u} is differentiable at \mathcal{L}^1 -a.e. point of I , denoted by \bar{u}' , which coincides with the density of Du with respect to \mathcal{L}^1 .*

The measure Du is a Radon measure and therefore the set A is at most countable. By the Radon-Nikodým theorem, we can split Du into the absolutely continuous part $D^a u$ with respect to $\mathcal{L}^1(0, 1)$ and the singular part $D^s u$. Further, we define the jump part $D^j u = D^s u \llcorner A$ and the Cantor part $D^c u = D^s u \llcorner (I \setminus A)$. In this way, we obtain

$$Du = D^a u + D^s u = D^a u + D^j u + D^c u.$$

The decomposition is unique. According to this, we call $u \in BV(I)$ a jump function if $Du = D^j u$, i.e. Du is a purely atomic measure, and we call u a Cantor function if $Du = D^c u$, i.e. Du is a singular measure without atoms. This leads us to a decomposition theorem of BV functions.

Corollary 2.7 ([5, Cor. 3.33]). *Let $I = (a, b) \subset \mathbb{R}$ be a bounded interval. Then, any $u \in BV(I)$ can be represented by $u^a + u^j + u^c$, where $u^a \in W^{1,1}(I)$, u^j is a jump function and u^c is a Cantor function. The three functions are uniquely determined up to additive constants and*

$$|Du|(I) = |Du^a|(I) + |Du^j|(I) + |Du^c|(I) = \int_a^b |\bar{u}'| dt + \sum_{t \in A} |\bar{u}(t^+) - \bar{u}(t^-)| + |Du^c|(I),$$

where \bar{u} is any good representative of u .

This decomposition only works for BV functions of one variable and not for BV functions of two or more variables. As an abbreviation, we set

$$[u](x) := u(x^+) - u(x^-)$$

and define the jump set

$$S_u = \{x \in (0, 1) : [u](x) \neq 0\}$$

for $u \in BV(0, 1)$, as well as for $u \in SBV(0, 1)$ (introduced below). This jump set S_u coincides with the set of atoms A of the measure Du . According to the previous results and definitions, we get for the absolute continuous part

$$D^a u = u' \mathcal{L}^1,$$

and for the jump part

$$D^j u = \sum_{x \in S_u} (u^+(x) - u^-(x)) \delta_x = \sum_{x \in S_u} [u](x) \delta_x,$$

since the set S_u is at most countable.

The next proposition is a relaxation result of a special kind of BV functionals in one dimension which we will often make use of. The proposition is deduced from [63, Thm. 1.62] and proven in [102].

Proposition 2.8. *Let $f : \mathbb{R} \rightarrow \mathbb{R} \cup \{+\infty\}$ be convex, lower semicontinuous, monotone decreasing with*

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

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

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

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

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

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

2.2.2 Special functions of bounded variation

The set of special functions of bounded variation has been singled out by E. De Giorgi and L. Ambrosio as a good space for variational problems where both volume and surface energies are involved. This overview again follows [5].

We say that $u \in BV(I)$ is a special function of bounded variation, and write $u \in SBV(I)$, if the Cantor part of its derivative $D^c u$ is zero. We obtain

$$Du = D^a u + D^j u = u' \mathcal{L}^1 + \sum_{x \in S_u} (u^+(x) - u^-(x)) \delta_x \quad \forall u \in SBV(I).$$

The Sobolev space $W^{1,1}(I)$ is contained in $SBV(I)$ and this inclusion is strict. For instance if $u = \chi_{(a,b/2)}$ for $I = (a,b)$, then $u \in SBV(I)$ but u is not a Sobolev function. We state a useful result about the space $SBV(I)$.

Proposition 2.9 ([5, Prop. 4.2]). *Any $u \in BV(I)$ belongs to $SBV(I)$ if and only if $D^s u$ is concentrated on a Borel set σ -finite with respect to \mathcal{H}^0 .*

The following two theorems are a closure and a compactness theorem for $SBV(I)$.

Theorem 2.10 (Closure of SBV , [5, Thm. 4.7]). *Let $\varphi : [0, \infty) \rightarrow [0, \infty]$, $\theta : (0, \infty) \rightarrow (0, \infty]$ be lower semicontinuous increasing functions and assume that*

$$\lim_{t \rightarrow \infty} \frac{\varphi(t)}{t} = \infty, \quad \lim_{t \rightarrow 0} \frac{\theta(t)}{t} = \infty.$$

Let $I \subset \mathbb{R}$ be open and bounded, and let $(u_h) \subset SBV(I)$ be such that

$$\sup_h \left\{ \int_I \varphi(|u'_h|) \, dx + \sum_{S_{u_h}} \theta(|u_h^+ - u_h^-|) \right\} < \infty. \quad (2.1)$$

If (u_h) weakly converges in $BV(I)$ to u , then $u \in SBV(I)$, the approximate gradients u'_h weakly converge to u' in $L^1(I)$, $D^j u_h$ weakly* converges to $D^j u$ in I and*

$$\begin{aligned} \int_I \varphi(|u'|) \, dx &\leq \liminf_{h \rightarrow \infty} \int_I \varphi(|u'_h|) \, dx \quad \text{if } \varphi \text{ is convex,} \\ \sum_{S_u} \theta(|u^+ - u^-|) &\leq \liminf_{h \rightarrow \infty} \sum_{S_{u_h}} \theta(|u_h^+ - u_h^-|) \quad \text{if } \theta \text{ is convex.} \end{aligned}$$

Theorem 2.11 (Compactness of SBV , [5, Thm. 4.8]). *Let φ, θ, I be as in Theorem 2.10. Let $(u_h) \subset SBV(I)$ satisfy (2.1) and assume, in addition, that $\|u_h\|_\infty$ is uniformly bounded in h . Then, there exists a subsequence $(u_{h(k)})$ weakly* converging in $BV(I)$ to $u \in SBV(I)$.*

2.2.3 Boundary values in BV and SBV

In this thesis, we often work with Dirichlet boundary values. In order to include boundary values in the context of BV and SBV functions, an appropriate function space has to be defined. This is done in compliance with previous works, see, e.g., [26, 100].

For $\ell > 0$, the space $BV^\ell(0, 1)$ is defined as the space of functions of bounded variation in $(0, 1)$ satisfying $u(0^-) = 0$ and $u(1^+) = \ell$. Note that $BV^\ell(0, 1)$ is not weakly closed. However, in order to give some meaning to the boundary values, we will extend functions in $BV^\ell(0, 1)$ outside of $(0, 1)$. The space of special functions of bounded variation in $(0, 1)$ is extended in the same fashion to $SBV^\ell(0, 1)$. As a remark, note that $BV^\ell(0, 1)$ or $SBV^\ell(0, 1)$ can be identified with the space of functions $u \in BV_{\text{loc}}(\mathbb{R})$ or $u \in SBV_{\text{loc}}(\mathbb{R})$, respectively, fulfilling $u = 0$ on $(-\infty, 0)$ and $u = \ell$ on

$(1, \infty)$. Further, we extend $D^s u$ to $[0, 1]$ by

$$D^s u := \sum_{x \in S_u} [u](x) \delta_x + D^c u,$$

and the jump set by

$$S_u = \{x \in [0, 1] \mid [u](x) \neq 0\},$$

for every $u \in BV^\ell(0, 1)$ as well as $u \in SBV^\ell(0, 1)$, respectively.

2.3 Ergodic theorems

We deal with random structures in our model by considering stochastically distributed interaction potentials. The interaction potentials are defined and discussed in Chapter 3. The underlying stochastic setting is given here, defined in a way that is common in the theory of stochastic homogenization, see, e.g., [4]. Further, the main theorems of ergodic theory, which we are going to use in the proofs, are presented. Of course, this is just a brief excerpt of the full theory, but enough to follow the rest of the thesis.

Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space and let $(\tau_i)_{i \in \mathbb{Z}}$ be a family of measurable mappings $\tau_i : \Omega \rightarrow \Omega$ which is an additive group action, i.e.

- (group property) $\tau_0 \omega = \omega$ for all $\omega \in \Omega$ and $\tau_{i_1+i_2} = \tau_{i_1} \tau_{i_2}$ for all $i_1, i_2 \in \mathbb{Z}$.

Additionally, the group action is assumed to be stationary and ergodic, i.e.

- (stationarity) the group action is measure preserving, i.e. $\mathbb{P}(\tau_i B) = \mathbb{P}(B)$ for every $B \in \mathcal{F}$, $i \in \mathbb{Z}$
- (ergodicity) for all $B \in \mathcal{F}$, the following holds true: If $\tau_i(B) = B$ for all $i \in \mathbb{Z}$ then it is $\mathbb{P}(B) = 0$ or $\mathbb{P}(B) = 1$.

First of all, we state the classical Birkhoff's ergodic theorem, which of the proof can be found in [79, §1.2, Thm. 2.3].

Theorem 2.12 (Birkhoff's ergodic theorem). *Let $\{\tau_z\}_{z \in \mathbb{Z}}$ be a measure preserving ergodic group action. For all $f \in L^1(\Omega)$ there exists a set of full measure $\Omega_f \subset \Omega$ such that*

$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{i=0}^{n-1} f(\tau_i \omega) = \mathbb{E}[f] \quad \text{for all } \omega \in \Omega_f$$

holds true.

Birkhoff's theorem can be generalized in different ways. For this, we have to introduce the definition of regular families of sets. Let $\mathcal{I} = \{[a, b] : a, b \in \mathbb{Z}, a \neq b\}$.

Definition 2.13. *Let $\{I_k\}_{k \in \mathbb{N}}$ be a family of sets in \mathcal{I} . Then $\{I_k\}$ is called regular if there exist a constant $C > 0$ and another family $\{I'_k\}_{k \in \mathbb{N}}$ of sets in \mathcal{I} such that*

- (i) $I_k \subset I'_k$ for all k ,
- (ii) $I'_k \subset I'_h$ whenever $k < h$,
- (iii) $0 < |I'_k| \leq C |I_k|$ for all k .

Furthermore, if $\{I'_k\}$ can be chosen in such a way that $\mathbb{R} = \bigcup_k I'_k$ then we write $\lim_{k \rightarrow \infty} I_k = \mathbb{R}$.

The first generalization of Birkhoff's theorem is Tempel'man's ergodic theorem, see [106] or [79, §6.2, Thm. 2.8] for a proof. It broadens the allowed range of summation.

Theorem 2.14 (Tempel'man's ergodic theorem). *Let $\{I_k\}_{k \in \mathbb{N}}$ be a regular family of sets in \mathcal{I} with $\lim_{k \rightarrow \infty} I_k = \mathbb{R}$ and let $\{\tau_z\}_{z \in \mathbb{Z}}$ be a measure preserving ergodic group action. Then for \mathbb{P} -almost every ω*

$$\lim_{k \rightarrow \infty} \frac{1}{|I_k|} \sum_{i \in I_k \cap \mathbb{Z}} f(\tau_i \omega) = \mathbb{E}[f], \quad \text{for all } f \in L^p(\Omega), 1 \leq p < \infty.$$

The second generalisation of Birkhoff's theorem is the subadditive ergodic theorem due to Akcoglu and Krengel. It allows also for subadditive processes, while Birkhoff's theorem includes only additive ones. First, we give the definition of a subadditive process.

Definition 2.15. *We say that $F : \mathcal{I} \rightarrow L^1(\Omega)$ is a subadditive stochastic process if \mathbb{P} -almost surely the following two properties hold:*

(i) *For every $I \in \mathcal{I}$ and for every finite family $(I_m)_{m \in M}$ in \mathcal{I} , with $M \subset \mathbb{N}$, such that*

$$I_k \cap I_m = \emptyset \quad \forall k, m \in M, k \neq m, \quad I = \bigcup_{m \in M} I_m,$$

it holds that

$$F(I; \omega) \leq \sum_{m \in M} F(I_m; \omega).$$

$$(ii) \inf \left\{ \frac{1}{|I|} \int_{\Omega} F(I; \omega) d\mathbb{P}(\omega) : I \in \mathcal{I} \right\} > -\infty$$

Now, we can state the subadditive ergodic theorem, see [2] or [79, §6.2, Thm. 2.9] for a proof.

Theorem 2.16 (Akcoglu and Krengel, subadditive ergodic theorem). *Let $F : \mathcal{I} \rightarrow L^1(\Omega)$ be a subadditive stochastic process and let $\{I_k\}_{k \in \mathbb{N}}$ be a regular family of sets in \mathcal{I} with $\lim_{k \rightarrow \infty} I_k = \mathbb{R}$. If F is stationary w.r.t. a measure preserving group action $\{\tau_z\}_{z \in \mathbb{Z}}$, i.e. for all $I \in \mathcal{I}$ and all $z \in \mathbb{Z}$*

$$F(I + z; \omega) = F(I; \tau_z \omega) \quad \text{almost surely,}$$

then there exists $\phi : \Omega \rightarrow \mathbb{R}$ such that for \mathbb{P} -almost every ω

$$\lim_{k \rightarrow \infty} \frac{F(I_k; \omega)}{|I_k|} = \phi(\omega).$$

Further, if $\{\tau_z\}_{z \in \mathbb{Z}}$ is ergodic, then ϕ is constant.

Although it is not an ergodic theorem, we recall a result from the theory of subadditive functions. It can be found in [70, Thm. 7.6.1].

Theorem 2.17. *If $f(t)$ is subadditive and finite in (a, ∞) , $a \geq 0$, then*

$$\lim_{t \rightarrow \infty} \frac{f(t)}{t} = \inf_{t > a} \frac{f(t)}{t} < \infty.$$

2.4 Γ -convergence

In the 1970's, De Giorgi introduced a new kind of variational convergence, the so called Γ -convergence. Here, we give a brief introduction and summarize the main results, following the overview given in [21]. For further details, see also [46].

The starting point of many mathematical or physical models is an energy functional depending on a small parameter. This parameter may arise from an approximation process or a discretization argument, e.g., and can represent the periodicity length of a lamination or the thickness of a plate. The smaller this parameter gets the more complex the problem can be. In the vanishing parameter limit, it may even be degenerate. Therefore, the aim is to replace the problem by a simplified version.

Γ -convergence addresses this issue by providing a limiting functional, which substitutes the original problem while keeping minimizers. This will be explained later in this section in detail. First, we give the definition of Γ -convergence.

Definition 2.18 ([21, Def. 1.5]). *Let X be a metric space equipped with distance d . We say that a sequence of functions $f_j : X \rightarrow \overline{\mathbb{R}}$ Γ -converges in X to $f_\infty : X \rightarrow \overline{\mathbb{R}}$ if for all $x \in X$ we have*

(i) (liminf-inequality) for every sequence (x_j) converging to x

$$f_\infty(x) \leq \liminf_j f_j(x_j),$$

(ii) (limsup-inequality) there exists a sequence, which we call recovery sequence, (x_j) converging to x such that

$$f_\infty(x) \geq \limsup_j f_j(x_j).$$

The function f_∞ is called the Γ -limit of (f_j) , and we write $f_\infty = \Gamma\text{-lim}_j f_j$.

Clearly, the existence of the Γ -limit depends on the metric d , since the set of converging sequences for different metrics can be different.

For Γ -convergence, there also exist upper and lower Γ -limits, which we want to define in the following.

Definition 2.19 ([21, Def. 1.24]). *Let $f_j : X \rightarrow \overline{\mathbb{R}}$, $j \in \mathbb{N}$ and let $x \in X$. The quantity*

$$\Gamma\text{-lim inf}_j f_j(x) = \inf \left\{ \liminf_j f_j(x_j) : x_j \rightarrow x \right\}$$

is called the Γ -lower limit of the sequence (f_j) at x . The quantity

$$\Gamma\text{-lim sup}_j f_j(x) = \inf \left\{ \limsup_j f_j(x_j) : x_j \rightarrow x \right\}$$

is called the Γ -upper limit of the sequence (f_j) at x . If we have the equality

$$\Gamma\text{-lim inf}_j f_j(x) = \lambda = \Gamma\text{-lim sup}_j f_j(x)$$

for some $\lambda \in [-\infty, +\infty]$, then we write

$$\lambda = \Gamma\text{-}\lim_j f_j(x),$$

and we say that λ is the Γ -limit of the sequence (f_j) at x .

A useful observation is phrased in the following remark.

Remark 2.20 ([21, Rem. 1.7]). *An important property of Γ -convergence is its stability under continuous perturbations: if (f_j) Γ -converges to f_∞ and $g : X \rightarrow [-\infty, +\infty]$ is a d -continuous function then $(f_j + g)$ Γ -converges to $f_\infty + g$. This is an immediate consequence of the definition.*

Next, we introduce the coerciveness conditions, that will be used in the main theorem of Γ -convergence.

Definition 2.21 ([21, Def. 1.19]). *A function $f : X \rightarrow \overline{\mathbb{R}}$ is coercive if for all $t \in \mathbb{R}$ the set $\{f \leq t\}$ is precompact. A function $f : X \rightarrow \overline{\mathbb{R}}$ is mildly coercive if there exists a non-empty compact set $K \subset X$ such that $\inf_X f = \inf_K f$. A sequence (f_j) is equi-mildly coercive if there exists a non-empty compact set $K \subset X$ such that $\inf_X f_j = \inf_K f_j$ for all j .*

If f is coercive then it is mildly coercive. The reverse implication is not true, which can be seen by considering any periodic function $f : \mathbb{R}^n \rightarrow \mathbb{R}$.

Now, we state the main theorem of Γ -convergence.

Theorem 2.22 ([21, Thm. 1.21]). *Let (X, d) be a metric space, let (f_j) be a sequence of equi-mildly coercive functions on X , and let $f_\infty = \Gamma\text{-}\lim_j f_j$. Then*

$$\exists \min_X f_\infty = \lim_j \inf_X f_j.$$

Moreover, if (x_j) is a precompact sequence such that $\lim_j f_j(x_j) = \lim_j \inf_X f_j$, then every limit of a subsequence of (x_j) is a minimum point for f_∞ .

This theorem shows that under suitable coercivity conditions, minimizers of the original problem converge to minimizers of the limiting problem. Since energy minimization is one of the main tasks in physical problems, Γ -convergence is a suitable convergence tool to replace the original sequence of functionals by its Γ -limit without losing the essential information. The advantage is that the limiting functional often uses only a few variables and is easier to handle. A drawback is that Γ -convergence only provides information about the global minimizers and not about local ones, see [23] for further discussion.

2.5 Miscellaneous

We state the Attouch-Lemma and refer to [7, Cor. 1.16] for its proof. We will use this several times in the construction of the recovery sequence for merging two parameters.

Lemma 2.23. *Let $(a_{n,m})_{n \in \mathbb{N}, m \in \mathbb{N}}$ be a doubly indexed sequence in $\overline{\mathbb{R}}$. Then, there exists a mapping $n \mapsto m(n)$, increasing to $+\infty$, such that*

$$\limsup_{n \rightarrow \infty} a_{n, m(n)} \leq \limsup_{m \rightarrow \infty} \left(\limsup_{n \rightarrow \infty} a_{n, m} \right).$$

Finally, we state and prove a lemma on quadratic minimum problems, which we will make use of in this thesis at various occasions.

Lemma 2.24. *Let $z \in \mathbb{R}$ and $a, b \in \mathbb{N}$ with $a < b$. Further, let $0 < \rho_i \in \mathbb{R}$ for all $i \in \mathbb{Z}$. Then it holds true that*

$$\min \left\{ (b-a) \sum_{i=a}^{b-1} \rho_i z_i^2 : \sum_{i=a}^{b-1} z_i = z \right\} = (b-a) \left(\sum_{i=a}^{b-1} \frac{1}{\rho_i} \right)^{-1} z^2. \quad (2.2)$$

Proof. **Step 1:** We show

$$\min \left\{ (b-a) \sum_{i=a}^{b-1} \rho_i z_i^2 : \sum_{i=a}^{b-1} z_i = z \right\} \geq (b-a) \left(\sum_{i=a}^{b-1} \frac{1}{\rho_i} \right)^{-1} z^2. \quad (2.3)$$

For this, we calculate by using the Cauchy inequality

$$|z| = \left| \sum_{i=a}^{b-1} z_i \right| = \left| \sum_{i=a}^{b-1} \left(\rho_i^{\frac{1}{2}} z_i \right) \frac{1}{\rho_i^{\frac{1}{2}}} \right| \leq \sum_{i=a}^{b-1} \left| \rho_i^{\frac{1}{2}} z_i \right| \left| \frac{1}{\rho_i^{\frac{1}{2}}} \right| \leq \left(\sum_{i=a}^{b-1} \rho_i z_i^2 \right)^{\frac{1}{2}} \left(\sum_{i=a}^{b-1} \frac{1}{\rho_i} \right)^{\frac{1}{2}}.$$

Since all terms are positive, we can square both sides and get

$$z^2 \leq \left(\sum_{i=a}^{b-1} \rho_i z_i^2 \right) \left(\sum_{i=a}^{b-1} \frac{1}{\rho_i} \right).$$

This means that we have

$$\sum_{i=a}^{b-1} \rho_i z_i^2 \geq z^2 \left(\sum_{i=a}^{b-1} \frac{1}{\rho_i} \right)^{-1}$$

for all $\sum_{i=a}^{b-1} z_i = z$ and this proves (2.3).

Step 2: We apply the method of Lagrange multipliers. Let

$$\mathcal{L}(z_a, \dots, z_i, \dots, z_b, \lambda) = (b-a) \sum_{i=a}^{b-1} \rho_i z_i^2 + \lambda \left(z - \sum_{i=a}^{b-1} z_i \right),$$

then we calculate

$$\frac{d\mathcal{L}}{dz_i} = 2(b-a)\rho_i z_i - \lambda = 0 \quad \Leftrightarrow \quad 2(b-a)\rho_i z_i = \lambda, \quad (2.4)$$

$$\frac{d\mathcal{L}}{d\lambda} = z - \sum_{i=a}^{b-1} z_i = 0 \quad \Leftrightarrow \quad z = \sum_{i=a}^{b-1} z_i. \quad (2.5)$$

From (2.4) we get $z_i = \frac{1}{2}\lambda(b-a)^{-1}\rho_i^{-1}$, which can be inserted into (2.5) to get

$$\lambda = 2(b-a)z \left(\sum_{i=a}^{b-1} \frac{1}{\rho_i} \right)^{-1}.$$

Again together with (2.4) this yields

$$z_i = \left(\sum_{i=a}^{b-1} \frac{1}{\rho_i} \right)^{-1} z \frac{1}{\rho_i}.$$

With this candidate for the extremal value, we get

$$\begin{aligned} (b-a) \sum_{i=a}^{b-1} \rho_i z_i^2 &= (b-a) \sum_{i=a}^{b-1} \rho_i \left(\sum_{i=a}^{b-1} \frac{1}{\rho_i} \right)^{-2} z^2 \frac{1}{\rho_i^2} = (b-a) z^2 \left(\sum_{i=a}^{b-1} \frac{1}{\rho_i} \right)^{-2} \sum_{i=a}^{b-1} \frac{1}{\rho_i} \\ &= (b-a) z^2 \left(\sum_{i=a}^{b-1} \frac{1}{\rho_i} \right)^{-1}, \end{aligned}$$

which is a global minimum due to Step 1. Hence, (2.2) follows. \square

3 The discrete model: microscopic scale

We describe the main model of this thesis, which is a one-dimensional chain of particles. This is the same model as in the article in [81], that I published jointly with S. Neukamm, M. Schäffner and A. Schlömerkemper. For the reference configuration, consider a lattice given by $\lambda_n \mathbb{Z} \cap [0, 1]$, where $n \in \mathbb{N}$ and $\lambda_n = \frac{1}{n}$. Each of the $n + 1$ particles is assigned to one of these lattice points. Therefore, the reference position of the i -th atom is referred to as $x_n^i := i\lambda_n$. A sketch of the chain can be found in Figure 3.1, including the interaction potentials J described in the following.

The deformation of the atoms, and therefore the deformed configuration, is defined by $u : \lambda_n \mathbb{Z} \cap [0, 1] \rightarrow \mathbb{R}$ and we write $u(x_n^i) = u^i$ for a better readability. In order to deal with the passage from discrete systems to their continuous counterparts, we identify the discrete functions with their piecewise affine interpolations. So we define

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

as the set of all piecewise affine functions which are continuous.

3.1 Lennard-Jones type potentials: (LJ1)–(LJ3)

The interaction potentials we deal with are of a special class $\mathcal{J}(\alpha, b, d, \Psi)$ of functions, which are called Lennard-Jones type potentials and include the classical Lennard-Jones potential.

Definition 3.1. Fix $\alpha \in (0, 1]$, $b > 0$, $d \in (1, +\infty)$ and a convex function $\Psi : \mathbb{R} \rightarrow [0, +\infty]$ satisfying

$$\lim_{z \rightarrow 0^+} \Psi(z) = +\infty. \quad (3.2)$$

We denote by $\mathcal{J} = \mathcal{J}(\alpha, b, d, \Psi)$ the class of functions $J : \mathbb{R} \rightarrow \mathbb{R} \cup \{+\infty\}$ which satisfies the following properties:

(LJ1) (Regularity and asymptotic decay) The function J is lower semicontinuous, $J \in C_{loc}^{0,\alpha}(0, \infty)$ and

$$\lim_{z \rightarrow 0^+} J(z) = \infty \quad \text{as well as} \quad J(z) = \infty \quad \text{for } z \leq 0.$$

(LJ2) (Convex bound, minimum and minimizer) J has a unique minimizer δ with $\delta \in (\frac{1}{d}, d)$ and $J(\delta) < 0$, and J is strictly convex on $(0, \delta)$. Moreover, $\|J\|_{L^\infty(\delta, \infty)} < b$ and it holds

$$\frac{1}{d}\Psi(z) - d \leq J(z) \leq d \max\{\Psi(z), |z|\} \quad \text{for all } z \in (0, +\infty). \quad (3.3)$$

(LJ3) (Asymptotic behaviour) It holds

$$\lim_{z \rightarrow \infty} J(z) = 0.$$

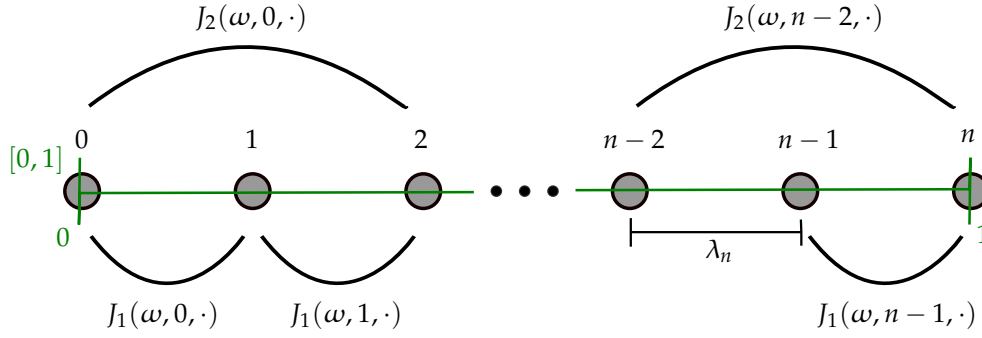


Figure 3.1 | Chain of $n + 1$ atoms with reference position $x_n^i = i\lambda_n$. The potentials $J_j(\omega, i, \cdot)$ describe the interaction between atom i and $i + j$. The characteristic length scale is $\lambda_n = \frac{1}{n}$ and the macroscopic interval is $[0, 1]$.

Remark 3.2. (i) The choice of the assumptions allows *inter alia* for the classical Lennard-Jones potential as well as for a potential with a hard core, described in Section 2. The hard core is achieved by a shift of the domain from $(0, +\infty)$ to $(z_0, +\infty)$, with $z_0 > 0$. This can be easily done by shifting the Lennard-Jones potentials as $J(z - z_0)$, which does not affect the Γ -convergence result. More generally, the result holds true for any shift of the domain from $(0, +\infty)$ to $(z_0, +\infty)$, with $z_0 \in \mathbb{R}$.

(ii) If one uses $\text{dom} J = [0, +\infty)$ instead of $\text{dom} J = (0, +\infty)$, the proofs become much easier, because then we have $J(\omega, \cdot) \in C^{0,\alpha}(0, +\infty)$, $0 < \alpha \leq 1$, on its domain, in particular J is bounded on $[0, +\infty)$. This simplifies the handling of the ergodic theorems and the approximation (introduced below) is not necessary. Therefore, J_{hom} can be derived from the ergodic theorems and the Γ -convergence result remains the same.

(iii) Since we deal with a countable or even uncountable set of functions, the condition (LJ2) gives common bounds for the minimizers and the decay at $+\infty$, respectively.

By defining the class of Lennard-Jones type potentials not only the classical Lennard-Jones potentials, but a wide range of potentials is covered. Further examples include the double Yukawa potentials, Mie potentials and Gay-Berne potentials. For a more detailed discussion we refer to Section 2.1. As discussed in the introduction, the Lennard-Jones type potentials describe long-range interactions, since their modulus decays more slowly than exponential.

3.2 Random interaction potentials

Our system is allowed to be heterogeneous, i.e. the different particles in the chain need not to be identical. With this, composite materials can be modelled, where two or more different kinds of particles are involved, see, e.g., Figure 3.2. Further, this can be used to model particles with ellipsoidal shape, where the interaction potential between two particles depends on the orientation they have to each other, no matter if the single particles are different or all of the same type. For a more detailed description, see the discussion about Gay-Berne potentials in Section 2.1.

There are different kinds of heterogeneous systems. Here, we on the one hand assume a periodic structure and on the other hand we consider a random distribution of particles. The periodic setting is discussed as a special case in Chapter 6. In general, we discuss the fully random case in this thesis.

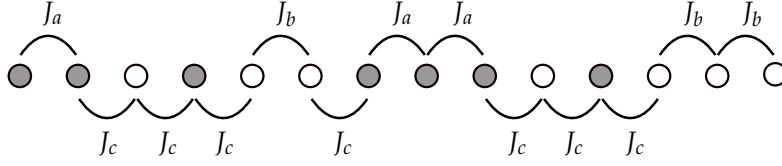


Figure 3.2 | Randomly arranged chain of atoms. The nearest neighbour interaction potential of two grey atoms is labelled by J_a , that of two white atoms by J_b and that between a white and a grey one by J_c . Since the atoms are randomly distributed, this holds for the potentials as well.

The heterogeneity, and therefore the randomness, enters our model through the interaction potentials. On the chain of atoms described above, we consider random interactions up to order K , with $K \in \mathbb{N}$. This is one way of modelling random systems, while other authors use approaches by random lattices or random diffeomorphisms, e.g. [4, 17].

The random interaction potentials are given by $\{J_j(\omega, i, \cdot)\}_{i \in \mathbb{Z}, j=1, \dots, K}$, with $J_j(\omega, i, \cdot) : \mathbb{R} \rightarrow (-\infty, +\infty]$, for a lattice site i and for neighbouring particles from $j = 1$ up to $j = K$. Again, we refer to Figure 3.1 for an illustration. The potentials are of Lennard-Jones type, specified in Section 3.1. They are assumed to be statistically homogeneous and ergodic. This is a standard way in the theory of stochastic homogenization, see, e.g., [4].

This assumptions are phrased as follows, cf. Section 2.3: Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space. We emphasize that this space can be discrete or continuous with uncountably many different elements in the set Ω . This is one of the main differences between our setting and the work in [73]. We assume that the family $(\tau_i)_{i \in \mathbb{Z}}$ of measurable mappings $\tau_i : \Omega \rightarrow \Omega$ is an additive group action, i.e.

- (group property) $\tau_0 \omega = \omega$ for all $\omega \in \Omega$ and $\tau_{i_1+i_2} = \tau_{i_1} \tau_{i_2}$ for all $i_1, i_2 \in \mathbb{Z}$.

Additionally, the group action is assumed to be stationary and ergodic, which reads:

- (stationarity) The group action is measure preserving, i.e. $\mathbb{P}(\tau_i B) = \mathbb{P}(B)$ for every $B \in \mathcal{F}$, $i \in \mathbb{Z}$.
- (ergodicity) For all $B \in \mathcal{F}$, the following holds true: If $\tau_i(B) = B$ for all $i \in \mathbb{Z}$ then it is $\mathbb{P}(B) = 0$ or $\mathbb{P}(B) = 1$.

For each $j = 1, \dots, K$ we define the random variable $\tilde{J}_j : \Omega \rightarrow \mathcal{J}(\alpha, b, d, \Psi)$, $\omega \mapsto \tilde{J}_j(\omega)(\cdot) =: \tilde{J}_j(\omega, \cdot)$, measurable in ω . This maps the sample space into the set of Lennard-Jones potentials. Then, we define

$$J_j(\omega, i, \cdot) := \tilde{J}_j(\tau_i \omega, \cdot) \quad \text{for all } i \in \mathbb{Z}, \omega \in \Omega, j = 1, \dots, K. \quad (3.4)$$

This means that every mapping $\tau_i : \Omega \rightarrow \Omega$ of the group action is assigned to an atom of the chain and is used to relate the different atoms to different elements of the sample space and therefore to different interaction potentials. In the following, we denote \tilde{J}_j simply by J_j , for better readability. This is not precise, but the two functions can be easily distinguished by their variables. We fix the following notation for the minimizers. For each $\omega \in \Omega$ we set

$$\delta_j(\omega) := \operatorname{argmin}_{z \in \mathbb{R}} \{J_j(\omega, z)\}, \quad \text{for all } j = 1, \dots, K.$$

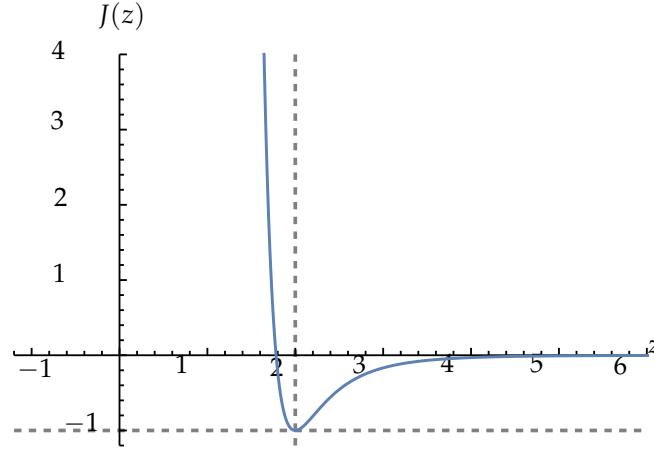


Figure 3.3 | Lennard-Jones potential J_{LJ} , with $\delta = 2$ and $\epsilon = 1$.

As mentioned above, a potential which satisfies the assumptions of the Lennard-Jones type class is, e.g., the classical Lennard-Jones potential

$$J_{LJ}(z) = \epsilon \left(\frac{\delta}{z} \right)^6 \left[\left(\frac{\delta}{z} \right)^6 - 2 \right],$$

where $\delta > 0$ is the minimizer and $-\epsilon < 0$ is the minimum of the potential. A representation is shown in Figure 3.3. In order to illustrate the stochastic setting, we recall the example shown in the introduction. Let the set Ω be defined as $\Omega = \{(\delta, \epsilon), \delta \in [1, 2], \epsilon \in [3, 4]\}$. Accordingly, ω is related to the parameters δ and ϵ of the minimizer and the minimum of the potential. This means that all potentials in this example have a minimizer in the interval $[1, 2]$ and a minimum in the interval $[-4, -3]$, randomly chosen by the random variable $J_j(\omega, \cdot)$ for every particle of the chain.

The potentials have to fulfil some more properties, coming along with the stochastic setting. To be precise, the assumptions are not on the potentials themselves, but on the random variable J_j . In Theorem 4.14 and all related propositions, only one additional assumption is needed. For Theorem 5.8, we use a second additional assumption, which will be formulated in the corresponding chapter. Before we can phrase first assumptions, we need to define some notation. Let $[f]_{C^{0,\alpha}(A)}$ be the Hölder semi-norm of $f \in C^{0,\alpha}(A)$. Now, the assumption is:

(H1) (Hölder coefficient) For every $j = 1, \dots, K$ it holds true that $\mathbb{E} \left[[J_j]_{C^{0,\alpha}(\delta_j, +\infty)} \right] < \infty$.

This condition occurs with respect to the infinite set of potentials. When dealing with finitely many different potentials, this property is fulfilled automatically. Especially, (H1) is fulfilled if the Hölder coefficients on $(\delta, +\infty)$ of all functions $J \in \mathcal{J}$ are uniformly bounded.

The stochastic setting of the chain with Lennard-Jones type interaction potentials is collected in the following assumption.

Assumption 3.3. Fix $K \in \mathbb{N}$, $\alpha \in (0, 1]$, $b > 0$, $d \in (1, \infty)$ and a convex function $\Psi : \mathbb{R} \rightarrow [0, \infty]$ satisfying (3.2). Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space and $(\tau_i)_{i \in \mathbb{Z}}$ be a family of stationary and ergodic group actions in the sense of the definitions on page 29. For every $j \in \{1, \dots, K\}$, we suppose that the random variable $J_j : \Omega \rightarrow \mathcal{J}(a, b, d, \Psi)$ from (3.4), is measurable and (H1) is satisfied, with $J(a, b, d, \Psi)$ as in Definition 3.1.

Remark 3.4. (LJ2) provides a uniform bound of $\delta_j(\omega)$ and of $J_j(\omega, \delta_j(\omega))$. Therefore, the random variables $\delta_j(\omega)$ and $J_j(\omega, \delta_j(\omega))$ are integrable. By definition of integrability, the expectation value exists for both random variables, which we denote by $\mathbb{E}[\delta_j]$ and $\mathbb{E}[J_j(\delta_j)]$. Regarding the expectation value as an ensemble mean, we can also say something about the sample average. This connection is strongly related to ergodicity and is explained in the next proposition.

Define, for better readability, the random variable

$$C_j^H(\omega) := [J_j(\omega, \cdot)]_{C^{0,\alpha}(\delta_j(\omega), +\infty)},$$

that is the Hölder semi-norm of the function $J_j(\omega, \cdot)$ on $(\delta_j(\omega), \infty)$. We define some functions, which represent sample averages of the quantities δ_j , $J_j(\delta_j)$, α_j^{-1} and C_j^H , since in the convergence theorem, we have to deal with this sample averages and their limits. Therefore, the next proposition shows the limiting behaviour of the sample averages. We define for an arbitrary $N \in \mathbb{N}$

$$\begin{aligned} \delta_j^{(N)}(\omega, A) &:= \frac{1}{|NA \cap \mathbb{Z}|} \sum_{i \in NA \cap \mathbb{Z}} \delta_j(\tau_i \omega), \\ J_j(\delta_j)^{(N)}(\omega, A) &:= \frac{1}{|NA \cap \mathbb{Z}|} \sum_{i \in NA \cap \mathbb{Z}} J_j(\omega, i, \delta_j(\tau_i \omega)), \\ C_j^{H,(N)}(\omega, A) &:= \frac{1}{|NA \cap \mathbb{Z}|} \sum_{i \in NA \cap \mathbb{Z}} C_j^H(\tau_i \omega). \end{aligned} \quad (3.5)$$

Proposition 3.5. Let Assumption 3.3 be satisfied. Then there exists an $\Omega' \subset \Omega$ with $\mathbb{P}(\Omega') = 1$ such that for all $\omega \in \Omega'$, all $j = 1, \dots, K$ and for all $A = [a, b]$ with $a, b \in \mathbb{R}$ the limits

$$\begin{aligned} \mathbb{E}[\delta_j] &= \lim_{N \rightarrow \infty} \delta_j^{(N)}(\omega, A), \\ \mathbb{E}[J_j(\delta_j)] &= \lim_{N \rightarrow \infty} J_j(\delta_j)^{(N)}(\omega, A), \\ \mathbb{E}[C_j^H] &= \lim_{N \rightarrow \infty} C_j^{H,(N)}(\omega, A) \end{aligned}$$

exist in $\overline{\mathbb{R}}$ and are independent of ω and the interval A .

Proof. For notational simplicity we omit the j -dependence in the whole proof. We prove the claim of the proposition first for $\delta^{(N)}(\omega, A)$ and explain the adaptations of the proof for the other random variables in the last step.

Step 1. Intervals $A = [a, b]$ with $a, b \in \mathbb{Z}$.

Due to the Birkhoff ergodic theorem (see Thm. 2.12), integrability of the random variables (see Remark 3.4 and (H1)) and ergodicity of the group action provide the existence of $\Omega_{\delta, A} \subset \Omega$ with $\mathbb{P}(\Omega_{\delta, A}) = 1$ for a fixed A with $a, b \in \mathbb{Z}$, such that for every $\omega \in \Omega_{\delta, A}$ it holds true that

$$\mathbb{E}[\delta] = \lim_{N \rightarrow \infty} \delta^{(N)}(\omega, A). \quad (3.6)$$

By defining $\Omega_\delta := \bigcap_{a, b \in \mathbb{Z}} \Omega_{\delta, A}$, we get (3.6) for all $\omega \in \Omega_\delta$ and for all A with $a, b \in \mathbb{Z}$, while it still holds true that $\mathbb{P}(\Omega_\delta) = 1$.

Step 2. Technical interlude.

We will prove in this step the following claim: Let $T \in \mathbb{R}$, $T > 0$ and A be an interval. Assume that $\lim_{t \rightarrow \infty} \delta^{(t)}(\omega, TA)$ exists, where we extend the definition of $\delta^{(N)}(\omega, A)$ in (3.5) from the integers to the real line, with $t \in \mathbb{R}$. Then it holds true that

$$\lim_{t \rightarrow \infty} \delta^{(t)}(\omega, TA) = \lim_{N \rightarrow \infty} \delta^{(N)}(\omega, A). \quad (3.7)$$

Proof of this claim: By definition of $\delta^{(N)}(\omega, A)$ and its extension to the real line, it holds true that

$$\delta^{(N)}(\omega, A) = \frac{1}{|NA \cap \mathbb{Z}|} \sum_{i \in NA \cap \mathbb{Z}} \delta(\tau_i \omega) = \delta^{(N/T)}(\omega, TA) \quad (3.8)$$

for all $N \in \mathbb{N}$. By definition of the limit inferior, it exists a subsequence (N_k) with

$$\liminf_{N \rightarrow \infty} \delta^{(N)}(\omega, A) = \lim_{k \rightarrow \infty} \delta^{(N_k)}(\omega, A) \stackrel{(3.8)}{=} \lim_{k \rightarrow \infty} \delta^{(N_k/T)}(\omega, TA) \geq \liminf_{t \rightarrow \infty} \delta^{(t)}(\omega, TA). \quad (3.9)$$

Further by definition of the limit superior, it exists a subsequence (N_k) with

$$\limsup_{N \rightarrow \infty} \delta^{(N)}(\omega, A) = \lim_{k \rightarrow \infty} \delta^{(N_k)}(\omega, A) \stackrel{(3.8)}{=} \lim_{k \rightarrow \infty} \delta^{(N_k/T)}(\omega, TA) \leq \limsup_{t \rightarrow \infty} \delta^{(t)}(\omega, TA). \quad (3.10)$$

Together with the assertion that $\lim_{t \rightarrow \infty} \delta^{(t)}(\omega, TA)$ exists, (3.9) and (3.10) yield

$$\lim_{t \rightarrow \infty} \delta^{(t)}(\omega, TA) = \lim_{N \rightarrow \infty} \delta^{(N)}(\omega, A),$$

which proofs the claim.

Step 3. Intervals $A = [a, b)$ with $a, b \in \mathbb{R}$.

To pass to general intervals with $a, b \in \mathbb{R}$, we argue as in [47, Proposition 1]. For every $\epsilon > 0$, there exists T big enough and intervals $A_\epsilon^- := [a_\epsilon^-, b_\epsilon^-)$ and $A_\epsilon^+ := [a_\epsilon^+, b_\epsilon^+)$ with $a_\epsilon^-, b_\epsilon^-, a_\epsilon^+, b_\epsilon^+ \in \mathbb{Z}$ such that it holds true

$$A_\epsilon^- \subset TA \subset A_\epsilon^+, \quad \frac{|A_\epsilon^-|}{|TA|} \geq 1 - \epsilon, \quad \frac{|TA|}{|A_\epsilon^+|} \geq 1 - \epsilon. \quad (3.11)$$

Since $\delta(\omega) \leq C$ due to (LJ3), we get for all intervals $B \subset A$ the inequality

$$\delta^{(N)}(\omega, A) \leq \delta^{(N)}(\omega, B) + \frac{|N(A \setminus B) \cap \mathbb{Z}|}{|N(A) \cap \mathbb{Z}|} C, \quad (3.12)$$

which can be seen by the calculation

$$\begin{aligned} \delta^{(N)}(\omega, A) &= \frac{1}{|NA \cap \mathbb{Z}|} \sum_{i \in NA \cap \mathbb{Z}} \delta(\tau_i \omega) \leq \frac{1}{|NA \cap \mathbb{Z}|} \sum_{i \in NB \cap \mathbb{Z}} \delta(\tau_i \omega) + \frac{1}{|NA \cap \mathbb{Z}|} \sum_{i \in N(A \setminus B) \cap \mathbb{Z}} C \\ &\leq \frac{1}{|NB \cap \mathbb{Z}|} \sum_{i \in NB \cap \mathbb{Z}} \delta(\tau_i \omega) + \frac{|N(A \setminus B) \cap \mathbb{Z}|}{|N(A) \cap \mathbb{Z}|} C. \end{aligned}$$

Now, we get from Step 1

$$\begin{aligned}
 \mathbb{E}[\delta] &= \lim_{N \rightarrow \infty} \delta^{(N)}(\omega, A_\epsilon^+) \stackrel{(3.12)}{\leq} \liminf_{N \rightarrow \infty} \delta^{(N)}(\omega, TA) + \liminf_{N \rightarrow \infty} \frac{|N(A_\epsilon^+ \setminus TA) \cap \mathbb{Z}|}{|N(A_\epsilon^+) \cap \mathbb{Z}|} C \\
 &= \liminf_{N \rightarrow \infty} \delta^{(N)}(\omega, TA) + \frac{|(A_\epsilon^+ \setminus TA)|}{|(A_\epsilon^+)|} C \stackrel{(3.11)}{\leq} \limsup_{N \rightarrow \infty} \delta^{(N)}(\omega, TA) + \epsilon C \\
 &\stackrel{(3.12)}{\leq} \lim_{N \rightarrow \infty} \delta^{(N)}(\omega, A_\epsilon^-) + \left(\epsilon + \frac{|(TA \setminus A_\epsilon^-)|}{|(TA)|} \right) C \stackrel{(3.11)}{=} \mathbb{E}[\delta] + 2\epsilon C.
 \end{aligned}$$

This shows that

$$\mathbb{E}[\delta] = \lim_{N \rightarrow \infty} \delta^{(N)}(\omega, TA)$$

for $A = [a, b]$ with $a, b \in \mathbb{R}$, since $\epsilon > 0$ was chosen arbitrarily. With the result (3.7) from Step 2 we get

$$\mathbb{E}[\delta] = \lim_{N \rightarrow \infty} \delta^{(N)}(\omega, TA) = \lim_{N \rightarrow \infty} \delta^{(N)}(\omega, A),$$

for every $T > 0$, which concludes Step 3.

Step 4. Adaptation to the other random variables.

The proof for $J(\delta)^{(N)}(\omega, A)$ is exactly the same, replacing Ω_δ by $\Omega_{J(\delta)}$, since it also holds true that $J(\delta)^{(N)}(\omega, A)$ is bounded due to (LJ2). This was important for the analogue of (3.12).

The proof for $C^{H,(N)}(\omega, A)$ can be done analogously with the set Ω_{CH} instead of Ω_δ and with a different estimate replacing (3.12). The new estimate can be derived, using $C^H(\omega) > 0$, as follows:

$$\begin{aligned}
 C^{H,(N)}(\omega, A) &= \frac{1}{|NA \cap \mathbb{Z}|} \sum_{i \in NA \cap \mathbb{Z}} C^H(\tau_i \omega) \geq \frac{1}{|NA \cap \mathbb{Z}|} \sum_{i \in NB \cap \mathbb{Z}} C^H(\tau_i \omega) \\
 &= \frac{|NB \cup \mathbb{Z}|}{|NA \cup \mathbb{Z}|} C^{H,(N)}(\omega, B).
 \end{aligned}$$

In the end, we define $\Omega' := \Omega_\delta \cap \Omega_{J(\delta)} \cap \Omega_{CH}$, which yields the assertion of the proposition. \square

3.3 Energy of the system

So far, we defined the one-dimensional chain of particles, the class of interaction potentials and the random setting. Next, we consider the energy of this model. Let $u \in \mathcal{A}_n(0, 1)$ be a given deformation with $n \in \mathbb{N}$. Then we define the energy of interactions up to order K for a given deformation $u \in \mathcal{A}_n(0, 1)$ as

$$H_n(\omega, u) := \sum_{j=1}^K \sum_{i=0}^{n-j} \lambda_n J_j \left(\omega, i, \frac{u^{i+j} - u^i}{j \lambda_n} \right). \quad (3.13)$$

As discussed in the introduction, using interactions beyond nearest neighbours is one possible notion of long-range potentials. For a given $\ell > 0$, we take Dirichlet boundary conditions into account by considering the functional $H_n^\ell : \Omega \times L^1(0, 1) \rightarrow (-\infty, +\infty]$ defined by

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

In the Γ -limit of zeroth order, fixing not only the first and last atom, but also the first K and the last K atoms would not change the result for the limiting energy. This becomes interesting as a modelling aspect when considering the Γ -limit of first or higher order. Then, the limiting energy contains the additional boundary constraints as additional degrees of freedom. This is discussed, e.g., in [24, 103].

In the following, we are interested in the Γ -limit of the energy in (3.13). To this end, we introduce the function $J_{\text{hom}} : \mathbb{R} \rightarrow (-\infty, +\infty]$, which will play an important role in the Γ -convergence result. It is defined by

$$J_{\text{hom}}(z) := \inf_{N \in \mathbb{N}} \mathbb{E} \left[J_{\text{hom}}^{(N)}(\cdot, z) \right], \quad (3.14)$$

with $N \in \mathbb{N}$ and

$$J_{\text{hom}}^{(N)}(\omega, z) := \frac{1}{N} \inf \left\{ \sum_{j=1}^K \sum_{i=0}^{N-j} J_j \left(\omega, i, z + \frac{\phi^{i+j} - \phi^i}{j} \right), \phi^i \in \mathbb{R}, \phi^s = \phi^{N-s} = 0 \right. \\ \left. \text{for } s = 0, \dots, K-1 \right\}.$$

One of the main results on the way to the limiting energy in Theorem 4.14 is that

$$J_{\text{hom}}(z) = \lim_{N \rightarrow \infty} J_{\text{hom}}^{(N)}(\omega, z). \quad (3.15)$$

Before we address the Γ -convergence of the energy, we first provide a characterization of $J_{\text{hom}}^{(N)}(\omega, z)$, which we frequently use in the following proofs.

Lemma 3.6. *For $z \in \mathbb{R}$ and $N \in \mathbb{N}$, it holds true that*

$$J_{\text{hom}}^{(N)}(\omega, z) = \inf \left\{ \sum_{j=1}^K \sum_{i=0}^{N-j} J_j \left(\omega, i, \frac{1}{j} \sum_{k=i}^{i+j-1} z^k \right) : z^i \in \mathbb{R}, \sum_{i=0}^{N-1} z^i = Nz, z^s = z^{N-s-1} = z \text{ for } s = 0, \dots, K-2 \right\}.$$

Proof. For fixed $N \in \mathbb{N}$ and $\omega \in \Omega$, we define for the term on the right-hand side

$$p(z) := \inf \left\{ \sum_{j=1}^K \sum_{i=0}^{N-j} J_j \left(\omega, i, \frac{1}{j} \sum_{k=i}^{i+j-1} p^k \right) : p^i \in \mathbb{R}, \sum_{i=0}^{N-1} p^i = Nz, p^s = p^{N-s-1} = z \right. \\ \left. \text{for } s = 0, \dots, K-2 \right\},$$

and for the right-hand side we have by definition

$$q(z) := \inf \left\{ \sum_{j=1}^K \sum_{i=0}^{N-j} J_j \left(\omega, i, z + \frac{q^{i+j} - q^i}{j} \right) : q^i \in \mathbb{R}, q^s = q^{N-s} = 0 \text{ for } s = 0, \dots, K-1 \right\} \\ = J_{\text{hom}}^{(N)}(\omega, z).$$

Given a minimizer $p = (p^0, \dots, p^{N-1})$ of $p(z)$, we set

$$q^i := \sum_{k=0}^{i-1} p^k - iz$$

for $i = 0, \dots, N$. Then for $s = 0, \dots, K-1$, it holds true that

$$q^s = \sum_{k=0}^{s-1} p^k - sz = sz - sz = 0$$

and

$$q^{N-s} = \sum_{k=0}^{N-s-1} p^k - (N-s)z = \sum_{k=0}^{N-1} p^k - \sum_{k=N-s}^{N-1} p^k - (N-s)z = Nz - sz - (N-s)z = 0.$$

Thus, $q = (q^0, \dots, q^N)$ is a candidate for the minimum problem related to $q(z)$. Further, we have

$$\frac{q^{i+j} - q^i}{j} + z = \frac{1}{j} \left(\sum_{k=0}^{i+j-1} p^k - (i+j)z - \sum_{k=0}^{i-1} p^k + iz \right) + z = \frac{1}{j} \sum_{k=i}^{i+j-1} p^k$$

for $i = 0, \dots, N-j$. This yields

$$J_j \left(\omega, i, \frac{1}{j} \sum_{k=i}^{i+j-1} p^k \right) = J_j \left(\omega, i, z + \frac{q^{i+j} - q^i}{j} \right),$$

which shows $p(z) \geq q(z)$.

On the other hand, given a minimizer $q = (q^0, \dots, q^N)$ of $q(z)$, we define

$$p^i := q^{i+1} - q^i + z$$

for $i = 0, \dots, N-1$. Then, it holds true that

$$\sum_{k=0}^{N-1} p^k = \sum_{k=0}^{N-1} (q^{k+1} - q^k + z) = q^N - q^0 + Nz = Nz,$$

and for $s = 0, \dots, K-2$, that $p^s = q^{s+1} - q^s + z = z$ and $p^{N-s} = q^{N-s+1} - q^{N-s} + z = z$. Thus, $p = (p^0, \dots, p^{N-1})$ is a candidate for the minimum problem of $p(z)$. Further, it holds true that

$$\frac{1}{j} \sum_{k=i}^{i+j-1} p^k = \frac{1}{j} \sum_{k=i}^{i+j-1} (q^{k+1} - q^k + z) = \frac{1}{j} (q^{i+j} - q^i) + z.$$

Therefore, we get

$$J_j \left(\omega, i, \frac{1}{j} \sum_{k=i}^{i+j-1} p^k \right) = J_j \left(\omega, i, z + \frac{q^{i+j} - q^i}{j} \right),$$

which yields $p(z) \leq q(z)$. This proves $p(z) = q(z)$.

□

4 Variational limit: macroscopic scale

In the previous chapter, we have set up the model under consideration. In essence, the discrete model is a one-dimensional chain of atoms or particles, equi-distributed on the continuous interval $[0, 1]$. The elements of the chain are linked by randomly distributed interactions potentials of Lennard-Jones type, up to order K . The latter means that we consider not only nearest and next-to-nearest neighbour interactions, referring to $K = 1$ and $K = 2$, but up to K -interacting neighbours.

We now let the number n of particles in this chain go to infinity. This corresponds to the passage from the discrete system to its continuous counterpart. The limiting procedure is performed in the sense of Γ -convergence. As we are interested in minimizers of the energy, this variational convergence is the method of choice. As pointed out in Section 2.4, Γ -convergence together with proper coercivity yields not only a limiting energy but also a convergence of minimizers.

This chapter is dealing with the Γ -limit of the energy of our model. Section 4.1 starts with an approximation procedure of the interaction potential. The approximated potentials are Lipschitz continuous and allow therefore for an application of the ergodic theorems. The homogenized energy density is first derived in the case of the approximated potentials. Then, the homogenization formula with the original potentials are recovered by a limiting analysis for the approximation. In the end, Section 4.2 shows existence and properties of the homogenized energy density. This homogenization formula turns out to be the density in the limiting energy functional, which is stated and proven in Section 4.3.

The results of this chapter have been already published by myself in [81], together with S. Neukamm, M. Schäffner and A. Schlömerkemper. Here, the proofs and the discussions are given in more detail.

4.1 Lipschitz approximation of the interaction potentials

The first main issue in the proof of the main Theorem 4.14 is the existence of the limit function $J_{\text{hom}} = \lim_{N \rightarrow \infty} J_{\text{hom}}^{(N)}(\omega, \cdot)$ for every $\omega \in \Omega'$ with $\mathbb{P}(\Omega') = 1$. A key ingredient of the proof is the ergodic theorem 2.16 due to Akcoglu and Krengel. By applying it to $J_{\text{hom}}^{(N)}(\omega, z)$, we get that for every $z \in \mathbb{R}$ there exists $\Omega_z \subset \Omega$ with $\mathbb{P}(\Omega_z) = 1$ such that for every $\omega \in \Omega_z$ the limit

$$\lim_{N \rightarrow \infty} J_{\text{hom}}^{(N)}(\omega, z)$$

exists and is independent of ω . This already seems to be the proof of the existence of the limit J_{hom} , however it is not. The problem is the dependence of the set Ω_z on the variable z . Since we want to have the result proven for all $z \in \mathbb{R}$, we have to consider the intersection $\Omega' = \bigcap_{z \in \mathbb{R}} \Omega_z$ of all these sets, which is an intersection of uncountably many sets, and hence does not conserve the property $\mathbb{P}(\Omega') = 1$.

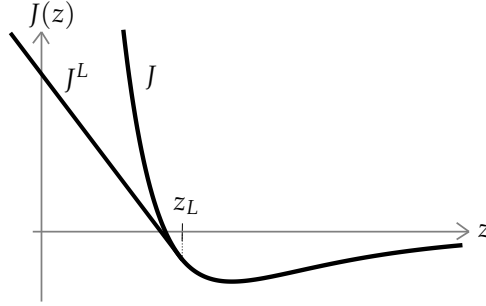


Figure 4.1 | The function J is a typical representant of a Lennard-Jones type potential and J^L its z_L -approximation function.

If we had a polynomial growth from above on the interaction potentials, this problem could be solved by a continuity argument, see e.g. [47, 94]. However, polynomial growth does not hold true due to the blow up at zero. The blow-up combined with the non-convexity of the potentials prevents to use well-established homogenization methods. Therefore, our approach is an approximation of the Lennard-Jones type potentials by functions that exhibit a linear growth at $z \rightarrow -\infty$. This approximation allows the application of the ergodic theorem. A drawback is that removing this approximation in order to get back to the original potentials will bring up certain challenges.

The following definition provides the approximation, as described above, with linear growth at $z \rightarrow -\infty$, and is used as a technical tool. Especially in Proposition 4.6, the advantage of the approximation in contrast to the original function, takes effect, which is summarized in Remark 4.7 in detail.

Definition 4.1. Fix a decreasing sequence $(z_L)_{L \in \mathbb{N}} \subset \mathbb{R}$ satisfying $z_L \rightarrow 0$ as $L \rightarrow \infty$ and $z_L < \frac{1}{d}$ for every $L \in \mathbb{N}$ (see (LJ2)). The z_L -approximation $J_j^L(\omega, \cdot)$ of $J_j(\omega, \cdot)$ is defined as

$$J_j^L(\omega, z) := \begin{cases} m_j^L(\omega)(z - z_L) + J_j(\omega, z_L) & \text{for } z < z_L, \\ J_j(\omega, z) & \text{for } z \geq z_L, \end{cases}$$

where $m_j^L(\omega) \in \mathbb{R}$ is the smallest element of the subdifferential $\partial J_j(\omega, z_L)$.

Since $J_j(\omega, \cdot)$ is convex in $(0, \delta_j(\omega))$ and $\frac{1}{d} \leq \delta_j(\omega)$, the subdifferential $\partial J_j(\omega, z_L)$ is a nonempty compact interval. By definition, the approximating function $J_j^L(\omega) : \mathbb{R} \rightarrow \mathbb{R}$ is continuous. More precisely it is Hölder-continuous on $(z_L, +\infty)$ and Lipschitz-continuous on $(-\infty, z_L)$. A sketch of a Lennard-Jones type potential, together with one of its approximating functions is shown in Figure 4.1.

Remark 4.2. (i) By Definition 4.1, it holds true that $J_j^L(\omega, z) \leq J_j(\omega, z)$ for every $z \in \mathbb{R}$ and every $L \in \mathbb{N}$.

(ii) For the approximation J_j^L , a corresponding condition as in (3.3) in (LJ2) does not hold true any more. However, we have

$$-d \leq J_j^L(\omega, z) \leq d \max\{\Psi(z), |z|\} \quad \text{for all } z \in \mathbb{R}, j = 1, \dots, K, \omega \in \Omega, \quad (4.1)$$

by construction.

Whenever we use the approximation $J_j^L(\omega, i, z)$ instead of each $J_j(\omega, i, z)$ we indicate this with a superscript of the letter L , that means

$$J_{\text{hom}}^L(z) := \inf_{N \in \mathbb{N}} \mathbb{E} \left[J_{\text{hom}}^{L,(N)}(\cdot, z) \right],$$

with $N \in \mathbb{N}$ and

$$J_{\text{hom}}^{L,(N)}(\omega, z) := \frac{1}{N} \inf \left\{ \sum_{j=1}^K \sum_{i=0}^{N-j} J_j^L \left(\omega, i, z + \frac{\phi^{i+j} - \phi^i}{j} \right) : \phi^i \in \mathbb{R}, \right. \\ \left. \phi^s = \phi^{N-s} = 0 \text{ for } s = 0, \dots, K-1 \right\}.$$

While using the approximation, we are able to prove the counterpart to (3.15), which reads

$$J_{\text{hom}}^L(z) = \lim_{N \rightarrow \infty} J_{\text{hom}}^{L,(N)}(\omega, z).$$

Before we prove the existence of the above limit in the next section, we have to work out special properties of the Lennard-Jones type potentials and their approximating functions. This is done in the following propositions. The first one shows that J is (locally) Lipschitz continuous in $(0, \delta)$, by a combination of the convexity and monotonicity of $J \in \mathcal{J}$ on $(0, \delta)$ together with the growth condition (3.3). The second one deals with an upper bound on the slopes in the approximation regime and the third one combines the Lipschitz and the Hölder continuity together in one estimate.

Proposition 4.3. Fix $\alpha \in (0, 1]$, $b > 0$, $d \in (1, \infty)$ and a convex function $\Psi : \mathbb{R} \rightarrow [0, \infty]$ satisfying (3.2). Let the approximating function be defined as above. Let $A = [a, b]$, $a, b \in \mathbb{R}$, be an interval, and $A_N := NA \cap \mathbb{Z}$ with $N \in \mathbb{N}$.

(i) There exists a function $C_{\text{Lip}} : (0, d) \rightarrow [0, \infty)$ depending only on d and Ψ such that the following is true. Let $J \in \mathcal{J}(\alpha, b, d, \Psi)$ be given and let δ be its unique minimizer. Then it holds

$$\|J\|_{\text{Lip}(\rho, \delta)} := \sup_{\substack{x, y \in (\rho, \delta) \\ x \neq y}} \left| \frac{J(y) - J(x)}{y - x} \right| \leq C_{\text{Lip}}(\rho).$$

(ii) There exists L^* such that for all $L > L^*$ it holds true that

$$m_j^L(\omega) \leq -M_L,$$

with a constant $M_L > 0$ independent of j and ω . Further, we have that

$$M_L \rightarrow \infty \quad \text{as } L \rightarrow \infty. \quad (4.2)$$

(iii) There exists an $\Omega' \subset \Omega$ with $\mathbb{P}(\Omega') = 1$ such that for all $\omega \in \Omega'$, all $j = 1, \dots, K$, it holds true that

$$\frac{1}{|A_N|} \sum_{j=1}^K \sum_{i \in A_N} \left| J_j^L(\omega, i, x) - J_j^L(\omega, i, y) \right| \leq C^{L,H,(N)}(\omega) \max \{|x - y|^\alpha, |x - y|\}, \quad (4.3)$$

for every $x, y \in \mathbb{R}$ and independent of the choice of A , and some constant $0 < C^{L,H,(N)}(\omega) \rightarrow C^{L,H}$ as $N \rightarrow \infty$.

Proof. **Step 1.** Proof of (i).

Since J is decreasing on $(0, \delta)$ we obviously have

$$\frac{J(y) - J(x)}{y - x} \leq 0 \quad (4.4)$$

for every $0 < x < y \leq \delta$. Further, for every $\alpha, \beta, \gamma \in (0, \delta)$ with $\alpha < \beta < \gamma$ it holds true that

$$\frac{J(\beta) - J(\alpha)}{\beta - \alpha} \leq \frac{J(\gamma) - J(\alpha)}{\gamma - \alpha} \leq \frac{J(\gamma) - J(\beta)}{\gamma - \beta}, \quad (4.5)$$

which can be seen as follows: Choose $t \in (0, 1)$ such that $\beta = t\alpha + (1-t)\gamma$, i.e. $t = \frac{\gamma - \beta}{\gamma - \alpha}$. Convexity yields $J(\beta) \leq tJ(\alpha) + (1-t)J(\gamma)$ and thus the two equations

$$\begin{aligned} J(\beta) - J(\alpha) &\leq (1-t)(J(\gamma) - J(\alpha)) = \frac{\beta - \alpha}{\gamma - \alpha}(J(\gamma) - J(\alpha)), \\ J(\gamma) - J(\beta) &\geq J(\gamma) - tJ(\alpha) - (1-t)J(\gamma) \geq t(J(\gamma) - J(\alpha)) = \frac{\gamma - \beta}{\gamma - \alpha}(J(\gamma) - J(\alpha)) \end{aligned}$$

hold true, and imply (4.5).

Next we apply (4.5) to $\alpha = \frac{1}{2R}$, $\beta = \frac{1}{R}$, $\gamma = y$ as well as to $\alpha = \frac{1}{R}$, $\beta = x$, $\gamma = y$ and get

$$\begin{aligned} \frac{J\left(\frac{1}{R}\right) - J\left(\frac{1}{2R}\right)}{\frac{1}{2R}} &\leq \frac{J(y) - J\left(\frac{1}{2R}\right)}{y - \frac{1}{2R}} \leq \frac{J(y) - J\left(\frac{1}{R}\right)}{y - \frac{1}{R}}, \\ \frac{J(x) - J\left(\frac{1}{R}\right)}{x - \frac{1}{R}} &\leq \frac{J(y) - J\left(\frac{1}{R}\right)}{y - \frac{1}{R}} \leq \frac{J(y) - J(x)}{y - x}. \end{aligned}$$

A combination of the obtained chains of inequalities yields

$$\frac{J\left(\frac{1}{R}\right) - J\left(\frac{1}{2R}\right)}{\frac{1}{2R}} \leq \frac{J(y) - J\left(\frac{1}{R}\right)}{y - \frac{1}{R}} \leq \frac{J(y) - J(x)}{y - x} \leq 0,$$

where boundedness from above is due to (4.4). By (LJ2),

$$\frac{J\left(\frac{1}{R}\right) - J\left(\frac{1}{2R}\right)}{\frac{1}{2R}} \geq -2Rd \left(1 + \left(\Psi\left(\frac{1}{2R}\right) + \frac{1}{2R} \right) \right).$$

Hence, for every $\frac{1}{R} < x < y < \delta$ it holds

$$\left| \frac{J(y) - J(x)}{y - x} \right| \leq 2Rd \left(1 + \left(\Psi\left(\frac{1}{2R}\right) + \frac{1}{2R} \right) \right),$$

which implies the assertion.

Step 2. Proof of (ii).

By definition of the subdifferential, it holds true that

$$J_j(\omega, y) \geq J_j(\omega, x) + m_j^L(\omega)(y - x),$$

for every $x, y \in (0, \frac{1}{d}]$. Setting $y = \frac{1}{d}$ and $x = z_L$, we get

$$m_j^L(\omega) \leq \frac{J_j\left(\omega, \frac{1}{d}\right) - J_j(\omega, z_L)}{\frac{1}{d} - z_L} \leq \frac{d \max\left\{\Psi\left(\frac{1}{d}\right), \left|\frac{1}{d}\right|\right\} - \left(\frac{1}{d}\Psi(z_L) - d\right)}{\frac{1}{d} - z_L}.$$

The denominator is always positive and $\Psi(z_L) \rightarrow \infty$ as $L \rightarrow \infty$. Note that m_j^L is always negative, by definition. The right hand side gets smaller and negative as $L \rightarrow \infty$. Therefore, there exists L^* such that for all $L > L^*$ it holds true that $m_j^L(\omega) \leq -M_L$, with a constant $M_L > 0$ independent of j and ω . Further, by (LJ2), we have that $M_L \rightarrow \infty$ as $L \rightarrow \infty$, which proves (ii).

Step 3. Proof of (iii).

It holds true for every $x, y \in \mathbb{R}$ that

$$\begin{aligned} & \frac{1}{|A_N|} \sum_{j=1}^K \sum_{i \in A_N} \left| J_j^L(\omega, i, x) - J_j^L(\omega, i, y) \right| \\ & \leq 2 \max \left\{ KC_{\text{Lip}}(z_L), \sum_{j=1}^K \frac{1}{|A_N|} \sum_{i \in A_N} C_j^H(\tau_i \omega) \right\} \max\{|x - y|^\alpha, |x - y|\}. \end{aligned}$$

This estimate can be derived as follows: recall that for a fixed L , the Lipschitz constant of $J_j^L(\omega, i, \cdot)$ on (z_L, δ) is bounded by $C_{\text{Lip}}(z_L)$ due to Lemma 4.3 (i). By monotonicity and convexity of $J_j(\omega, i, \cdot)$, the Lipschitz constant of $J_j^L(\omega, i, \cdot)$ on $(-\infty, z_L)$ is also bounded by $C_{\text{Lip}}(z_L)$, by construction of the approximating function. Further, $C_j^H(\tau_i \omega)$ is the Hölder constant of $J_j^L(\omega, i, \cdot)$ on $[\delta_j(\tau_i \omega), +\infty)$, by definition (see Proposition 3.5 and the related definitions). Now, we have to distinguish between three cases: (a) x and y are both greater than $\delta_j(\tau_i \omega)$, (b) both are less than $\delta_j(\tau_i \omega)$ and (c) one is less and one is greater than $\delta_j(\tau_i \omega)$. In the first case (a) the Hölder estimate holds, in the second one (b) we can use the Lipschitz estimate and in the third one (c) we can insert $\pm J_j^L(\omega, i, \delta_j(\tau_i \omega))$ and use the triangle inequality, which results in the factor 2. Since the constants $C_{\text{Lip}}(z_L)$ and C_j^H are all positive, we still increase the estimate, if we sums over the whole set A_N .

Due to (H1) and Proposition 3.5, there exists a set $\Omega' \subset \Omega$ with $\mathbb{P}(\Omega') = 1$ such that for all $\omega \in \Omega'$, all $j = 1, \dots, K$, the sum on the right hand side is convergent. Therefore, we finally obtain

$$\frac{1}{|A_N|} \sum_{j=1}^K \sum_{i \in A_N} \left| J_j^L(\omega, i, x) - J_j^L(\omega, i, y) \right| \leq C^{L,H,(N)}(\omega) \max\{|x - y|^\alpha, |x - y|\},$$

for every $x, y \in \mathbb{R}$ and independent of the choice of A , with $C^{L,H,(N)}(\omega) \rightarrow C^{L,H}$ almost everywhere as $N \rightarrow \infty$. This proves (iii). □

4.1.1 Approximated homogenized energy density

The approximation introduced in Section 4.1 was said to be a suitable approach with respect to an application of the ergodic theorem by Akcoglu and Krengel and accordingly to the existence of the limit J_{hom}^L . This will be specified and worked out now, in Section 4.1.1. Further, we derive some properties of this limit J_{hom}^L . These results will be used as technical tools in subsequent propositions and theorems.

We start with establishing the existence of the function J_{hom}^L . This is done by proving that the limit $N \rightarrow \infty$ of $J_{\text{hom}}^{L,(N)}(\omega, z)$ exists and is indeed independent of ω . The assertion is formulated in a more general way, because we need the convergence result in this general form in subsequent proofs. Let $A = [a, b)$, $a, b \in \mathbb{R}$ be an interval. Throughout the entire thesis, the notation

$$i_{\min}^A := \min\{i : i \in NA \cap \mathbb{Z}\} \quad \text{and} \quad i_{\max}^A := \max\{i : i \in NA \cap \mathbb{Z}\},$$

as $N \in \mathbb{N}$, is frequently used. We define a localized version of $J_{\text{hom}}^{L,(N)}(\omega, z)$ by

$$J_{\text{hom}}^{L,(N)}(\omega, z, A) := \frac{1}{|NA \cap \mathbb{Z}|} \inf \left\{ \sum_{j=1}^K \sum_{\substack{i \in NA \cap \mathbb{Z} \\ i+j-1 \in NA}} J_j^L \left(\omega, i, z + \frac{\phi^{i+j} - \phi^i}{j} \right) : \phi \in \mathcal{A}_{N,K}^0(A) \right\},$$

as well as a localized version of $J_{\text{hom}}^{(N)}(\omega, z)$ by

$$J_{\text{hom}}^{(N)}(\omega, z, A) := \frac{1}{|NA \cap \mathbb{Z}|} \inf \left\{ \sum_{j=1}^K \sum_{\substack{i \in NA \cap \mathbb{Z} \\ i+j-1 \in NA}} J_j \left(\omega, i, z + \frac{\phi^{i+j} - \phi^i}{j} \right) : \phi \in \mathcal{A}_{N,K}^0(A) \right\},$$

where

$$\mathcal{A}_{N,K}^0(A) := \left\{ \phi : \mathbb{Z} \rightarrow \mathbb{R} : \phi^i = 0 \text{ for } \left| \min_{j \in AN \cap \mathbb{Z}} \{j\} - i \right| < K \text{ or } \left| \max_{j \in AN \cap \mathbb{Z}} \{j\} + 1 - i \right| < K \right\}. \quad (4.6)$$

Note that $J_{\text{hom}}^{L,(N)}(\omega, z)$ and $J_{\text{hom}}^{(N)}(\omega, z)$ are obtained when taking $A = [0, 1)$.

In view of an application of the ergodic theorem by Akcoglu and Krengel, we prove that $J_{\text{hom}}^{L,(N)}(\omega, z, A)$ as well as $J_{\text{hom}}^{(N)}(\omega, z, A)$ are indeed, in a slightly modified version, subadditive.

Proposition 4.4. *Let Assumption 3.3 be satisfied. Set $\mathcal{I} := \{[a, b) : a, b \in \mathbb{Z}\}$ and denote by \mathcal{L}^1 the class of integrable functions on the probability space $(\Omega, \mathcal{F}, \mathbb{P})$. Then,*

$$f_z^L(\omega) : \mathcal{I} \rightarrow \mathcal{L}^1, \quad A \mapsto |NA \cap \mathbb{Z}| J_{\text{hom}}^{L,(N)}(\cdot, z, A) + K^2 d \max\{\Psi(z), |z|\},$$

as well as

$$f_z(\omega) : \mathcal{I} \rightarrow \mathcal{L}^1, \quad A \mapsto |NA \cap \mathbb{Z}| J_{\text{hom}}^{(N)}(\cdot, z, A) + K^2 d \max\{\Psi(z), |z|\},$$

define subadditive processes, cf. Definition 2.15.

Proof. We give the proof for $f_z(\omega)$ and highlight the differences in proving the corresponding result for $f_z^L(\omega)$.

Step 1. $f_z(\omega)$ defines a set function from \mathcal{I} to \mathcal{L}^1 .

By the deterministic upper bound due to (LJ2), or due to (4.1) for the approximation, respectively,

and with $\phi^i = 0$ for all $i = 0, \dots, n-1$ being a competitor for the infimum problem, we get

$$\begin{aligned} 0 \leq \mathbb{E}[f_z(\omega)(A)] &\leq \mathbb{E} \left[\sum_{j=1}^K \sum_{\substack{i \in NA \cap \mathbb{Z} \\ i+j-1 \in NA}} J_j(\omega, i, z) + K^2 d \max\{\Psi(z), |z|\} \right] \\ &\leq |NA \cap \mathbb{Z}| K d \max\{\Psi(z), |z|\} + K^2 d \max\{\Psi(z), |z|\} < +\infty. \end{aligned}$$

Step 2. Bound from below.

By the deterministic lower bound due to (LJ2), or due to (4.1) for the approximation, respectively, we obtain

$$\inf_{A \in \mathcal{I}} \left\{ \frac{1}{|NA \cap \mathbb{Z}|} \mathbb{E} \left[f_z(\omega)(A) + K^2 d \max\{\Psi(z), |z|\} \right] \right\} \geq -Kd + K^2 d \max\{\Psi(z), |z|\} > -\infty.$$

Step 3. $f_z(\omega)$ is subadditive.

Let $A_1, \dots, A_M \subset \mathcal{I}$ be such that $A_h \cap A_m = \emptyset$ for all $h, m \in \{1, \dots, M\}$ with $h \neq m$ and with $\bigcup_{m=1}^M A_m =: A \in \mathcal{I}$. Then, for every A_m there exists a minimizer $\phi_m \in \mathcal{A}_{N,K}^0(A_m)$ of $J_{\text{hom}}^{(N)}(\omega, i, A_m)$, that is

$$J_{\text{hom}}^{(N)}(\omega, i, A_m) = \frac{1}{|NA_m \cap \mathbb{Z}|} \sum_{j=1}^K \sum_{\substack{i \in NA_m \cap \mathbb{Z} \\ i+j-1 \in NA_m}} J_j \left(\omega, i, z + \frac{\phi_m^{i+j} - \phi_m^i}{j} \right).$$

We set $\phi_A := \sum_{m=1}^M \phi_m \in \mathcal{A}_{N,K}^0(A)$. Due to the zero boundary constraint in the definition of $\mathcal{A}_{N,K}^0(A)$ it holds true that $\phi_A = \phi_m$ on A_m for all $m = 1, \dots, M$. Since ϕ_A is a competitor of $J_{\text{hom}}^{(N)}(\omega, z, A)$ and due to the zero boundary condition of ϕ_m , we obtain

$$\begin{aligned} f_z(\omega)(A) &\leq \sum_{j=1}^K \sum_{\substack{i \in NA \cap \mathbb{Z} \\ i+j-1 \in NA}} J_j \left(\omega, i, z + \frac{\phi_A^{i+j} - \phi_A^i}{j} \right) + K^2 d \max\{\Psi(z), |z|\} \\ &= \sum_{m=1}^M \sum_{j=1}^K \sum_{\substack{i \in NA_m \cap \mathbb{Z} \\ i+j-1 \in NA_m}} J_j \left(\omega, i, z + \frac{\phi_m^{i+j} - \phi_m^i}{j} \right) + \sum_{m=1}^{M-1} \sum_{j=2}^K \sum_{s=0}^{j-2} J_j \left(\omega, i_{\max}^m - s, z \right) + K^2 d \max\{\Psi(z), |z|\} \\ &\stackrel{(*)}{\leq} \sum_{m=1}^M \sum_{j=1}^K \sum_{\substack{i \in NA_m \cap \mathbb{Z} \\ i+j-1 \in NA_m}} J_j \left(\omega, i, z + \frac{\phi_m^{i+j} - \phi_m^i}{j} \right) + \sum_{m=1}^M K^2 d \max\{\Psi(z), |z|\} = \sum_{m=1}^M f_z(\omega)(A_m), \end{aligned}$$

where inequality $(*)$ holds true due to (LJ2), or due to (4.1) for the approximation, respectively, and since $\Psi(z) \geq 0$ for all $z \in \mathbb{R}$. Thus, subadditivity is proven. \square

Remark 4.5. We show in the following the existence of the function J_{hom}^L . One ingredient of the proof is the subadditive ergodic theorem by Akcoglu and Krengel. Since J_{hom}^L itself is not subadditive, the ergodic theorem can only be applied to $f_z^L(\omega)$, or $f_z(\omega)$, respectively, and we obtain

$$\frac{f_z^L(\omega)(A)}{|NA_m \cap \mathbb{Z}|} \rightarrow f(z)$$

pointwise almost everywhere in Ω as $N \rightarrow \infty$ to a limit independent of ω and A . Further, it holds true that

$$J_{\text{hom}}^L(\omega, z, A) = \frac{f_z^L(\omega)(A)}{|NA_m \cap \mathbb{Z}|} - \frac{1}{N} K^2 d \max\{\Psi(z), |z|\} \rightarrow f(z) - 0$$

as $N \rightarrow \infty$. Therefore, $f_z^L(\omega)$ and J_{hom}^L yield the same limit. In order to simplify the proofs, we consider J_{hom}^L instead of the modified function $f_z^L(\omega)$ and call it subadditive, although we have only proven that $f_z^L(\omega)$ is subadditive. We proceed in the case of J_{hom} in the same way.

The existence of the function J_{hom}^L , that we show in the next proposition, is mainly based on the subadditivity, shown in the previous proposition, because it allows to use the subadditive ergodic theorem by Akcoglu and Krengel.

Proposition 4.6. *Let Assumption 3.3 be satisfied. There exists an $\Omega' \subset \Omega$ with $\mathbb{P}(\Omega') = 1$ such that the following is true: For all $\omega \in \Omega'$, $z \in \mathbb{R}$ and $A := [a, b]$ with $a, b \in \mathbb{R}$ it holds*

$$J_{\text{hom}}^L(z) = \lim_{N \rightarrow \infty} \mathbb{E} \left[J_{\text{hom}}^{L,(N)}(\cdot, z, [0, 1]) \right] = \lim_{N \rightarrow \infty} J_{\text{hom}}^{L,(N)}(\omega, z, A). \quad (4.7)$$

Proof. In the following Steps 1–3, we will prove that $J_{\text{hom}}^{L,(N)}(\cdot, z, A)$ converges pointwise almost everywhere on Ω' to a function $f(z)$ independent of ω and A . Given this result, the upper bound from (LJ2) together with the dominated convergence theorem then yields

$$\lim_{N \rightarrow \infty} \mathbb{E} \left[J_{\text{hom}}^{L,(N)}(\cdot, z, [0, 1]) \right] = \mathbb{E}[f(z)] = f(z),$$

where the last equality holds true since $f(z)$ is independent of ω . This shows the second equality in (4.7).

Further, $NJ_{\text{hom}}^{L,(N)}(\cdot, z, [0, 1])$ is subadditive in view of Proposition 4.4 and Remark 4.5. Because of linearity and monotonicity of the expectation value, it also holds true that $\mathbb{E} \left[NJ_{\text{hom}}^{L,(N)}(\cdot, z, [0, 1]) \right]$ is subadditive. Thus, we can apply Theorem 2.17, a result from the theory of subadditive functions, to get (again with linearity of the expectation value)

$$\begin{aligned} J_{\text{hom}}^L(z) &= \inf_{N \in \mathbb{N}} \mathbb{E} \left[J_{\text{hom}}^{L,(N)}(\cdot, z, [0, 1]) \right] = \inf_{N \in \mathbb{N}} \frac{\mathbb{E} \left[NJ_{\text{hom}}^{L,(N)}(\cdot, z, [0, 1]) \right]}{N} \\ &= \lim_{N \rightarrow \infty} \frac{\mathbb{E} \left[NJ_{\text{hom}}^{L,(N)}(\cdot, z, [0, 1]) \right]}{N} = \lim_{N \rightarrow \infty} \mathbb{E} \left[J_{\text{hom}}^{L,(N)}(\cdot, z, [0, 1]) \right]. \end{aligned}$$

This shows the first equality in (4.7) and justifies $f(z) = J_{\text{hom}}^L(z)$.

At this point, it is left to show the existence of the limit $\lim_{N \rightarrow \infty} J_{\text{hom}}^{L,(N)}(\omega, z, A)$ pointwise almost everywhere, which is done in the following three steps. As indicated at the beginning of Section 4.1, the ergodic theorem 2.16 due to Akcoglu and Krengel yields, for every $z \in \mathbb{R}$ and for every A , the existence of $\Omega_{z,A} \subset \Omega$ with $\mathbb{P}(\Omega_{z,A}) = 1$ such that for every $\omega \in \Omega_{z,A}$ the limit

$$\lim_{N \rightarrow \infty} J_{\text{hom}}^{L,(N)}(\omega, z, A)$$

exists and is independent of ω and A . This already seems to be the proof of the theorem, however it is not. The difference to the assertion we need to prove is hidden in the type and order of the

quantifiers for z , A and Ω . The ergodic theorem provides the assertion with a different type and order of quantifiers. Therefore, we have to do some work to correct and rearrange.

Step 1. The case of a fixed $z \in \mathbb{R}$ and intervals $A = [a, b)$ with $a, b \in \mathbb{Z}$.

We prove pointwise convergence almost everywhere for a fixed $z \in \mathbb{R}$. As $|NA \cap \mathbb{Z}| J_{\text{hom}}^{L,(N)}(\omega, z, \cdot)$ is subadditive in view of Proposition 4.4 and Remark 4.5, and $J_{\text{hom}}^{L,(N)}$ is stationary and ergodic due to the stationarity and ergodicity of the group action, the ergodic theorem 2.16 by Akcoglu and Krengel can be applied. Thus, there exists $\Omega_z \subset \Omega$ with $\mathbb{P}(\Omega_z) = 1$ such that for every $\omega \in \Omega_z$ and for every $A = [a, b)$ with $a, b \in \mathbb{Z}$, the limit

$$\lim_{N \rightarrow \infty} J_{\text{hom}}^{L,(N)}(\omega, z, A)$$

exists and is independent of ω and A . Note that this holds true because of the countability of the intervals, since we only demand for $a, b \in \mathbb{Z}$. Otherwise, the property $\mathbb{P}(\Omega_z) = 1$ cannot be ensured. More precisely, it holds true that $\Omega_z = \bigcap_{a,b \in \mathbb{Z}} \Omega_A$, with $\Omega_A \subset \Omega$ being the set on which the ergodic theorem holds true for a fixed A . Considering $A = [0, N)$, we get

$$J_{\text{hom}}^L(z) = \lim_{N \rightarrow \infty} J_{\text{hom}}^{L,(N)}(\omega, z, A).$$

Step 2. The case of a fixed $z \in \mathbb{R}$ and intervals $A = [a, b)$ with $a, b \in \mathbb{R}$.

In order to pass to general intervals with $a, b \in \mathbb{R}$, we argue as in Proposition 3.5, Step 2 and in [47, Proposition 1]. For every $\epsilon > 0$, there exists $T > 0$ large enough and intervals $A_\epsilon^- := [a_\epsilon^-, b_\epsilon^-]$, $A_\epsilon^+ := [a_\epsilon^+, b_\epsilon^+]$ with $a_\epsilon^-, b_\epsilon^-, a_\epsilon^+, b_\epsilon^+ \in \mathbb{Z}$ such that

$$A_\epsilon^- \subset TA \subset A_\epsilon^+, \quad \frac{|A_\epsilon^-|}{|TA|} \geq 1 - \epsilon, \quad \frac{|TA|}{|A_\epsilon^+|} \geq 1 - \epsilon. \quad (4.8)$$

From (LJ2), we get for all intervals $B \subset A$ and N large enough the inequality

$$J_{\text{hom}}^{L,(N)}(\omega, z, A) \leq J_{\text{hom}}^{L,(N)}(\omega, z, B) + \frac{|N(A \setminus B) \cap \mathbb{Z}|}{|N(A) \cap \mathbb{Z}|} C \max\{\Psi(z), |z|\}, \quad (4.9)$$

which can be seen as follows. Taking a minimizer ϕ of the minimum problem related to B , one has

$$\begin{aligned} & J_{\text{hom}}^{L,(N)}(\omega, z, A) \\ & \leq \frac{1}{|NB \cap \mathbb{Z}|} \sum_{j=1}^K \sum_{i=i_{\min}^B}^{i_{\max}^B+1-j} J_j^L \left(\omega, i, z + \frac{\phi^{i+j} - \phi^i}{j} \right) + \frac{1}{|NA \cap \mathbb{Z}|} \sum_{j=1}^K \sum_{\substack{i=i_{\min}^{A \setminus B} \\ i \in N(A \setminus B) \cap \mathbb{Z}}}^{i_{\max}^{A \setminus B}+1-j} J_j^L(\omega, i, z) \\ & \quad + \frac{1}{|NA \cap \mathbb{Z}|} \sum_{j=2}^K \sum_{i=i_{\max}^B+2-j}^{i_{\max}^B} J_j^L(\omega, i, z) \\ & \stackrel{(LJ2)}{\leq} J_{\text{hom}}^{L,(N)}(\omega, z, B) + \frac{1}{|NA \cap \mathbb{Z}|} \sum_{j=1}^K \sum_{\substack{i=i_{\min}^{A \setminus B} \\ i \in N(A \setminus B) \cap \mathbb{Z}}}^{i_{\max}^{A \setminus B}+1-j} d \max\{\Psi(z), |z|\} \end{aligned}$$

$$\begin{aligned}
 & + \frac{1}{|NA \cap \mathbb{Z}|} \sum_{j=2}^K \sum_{i=i_{\max}^B+2-j}^{i_{\max}^B} d \max\{\Psi(z), |z|\} \\
 & \leq J_{\text{hom}}^{L,(N)}(\omega, z, B) + \frac{1}{|NA \cap \mathbb{Z}|} d \max\{\Psi(z), |z|\} \left(K|N(A \setminus B) \cap \mathbb{Z}| + \frac{1}{2}(K+1)K \right) \\
 & \leq J_{\text{hom}}^{L,(N)}(\omega, z, B) + \frac{1}{|NA \cap \mathbb{Z}|} d \max\{\Psi(z), |z|\} \left(\left(K + \frac{1}{2}(K+1)K \right) |N(A \setminus B) \cap \mathbb{Z}| \right),
 \end{aligned}$$

where the last inequality holds true for N large enough. Now, we get from Step 1

$$\begin{aligned}
 J_{\text{hom}}^L(z) & = \lim_{N \rightarrow \infty} J_{\text{hom}}^{L,(N)}(\omega, z, A_\epsilon^+) \\
 & \stackrel{(4.9)}{\leq} \liminf_{N \rightarrow \infty} J_{\text{hom}}^{L,(N)}(\omega, z, TA) + \liminf_{N \rightarrow \infty} \frac{|N(A_\epsilon^+ \setminus TA) \cap \mathbb{Z}|}{|N(A_\epsilon^+) \cap \mathbb{Z}|} C \max\{\Psi(z), |z|\} \\
 & = \liminf_{N \rightarrow \infty} J_{\text{hom}}^{L,(N)}(\omega, z, TA) + \frac{|(A_\epsilon^+ \setminus TA)|}{|(A_\epsilon^+)|} C \max\{\Psi(z), |z|\} \\
 & \stackrel{(4.8)}{\leq} \limsup_{N \rightarrow \infty} J_{\text{hom}}^{L,(N)}(\omega, z, TA) + \epsilon C \max\{\Psi(z), |z|\} \\
 & \stackrel{(4.9)}{\leq} \lim_{N \rightarrow \infty} J_{\text{hom}}^{L,(N)}(\omega, z, A_\epsilon^-) + \left(\epsilon + \frac{|(TA \setminus A_\epsilon^-)|}{|(TA)|} \right) C \max\{\Psi(z), |z|\} \\
 & \stackrel{(4.8)}{=} J_{\text{hom}}^L(z) + 2C\epsilon \max\{\Psi(z), |z|\}.
 \end{aligned}$$

This shows

$$J_{\text{hom}}^L(z) = \lim_{N \rightarrow \infty} J_{\text{hom}}^{L,(N)}(\omega, z, TA),$$

for $A = [a, b]$ with $a, b \in \mathbb{R}$, since we can pass to the limit $\epsilon \rightarrow 0$. With the result (3.7) from Step 2 of Proposition 3.5 we get

$$J_{\text{hom}}^L(z) = \lim_{N \rightarrow \infty} J_{\text{hom}}^{L,(N)}(\omega, z, TA) = \lim_{N \rightarrow \infty} J_{\text{hom}}^{L,(N)}(\omega, z, A),$$

for every $T > 0$, which concludes Step 2.

Step 3. The case of arbitrary $z \in \mathbb{R}$ and intervals $A = [a, b]$ with $a, b \in \mathbb{R}$.

With the definition of Ω_z from the previous steps, we define $\Omega' := \bigcap_{z \in \mathbb{Q}} \Omega_z$. It holds true that $\mathbb{P}(\Omega') = 1$ and that we have for every $\omega \in \Omega'$

$$J_{\text{hom}}^L(z) = \lim_{N \rightarrow \infty} J_{\text{hom}}^{L,(N)}(\omega, z, A), \quad (4.10)$$

for arbitrary A and all $z \in \mathbb{Q}$. This was shown in the previous steps.

Next, we derive the existence of the limit of $J_{\text{hom}}^{L,(N)}(\omega, z, A)$ also for $z \in \mathbb{R} \setminus \mathbb{Q}$ and $\omega \in \Omega'$. Note, that the ergodic theorem provides existence of that limit only for $\omega \in \Omega_z$ and not for $\omega \in \Omega'$. For this, let $z \in \mathbb{R} \setminus \mathbb{Q}$ and $(z_k)_{k \in \mathbb{N}} \subset \mathbb{Q}$ be a sequence with $z_k \rightarrow z$. Strictly speaking, we can also assume $z \in \mathbb{R}$, but it is not necessary, because we have already dealt with the case $z \in \mathbb{Q}$. By

contrast, the assumption $(z_k)_{k \in \mathbb{N}} \subset \mathbb{Q}$ is essential, because it allows us to use the result (4.10) for z_n in what follows, since (4.10) was only proven for $z \in \mathbb{Q}$.

We denote the minimizer related to the minimum problem of $J_{\text{hom}}^{L,(N)}(\omega, z, A)$ by $\phi_{N,z} : (NA \cap \mathbb{Z}) \cup \{i_{\max}^A + 1\} \rightarrow \mathbb{R}$ with $\phi_{N,z}^{i_{\min}^A} = 0 = \phi_{N,z}^{i_{\max}^A + 1}$ (we drop the index A for the minimizer for better readability), which means that

$$J_{\text{hom}}^{L,(N)}(\omega, z, A) = \frac{1}{|NA \cap \mathbb{Z}|} \sum_{j=1}^K \sum_{i=i_{\min}^A}^{i_{\max}^A+1-j} J_j^L \left(\omega, i, z + \frac{\phi_{N,z}^{i+j} - \phi_{N,z}^i}{j} \right). \quad (4.11)$$

Consequently, we have

$$\begin{aligned} J_{\text{hom}}^{L,(N)}(\omega, z, A) &= \frac{1}{|NA \cap \mathbb{Z}|} \sum_{j=1}^K \sum_{i=i_{\min}^A}^{i_{\max}^A+1-j} J_j^L \left(\omega, i, z + \frac{\phi_{N,z}^{i+j} - \phi_{N,z}^i}{j} \right) \\ &= \frac{1}{|NA \cap \mathbb{Z}|} \sum_{j=1}^K \sum_{i=i_{\min}^A}^{i_{\max}^A+1-j} J_j^L \left(\omega, i, z_k + \frac{\phi_{N,z}^{i+j} - \phi_{N,z}^i}{j} \right) \\ &\quad + \frac{1}{|NA \cap \mathbb{Z}|} \sum_{j=1}^K \sum_{i=i_{\min}^A}^{i_{\max}^A+1-j} \left(J_j^L \left(\omega, i, z + \frac{\phi_{N,z}^{i+j} - \phi_{N,z}^i}{j} \right) - J_j^L \left(\omega, i, z_k + \frac{\phi_{N,z}^{i+j} - \phi_{N,z}^i}{j} \right) \right), \end{aligned}$$

which can be estimated by

$$\begin{aligned} J_{\text{hom}}^{L,(N)}(\omega, z, A) &\geq J_{\text{hom}}^{L,(N)}(\omega, z_k, A) \\ &\quad - \frac{1}{|NA \cap \mathbb{Z}|} \sum_{j=1}^K \sum_{i=i_{\min}^A}^{i_{\max}^A+1-j} \left| J_j^L \left(\omega, i, z + \frac{\phi_{N,z}^{i+j} - \phi_{N,z}^i}{j} \right) - J_j^L \left(\omega, i, z_k + \frac{\phi_{N,z}^{i+j} - \phi_{N,z}^i}{j} \right) \right|. \end{aligned}$$

Since $|z - z_k| \leq |z - z_k|^\alpha$ for k large enough, we continue with this estimate by using (4.3) and get

$$J_{\text{hom}}^{L,(N)}(\omega, z, A) \geq J_{\text{hom}}^{L,(N)}(\omega, z_k, A) - C^{L,H,(N)}(\omega) |z - z_k|^\alpha. \quad (4.12)$$

Next we take the limit $\liminf_{N \rightarrow \infty}$ of (4.12). Recalling that $C^{L,H,(N)}(\omega) \rightarrow C^{L,H}$ in the limit $N \rightarrow \infty$ by (4.3), we obtain

$$\begin{aligned} \liminf_{N \rightarrow \infty} J_{\text{hom}}^{L,(N)}(\omega, z, A) &\geq \liminf_{N \rightarrow \infty} J_{\text{hom}}^{L,(N)}(\omega, z_k, A) - \lim_{N \rightarrow \infty} C^{L,H,(N)}(\omega) |z - z_k|^\alpha \\ &= J_{\text{hom}}^L(z_k) - C^{L,H} |z - z_k|^\alpha, \end{aligned}$$

where the last equality holds true due to (4.10), by using the assumption $(z_k)_{k \in \mathbb{N}} \subset \mathbb{Q}$. Subsequently we take the limit $\limsup_{k \rightarrow \infty}$, which yields, by the assumption $z_k \rightarrow z$ as $k \rightarrow \infty$,

$$\liminf_{N \rightarrow \infty} J_{\text{hom}}^{L,(N)}(\omega, z, A) \geq \limsup_{k \rightarrow \infty} J_{\text{hom}}^L(z_k).$$

Now, we can repeat the whole calculation, from (4.11) onwards, by changing the roles of z and z_k . Hence, the limits which have to be taken are first $\limsup_{N \rightarrow \infty}$ and subsequently $\liminf_{k \rightarrow \infty}$. By

this, we get analogously

$$\liminf_{k \rightarrow \infty} J_{\text{hom}}^L(z_k) \geq \limsup_{N \rightarrow \infty} J_{\text{hom}}^{L,(N)}(\omega, z, A).$$

Together, the two inequalities yield

$$\begin{aligned} J_{\text{hom}}^L(z) &= \lim_{N \rightarrow \infty} J_{\text{hom}}^{L,(N)}(\omega, z, A) \\ &= \lim_{k \rightarrow \infty} J_{\text{hom}}^L(z_k), \quad \text{for all } z \in \mathbb{R} \setminus \mathbb{Q} \text{ and all } (z_k)_k \subset \mathbb{Q}. \end{aligned} \tag{4.13}$$

This shows that for $\omega \in \Omega'$ the limit of $J_{\text{hom}}^{L,(N)}(\omega, z, A)$ exists and is independent of ω and A for all $z \in \mathbb{R} \setminus \mathbb{Q}$. Altogether, we have that the limit of $J_{\text{hom}}^{L,(N)}(\omega, z, A)$ exists for every $z \in \mathbb{R}$, is independent of ω and A , and equals $J_{\text{hom}}^L(z)$. This finally proves (4.7). \square

Remark 4.7. *The basic difficulty of the proof of Proposition 4.6 is to extend the result, after applying the ergodic theorem, in such way that we obtain the limit of $J_{\text{hom}}^{L,(N)}(\omega, z, A)$ for all $z \in \mathbb{R}$ and an arbitrary interval A . A main ingredient used in the proofs is the Lipschitz-continuity of the approximating functions, which yields estimate (4.12). Without this regularity, it is not readily apparent whether the line of arguments can be adopted. Herein lies the reason of considering the approximation functions $J_j^L(\omega, i, z)$ instead of the original functions $J_j(\omega, i, z)$ as a technical tool. Likewise, the Lipschitz-continuity is useful in Proposition 4.8. Estimate (4.12) also shows the importance of the Hölder-regularity.*

After proving the existence of the limit J_{hom}^L , we now want to shed some light on the shape and properties of this function. The following proposition gives some useful technical properties of the limiting function J_{hom}^L , in particular continuity and convexity of J_{hom}^L , as well as its Γ -limit.

Note that equation (4.13) does not show continuity yet, because it is only valid for sequences $(z_n) \subset \mathbb{Q}$ and $z \in \mathbb{R} \setminus \mathbb{Q}$. As already mentioned in the proof, $z \in \mathbb{R} \setminus \mathbb{Q}$ is not a necessary restriction. The result holds true also for $z \in \mathbb{R}$. The only real limitation is $(z_n) \subset \mathbb{Q}$ and this is not enough to obtain continuity.

Proposition 4.8. *Let Assumption 3.3 be satisfied. The map $z \mapsto J_{\text{hom}}^L(z)$ is continuous and convex. Moreover, there exists an $\Omega' \subset \Omega$ with $\mathbb{P}(\Omega') = 1$ such that the following is true: For all $\omega \in \Omega'$ and every $A = [a, b]$, $a, b \in \mathbb{R}$ it holds*

$$\Gamma\text{-}\lim_{N \rightarrow \infty} J_{\text{hom}}^{L,(N)}(\omega, \cdot, A) = J_{\text{hom}}^L.$$

Proof. We prove the three assertions of the proposition, namely continuity, convexity and the Γ -limit result, separately in the following three steps.

Step 1. Continuity.

Let $(z_k)_{k \in \mathbb{N}} \subset \mathbb{R}$ be a sequence converging to $z \in \mathbb{R}$. Let $\phi_{N,z}$ be a minimizing sequence such that it holds true $\phi_{N,z}^N = \phi_{N,z}^0 = 0$ and

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{j=1}^K \sum_{i=0}^{N-j} J_j^L \left(\omega, i, z + \frac{\phi_{N,z}^{i+j} - \phi_{N,z}^i}{j} \right) = J_{\text{hom}}^L(z) \tag{4.14}$$

for $\omega \in \Omega'$ defined in Proposition 4.6. We estimate the term on the left-hand side of this equation

and obtain

$$\begin{aligned} \frac{1}{N} \sum_{j=1}^K \sum_{i=0}^{N-j} J_j^L \left(\omega, i, z + \frac{\phi_{N,z}^{i+j} - \phi_{N,z}^i}{j} \right) &= \frac{1}{N} \sum_{j=1}^K \sum_{i=0}^{N-j} J_j^L \left(\omega, i, z_k + \frac{\phi_{N,z}^{i+j} - \phi_{N,z}^i}{j} \right) \\ &+ \frac{1}{N} \sum_{j=1}^K \sum_{i=0}^{N-j} \left(J_j^L \left(\omega, i, z + \frac{\phi_{N,z}^{i+j} - \phi_{N,z}^i}{j} \right) - J_j^L \left(\omega, i, z_k + \frac{\phi_{N,z}^{i+j} - \phi_{N,z}^i}{j} \right) \right) \end{aligned}$$

With this equality, we can estimate (4.14) by

$$J_{\text{hom}}^L(z) \geq J_{\text{hom}}^{L,(N)}(\omega, z_k) - C^{L,H,(N)}(\omega) |z - z_k|^\alpha, \quad (4.15)$$

due to (4.3) and since $|z - z_k| \leq |z - z_k|^\alpha$ for k large enough. Next we take the limit $N \rightarrow \infty$ of (4.15). Recalling that $C^{L,H,(N)}(\omega) \rightarrow C^{L,H}$ in the limit $N \rightarrow \infty$ by (4.3), we obtain

$$J_{\text{hom}}^L(z) \geq J_{\text{hom}}^L(z_k) - C^{L,H} |z - z_k|^\alpha,$$

by the result of Proposition 4.6. Subsequently we take the limit $\limsup_{k \rightarrow \infty}$, which yields, by the assumption $z_k \rightarrow z$ as $k \rightarrow \infty$,

$$J_{\text{hom}}^L(z) \geq \limsup_{k \rightarrow \infty} J_{\text{hom}}^L(z_k).$$

Restarting the whole calculation, from (4.14) onwards, by changing the roles of z and z_k , we get analogously by first taking the limit $N \rightarrow \infty$ and subsequently $\liminf_{k \rightarrow \infty}$

$$J_{\text{hom}}^L(z) \leq \liminf_{k \rightarrow \infty} J_{\text{hom}}^L(z_k).$$

Together, this shows $J_{\text{hom}}^L(z) = \lim_{k \rightarrow \infty} J_{\text{hom}}^L(z_k)$ and therefore J_{hom}^L is continuous.

Step 2. Convexity.

We need to show

$$J_{\text{hom}}^L(tz_1 + (1-t)z_2) \leq tJ_{\text{hom}}^L(z_1) + (1-t)J_{\text{hom}}^L(z_2)$$

for every $t \in [0, 1]$ and every $z_1, z_2 \in (0, +\infty)$. Otherwise, the proof of the inequality is trivial. Fix $t \in [0, 1]$. Let $\phi_{N,z_1} : N[0, t + \frac{1}{N}] \cap \mathbb{Z} \rightarrow \mathbb{R}$ be a minimizer related to the minimum problem of $J_{\text{hom}}^{L,(N)}(\omega, z_1, [0, t])$, i.e. $\phi_{N,z_1}^s = 0 = \phi_{N,z_1}^{i_{\max}^{(0,t)}+1-s}$ for $s = 0, \dots, K-1$ and

$$J_{\text{hom}}^{L,(N)}(\omega, z_1, [0, t]) = \frac{1}{|N[0, t] \cap \mathbb{Z}|} \sum_{j=1}^K \sum_{i=0}^{i_{\max}^{(0,t)}+1-j} J_j^L \left(\omega, i, z_1 + \frac{\phi_{N,z_1}^{i+j} - \phi_{N,z_1}^i}{j} \right).$$

Further, let $\phi_{N,z_2} : N[t, N] \cap \mathbb{Z} \rightarrow \mathbb{R}$ be a minimizer of the minimum problem of $J_{\text{hom}}^{L,(N)}(\omega, z_2, [t, 1])$,

i.e. $\phi_{N,z_2}^{i_{\min}^{[t,1]}+s} = 0 = \phi_{N,z_2}^{N-s}$ for $s = 0, \dots, K-1$ and

$$J_{\text{hom}}^{L,(N)}(\omega, z_2, [t, 1]) = \frac{1}{|N[t, 1] \cap \mathbb{Z}|} \sum_{j=1}^K \sum_{i=i_{\min}^{[t,1]}}^{N-j} J_j^L \left(\omega, i, z_2 + \frac{\phi_{N,z_2}^{i+j} - \phi_{N,z_2}^i}{j} \right).$$

This given, we define a new competitor

$$\tilde{\phi}_N^i := \begin{cases} \phi_{N,z_1}^i = 0 & \text{for } 0 \leq i \leq K-1, \\ \phi_{N,z_1}^i + (i-K)(z_1-z_2)(1-t) & \text{for } K \leq i \leq i_{\max}^{[0,t]} + 1 - K, \\ i_{\max}^{[0,t]}(z_1-z_2)(1-t) & \text{for } i_{\max}^{[0,t]} + 2 - K \leq i \leq i_{\min}^{[t,1]} - 1 + K, \\ \phi_{N,z_2}^i + (N-i)(z_1-z_2)t & \text{for } i_{\min}^{[t,1]} + K \leq i \leq N-K, \\ \phi_{N,z_2}^i = 0 & \text{for } N+1-K \leq i \leq N. \end{cases}$$

Indeed, $\tilde{\phi}_N$ fulfils the constraints of the infimum problem of $J_{\text{hom}}^{L,(N)}$, because $\tilde{\phi}_N^i = 0$ for $i = 0, \dots, K-1$ and $i = N+1-K, \dots, N$ by definition. In addition, the second and fourth line in the definition of $\tilde{\phi}_N$ is chosen in such a way that in these regimes

$$\begin{aligned} tz_1 + (1-t)z_2 + \frac{\tilde{\phi}_N^{i+j} - \tilde{\phi}_N^i}{j} &= z_1 + \frac{\phi_{N,z_1}^{i+j} - \phi_{N,z_1}^i}{j}, \\ tz_1 + (1-t)z_2 + \frac{\tilde{\phi}_N^{i+j} - \tilde{\phi}_N^i}{j} &= z_2 + \frac{\phi_{N,z_2}^{i+j} - \phi_{N,z_2}^i}{j}, \end{aligned} \quad (4.16)$$

respectively. Since $\tilde{\phi}_N$ is a competitor, it can be used to estimate

$$\begin{aligned} J_{\text{hom}}^{L,(N)}(\omega, tz_1 + (1-t)z_2) &\leq \frac{1}{N} \sum_{j=1}^K \sum_{i=0}^{N-j} J_j^L \left(\omega, i, tz_1 + (1-t)z_2 + \frac{\tilde{\phi}_N^{i+j} - \tilde{\phi}_N^i}{j} \right) \\ &= \frac{1}{N} \sum_{j=1}^K \sum_{i=0}^{i_{\max}^{[0,t]}+1-j} J_j^L \left(\omega, i, tz_1 + (1-t)z_2 + \frac{\tilde{\phi}_N^{i+j} - \tilde{\phi}_N^i}{j} \right) \\ &\quad + \frac{1}{N} \sum_{j=1}^K \sum_{i=i_{\min}^{[t,1]}}^{N-j} J_j^L \left(\omega, i, tz_1 + (1-t)z_2 + \frac{\tilde{\phi}_N^{i+j} - \tilde{\phi}_N^i}{j} \right) \\ &\quad + \frac{1}{N} \sum_{j=2}^K \sum_{s=0}^{j-2} J_j^L \left(\omega, i_{\max}^{[0,t]} - s, tz_1 + (1-t)z_2 + \frac{\tilde{\phi}_N^{i_{\max}^{[0,t]}-s+j} - \tilde{\phi}_N^{i_{\max}^{[0,t]}-s}}{j} \right). \end{aligned} \quad (4.17)$$

We consider all three terms of the right-hand side of (4.17) individually in Step A-C and bring it together in Step D.

Step A: First term of (4.17).

Using (4.16), we start with the first term of (4.17), that is

$$\begin{aligned}
 & \frac{1}{N} \sum_{j=1}^K \sum_{i=0}^{i_{\max}^{[0,t]}+1-j} J_j^L \left(\omega, i, tz_1 + (1-t)z_2 + \frac{\tilde{\phi}_N^{i+j} - \tilde{\phi}_N^i}{j} \right) \\
 &= \frac{1}{N} \sum_{j=1}^K \sum_{i=0}^{i_{\max}^{[0,t]}+1-j} J_j^L \left(\omega, i, z_1 + \frac{\phi_{N,z_1}^{i+j} - \phi_{N,z_1}^i}{j} \right) \\
 &+ \frac{1}{N} \sum_{j=1}^K \sum_{i=0}^{K-1} \left(J_j^L \left(\omega, i, tz_1 + (1-t)z_2 + \frac{\tilde{\phi}_N^{i+j} - \tilde{\phi}_N^i}{j} \right) - J_j^L \left(\omega, i, z_1 + \frac{\phi_{N,z_1}^{i+j} - \phi_{N,z_1}^i}{j} \right) \right) \\
 &+ \frac{1}{N} \sum_{j=1}^K \sum_{i=i_{\max}^{[0,t]}+2-K-j}^{i_{\max}^{[0,t]}+1-j} \left(J_j^L \left(\omega, i, tz_1 + (1-t)z_2 + \frac{\tilde{\phi}_N^{i+j} - \tilde{\phi}_N^i}{j} \right) - J_j^L \left(\omega, i, z_1 + \frac{\phi_{N,z_1}^{i+j} - \phi_{N,z_1}^i}{j} \right) \right).
 \end{aligned} \tag{4.18}$$

The second and third term on the right-hand side take into account all contributions that have at least one $\tilde{\phi}_N^k$, $k = i$ or $k = i + j$, in the first or third line in the definition of $\tilde{\phi}_N$. For $0 \leq i \leq K - 1$, it holds true that $\phi_{N,z_1}^i = \tilde{\phi}_N^i = 0$ and ϕ_{N,z_1}^{i+j} and $\tilde{\phi}_N^{i+j}$ are either both equal to zero or $\tilde{\phi}_N^{i+j} - \phi_{N,z_1}^{i+j} = (i - K + j)(z_1 - z_2)(1 - t)$. This yields

$$\begin{aligned}
 \left| \frac{\tilde{\phi}_N^{i+j} - \tilde{\phi}_N^i}{j} - \frac{\phi_{N,z_1}^{i+j} - \phi_{N,z_1}^i}{j} \right| &\leq \left| \frac{(i - K + j)(z_1 - z_2)(1 - t)}{j} \right| \\
 &\leq (K + 1) |(z_1 - z_2)(1 - t)| =: C_1.
 \end{aligned}$$

For $i_{\max}^{[0,t]} + 2 - K - j \leq i \leq i_{\max}^{[0,t]} + 1 - j$, it holds true that $\tilde{\phi}_N^{i+j} = i_{\max}^{[0,t]}(z_1 - z_2)(1 - t)$, $\phi_{N,z_1}^{i+j} = 0$ and $\tilde{\phi}_N^i$ and ϕ_{N,z_1}^i are either also $i_{\max}^{[0,t]}(z_1 - z_2)(1 - t)$ and 0 or $\tilde{\phi}_N^i - \phi_{N,z_1}^i = (i - K)(z_1 - z_2)(1 - t)$. This yields

$$\begin{aligned}
 \left| \frac{\tilde{\phi}_N^{i+j} - \tilde{\phi}_N^i}{j} - \frac{\phi_{N,z_1}^{i+j} - \phi_{N,z_1}^i}{j} \right| &\leq \left| \frac{(K - i + i_{\max}^{[0,t]})(z_1 - z_2)(1 - t)}{j} \right| \\
 &\leq (3K - 2) |(z_1 - z_2)(1 - t)| =: C_2.
 \end{aligned}$$

Thus, we can estimate (4.18) with $\epsilon > 0$ and $I_\epsilon(x) := [x - \epsilon, x + \epsilon] \cap [0, 1]$ for N large enough by

$$\begin{aligned}
 & \frac{1}{N} \sum_{j=1}^K \sum_{i=0}^{i_{\max}^{[0,t]}+1-j} J_j^L \left(\omega, i, tz_1 + (1-t)z_2 + \frac{\tilde{\phi}_N^{i+j} - \tilde{\phi}_N^i}{j} \right) \\
 &\leq \left(t + \frac{2}{N} \right) J_{\text{hom}}^{L,(N)}(\omega, z_1, [0, t]) + \frac{|NI_\epsilon(0) \cap \mathbb{Z}|}{N} C_1 C^{L,H,(N)}(\omega) + \frac{|NI_\epsilon(t) \cap \mathbb{Z}|}{N} C_2 C^{L,H,(N)}(\omega),
 \end{aligned} \tag{4.19}$$

where the last two steps are due to (4.3).

Step B: Second term of (4.17).

The second term of (4.17) can be estimated, using (4.16), as

$$\begin{aligned}
 & \frac{1}{N} \sum_{j=1}^K \sum_{i=i_{\min}^{[t,1]}}^{N-j} J_j^L \left(\omega, i, tz_1 + (1-t)z_2 + \frac{\tilde{\phi}_N^{i+j} - \tilde{\phi}_N^i}{j} \right) \\
 &= \frac{1}{N} \sum_{j=1}^K \sum_{i=i_{\min}^{[t,1]}}^{N-j} J_j^L \left(\omega, i, z_2 + \frac{\phi_{N,z_2}^{i+j} - \phi_{N,z_2}^i}{j} \right) \\
 &+ \frac{1}{N} \sum_{j=1}^K \sum_{i=i_{\min}^{[t,1]}}^{i_{\min}^{[t,1]}-1+K} \left(J_j^L \left(\omega, i, tz_1 + (1-t)z_2 + \frac{\tilde{\phi}_N^{i+j} - \tilde{\phi}_N^i}{j} \right) - J_j^L \left(\omega, i, z_2 + \frac{\phi_{N,z_2}^{i+j} - \phi_{N,z_2}^i}{j} \right) \right) \\
 &+ \frac{1}{N} \sum_{j=1}^K \sum_{i=i_{\min}^{[t,1]}}^{N-j} \left(J_j^L \left(\omega, i, tz_1 + (1-t)z_2 + \frac{\tilde{\phi}_N^{i+j} - \tilde{\phi}_N^i}{j} \right) - J_j^L \left(\omega, i, z_2 + \frac{\phi_{N,z_2}^{i+j} - \phi_{N,z_2}^i}{j} \right) \right). \tag{4.20}
 \end{aligned}$$

The second and third term on the right-hand side take into account all contributions that have at least one $\tilde{\phi}_N^k$, $k = i$ or $k = i + j$, in the third or fifth line in the definition of $\tilde{\phi}_N$. For $i = i_{\min}^{[t,1]} \leq i \leq i_{\min}^{[t,1]} - 1 + K$, it holds true that $\tilde{\phi}_N^i = i_{\max}^{[0,t]}(z_1 - z_2)(1-t)$, $\phi_{N,z_1}^i = 0$ and $\tilde{\phi}_N^{i+j}$ and ϕ_{N,z_1}^{i+j} are either also $i_{\max}^{[0,t]}(z_1 - z_2)(1-t)$ and 0 or $\tilde{\phi}_N^{i+j} - \phi_{N,z_1}^{i+j} = (i - i_{\max}^{[0,t]} + j)(z_2 - z_1)t + (N - i_{\max}^{[0,t]})(z_1 - z_2)t$. This yields

$$\begin{aligned}
 & \left| \frac{\tilde{\phi}_N^{i+j} - \tilde{\phi}_N^i}{j} - \frac{\phi_{N,z_1}^{i+j} - \phi_{N,z_1}^i}{j} \right| \leq \left| \frac{(i - i_{\max}^{[0,t]} + j)(z_2 - z_1)t + (z_2 - z_1)(i_{\max}^{[0,t]} - tN)}{j} \right| \\
 & \leq (2K + 1) |(z_2 - z_1)t| + \left| \frac{((z_2 - z_1)(i_{\max}^{[0,t]} \lambda_N - t))}{j \lambda_N} \right| \leq (2K + 1) |(z_2 - z_1)t| + \left| (z_2 - z_1) \frac{\lambda_N}{j \lambda_N} \right| \\
 & \leq (2K + 1) |(z_2 - z_1)t| + |(z_2 - z_1)| =: C_3.
 \end{aligned}$$

For $N - K + 1 - j \leq i \leq N - j$, it holds true that $\tilde{\phi}_N^{i+j} = \phi_{N,z_1}^{i+j} = 0$ and ϕ_{N,z_1}^i and $\tilde{\phi}_N^i$ are either both equal to zero or $\tilde{\phi}_N^i - \phi_{N,z_1}^i = (i - N)(z_2 - z_1)t$. This yields

$$\left| \frac{\tilde{\phi}_N^{i+j} - \tilde{\phi}_N^i}{j} - \frac{\phi_{N,z_1}^{i+j} - \phi_{N,z_1}^i}{j} \right| \leq \left| \frac{(N - i)(z_2 - z_1)t}{j} \right| \leq (2K - 1) |(z_2 - z_1)t| =: C_4.$$

This result can be used to estimate (4.20) with $\epsilon > 0$ and $I_\epsilon(x) := [x - \epsilon, x + \epsilon] \cap [0, 1]$ for N large enough and together with (4.3), by

$$\begin{aligned}
 & \frac{1}{N} \sum_{j=1}^K \sum_{i=i_{\min}^{[t,1]}}^{N-j} J_j^L \left(\omega, i, tz_1 + (1-t)z_2 + \frac{\tilde{\phi}_N^{i+j} - \tilde{\phi}_N^i}{j} \right) \\
 & \leq \left(1 - t + \frac{2}{N} \right) J_{\text{hom}}^{L,(N)}(\omega, z_2, [t, 1]) + \frac{|NI_\epsilon(t) \cap \mathbb{Z}|}{N} C_3 C^{L,H,(N)}(\omega) + \frac{|NI_\epsilon(1) \cap \mathbb{Z}|}{N} C_4 C^{L,H,(N)}(\omega). \tag{4.21}
 \end{aligned}$$

Step C: Third term of (4.17).

The third term of (4.17) is

$$\frac{1}{N} \sum_{j=2}^K \sum_{s=0}^{j-2} J_j^L \left(\omega, i_{\max}^{[0,t]} - s, tz_1 + (1-t)z_2 + \frac{\tilde{\phi}_{N, i_{\max}^{[0,t]}-s+j}^{[0,t]} - \tilde{\phi}_{N, i_{\max}^{[0,t]}-s}^{[0,t]}}{j} \right).$$

For the given values of s and j , it holds true that $\tilde{\phi}_N^{i+j} - \tilde{\phi}_N^i = 0$ because of $i_{\max}^{[0,t]} + 2 - K \leq i \leq i_{\max}^{[0,t]} + K$. This yields

$$\begin{aligned} & \frac{1}{N} \sum_{j=2}^K \sum_{s=0}^{j-2} J_j^L \left(\omega, i_{\max}^{[0,t]} - s, tz_1 + (1-t)z_2 + \frac{\tilde{\phi}_{N, i_{\max}^{[0,t]}-s+j}^{[0,t]} - \tilde{\phi}_{N, i_{\max}^{[0,t]}-s}^{[0,t]}}{j} \right) \\ & \leq \frac{1}{N} \sum_{j=2}^K \sum_{s=0}^{j-2} d \max \{ \Psi(tz_1 + (1-t)z_2), |tz_1 + (1-t)z_2| \} \\ & \leq \frac{1}{N} \frac{1}{2} (K+1) KC \rightarrow 0 \quad \text{as } N \rightarrow \infty. \end{aligned} \tag{4.22}$$

Step D: Conclusion of (4.17).

Bringing together all previous estimates (4.19), (4.21) and (4.22), we perform the limit $N \rightarrow \infty$ in (4.17) and get, with the convergence of the constant $C^{L,H,(N)}(\omega) \rightarrow C^{L,H}$ from (4.3),

$$J_{\text{hom}}^L(tz_1 + (1-t)z_2) \leq tJ_{\text{hom}}^L(z_1) + (1-t)J_{\text{hom}}^L(z_2) + \epsilon(C_1 + 2C_2 + 2C_3 + C_4)C^{L,H},$$

where Proposition 4.6 yields the existence of $\Omega' \subset \Omega$ with $\mathbb{P}(\Omega') = 1$ such that the above calculated limit exists for all $\omega \in \Omega'$ and all $z_1, z_2 \in \mathbb{R}$. Finally, we can perform the limit $\epsilon \rightarrow 0$ and get

$$J_{\text{hom}}^L(tz_1 + (1-t)z_2) \leq tJ_{\text{hom}}^L(z_1) + (1-t)J_{\text{hom}}^L(z_2),$$

which shows convexity.

Step 3. Γ -limit.

Let $(z_N)_{N \in \mathbb{N}}$ be a sequence converging to z . Then, for every $N \in \mathbb{N}$ we denote a minimizer related to the minimum problem of $J_{\text{hom}}^{L,(N)}(\omega, z_N, A)$ by $\phi_{N, z_N} : (NA \cap \mathbb{Z}) \rightarrow \mathbb{R}$, i.e.

$$J_{\text{hom}}^{L,(N)}(\omega, z_N, A) = \frac{1}{|NA \cap \mathbb{Z}|} \sum_{j=1}^K \sum_{\substack{i \in NA \cap \mathbb{Z} \\ i+j-1 \in NA}} J_j^L \left(\omega, i, z_N + \frac{\phi_{N, z_N}^{i+j} - \phi_{N, z_N}^i}{j} \right).$$

Now, we have

$$\begin{aligned} J_{\text{hom}}^{L,(N)}(\omega, z_N, A) &= \frac{1}{|NA \cap \mathbb{Z}|} \sum_{j=1}^K \sum_{\substack{i \in NA \cap \mathbb{Z} \\ i+j-1 \in NA}} J_j^L \left(\omega, i, z + \frac{\phi_{N, z_N}^{i+j} - \phi_{N, z_N}^i}{j} \right) \\ &+ \frac{1}{|NA \cap \mathbb{Z}|} \sum_{j=1}^K \sum_{\substack{i \in NA \cap \mathbb{Z} \\ i+j-1 \in NA}} \left(J_j^L \left(\omega, i, z_N + \frac{\phi_{N, z_N}^{i+j} - \phi_{N, z_N}^i}{j} \right) - J_j^L \left(\omega, i, z + \frac{\phi_{N, z_N}^{i+j} - \phi_{N, z_N}^i}{j} \right) \right) \end{aligned}$$

$$\geq J_{\text{hom}}^{L,(N)}(\omega, z, A) - C^{L,H,(N)}(\omega)|z - z_N|^\alpha,$$

where the last step is due to (4.3) and since $|z - z_N| \leq |z - z_N|^\alpha$ for N large enough. Recalling that $z_N \rightarrow z$ and $C^{L,H,(N)}(\omega) \rightarrow C^{L,H}$ in the limit $N \rightarrow \infty$ by (4.3) and with Proposition 4.6, we get for $\omega \in \Omega'$, by taking the limit $\liminf_{N \rightarrow \infty}$,

$$\begin{aligned} \liminf_{N \rightarrow \infty} J_{\text{hom}}^{L,(N)}(\omega, z_N, A) &\geq \liminf_{N \rightarrow \infty} J_{\text{hom}}^{L,(N)}(\omega, z, A) - \limsup_{N \rightarrow \infty} \left(C^{L,H,(N)}(\omega)|z - z_N|^\alpha \right) \\ &= J_{\text{hom}}^L(z), \end{aligned}$$

which shows the liminf-inequality. We can take for every $z \in \mathbb{R}$ the constant recovery sequence $z_N := z$ and get

$$\limsup_{N \rightarrow \infty} J_{\text{hom}}^{L,(N)}(\omega, z_N, A) = \limsup_{N \rightarrow \infty} J_{\text{hom}}^{L,(N)}(\omega, z, A) = J_{\text{hom}}^L(z),$$

due to Proposition 4.6. This shows the limsup-inequality and completes the proof of the Γ -limit. \square

4.1.2 Limiting functional of the approximation

So far, we have established the limit J_{hom}^L and have worked out properties of this function. Now, we want to recover the homogenization formula for the original Lennard-Jones type potentials. This means that we have to pass to the limit $L \rightarrow \infty$ in the approximation functions, with the limit being J_{hom} . The rest of this section is devoted to the proof of the approximation limit, which establishes J_{hom} as the limit of the homogenization formula of the approximation.

We start with a technical lemma, preparing the proof of the limit as $L \rightarrow \infty$. Even though it is only a technical tool, it is the crucial step towards removing the approximation.

Lemma 4.9. *Let Assumption 3.3 be satisfied. There exists an $\Omega' \subset \Omega$ with $\mathbb{P}(\Omega') = 1$ such that for every $z \in (0, +\infty)$ and $\omega \in \Omega'$ it holds true that*

$$\liminf_{L \rightarrow \infty} J_{\text{hom}}^L(z) \geq \limsup_{N \rightarrow \infty} J_{\text{hom}}^{L,(N)}(\omega, z, A). \quad (4.23)$$

Proof. We present the proof for $A = [0, 1]$; the proof for a general interval is essentially the same. First, note that the assumption $z \in (0, +\infty)$ implies finite values of the energy. To show (4.23), we start for a given z with a minimizer related to the minimum problem of $J_{\text{hom}}^{L,(N)}(\omega, z)$, which we call $\bar{z}_{L,N} = (\bar{z}_{L,N}^0, \dots, \bar{z}_{L,N}^{N-1})$, i.e.

$$J_{\text{hom}}^{L,(N)}(\omega, z, [0, 1]) = \frac{1}{N} \sum_{j=1}^K \sum_{i=0}^{N-j} J_j^L \left(\omega, i, \frac{1}{j} \sum_{k=i}^{i+j-1} \bar{z}_{L,N}^k \right).$$

We define the set of all indices i with $\bar{z}_{L,N}^i$ being in the regime where J_j and its approximation J_j^L differ by

$$I_{L,N} := \{i : \bar{z}_{L,N}^i < z_L\}, \quad \text{for all } L, N \in \mathbb{N}.$$

Step 1. We claim that

$$\lim_{L \rightarrow \infty} \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i \in I_{L,N}} (z_L - \hat{z}_{L,N}^i) = 0. \quad (4.24)$$

By definition of $I_{L,N}$, every term in the sum in (4.24) is non-negative. Suppose that for some $\epsilon > 0$ it holds

$$\limsup_{L \rightarrow \infty} \limsup_{N \rightarrow \infty} \frac{1}{N} \sum_{i \in I_{L,N}} (z_L - \hat{z}_{L,N}^i) \geq \epsilon. \quad (4.25)$$

We recall that $m_j^L(\omega)$ is the slope of J_j^L in the regime $z \leq z_L$ due to Definition 4.1. Using Proposition 4.6 and (LJ2), we obtain

$$\begin{aligned} J_{\text{hom}}^L(z) &= \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{j=1}^K \sum_{i=0}^{N-j} J_j \left(\tau_i \omega, \frac{1}{j} \sum_{k=i}^{i+j-1} \hat{z}_{L,N}^k \right) \\ &= \limsup_{N \rightarrow \infty} \frac{1}{N} \sum_{j=2}^K \sum_{i=0}^{N-j} J_j \left(\tau_i \omega, \frac{1}{j} \sum_{k=i}^{i+j-1} \hat{z}_{L,N}^k \right) + \limsup_{N \rightarrow \infty} \frac{1}{N} \sum_{i \notin I_{L,N}} J_1 \left(\tau_i \omega, \hat{z}_{L,N}^i \right) \\ &\quad + \limsup_{N \rightarrow \infty} \frac{1}{N} \sum_{i \in I_{L,N}} J_1 \left(\tau_i \omega, z_L \right) + \limsup_{N \rightarrow \infty} \frac{1}{N} \sum_{i \in I_{L,N}} m_1^L(\tau_i \omega) (\hat{z}_{L,N}^i - z_L) \\ &\geq -Kd + \limsup_{N \rightarrow \infty} \frac{1}{N} \sum_{i \in I_{L,N}} m_1^L(\tau_i \omega) (\hat{z}_{L,N}^i - z_L) \geq -Kd + M^L \limsup_{N \rightarrow \infty} \frac{1}{N} \sum_{i \in I_{L,N}} (z_L - \hat{z}_{L,N}^i), \end{aligned}$$

where the last inequality is due to Proposition 4.3 (ii). Hence, a combination of (4.2) and the assumption (4.25) yields

$$\limsup_{L \rightarrow \infty} J_{\text{hom}}^L(z) = \infty.$$

This is absurd in view of the estimate

$$J_{\text{hom}}^L(z) \leq Kd \max\{\Psi(z), |z|\} < \infty,$$

valid for every $L \in \mathbb{N}$. Thus the claim is proven.

Step 2. Conclusion

We provide a new sequence of competitors $(\hat{z}_{L,N})$ for the minimization problem in $J_{\text{hom}}^{L,(N)}(\omega, z)$ satisfying $\hat{z}_{L,N}^i \geq z_L$ for all $i \in \{0, \dots, N-1\}$ and

$$\lim_{L \rightarrow \infty} \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{j=1}^K \sum_{i=0}^{N-j} \left(J_j^L \left(\tau_i \omega, \frac{1}{j} \sum_{k=i}^{i+j-1} \hat{z}_{L,N}^k \right) - J_j^L \left(\tau_i \omega, \frac{1}{j} \sum_{k=i}^{i+j-1} \hat{z}_{L,N}^k \right) \right) \geq 0. \quad (4.26)$$

Obviously (4.26) and $\hat{z}_{L,N}^i \geq z_L$ for all $i \in \{0, \dots, N-1\}$ imply the claim (4.23), due to

$$\begin{aligned} 0 &\leq \lim_{L \rightarrow \infty} \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{j=1}^K \sum_{i=0}^{N-j} \left(J_j^L \left(\tau_i \omega, \frac{1}{j} \sum_{k=i}^{i+j-1} \hat{z}_{L,N}^k \right) - J_j^L \left(\tau_i \omega, \frac{1}{j} \sum_{k=i}^{i+j-1} \hat{z}_{L,N}^k \right) \right) \\ &= \liminf_{L \rightarrow \infty} \liminf_{N \rightarrow \infty} \frac{1}{N} \sum_{j=1}^K \sum_{i=0}^{N-j} \left(J_j^L \left(\tau_i \omega, \frac{1}{j} \sum_{k=i}^{i+j-1} \hat{z}_{L,N}^k \right) - J_j \left(\tau_i \omega, \frac{1}{j} \sum_{k=i}^{i+j-1} \hat{z}_{L,N}^k \right) \right) \end{aligned}$$

$$\begin{aligned}
 & \stackrel{(*)}{=} \liminf_{L \rightarrow \infty} \left(J_{\text{hom}}^L(z) - \limsup_{N \rightarrow \infty} \frac{1}{N} \sum_{j=1}^K \sum_{i=0}^{N-j} J_j \left(\tau_i \omega, \frac{1}{j} \sum_{k=i}^{i+j-1} \hat{z}_{L,N}^k \right) \right) \\
 & \leq \liminf_{L \rightarrow \infty} \left(J_{\text{hom}}^L(z) - \limsup_{N \rightarrow \infty} J_{\text{hom}}^{(N)}(\omega, z) \right) \stackrel{(**)}{\leq} \liminf_{L \rightarrow \infty} J_{\text{hom}}^L(z) - \limsup_{N \rightarrow \infty} \frac{1}{N} \sum_{j=1}^K \sum_{i=0}^{N-j} J_{\text{hom}}^{(N)}(\omega, z),
 \end{aligned}$$

where the last step $(**)$ holds because $J_{\text{hom}}^{(N)}(\omega, z)$ is independent of L , and in $(*)$ Proposition 4.6, together with $\liminf_{k \rightarrow \infty} (a_k + b_k) = a + \liminf b_k$ if $a_k \rightarrow a$, was used. Indeed, it holds true that $-a + \liminf (a_k + b_k) = \liminf(-a_k) + \liminf(a_k + b_k) \leq \liminf(b_k)$ and thus $\liminf(a_k + b_k) \leq a + \liminf(b_k)$. The reverse inequality is trivial, since $\liminf(a_k + b_k) \geq \liminf(a_k) + \liminf(b_k) = a + \liminf(b_k)$.

Since $z_L \rightarrow 0$ as $L \rightarrow \infty$, it holds true that $z_L < z$ for L big enough. Especially the constraint $\bar{z}_N^s = \bar{z}_N^{N-s-1} = z$ for $s = 0, \dots, K-2$ creates no conflict regarding the purpose of constructing a minimizer with $\hat{z}_N^i > z_L$ for every $i \in \{0, \dots, N\}$.

In what follows we suppose that there exists $i \in \{0, \dots, N-1\}$ such that $\hat{z}_{L,N}^i < z_L$ (the other case is trivial). The constraint $\sum_{i=0}^{N-1} (\hat{z}_N^i - z) = 0$, implies $I_{L,N,z} := \{i : z < \hat{z}_{L,N}^i\} \neq \emptyset$ and we obtain

$$\begin{aligned}
 0 &= \sum_{i=0}^{N-1} (\hat{z}_{L,N}^i - z) \leq \sum_{i \in I_{L,N,z}} (\hat{z}_{L,N}^i - z) + \sum_{i \in I_{L,N}} (\hat{z}_{L,N}^i - z) \\
 \Leftrightarrow & \sum_{i \in I_{L,N}} (z - \hat{z}_{L,N}^i) \leq \sum_{i \in I_{L,N,z}} (\hat{z}_{L,N}^i - z).
 \end{aligned} \tag{4.27}$$

Combining (4.27) and the assumption $z_L < z$, we find v_N^i for $i = 0, \dots, N-1$ with $0 \leq v_N^i \leq \max\{\hat{z}_N^i - z, 0\}$ and

$$\sum_{i \in I_{L,N}} (z_L - \hat{z}_{L,N}^i) = \sum_{i=0}^{N-1} v_N^i. \tag{4.28}$$

Notice that by construction $v_N^i = 0$ whenever $i \notin I_{L,N,z}$. Next, we define $\hat{z}_{L,N}$ by

$$\hat{z}_{L,N}^i = \begin{cases} z_L & \text{for } i \in I_{L,N}, \\ \hat{z}_{L,N}^i - v_N^i & \text{for } i \notin I_{L,N}. \end{cases}$$

By definition it holds $\hat{z}_{L,N}^i \geq z_L$ for every i and $\hat{z}_{L,N}$ is a competitor for the minimization problem in the definition of $J_{\text{hom}}^{L,(N)}$. Indeed, $\hat{z}_{L,N}^i = \hat{z}_{L,N}^i = z$ for all $i \in \{0, \dots, K-1\} \cup \{N-K+1, \dots, N-1\}$ and this competitor also fulfils the boundary constraint, which can be seen by

$$\begin{aligned}
 \sum_{i=0}^{N-1} (\hat{z}_N^i - z) &= \sum_{i \in I_L} (z_L - z) + \sum_{i \notin I_L} (\hat{z}_N^i - v_N^i - z) \\
 &= \sum_{i \in I_L} (z_L - z) - \sum_{i \in I_L} (\hat{z}_N^i - z) + \sum_{i=0}^{N-1} (\hat{z}_N^i - z) - \sum_{i=0}^{N-1} v_N^i = \sum_{i \in I_L} (z_L - \hat{z}_N^i) - \sum_{i=0}^{N-1} v_N^i \stackrel{(4.28)}{=} 0
 \end{aligned}$$

Fix $\hat{\rho} = \hat{\rho}(b, d, \Psi) \in (0, \frac{1}{d}]$ such that

$$\frac{1}{d}\Psi(z) - d \geq b \quad \text{for all } z \leq \hat{\rho}, \quad (4.29)$$

where b, d and Ψ are the constants and the convex function from the definition of \mathcal{J} , respectively. Further, we define $\rho_z := \min\{\frac{z}{K}, \frac{1}{d}, \hat{\rho}\}$. We consider for all L sufficiently large such that $z_L < \rho_z$

$$\text{Diff}_{i,j}^{L,N} := J_j^L \left(\tau_i \omega, \frac{1}{j} \sum_{k=i}^{i+j-1} z_{L,N}^k \right) - J_j^L \left(\tau_i \omega, \frac{1}{j} \sum_{k=i}^{i+j-1} \hat{z}_{L,N}^k \right).$$

To show (4.26), we distinguish three cases:

- *Case (i)*: $\frac{1}{j} \sum_{k=i}^{i+j-1} z_{L,N}^k \leq \frac{1}{j} \sum_{k=i}^{i+j-1} \hat{z}_{L,N}^k \leq \delta_j(\tau_i \omega)$. Since $J_j^L(\tau_i \omega, \cdot)$ is monotonically decreasing on $(0, \delta_j(\tau_i \omega)]$ (see (LJ2)) it follows $\text{Diff}_{i,j}^{L,N} \geq 0$.
- *Case (ii)*: $\frac{1}{j} \sum_{k=i}^{i+j-1} z_{L,N}^k \geq \delta_j(\tau_i \omega)$. It is $\text{Diff}_{i,j}^{L,N} \geq \frac{1}{d}\Psi \left(\frac{1}{j} \sum_{k=i}^{i+j-1} z_{L,N}^k \right) - d - b$. By the definition of $\hat{\rho}$ (see (4.29)), we have either $\text{Diff}_{i,j}^{L,N} \geq 0$ or $\frac{1}{j} \sum_{k=i}^{i+j-1} z_{L,N}^k \geq \hat{\rho} \geq z_L$.
- *Case (iii)*: $\frac{1}{j} \sum_{k=i}^{i+j-1} z_{L,N}^k \leq \delta_j(\tau_i \omega)$ and $\frac{1}{j} \sum_{k=i}^{i+j-1} z_{L,N}^k \leq \frac{1}{j} \sum_{k=i}^{i+j-1} \hat{z}_{L,N}^k$. By the definition of \hat{z} , there exists $\hat{k} \in \{i, \dots, i+j-1\}$ such that $\hat{z}_{L,N}^{\hat{k}} \geq z$ and thus $\frac{1}{j} \sum_{k=i}^{i+j-1} \hat{z}_{L,N}^k \geq \frac{1}{K}z$, since $\hat{z}_{L,N}^k \geq 0$ due to the finite value of the energy.

Those indices i where $\text{Diff}_{i,j}^{L,N} \geq 0$ holds true, do not cause a problem regarding the proof of (4.26). In order to conclude the proof of (4.26), we have to further consider *Case (iii)* and the part of *Case (ii)* where $\frac{1}{j} \sum_{k=i}^{i+j-1} z_{L,N}^k \geq \hat{\rho}$. As an abbreviation, we name the set of those remaining indices I_{rem} . For this, we need a finer estimation and define sets of *small* and *big* shifts. Let $\mu > 0$, then we get

$$\begin{aligned} I_{L,N;j} &:= \{i \in \{0, \dots, N-j\} : \{i, \dots, i+j-1\} \cap I_L \neq \emptyset\}, \\ I_{L,N;j}^s &:= \{i \in \{0, \dots, N-j\} \setminus I_{L,N;j} : v_N^k < \mu \text{ for all } k = i, \dots, i+j-1\}, \\ I_{L,N;j}^b &:= \{0, \dots, N-j\} \setminus (I_{L,N;j} \cup I_{L,N;j}^s), \\ \tilde{I}_{L,N;j}^s &:= \{i \in I_{L,N;j} : |z_N^k - \hat{z}_N^k| < \mu \text{ for all } k = i, \dots, i+j-1\}, \\ \tilde{I}_{L,N;j}^b &:= I_{L,N;j} \setminus \tilde{I}_{L,N;j}^s \end{aligned}$$

We claim that for every $\mu > 0$ and for every $j = 1, \dots, K$ it holds true that

$$\lim_{L \rightarrow \infty} \lim_{N \rightarrow \infty} |I_{L,N;j}^b|/N = 0 \quad \text{and} \quad \lim_{L \rightarrow \infty} \lim_{N \rightarrow \infty} |\tilde{I}_{L,N;j}^b|/N = 0. \quad (4.30)$$

Indeed by definition, we have

$$0 \leq \frac{1}{N} \sum_{i \in I_{L,N,z}} v_N^i = \frac{1}{N} \sum_{i \in \tilde{I}_{L,N;1}^s} v_N^i + \frac{1}{N} \sum_{i \in I_{L,N;1}^b} v_N^i \stackrel{(4.28)}{=} \frac{1}{N} \sum_{i \in I_{L,N}} (z_L - \hat{z}_{L,N}^i),$$

and the asymptotic result $\lim_{L \rightarrow \infty} \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i \in I_{L,N}} (z_L - \bar{z}_{L,N}^i) = 0$ from (4.24). Therefore, we have $\lim_{L \rightarrow \infty} \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i \in I_s^1} v_N^i = 0$ as well as $\lim_{L \rightarrow \infty} \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i \in I_{L,N;1}^b} v_N^i = 0$, because of $v_n^i \geq 0$. In particular, since we have

$$0 \leq \frac{|I_{L,N;1}^b|}{N} \mu \leq \frac{1}{N} \sum_{i \in I_{L,N;1}^b} v_N^i,$$

it follows that for every $\mu > 0$ it holds true that $\lim_{L \rightarrow \infty} \lim_{N \rightarrow \infty} |I_{L,N;1}^b|/N = 0$. Since $|I_{L,N;j}^b| \leq K|I_{L,N;1}^b|$, we also get $\lim_{L \rightarrow \infty} \lim_{N \rightarrow \infty} |I_{L,N;j}^b|/N = 0$ for every $j = 1, \dots, K$. In an analogous way, we have

$$0 \leq \frac{1}{N} \sum_{i \in \tilde{I}_{L,N;1}^s} (z_L - \bar{z}_N^i) + \frac{1}{N} \sum_{i \in \tilde{I}_{L,N;1}^b} (z_L - \bar{z}_N^i) = \frac{1}{N} \sum_{i \in I_{L,N}} (z_L - \bar{z}_N^i),$$

and the asymptotic decay $\lim_{L \rightarrow \infty} \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i \in I_{L,N}} (z_L - \bar{z}_{L,N}^i) = 0$ from (4.24), which yields $\lim_{L \rightarrow \infty} \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i \in \tilde{I}_{L,N;1}^b} (z_L - \bar{z}_{L,N}^i) = 0$. Together with

$$0 \leq \frac{|\tilde{I}_{L,N;1}^b|}{N} \mu \leq \frac{1}{N} \sum_{i \in \tilde{I}_{L,N;1}^b} (z_L - \bar{z}_{L,N}^i),$$

this yields $\lim_{L \rightarrow \infty} \lim_{N \rightarrow \infty} |\tilde{I}_{L,N;1}^b|/N = 0$. Since $|\tilde{I}_{L,N;j}^b| \leq K|\tilde{I}_{L,N;1}^b| + K|I_{L,N;1}^b|$, we also get $\lim_{L \rightarrow \infty} \lim_{N \rightarrow \infty} |\tilde{I}_{L,N;j}^b|/N = 0$, for every $j = 1, \dots, K$. This concludes the proof of claim (4.30).

Now, we consider (4.26) for the remaining indices I_{rem} , separately for the previously defined small and big shift sets. We start with the big ones. By definition of *Case (ii) and (iii)* we get $\hat{z}_N^i \geq \rho_z$ for all $i \in I_{\text{rem}}$ and using (LJ2) yields

$$\text{Diff}_{i,j}^{L,N} = J_j^L \left(\omega, i, \frac{1}{j} \sum_{k=i}^{i+j-1} z_N^k \right) - J_j^L \left(\omega, i, \frac{1}{j} \sum_{k=i}^{i+j-1} \hat{z}_N^k \right) \geq -d - d \max \{ \Psi(\rho_z), |\rho_z|, b \} =: -C_z$$

and therefore for (4.26)

$$\begin{aligned} & \frac{1}{N} \sum_{j=1}^K \sum_{i \in (I_{L,N;j}^b \cup \tilde{I}_{L,N;j}^b) \cap I_{\text{rem}}} \left(J_j^L \left(\omega, i, \frac{1}{j} \sum_{k=i}^{i+j-1} z_N^k \right) - J_j^L \left(\omega, i, \frac{1}{j} \sum_{k=i}^{i+j-1} \hat{z}_N^k \right) \right) \\ & \geq \frac{1}{N} \sum_{j=1}^K \sum_{i \in (I_{L,N;j}^b \cup \tilde{I}_{L,N;j}^b) \cap I_{\text{rem}}} -C_z \geq -\frac{|I_{L,N;j}^b| + |\tilde{I}_{L,N;j}^b|}{N} K(-C_z). \end{aligned}$$

Together with (4.30) this shows (4.26) for the big shift sets. The small shift sets yield by definition $\hat{z}_N^i \geq \rho_z$ and $\bar{z}_N^i \geq \rho_z$ and allow for the following calculation: with (4.3) and for $\mu < 1$ we get

$$\frac{1}{N} \sum_{j=1}^K \sum_{i \in (I_{L,N;j}^s \cup \tilde{I}_{L,N;j}^s) \cap I_{\text{rem}}} \left(J_j^L \left(\omega, i, \frac{1}{j} \sum_{k=i}^{i+j-1} z_N^k \right) - J_j^L \left(\omega, i, \frac{1}{j} \sum_{k=i}^{i+j-1} \hat{z}_N^k \right) \right)$$

$$\begin{aligned}
 &\geq -\frac{1}{N} \sum_{j=1}^K \sum_{i \in (I_{L,N;j}^s \cup \tilde{I}_{L,N;j}^s) \cap I_{\text{rem}}} \left| J_j^L \left(\omega, i, \frac{1}{j} \sum_{k=i}^{i+j-1} \bar{z}_N^k \right) - J_j^L \left(\omega, i, \frac{1}{j} \sum_{k=i}^{i+j-1} \hat{z}_N^k \right) \right| \\
 &\geq -\frac{1}{N} \sum_{j=1}^K \sum_{i \in (I_{L,N;j}^s \cup \tilde{I}_{L,N;j}^s) \cap I_{\text{rem}}} [J_j(\tau_i \omega)]_{C^{0,\alpha}(\rho_z, \infty)} \mu^\alpha \geq -\frac{1}{N} \sum_{j=1}^K \sum_{i=0}^{N-1} [J_j(\tau_i \omega)]_{C^{0,\alpha}(\rho_z, \infty)} \mu^\alpha,
 \end{aligned}$$

because $|\bar{z}_N^k - \hat{z}_N^k| = v_N^k < \mu$ or $|\bar{z}_N^k - \hat{z}_N^k| = |\bar{z}_N^k - z_L| < \mu$, by the definition of the small shift set. Here, $[\cdot]_{C^{0,\alpha}(\rho_z, \infty)}$ is the Hölder seminorm. Now, (H1), Proposition 3.5 and Proposition 4.3 (i) yield for fixed $\mu > 0$

$$\lim_{L \rightarrow \infty} \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{j=1}^K \sum_{i=0}^{N-1} [J_j(\tau_i \omega)]_{C^{0,\alpha}(\rho_z, \infty)} \mu^\alpha = \lim_{L \rightarrow \infty} \mu^\alpha C(\rho_z) = \mu^\alpha C(\rho_z),$$

with a constant $C(\rho_z)$ independent of L . As this holds for every $\mu > 0$, we can take afterwards the limit $\mu \rightarrow 0$, which shows (4.26) for the small shift sets and concludes the proof. \square

Finally, we can state the result that the homogenization formula for the approximation converges to the original homogenization formula J_{hom} in the limit $L \rightarrow \infty$.

Proposition 4.10. *Let Assumption 3.3 be satisfied. There exists an $\Omega' \subset \Omega$ with $\mathbb{P}(\Omega') = 1$ such that the following is true: For all $\omega \in \Omega'$, $z \in \mathbb{R}$ and $A := [a, b]$ with $a, b \in \mathbb{R}$ it holds true that $\lim_{N \rightarrow \infty} J_{\text{hom}}^{(N)}(\omega, z, A)$ exists in \mathbb{R} and is independent of ω and A . Moreover, it is*

$$\lim_{N \rightarrow \infty} J_{\text{hom}}^{(N)}(\omega, z, A) = \lim_{L \rightarrow \infty} J_{\text{hom}}^L(z).$$

Proof. For $z \notin (0, +\infty)$, we have $\lim_{N \rightarrow \infty} J_{\text{hom}}^{(N)}(\omega, z, A) = \infty$ and $\lim_{L \rightarrow \infty} J_{\text{hom}}^L(z) = \infty$, because of (LJ1) and the definition of the regularization. Hence, the assertion is proven in this case.

Fix $\omega \in \Omega'$, $z \in (0, +\infty)$ and $A = [a, b]$, $a, b \in \mathbb{R}$. We prove two inequalities. The first one is simple to show. By the definition of the regularization J_j^L it obviously holds true that $J_{\text{hom}}^{L,(N)}(\omega, z, A) \leq J_{\text{hom}}^{(N)}(\omega, z, A)$ and thus by Proposition 4.6

$$J_{\text{hom}}^L(z) \leq \liminf_{N \rightarrow \infty} J_{\text{hom}}^{(N)}(\omega, z, A). \quad (4.31)$$

Lemma 4.9 yields for every $z \in \mathbb{R}$ the second inequality

$$\liminf_{L \rightarrow \infty} J_{\text{hom}}^L(z) \geq \limsup_{N \rightarrow \infty} J_{\text{hom}}^{(N)}(\omega, z, A). \quad (4.32)$$

The inequalities (4.31) and (4.32) together yield

$$\lim_{L \rightarrow \infty} J_{\text{hom}}^L(z) = \lim_{N \rightarrow \infty} J_{\text{hom}}^{(N)}(\omega, z, A),$$

which has a left-hand side independent of ω and A and therefore shows that $\lim_{N \rightarrow \infty} J_{\text{hom}}^{(N)}(\omega, z, A)$ exists and is independent of ω and A . Altogether, this shows the assertions of the proposition. \square

Remark 4.11. In [73], the authors deal with a situation similar to ours. Apart from the growth conditions ruling out e.g. the classical Lennard-Jones potential, the main difference is the number of potentials considered. In [73] a discrete probability density is considered, while in our case the set $\mathcal{J}(\alpha, b, d, \Psi)$ can be infinite, even uncountable, which refers to a continuous probability density. This continuous density requires the technical result of Lemma 4.9 as a main ingredient of our proof of Proposition 4.10.

4.2 Homogenized energy density

In the previous section, we have established the limit of $J_{\text{hom}}^{(N)}$ being equal to the limit of the homogenized energy density with respect to the approximations of the interaction potentials as $L \rightarrow \infty$. We are now in the position to prove the existence of the homogenization formula J_{hom} , which uses the unapproximated, original interaction potentials. Further, we derive a number of properties of J_{hom} . In particular, we prove in the following proposition convexity, lower semicontinuity, monotonicity and a blow up at zero, as well as a Γ -convergence result. The section is closed by a proposition showing special results for the case of nearest neighbour interactions.

J_{hom} will be an important ingredient of the Γ -limit. In Remark 4.15, some further observations about the homogenization formula are highlighted, additional to the following proposition.

Proposition 4.12. *Let Assumption 3.3 be satisfied. There exists an $\Omega' \subset \Omega$ with $\mathbb{P}(\Omega') = 1$ such that the following is true: For all $\omega \in \Omega'$, $z \in \mathbb{R}$ and $A := [a, b]$ with $a, b \in \mathbb{R}$ it holds*

$$J_{\text{hom}}(z) = \lim_{N \rightarrow \infty} \mathbb{E} \left[J_{\text{hom}}^{(N)}(\cdot, z, [0, 1]) \right] = \lim_{N \rightarrow \infty} J_{\text{hom}}^{(N)}(\omega, z, A). \quad (4.33)$$

The map $z \mapsto J_{\text{hom}}(z)$ is convex, lower semicontinuous, monotonically decreasing and satisfies

$$\lim_{z \rightarrow 0^+} J_{\text{hom}}(z) = +\infty. \quad (4.34)$$

Moreover, it holds for every $\omega \in \Omega'$ and $A := [a, b]$, $a, b \in \mathbb{R}$

$$\Gamma\text{-}\lim_{N \rightarrow \infty} J_{\text{hom}}^{(N)}(\omega, \cdot, A) = J_{\text{hom}}. \quad (4.35)$$

Proof. We prove the different claims separately in the next steps.

Step 1. Equation (4.33)

By Proposition 4.10 $J_{\text{hom}}^{(N)}(\cdot, z, A)$ converges pointwise almost everywhere on Ω in $\overline{\mathbb{R}}$ to a function $f(z)$ independent of ω and A . The upper bound from (LJ2) together with the dominated convergence theorem then yields

$$\lim_{N \rightarrow \infty} \mathbb{E} \left[J_{\text{hom}}^{(N)}(\cdot, z, [0, 1]) \right] = \mathbb{E}[f(z)] = f(z),$$

where the last equality holds true since $f(z)$ is independent of ω . This shows the second equality in (4.33).

Further in view of an application of the subadditive ergodic theorem of Akcoglu and Krengel, we note that $NJ_{\text{hom}}^{(N)}(\cdot, z, [0, 1])$ is subadditive in view of Proposition 4.4 and Remark 4.5. Because of linearity and monotonicity of the expectation value, it also holds true that $\mathbb{E} \left[NJ_{\text{hom}}^{(N)}(\cdot, z, [0, 1]) \right]$

is subadditive. Thus, we can apply Theorem 2.17, a result from the theory of subadditive functions, to get (again with linearity of the expectation value)

$$\begin{aligned} J_{\text{hom}}(z) &= \inf_{N \in \mathbb{N}} \mathbb{E} \left[J_{\text{hom}}^{(N)}(\cdot, z, [0, 1]) \right] = \inf_{N \in \mathbb{N}} \frac{\mathbb{E} \left[N J_{\text{hom}}^{(N)}(\cdot, z, [0, 1]) \right]}{N} \\ &= \lim_{N \rightarrow \infty} \frac{\mathbb{E} \left[N J_{\text{hom}}^{(N)}(\cdot, z, [0, 1]) \right]}{N} = \lim_{N \rightarrow \infty} \mathbb{E} \left[J_{\text{hom}}^{(N)}(\cdot, z, [0, 1]) \right]. \end{aligned}$$

This shows the first equality in (4.33) and justifies $f(z) = J_{\text{hom}}(z)$.

Step 2. This step deals with the properties of the map $z \mapsto J_{\text{hom}}(z)$, namely convexity, lower semicontinuity, monotonicity and the blow up at zero.

Convexity.

By Proposition 4.10, $J_{\text{hom}}(z) = \lim_{L \rightarrow \infty} J_{\text{hom}}^L(z)$ holds true, and $J_{\text{hom}}^L(z)$ is convex due to Proposition 4.8. Therefore, we get the convexity of $J_{\text{hom}}(z)$, because it is the pointwise limit of a sequence of convex functions and therefore convex itself.

Lower semicontinuity.

Due to convexity, $J_{\text{hom}}(z)$ is continuous on its domain, i.e. on $(0, +\infty)$. Further, we get from (3.2) the estimate

$$\lim_{z \rightarrow 0^+} J_{\text{hom}}(z) \stackrel{(4.38)}{\geq} \lim_{z \rightarrow 0^+} \left(\frac{1}{d} K \Psi(z) - Kd \right) \stackrel{(3.2)}{=} \infty. \quad (4.36)$$

This shows lower semicontinuity.

Monotonicity.

The map J_{hom} is bounded from below, which can be seen from (4.38) and $\Psi \geq 0$.

Next, we prove that J_{hom} is monotone decreasing. For this we fix $0 < \gamma < z < \infty$ and show $J_{\text{hom}}(\gamma) \geq J_{\text{hom}}(z)$. Let $z_N : \{0, \dots, N-1\} \rightarrow \mathbb{R}$ be a minimizer related to the minimum problem of $J_{\text{hom}}^{(N)}(\omega, \gamma)$, i.e. $z_N^s = z_N^{N-s-1} = \gamma$ for $s = 0, \dots, K-2$, $\sum_{i=0}^{N-1} z_N^i = N\gamma$ and

$$J_{\text{hom}}^{(N)}(\omega, \gamma) = \frac{1}{N} \sum_{j=1}^K \sum_{i=0}^{N-j} J_j \left(\omega, i, \frac{1}{j} \sum_{k=i}^{i+j-1} z_N^k \right).$$

Next, we manipulate z_N in order to construct a competitor for the minimum problem related to $J_{\text{hom}}^{(N)}(\omega, z)$. We set

$$z_N^i = \begin{cases} z & \text{for } i = 0, \dots, K-2 \text{ and } i = N-K+1, \dots, N-1, \\ (z - \gamma)(N/2 - K + 1) + z_N^{K-1} & \text{for } i = K-1, \\ (z - \gamma)(N/2 - K + 1) + z_N^{N-K} & \text{for } i = N-K, \\ z_N^i & \text{otherwise.} \end{cases}$$

Indeed, \bar{z}_N fulfils the constraints $\sum_{i=0}^{N-1} \bar{z}_N^i = Nz$ and $\bar{z}_N^s = \bar{z}_N^{N-s-1} = z$ for $s = 0, \dots, K-2$. Hence, we can estimate

$$\begin{aligned} J_{\text{hom}}^{(N)}(\omega, z) &\leq \frac{1}{N} \sum_{j=1}^K \sum_{i=0}^{N-j} J_j \left(\omega, i, \frac{1}{j} \sum_{k=i}^{i+j-1} \bar{z}_N^k \right) \\ &= J_{\text{hom}}^{(N)}(\omega, \gamma) + \frac{1}{N} \sum_{j=1}^K \sum_{\substack{i \in \{0, \dots, K-1\} \cup \\ \{N-K-j+1, \dots, N-1\}}} \left(J_j \left(\omega, i, \frac{1}{j} \sum_{k=i}^{i+j-1} \bar{z}_N^k \right) - J_j \left(\omega, i, \frac{1}{j} \sum_{k=i}^{i+j-1} z_N^k \right) \right). \end{aligned} \quad (4.37)$$

We now argue that the remainder converges to 0 as $N \rightarrow \infty$. The second part of the sum can be estimated by $-J_j \left(\omega, i, \frac{1}{j} \sum_{k=i}^{i+j-1} z_N^k \right) \leq d$, due to (LJ2). Since each sum contains at most K elements, the prefactor $\frac{1}{N}$ ensures the convergence to zero.

The first part of the sum needs a finer argument. Due to $\sup_N J_{\text{hom}}^{(N)}(\omega, \gamma) < \infty$, we have $z_N^i > 0$ for every $i = 0, \dots, N-1$. With this, we consider the first part of the sum $J_j \left(\omega, i, \frac{1}{j} \sum_{k=i}^{i+j-1} \bar{z}_N^k \right)$. Now it holds true that $\bar{z}_N^k = z$ for $k \leq K-2$ and $k \geq N-K+1$, and $\bar{z}_N^k \geq (z-\gamma)(N/2 - K + 1)$ for $k = K-1$ and $k = N-K$, and $\bar{z}_N^k \geq 0$ otherwise. This yields $\sum_{k=i}^{i+j-1} \bar{z}_N^k \geq z$ as N large enough. Therefore, $J_j \left(\omega, i, \frac{1}{j} \sum_{k=i}^{i+j-1} \bar{z}_N^k \right)$ is bounded, due to (3.3) from (LJ2). Since both sums contain at most K elements, the prefactor $\frac{1}{N}$ ensures the convergence to 0.

As the remainders in (4.37) vanish as $N \rightarrow \infty$, we get, using Proposition 4.10,

$$J_{\text{hom}}(z) = \lim_{N \rightarrow \infty} J_{\text{hom}}^{(N)}(\omega, z) \leq \lim_{N \rightarrow \infty} J_{\text{hom}}^{(N)}(\omega, \gamma) = J_{\text{hom}}(\gamma),$$

which is the desired result and finally shows that $J_{\text{hom}}(z) = J_{\text{hom}}(\gamma)$ for all $z \geq \gamma$. Together with (4.36), this shows that J_{hom} is monotonically decreasing.

Blow up at zero, proof of (4.34).

From the condition (LJ2) we have

$$\begin{aligned} J_{\text{hom}}^{(N)}(\omega, z, [0, 1]) &= \inf_{\phi \in \mathcal{A}_{N,K}^0([0,1])} \left\{ \frac{1}{N} \sum_{j=1}^K \sum_{i=0}^{N-j} J_j \left(\omega, i, z + \frac{\phi^{i+j} - \phi^i}{j} \right) \right\} \\ &\geq \frac{1}{d} \inf_{\phi \in \mathcal{A}_{N,K}^0([0,1])} \left\{ \sum_{j=1}^K \frac{1}{N} \sum_{i=0}^{N-j} \Psi \left(z + \frac{\phi^{i+j} - \phi^i}{j} \right) \right\} - Kd \geq \frac{1}{d} \sum_{j=1}^K \frac{N-j+1}{N} \Psi(z) - Kd, \end{aligned}$$

where we used in the last estimate Jensen's inequality and $\phi \in \mathcal{A}_{N,K}^0([0,1])$, see (4.6). By taking the limit and since we know from Proposition 4.10 that $J_{\text{hom}}(z)$ exists in $\bar{\mathbb{R}}$, we get

$$J_{\text{hom}}(z) = \lim_{N \rightarrow \infty} J_{\text{hom}}^{(N)}(\omega, z) \geq \frac{1}{d} K \Psi(z) - Kd. \quad (4.38)$$

Clearly, (3.2) and (4.38) imply (4.34).

Step 3. Γ -limit, equation (4.35).

For $z \in \mathbb{R}$, let (z_N) be a sequence with $z_N \rightarrow z$. Then, the definition of the approximation and

Proposition 4.8 yield

$$\liminf_{N \rightarrow \infty} J_{\text{hom}}^{(N)}(\omega, z_N, A) \geq \liminf_{N \rightarrow \infty} J_{\text{hom}}^{L, (N)}(\omega, z_N, A) \geq J_{\text{hom}}^L(z).$$

Further, taking the limit $L \rightarrow \infty$ we get with Proposition 4.10 that $\liminf_{N \rightarrow \infty} J_{\text{hom}}^{(N)}(\omega, z_N, A) \geq J_{\text{hom}}(z)$, which proves the liminf-inequality.

For $z \in \mathbb{Z}$, take the constant recovery sequence $(z_N)_{N \in \mathbb{N}}$ with $z_N := z$. Then it holds true that

$$\limsup_{N \rightarrow \infty} J_{\text{hom}}^{(N)}(\omega, z_N, A) = \limsup_{N \rightarrow \infty} J_{\text{hom}}^{(N)}(\omega, z, A) = J_{\text{hom}}(z),$$

which proves the limsup-inequality and completes the proof of the Γ -limit. \square

If we restrict ourselves to the case of only nearest neighbour interactions, i.e. $K = 1$, we can refine the previous proposition. This is the subject of the next proposition, cf. also Figure 4.2.

Proposition 4.13. *Suppose that Assumption 3.3 is satisfied and set $K = 1$. Then, J_{hom} given in (3.14) satisfies*

$$\min_{z \in \mathbb{R}} J_{\text{hom}}(z) = \mathbb{E}[J_1(\delta_1)] \quad \text{and} \quad J_{\text{hom}}(z) = \mathbb{E}[J_1(\delta_1)] \quad \text{for all } z \geq \mathbb{E}[\delta_1].$$

Proof. We claim

$$\min_{z \in \mathbb{R}} J_{\text{hom}}(z) = J_{\text{hom}}(\mathbb{E}[\delta_1]) = \mathbb{E}[J_1(\delta_1)]. \quad (4.39)$$

By (LJ2), we have $\min_{z \in \mathbb{R}} J_1(\omega, z) = J_1(\omega, \delta_1(\omega))$. Hence, for every $z \in \mathbb{R}$ and $\omega \in \Omega$ it holds

$$J_{\text{hom}}^{(N)}(\omega, z, [0, 1]) \geq \frac{1}{N} \sum_{i=0}^{N-1} J_1(\tau_i \omega, \delta_1(\tau_i \omega))$$

and thus by Propositions 4.12 and 3.5

$$J_{\text{hom}}(z) \geq \mathbb{E}[J_1(\delta_1)] \quad \text{for every } z \in \mathbb{R}.$$

Combining Proposition 3.5 in the form $\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i=0}^{N-1} \delta_1(\tau_i \omega) = \mathbb{E}[\delta_1]$ for \mathbb{P} -a.e. ω with the Γ -convergence statement (4.35) of Proposition 4.12, we obtain for \mathbb{P} -a.e. ω

$$\limsup_{N \rightarrow \infty} \frac{1}{N} \sum_{i=0}^{N-1} J_1(\tau_i \omega, \delta_1(\tau_i \omega)) \geq \liminf_{N \rightarrow \infty} J_{\text{hom}}^{(N)} \left(\omega, \frac{1}{N} \sum_{i=0}^{N-1} \delta_1(\tau_i \omega) \right) \geq J_{\text{hom}}(\mathbb{E}[\delta_1])$$

and thus (4.39) follows, which proves the proposition. \square

With all the previous results, we gathered enough information about the properties of the function J_{hom} . A sketch can be found in Figure 4.2. Next we state the convergence result.

4.3 Γ -limit of the energy

In this section, we finally prove the Γ -convergence result for the sequence $(H_n^\ell(\omega, \cdot))$ of our energy. The limit $n \rightarrow \infty$ refers to an increasing number n of particles in the chain and therefore is the

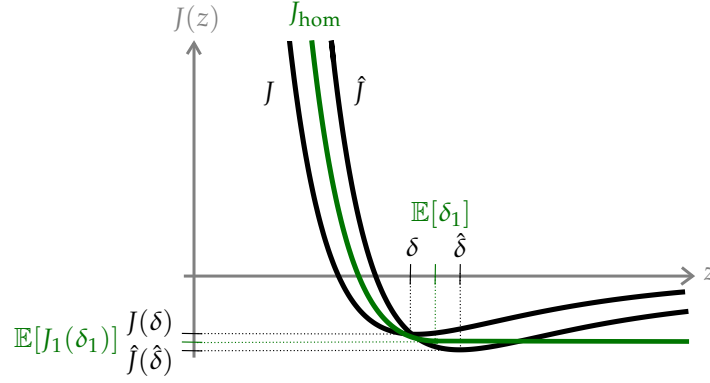


Figure 4.2 | The function J_{hom} for $K = 1$ in the case of two different potentials J and \hat{J} , which are equidistributed. Therefore the expectation values lies within the middle of both.

passage from the discrete to the continuous system. The density of the limiting energy functional turns out to be the homogenization formula J_{hom} which we established in the previous sections. Note that in the literature also the notion Γ -limit of zeroth order is used.

Theorem 4.14. *Let Assumption 3.3 be satisfied. Let $\ell > 0$. Then, there exists an $\Omega' \subset \Omega$ with $\mathbb{P}(\Omega') = 1$ such that for all $\omega \in \Omega'$ the Γ -limit of $H_n^\ell(\omega, \cdot)$ with respect to the $L^1(0, 1)$ -topology is $H_{\text{hom}}^\ell : L^1(0, 1) \rightarrow (-\infty, +\infty]$, given by*

$$H_{\text{hom}}^\ell(u) = \begin{cases} \int_0^1 J_{\text{hom}}(u'(x)) \, dx & \text{if } u \in BV^\ell(0, 1), D^s u \geq 0, \\ +\infty & \text{otherwise.} \end{cases}$$

with

$$J_{\text{hom}}(z) = \lim_{N \rightarrow \infty} \frac{1}{N} \inf \left\{ \sum_{j=1}^K \sum_{i=0}^{N-j} J_j \left(\omega, i, z + \frac{\phi^{i+j} - \phi^i}{j} \right) : \phi^i \in \mathbb{R}, \right. \\ \left. \phi^s = \phi^{N-s} = 0 \text{ for } s = 0, \dots, K-1 \right\}.$$

Moreover, the minimum values of $H_n^\ell(\omega, \cdot)$ and H_{hom}^ℓ satisfy

$$\lim_{n \rightarrow \infty} \inf_u H_n^\ell(\omega, u) = \min_u H_{\text{hom}}^\ell(u) = J_{\text{hom}}(\ell).$$

Remark 4.15. *Some remarks on the homogenization formula.*

- (i) We emphasize that the function J_{hom} is deterministic, i.e. it depends only on the variable z and not any more on the stochastic variable ω .
- (ii) We use Lennard-Jones type potentials because they allow for fracture in general. Indeed, the limit functional includes jumps since the energy is finite for deformations u in the space $BV^\ell(0, 1)$. Consequently, jumps are allowed.
- (iii) The limiting energy is only finite for $D^s u \geq 0$. This refers to positive jumps and guarantees that the chain shows no self interpenetration.
- (iv) The homogenized energy density is given by an asymptotic cell formula. This is a typical result in

stochastic homogenization, see, e.g., [4, 47, 94]. In Chapter 6, we consider the periodic case with nearest-neighbour interactions. There, the asymptotic cell formula reduces to a minimization problem on the periodicity cell.

- (v) The limiting energy reveals a major disadvantage. The jumps, which are allowed to occur, do not cost any energy, because the integrand J_{hom} only takes into account the absolute continuous part of the measure u' . Therefore, the chain can have arbitrarily many jumps without an increase of energy due to cracks. This problem will be overcome in Chapter 5 via a rescaling approach.
- (vi) In the case of only nearest neighbour interactions, i.e. $K = 1$, we can elaborate on the regime where jumps can occur. Due to Proposition 4.13, it holds true that $J_{\text{hom}}(\ell) = J_{\text{hom}}(\mathbb{E}[\delta_1])$ for $\ell > \mathbb{E}[\delta_1]$. Therefore, a minimizer of H_{hom}^ℓ can have a jump for $\ell > \mathbb{E}[\delta_1]$. Indeed, the limiting energy of $u_1(x) := \ell x$ and $u_2(x) := \mathbb{E}[\delta_1]x$ for $x \in [0, 1)$ and $u_2(1) := \ell$ is the same, while u_2 has a jump and u_1 has not.

In contrast, for $\ell \leq \mathbb{E}[\delta_1]$ no jump is possible, because here the function J_{hom} is monotonically decreasing, c.f. Proposition 4.12. Therefore, we call the regions of the boundary value ℓ separated by the value $\mathbb{E}[\delta_1]$ elastic and jump regime, respectively.

Proof. The existence of J_{hom} and some properties of that function were shown before in Proposition 4.12.

Step 1. Compactness.

Let $(u_n) \subset L^1(0, 1)$ be a sequence with $\sup_n H_n^\ell(\omega, u_n) < \infty$. Then, we have $u_n \in \mathcal{A}_n(0, 1)$ (cf. Definition 3.1) and $u_n(0) = 0$, $u_n(1) = \ell$ for every $n \in \mathbb{N}$, by definition. Since $\Psi(z) \geq 0$ for all $z \in \mathbb{R}$, we can estimate the energy from below by

$$\begin{aligned} C &\geq \sum_{j=1}^K \sum_{i=0}^{n-j} \lambda_n J_j \left(\omega, i, \frac{u_n^{i+j} - u_n^i}{j\lambda_n} \right) \stackrel{(LJ2)}{\geq} \frac{1}{d} \sum_{j=1}^K \sum_{i=0}^{n-j} \lambda_n \Psi \left(\frac{u_n^{i+j} - u_n^i}{j\lambda_n} \right) - d \sum_{j=1}^K \sum_{i=0}^{n-j} \lambda_n \\ &\geq \frac{1}{d} \sum_{i=0}^{n-1} \lambda_n \Psi \left(\frac{u_n^{i+1} - u_n^i}{\lambda_n} \right) - dK. \end{aligned} \quad (4.40)$$

By using the Jensen inequality, we obtain from (4.40)

$$\hat{C} \geq \frac{1}{d} \Psi \left(\sum_{i=0}^{n-1} \lambda_n \left(\frac{u_n^{i+1} - u_n^i}{\lambda_n} \right) \right) = \frac{1}{d} \Psi \left(\int_0^1 u_n'(x) \, dx \right). \quad (4.41)$$

We know from (3.2) that $\Psi(z) \rightarrow \infty$ as $z \rightarrow 0^+$. Since (4.41) shows that $\Psi \left(\int_0^1 u_n'(x) \, dx \right)$ is bounded, (3.2) tells us that $\int_0^1 u_n'(x) \, dx$ has to be bounded from below by zero, which reads

$$0 < \int_0^1 u_n'(x) \, dx.$$

In addition, the boundary conditions yield

$$0 < \int_0^1 u_n' \, dx = u_n(1) - u_n(0) = \ell.$$

This shows $\|u_n'\|_{L^1(0,1)} < \ell$. Since $u_n(0) = 0$, we get by the Poincaré inequality [21, Thm. A12] $\|u_n\|_{W^{1,1}(0,1)} < \tilde{C}$. Since $\|u_n\|_{W^{1,1}(0,1)}$ is equibounded, we can extract a subsequence (not relabelled)

(u_n) which weakly* converges in $BV(0,1)$ to $u \in BV(0,1)$ [5, Thm. 3.23]. By definition, we also have $u \in BV^\ell(0,1)$. This can be seen by defining the extension $\tilde{u}_n \in BV_{loc}(\mathbb{R})$ of u_n as

$$\tilde{u}_n^i = \begin{cases} 0 & \text{if } i \leq 0, \\ u_n^i & \text{if } 0 < i < n, \\ \ell & \text{if } i \geq n, \end{cases} \quad (4.42)$$

which is in $W^{1,\infty}(\mathbb{R})$ because it holds $u_n(0) = 0$ and $u_n(1) = \ell$ for every $n \in \mathbb{N}$. Then, \tilde{u}_n converges weakly* in $BV_{loc}(\mathbb{R})$ to the extension \tilde{u} of u . Therefore, we have

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

Since we need it in the following, we again go back to (4.40). The same calculation holds true if we consider a given partition $I_k = [c, d]$, $k = 0, 1, \dots, m$ and $c, d \in [0, 1]$, of $[0, 1]$, assuming $(nI_j \cap \mathbb{Z}) \cap (nI_k \cap \mathbb{Z}) = \emptyset$ for $j \neq k$ and for all $n \in \mathbb{N}$. Inequality (4.40) then becomes

$$\hat{C} \geq \frac{1}{d} \sum_{i=0}^{n-1} \lambda_n \Psi \left(\frac{u_n^{i+1} - u_n^i}{\lambda_n} \right) = \frac{1}{d} \sum_{k=0}^m \sum_{i \in nI_k \cap \mathbb{Z}} \lambda_n \Psi \left(\frac{u_n^{i+1} - u_n^i}{\lambda_n} \right).$$

Since all terms in the sum are positive due to $\Psi(z) \geq 0$ for all $z \in \mathbb{R}$, they all have to be bounded separately. That is, for every $k = 0, \dots, m$ and with the Jensen inequality, it holds true that

$$\begin{aligned} \hat{C} &\geq \frac{1}{d} \sum_{i \in nI_k \cap \mathbb{Z}} \lambda_n \Psi \left(\frac{u_n^{i+1} - u_n^i}{\lambda_n} \right) \geq \frac{1}{d} \left(\sum_{i \in nI_k \cap \mathbb{Z}} \lambda_n \right) \Psi \left(\frac{\sum_{i \in nI_k \cap \mathbb{Z}} \lambda_n \left(\frac{u_n^{i+1} - u_n^i}{\lambda_n} \right)}{\sum_{i \in nI_k \cap \mathbb{Z}} \lambda_n} \right) \\ &= \frac{1}{d} (|nI_k \cap \mathbb{Z}| \lambda_n) \Psi \left(\frac{\int_{I_k^+} u_n'(x) dx}{|nI_k \cap \mathbb{Z}| \lambda_n} \right), \end{aligned}$$

with $I_k^+ := \lambda_n [\min\{i : i \in nI_k \cap \mathbb{Z}\}, \max\{i : i \in nI_k \cap \mathbb{Z}\} + 1)$. Since we know that $\Psi(z) \rightarrow \infty$ for $z \rightarrow 0^+$ and with $a := \min\{x : x \in I_k \cap \frac{1}{n}\mathbb{Z}\}$ and $b := \max\{x : x \in I_k \cap \frac{1}{n}\mathbb{Z}\}$ we obtain

$$0 < \int_{I_k^+} u_n'(x) dx = u_n(b) - u_n(a).$$

With the same line of arguments as above, we then obtain

$$\|(u_n')\|_{L^1(I_k^-)} \leq u_n(b) - u_n(a). \quad (4.43)$$

The results will be applied in the proof of the limsup-inequality below.

Step 2. Liminf inequality.

Let $(u_n) \subset L^1(0,1)$ be a sequence with $u_n \rightarrow u$ in $L^1(0,1)$ and with $\sup_n H_n^\ell(\omega, u_n) < \infty$. From the compactness result, we know that $u_n \rightharpoonup^* u$ in $BV(0,1)$, $\|u_n'\|_{L^1(0,1)} < C$ and u fulfils the boundary conditions. We regard u as a good representative (cf. [5, Thm. 3.28] or Definition 2.6).

The aim is to show the liminf-inequality

$$\liminf_{n \rightarrow \infty} H_n^\ell(\omega, u_n) \geq \int_0^1 J_{\text{hom}}(u'(x)) \, dx. \quad (4.44)$$

We replace u_n with \hat{u}_n , which is the sequence (\hat{u}_n) of piecewise constant functions defined by $\hat{u}_n(i/n) = u_n(i/n)$ with \hat{u}_n being constant on $[i, i+1) \frac{1}{n}$, $i \in \{0, 1, \dots, n-1\}$. It is first shown that \hat{u}_n also weakly* converges to u in $BV(0, 1)$. For this, (i) $\|\hat{u}_n\|_{BV(0,1)} < \infty$ and (ii) $\hat{u}_n \rightarrow u$ in $L^1(0, 1)$ has to be proven.

For (i), we get with the Poincaré inequality in $BV(0, 1)$, see [5, p.152],

$$\begin{aligned} \|\hat{u}_n\|_{BV(0,1)} &= \int_0^1 |\hat{u}_n| \, dx + |D\hat{u}|(0, 1) \leq C|D\hat{u}|(0, 1) + |D\hat{u}|(0, 1) \\ &= \tilde{C} \sum_{i=0}^{n-1} \left| \hat{u}_n \left(\frac{i+1}{n} \right) - \hat{u}_n \left(\frac{i}{n} \right) \right| \\ &= \tilde{C} \sum_{i=0}^{n-1} \left| \int_{\frac{i}{n}}^{\frac{i+1}{n}} u'_n(x) \, dx \right| \leq \tilde{C} \sum_{i=0}^{n-1} \int_{\frac{i}{n}}^{\frac{i+1}{n}} |u'_n(x)| \, dx = \tilde{C} \|u'_n\|_{L^1(0,1)}. \end{aligned}$$

This term is bounded, which proves (i), because we assumed the norm to be equi-bounded.

For (ii), we have $\|\hat{u}_n - u\|_{L^1(0,1)} \leq \|\hat{u}_n - u_n\|_{L^1(0,1)} + \|u_n - u\|_{L^1(0,1)}$ due to the triangle inequality. Since $u_n \rightharpoonup^* u$ in $BV(0, 1)$, the second term converges to zero. Thus, we only have to consider the first one. It holds

$$\begin{aligned} \|\hat{u}_n - u_n\|_{L^1(0,1)} &= \int_0^1 |\hat{u}_n - u_n| \, dx = \sum_{i=1}^n \int_{\frac{i-1}{n}}^{\frac{i}{n}} |\hat{u}_n - u_n| \, dx \\ &= \sum_{i=1}^n \int_{\frac{i-1}{n}}^{\frac{i}{n}} \left| \hat{u}_n(x) - u_n \left(\frac{i-1}{n} \right) - \int_{\frac{i-1}{n}}^x u'_n(y) \, dy \right| \, dx \\ &= \sum_{i=1}^n \int_{\frac{i-1}{n}}^{\frac{i}{n}} \left| \left(x - \frac{i-1}{n} \right) u'_n(x) \right| \, dx \leq \frac{1}{n} \sum_{i=1}^n \int_{\frac{i-1}{n}}^{\frac{i}{n}} |u'_n(x)| \, dx = \frac{1}{n} \|u'_n\|_{L^1(0,1)}. \end{aligned}$$

As the norm of u'_n is equi-bounded, the right hand side converges to zero as $n \rightarrow \infty$. Altogether, this shows (ii).

The reason, why we can easily switch to \hat{u}_n instead of u_n is that it has the same discrete difference quotient as u_n , and therefore it holds true that

$$H_n^\ell(\omega, u_n) = \sum_{j=1}^K \sum_{i=0}^{n-j} \lambda_n J_j \left(\omega, i, \frac{u_n^{i+j} - u_n^i}{j\lambda_n} \right) = \sum_{j=1}^K \sum_{i=0}^{n-j} \lambda_n J_j \left(\omega, i, \frac{\hat{u}_n^{i+j} - \hat{u}_n^i}{j\lambda_n} \right).$$

With this, we pass to a subsequence (\hat{u}_{n_k}) with

$$\liminf_{n \rightarrow \infty} H_n^\ell(\omega, u_n) = \lim_{k \rightarrow \infty} \sum_{j=1}^K \sum_{i=0}^{n_k-j} \lambda_{n_k} J_j \left(\omega, i, \frac{\hat{u}_{n_k}^{i+j} - \hat{u}_{n_k}^i}{j\lambda_{n_k}} \right)$$

Since it holds $\hat{u}_{n_k} \rightarrow u$ in $L^1(0, 1)$, we can pass to a further subsequence $(\hat{u}_{n_{k_l}})$ such that $\hat{u}_{n_{k_l}} \rightarrow u$ pointwise almost everywhere. From now on, we relabel the subsequence $(\hat{u}_{n_{k_l}})$ and call it just (\hat{u}_n) .

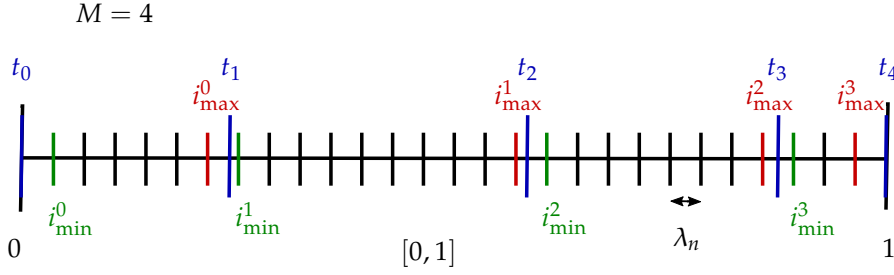


Figure 4.3 | Illustration of the definitions i_{\min}^m and i_{\max}^m for $M = 4$.

Step A: Introduction of the first additional and artificial scale.

As it is common in homogenization theory, we introduce an artificial coarser length scale δ and provide a liminf inequality of the form (4.44), where u on the right-hand side is replaced by a suitable piecewise affine interpolation u_δ of u . The claimed inequality (4.44) then follows by sending $\delta \rightarrow 0$ and a suitable relaxation result.

We define the coarser grid as follows: For a fixed $\delta > 0$, small enough, there always exists $M \in \mathbb{N}$ and $t_0, \dots, t_M \in [0, 1]$ such that $t_0 = 0$, $t_M = 1$, $\delta < t_{m+1} - t_m < 2\delta$, t_m is not in the jump set of u and $\hat{u}_n(t_m) \rightarrow \hat{u}(t_m)$ pointwise as $n \rightarrow \infty$ and for every $m = 0, 1, \dots, M$. With the definition

$$\begin{aligned} i_{\min}^m &:= \min \{i : i \in n[t_m, t_{m+1})\}, \\ i_{\max}^m &:= \max \{i : i \in n[t_m, t_{m+1})\}, \end{aligned}$$

illustrated in Figure 4.3, we can estimate

$$\begin{aligned} H_n^\ell(\omega, u_n) &= \sum_{j=1}^K \sum_{i=0}^{n-j} \lambda_n J_j \left(\omega, i, \frac{\hat{u}_n^{i+j} - \hat{u}_n^i}{j\lambda_n} \right) \\ &= \sum_{j=1}^K \sum_{m=0}^{M-1} \lambda_n \sum_{i=i_{\min}^m}^{i_{\max}^{m+1}-j} J_j \left(\omega, i, \frac{\hat{u}_n^{i+j} - \hat{u}_n^i}{j\lambda_n} \right) + \sum_{m=0}^{M-2} \sum_{j=2}^K \sum_{s=0}^{j-2} \lambda_n J_j \left(\omega, i_{\max}^m - s, \frac{\hat{u}_n^{i_{\max}^m - s + j} - \hat{u}_n^{i_{\max}^m - s}}{j\lambda_n} \right). \end{aligned} \quad (4.45)$$

The second term of (4.45) vanishes as $n \rightarrow \infty$, which can be seen as follows:

$$\begin{aligned} &\sum_{m=0}^{M-2} \sum_{j=2}^K \sum_{s=0}^{j-2} \lambda_n J_j \left(\omega, i_{\max}^m - s, \frac{\hat{u}_n^{i_{\max}^m - s + j} - \hat{u}_n^{i_{\max}^m - s}}{j\lambda_n} \right) \\ &\stackrel{(4.1)}{\geq} \sum_{m=0}^{M-2} \sum_{j=2}^K \sum_{s=0}^{j-2} \lambda_n (-d) \geq -\lambda_n d K^2 M \rightarrow 0 \quad \text{as } n \rightarrow \infty. \end{aligned} \quad (4.46)$$

Step B: Introduction of the second additional and artificial scale.

We want to continue with the first term of the right hand side of (4.45). In order to deal with the non-locality of the energy (due to the interaction beyond nearest neighbours) we introduce a second small scale $0 < \epsilon \ll \delta$ and manipulate u_n in a small boundary layer of size $\sim \epsilon$ at the boundary of the intervals (t_m, t_{m+1}) , see Figure 4.4 for illustration. This additional scale simplifies the calculation of the upcoming remainders.

The scale is defined as follows: Let $\epsilon > 0$ with $\epsilon \ll \delta$ (therefore it is reasonable to consider in the following first the limit $\epsilon \rightarrow 0$ and then $\delta \rightarrow 0$). Because of the pointwise convergence almost everywhere of \hat{u}_n , we can find for every $m = 0, \dots, M$ values $a_m \in \mathbb{R}$ and $b_m \in \mathbb{R}$ (explicitly, a_m and b_m depend also on M, n and ϵ , but we do not denote this for better readability) which are not in the jump set of u such that $t_m < a_m < b_m < t_{m+1}$, $\epsilon < a_m - t_m < 2\epsilon$, $\epsilon < t_{m+1} - b_m < 2\epsilon$ and $\hat{u}_n(a_m) \rightarrow u(a_m)$ and $\hat{u}_n(b_m) \rightarrow u(b_m)$ pointwise in \mathbb{R} as $n \rightarrow \infty$. With that, we define $h_n^{a_m} \in \mathbb{N}$ and $h_n^{b_m} \in \mathbb{N}$, with $0 \leq h_n^{a_m} \leq h_n^{b_m} \leq n$ such that $a_m \in \lambda_n[h_n^{a_m}, h_n^{a_m} + 1)$ and $b_m \in \lambda_n[h_n^{b_m}, h_n^{b_m} + 1)$. Note that for n large enough it always holds true that $i_{\min}^m + K \ll h_n^{a_m}$ and $h_n^{b_m} \ll i_{\max}^m - K$.

We further need a modified version \tilde{u}_n of the function \hat{u}_n , because \hat{u}_n does not fulfil the boundary constraint of the infimum problem of $J_{\text{hom}}^{L,(n)}$. Therefore we perform a minor modification, such that \tilde{u}_n becomes a competitor for the infimum problem. Recall that the discrete difference quotients of u_n and \hat{u}_n are the same, by construction, and can therefore be used equivalently. Now set

$$z_{n,m}^\epsilon := \frac{u_n^{h_n^{b_m}} - u_n^{h_n^{a_m}} + 2\epsilon}{\lambda_n(h_n^{b_m} - h_n^{a_m} + 2)},$$

which will be the average slope of \tilde{u}_n on the interval $\lambda_n[i_{\min}^m, i_{\max}^m + 1]$. Since (\hat{u}_n) is piecewise constant and by the definition of a_m and b_m , we get as $n \rightarrow \infty$

$$\begin{aligned} z_{n,m}^\epsilon &= \frac{u_n^{h_n^{b_m}} - u_n^{h_n^{a_m}} + 2\epsilon}{\lambda_n(h_n^{b_m} - h_n^{a_m} + 2)} = \frac{\hat{u}_n(b_m) - \hat{u}_n(a_m) + 2\epsilon}{\lambda_n(h_n^{b_m} - h_n^{a_m} + 2)} \\ &\rightarrow \frac{u(b_m) - u(a_m) + 2\epsilon}{b_m - a_m}. \end{aligned} \quad (4.47)$$

With this, we define \tilde{u}_n as the continuous and piecewise affine function with

$$\begin{aligned} \tilde{u}_n^0 &= 0, \\ \frac{\tilde{u}_n^{i+1} - \tilde{u}_n^i}{\lambda_n} &= z_{n,m}^\epsilon && \text{for } i_{\min}^m \leq i \leq h_n^{a_m} - 2 \text{ and } h_n^{b_m} + 1 \leq i \leq i_{\max}^m, \\ \tilde{u}_n^i &= \tilde{u}_n^{i-1} + \epsilon && \text{for } i = h_n^{a_m} \text{ and } i = h_n^{b_m} + 1, \\ \frac{\tilde{u}_n^{i+1} - \tilde{u}_n^i}{\lambda_n} &= \frac{u_n^{i+1} - u_n^i}{\lambda_n} && \text{for } h_n^{a_m} \leq i \leq h_n^{b_m} - 1. \end{aligned}$$

A sketch of this construction can be found in Figure 4.4. Note that the boundary constraints of the infimum problem of $J_{\text{hom}}^{(n)}$ are fulfilled, by definition. Further, note that the slopes of u_n and \tilde{u}_n are the same on the interval $h_n^{a_m} \leq i \leq h_n^{b_m} - 1$. The two parts where the slope is set equal to the value ϵ by definition of \tilde{u}_n are of technical reasons. They are designed in such a way that the remainders, which show up in the following, can easily be estimated. This can be seen in (4.50), where the presence of the jump ensures that the discrete gradients can be bounded from below by a positive value converging to $+\infty$.

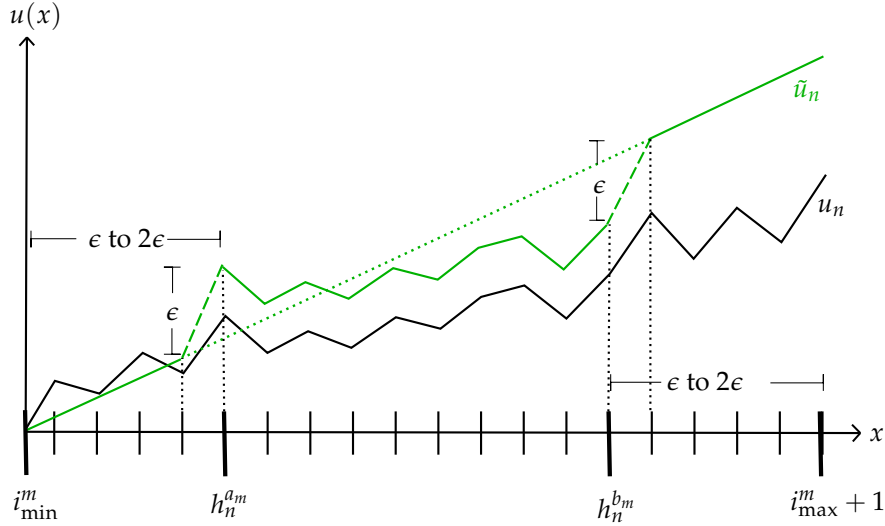


Figure 4.4 | Illustration of the definition of \tilde{u}_n .

Given this, and by definition of $J_{\text{hom}}^{(n)}$, we estimate the first term of the right-hand side of (4.45):

$$\begin{aligned}
 & \sum_{j=1}^K \sum_{m=0}^{M-1} \lambda_n \sum_{i=i_{\min}^m}^{i_{\max}^m+1-j} J_j \left(\omega, i, \frac{\hat{u}_n^{i+j} - \hat{u}_n^i}{j\lambda_n} \right) \\
 & \geq \sum_{m=0}^{M-1} \lambda_n |i_{\max}^m - i_{\min}^m + 1| J_{\text{hom}}^{(n)}(\omega, z_{n,m}^\epsilon, [t_m, t_{m+1})) \\
 & \quad + \sum_{m=0}^{M-1} \sum_{j=1}^K \sum_{i=i_{\min}^m}^{h_n^{a_m}-1} \lambda_n \left(J_j \left(\omega, i, \frac{\hat{u}_n^{i+j} - \hat{u}_n^i}{j\lambda_n} \right) - J_j \left(\omega, i, \frac{\tilde{u}_n^{i+j} - \tilde{u}_n^i}{j\lambda_n} \right) \right) \\
 & \quad + \sum_{m=0}^{M-1} \sum_{j=1}^K \sum_{i=h_n^{b_m}-j+1}^{i_{\max}^m+1-j} \lambda_n \left(J_j \left(\omega, i, \frac{\hat{u}_n^{i+j} - \hat{u}_n^i}{j\lambda_n} \right) - J_j \left(\omega, i, \frac{\tilde{u}_n^{i+j} - \tilde{u}_n^i}{j\lambda_n} \right) \right). \tag{4.48}
 \end{aligned}$$

Step C: Vanishing remainders.

Later on, we will continue with the first term of (4.48) in (4.51). Before, the second and third terms of (4.48) are considered in the limit $n \rightarrow \infty$. As the calculation and the arguments are the same, we only show them for the second one and leave out the analogous considerations for the third one. We show in the following that

$$\liminf_{n \rightarrow \infty} \sum_{m=0}^{M-1} \sum_{j=1}^K \sum_{i=i_{\min}^m}^{h_n^{a_m}-1} \lambda_n \left(J_j \left(\omega, i, \frac{\hat{u}_n^{i+j} - \hat{u}_n^i}{j\lambda_n} \right) - J_j \left(\omega, i, \frac{\tilde{u}_n^{i+j} - \tilde{u}_n^i}{j\lambda_n} \right) \right) \geq -C\epsilon, \tag{4.49}$$

for a constant $C > 0$. The first part of (4.49) can be estimated by using (4.1) as

$$\begin{aligned}
 & \sum_{m=0}^{M-1} \sum_{j=1}^K \sum_{i=i_{\min}^m}^{h_n^{a_m}-1} \lambda_n J_j \left(\omega, i, \frac{\hat{u}_n^{i+j} - \hat{u}_n^i}{j\lambda_n} \right) \geq \sum_{m=0}^{M-1} \sum_{j=1}^K \sum_{i=i_{\min}^m}^{h_n^{a_m}-1} \lambda_n (-d) \\
 & \geq -MK (h_n^{a_m} - i_{\min}^m) \lambda_n d \xrightarrow{n \rightarrow \infty} -MKd(a_m - t_m) \geq -2\epsilon MKd = -C_1\epsilon,
 \end{aligned}$$

with $C_1 > 0$. The second part of (4.49) reads

$$\sum_{m=0}^{M-1} \sum_{j=1}^K \sum_{i=i_{\min}^m}^{h_n^{a_m}-1} -\lambda_n J_j \left(\omega, i, \frac{\tilde{u}_n^{i+j} - \tilde{u}_n^i}{j\lambda_n} \right).$$

By construction of \tilde{u}_n and since we consider $i_{\min}^m \leq i \leq h_n^{a_m} - 1$, it holds true that

$$\frac{\tilde{u}_n^{i+j} - \tilde{u}_n^i}{j\lambda_n} = \left(\frac{\tilde{u}_n^{i+j} - \tilde{u}_n^{i+j-1}}{j\lambda_n} + \dots + \frac{\tilde{u}_n^{i+1} - \tilde{u}_n^i}{j\lambda_n} \right) = \frac{1}{j} \left(xz_{n,m}^\epsilon + \sum_{k=p}^q \frac{u_n^{k+1} - u_n^k}{\lambda_n} + y \frac{\epsilon}{\lambda_n} \right),$$

where $x \in \{0, \dots, j\}$, $p \geq h_n^{a_m}$, $q \leq h_n^{a_m} - 1 + j$, $q - p + 1 \leq j$, $y \in \{0, 1\}$ and from $y = 0$ follows $q < p$. Further, we know from (4.47) that $z_{n,m}^\epsilon$ converges and is therefore bounded by a constant $\hat{C} > 0$. Due to $\sup_n H_n^\ell(\omega, u_n) < \infty$, we have $\frac{u_n^{k+1} - u_n^k}{\lambda_n} \geq 0$ for every $k = 0, \dots, n-1$. Consequently, one of the following two cases holds true, namely either Case 1

$$\frac{\tilde{u}_n^{i+j} - \tilde{u}_n^i}{j\lambda_n} = \frac{1}{j} (jz_{n,m}^\epsilon) = z_{n,m}^\epsilon$$

or Case 2

$$\frac{\tilde{u}_n^{i+j} - \tilde{u}_n^i}{j\lambda_n} \geq \frac{1}{j} \left(-j\hat{C} + \frac{\epsilon}{\lambda_n} \right) = \frac{-\lambda_n \hat{C} + \epsilon/j}{\lambda_n} \geq \frac{\tilde{C}}{\lambda_n}, \quad (4.50)$$

for n large enough. In Case 1, we get

$$\begin{aligned} & \sum_{m=0}^{M-1} \sum_{j=1}^K \sum_{i=i_{\min}^m}^{h_n^{a_m}-1} -\lambda_n J_j \left(\omega, i, \frac{\tilde{u}_n^{i+j} - \tilde{u}_n^i}{j\lambda_n} \right) \geq \sum_{m=0}^{M-1} \sum_{j=1}^K \sum_{i=i_{\min}^m}^{h_n^{a_m}-1} -\lambda_n d \max \{ \Psi(z_{n,m}^\epsilon), |z_{n,m}^\epsilon| \} \\ & \geq \sum_{m=0}^{M-1} \sum_{j=1}^K \sum_{i=i_{\min}^m}^{h_n^{a_m}-1} -\lambda_n d \max \left\{ \max_{|z| \leq \hat{C}} \Psi(z), \max_{|z| \leq \hat{C}} |z| \right\} = \sum_{m=0}^{M-1} \sum_{j=1}^K \sum_{i=i_{\min}^m}^{h_n^{a_m}-1} -\lambda_n C_z \\ & \geq -MKC_z \lambda_n (h_n^{a_m} - i_{\min}^m) \xrightarrow{n \rightarrow \infty} -MKC_z (a_m - t_m) \geq -2\epsilon MKC_z = -C_2 \epsilon, \end{aligned}$$

with $C_z, C_2 > 0$. In this calculation, we assume that $z_{n,m}^\epsilon$ lies in the domain of Ψ . This is indeed the case, as can be made clear by (LJ2), from which we get (recall $\Psi(z) \geq 0$ for all $z \in \mathbb{R}$)

$$\begin{aligned} \infty & > \sup_n H_n^\ell(\omega, u_n) = \sup_n \sum_{j=1}^K \sum_{i=0}^{n-j} \lambda_n J_j \left(\omega, i, \frac{u_n^{i+j} - u_n^i}{j\lambda_n} \right) \\ & \geq \sup_n \sum_{j=1}^K \sum_{i=0}^{n-j} \lambda_n \left(\frac{1}{d} \Psi \left(\frac{u_n^{i+j} - u_n^i}{j\lambda_n} \right) - d \right) \geq \sup_n \sum_{i=0}^{n-1} \lambda_n \frac{1}{d} \Psi \left(\frac{u_n^{i+1} - u_n^i}{\lambda_n} \right) - dK, \end{aligned}$$

which shows that $\frac{u_n^{i+1} - u_n^i}{\lambda_n}$ for every $i = 0, \dots, n-1$ lies within the domain of Ψ . Then,

$$z_{n,m}^\epsilon = \frac{h_n^{b_m} - h_n^{a_m}}{h_n^{b_m} - h_n^{a_m} + 2} \frac{1}{h_n^{b_m} - h_n^{a_m}} \sum_{i=h_n^{a_m}}^{h_n^{b_m}-1} \frac{u_n^{i+1} - u_n^i}{\lambda_n} + \frac{2\epsilon}{\lambda_n (h_n^{b_m} - h_n^{a_m} + 2)},$$

where

$$\begin{aligned} \frac{h_n^{b_m} - h_n^{a_m}}{h_n^{b_m} - h_n^{a_m} + 2} &= \frac{1}{1 - \frac{2}{h_n^{b_m} - h_n^{a_m}}} \rightarrow 1, \\ \frac{2\epsilon}{2\delta} &\leq \lim_{n \rightarrow \infty} \left| \frac{2\epsilon}{\lambda_n (h_n^{b_m} - h_n^{a_m} + 2)} \right| \leq \frac{2\epsilon}{\delta}, \\ \min_{i=0, \dots, n-1} \frac{u_n^{i+1} - u_n^i}{\lambda_n} &\leq \frac{1}{h_n^{b_m} - h_n^{a_m}} \sum_{i=h_n^{a_m}}^{h_n^{b_m}-1} \frac{u_n^{i+1} - u_n^i}{\lambda_n} \leq \max_{i=0, \dots, n-1} \frac{u_n^{i+1} - u_n^i}{\lambda_n}. \end{aligned}$$

For ϵ small enough and n large enough, $z_{n,m}^\epsilon$ therefore also lies in the domain of Ψ , which proves the assumption.

In Case 2, we have $\frac{\tilde{u}_n^{i+j} - \tilde{u}_n^i}{j\lambda_n} \geq d$ for n large enough, with d from (LJ2). This yields, for n large enough, with (LJ2)

$$\begin{aligned} \sum_{m=0}^{M-1} \sum_{j=1}^K \sum_{i=i_{\min}^m}^{h_n^{a_m}-1} -\lambda_n J_j \left(\omega, i, \frac{\tilde{u}_n^{i+j} - \tilde{u}_n^i}{j\lambda_n} \right) &\geq \sum_{m=0}^{M-1} \sum_{j=1}^K \sum_{i=i_{\min}^m}^{h_n^{a_m}-1} -\lambda_n b \\ &\geq -MKb\lambda_n (h_n^{a_m} - i_{\min}^m) \xrightarrow{n \rightarrow \infty} -MKb(a_m - t_m) \geq -2MKb\epsilon = -C_3\epsilon, \end{aligned}$$

with $C_3 > 0$. Together this shows (4.49), by choosing $C := C_1 + C_2 + C_3$.

Step D: Conclusion and removal of the two artificial scales.

Now, we combine the previous results. By passing to the limit $\liminf_{n \rightarrow \infty}$ in (4.45) and with Proposition 4.12 (i.e. (4.35)), (4.46), (4.47), (4.48) and (4.49), we obtain

$$\begin{aligned} \liminf_{n \rightarrow \infty} H_n^\ell(\omega, u_n) &\geq \liminf_{n \rightarrow \infty} \sum_{m=0}^{M-1} \lambda_n |i_{\max}^m - i_{\min}^m + 1| J_{\text{hom}}^{(n)}(\omega, z_{n,m}^\epsilon, [t_m, t_{m+1}]) - 2C\epsilon \\ &\geq \sum_{m=0}^{M-1} |t_{m+1} - t_m| J_{\text{hom}} \left(\frac{u(b_m) - u(a_m) + 2\epsilon}{b_m - a_m} \right) - 2C\epsilon. \end{aligned} \tag{4.51}$$

For $\liminf_{\epsilon \rightarrow 0}$, we then get

$$\liminf_{\epsilon \rightarrow 0} \frac{u(b_m) - u(a_m) + 2\epsilon}{b_m - a_m} = \frac{u(t_{m+1}) - u(t_m)}{t_{m+1} - t_m},$$

as there is no jump in a_m , b_m and t_m and therefore u is absolutely continuous. Hence we can continue with (4.51) by

$$\begin{aligned} \liminf_{n \rightarrow \infty} H_n^\ell(\omega, u_n) &\geq \liminf_{\epsilon \rightarrow 0} \sum_{m=0}^{M-1} |t_{m+1} - t_m| J_{\text{hom}} \left(\frac{u(b_m) - u(a_m) + 2\epsilon}{b_m - a_m} \right) \\ &\geq \sum_{m=0}^{M-1} |t_{m+1} - t_m| J_{\text{hom}} \left(\frac{u(t_{m+1}) - u(t_m)}{t_{m+1} - t_m} \right), \end{aligned} \tag{4.52}$$

since J_{hom} is lower semicontinuous due to Proposition 4.12. We now define (w_M) as the piecewise

affine interpolation of u with grid points t_m , with $w_M(0) = 0$ and $w_M(1) = \ell$ for all M . We continue by estimating (4.52) as follows:

$$\begin{aligned} \liminf_{n \rightarrow \infty} H_n^\ell(\omega, u_n) &\geq \sum_{m=0}^M |t_{m+1} - t_m| J_{\text{hom}} \left(\frac{w_M(t_{m+1}) - w_M(t_m)}{t_{m+1} - t_m} \right) \\ &= \int_0^1 J_{\text{hom}}(w'_M(x)) \, dx. \end{aligned} \quad (4.53)$$

Note that J_{hom} fulfils all assumptions of Proposition 2.8 (see Proposition 4.12) and $w_M \rightharpoonup^* u$ in $BV(0, 1)$, which is discussed below. Therefore, we finally get, by taking the limit $\liminf_{M \rightarrow \infty}$ (which corresponds to $\delta \rightarrow 0$) on both sides in (4.53),

$$\liminf_{n \rightarrow \infty} H_n^\ell(\omega, u_n) \geq \liminf_{M \rightarrow \infty} \int_0^1 J_{\text{hom}}(w'_M(x)) \, dx \geq \int_0^1 J_{\text{hom}}(u'(x)) \, dx.$$

Due to $\infty > \liminf_{n \rightarrow \infty} H_n^\ell(\omega, u_n)$, Proposition 2.8 yields $D^s u \geq 0$ on $(0, 1)$.

Step E: Proof of $w_M \rightharpoonup^ u$ in $BV(0, 1)$.*

Finally, we sketch the argument for $w_M \rightharpoonup^* u$ in $BV(0, 1)$. Clearly it suffices to show that (i) $\sup_M \|w_M\|_{W^{1,1}(0,1)} < \infty$ and (ii) $w_M \rightarrow u$ in $L^1(0, 1)$. Regarding (i), we observe

$$\begin{aligned} \|w'_M\|_{L^1(0,1)} &= \int_0^1 |w'_M(x)| \, dx = \sum_{i=1}^M \int_{t_{i-1}}^{t_i} |w'_M(x)| \, dx \\ &= \sum_{i=1}^M \int_{t_{i-1}}^{t_i} \left| \frac{u(t_i) - u(t_{i-1})}{t_i - t_{i-1}} \right| \, dx = (t_i - t_{i-1}) \sum_{i=1}^M \left| \frac{u(t_i) - u(t_{i-1})}{t_i - t_{i-1}} \right| \\ &= \sum_{i=1}^M |u(t_i) - u(t_{i-1})| \leq \|\tilde{u}\|_{BV(-1,2)}, \end{aligned}$$

where \tilde{u} denotes the extension of $u \in BV^\ell(0, 1)$ satisfying $\tilde{u} = 0$ on $(-\infty, 0)$ and $\tilde{u} = \ell$ on $(1, \infty)$. Since $u \in BV^\ell(0, 1)$ implies $\|\tilde{u}\|_{BV(-1,2)} < \infty$, we obtain (i) by an application of the Poincaré inequality, together with $w_M(0) = 0$ for every M . It is left to provide the argument for (ii). The definition of w_M and the fundamental theorem of calculus yield

$$\begin{aligned} \|w_M - u\|_{L^1(0,1)} &= \sum_{i=1}^M \int_{t_{i-1}}^{t_i} |w_M(x) - u(x)| \, dx \\ &\leq \sum_{i=1}^M (t_i - t_{i-1}) \left(\int_{t_{i-1}}^{t_i} |w'_M(y)| \, dy + |Du|([t_{i-1}, t_i]) \right) \\ &\leq 2\delta (\|w'_M\|_{L^1(0,1)} + 2|Du|([0, 1])), \end{aligned}$$

where we used $t_i - t_{i-1} \leq 2\delta$ in the last step. Thus, (ii) follows from (i) and the fact that $|Du|([0, 1]) < \infty$, since $u \in BV^\ell(0, 1)$.

Remark on the two scales.

The two remainders showing up in (4.48) are the reason for introducing the second artificial scale ϵ . In the case of next-to-nearest neighbours, these remainders do not appear in the first place. Therefore, the second scale is not necessary in that case. It is only useful for the case $K \geq 2$.

Step F: Additional constraint $D^s u \geq 0$.

It is left to show $D^s u \geq 0$ on $[0, 1]$. For this, we argue as in [26, Thm. 4.2]. Set $I = (-1, 2)$ and extend the definition of $\mathcal{A}_n(0, 1)$ (cf. Definition 3.1) to $\mathcal{A}_n(I)$ as the space of continuous piecewise affine functions on the interval $I = (-1, 2)$. Further, define $F_n : L^1(I) \rightarrow (-\infty, +\infty]$ as

$$F_n(u) = \begin{cases} \sum_{i=-n}^{2n-1} \lambda_n \Psi \left(\frac{u_n^{i+1} - u_n^i}{\lambda_n} \right) & \text{if } u \in \mathcal{A}_n(I), \\ +\infty & \text{otherwise,} \end{cases}$$

with Ψ from (LJ2). From [29, Thm. 3.7] we get that the Γ -limit of F_n with respect to the convergence in $L^1_{loc}(-1, 2)$ is given by

$$F(u) = \begin{cases} \int_{-1}^2 \Psi^{**}(u'(x)) \, dx & \text{if } u \in BV_{loc}(-1, 2), [u] > 0 \text{ on } S(u), \\ +\infty & \text{otherwise in } L^1(-1, 2). \end{cases}$$

Now, for a sequence $(u_n) \subset L^1(0, 1)$ satisfying $\sup_n H_n^\ell(\omega, u_n) < +\infty$ and $u_n \rightarrow u$ in $L^1(0, 1)$, we define v_n as a continuous and piecewise affine extension of u_n as follows: Let $v_n(x) = u_n(x)$ for $x \in [0, 1]$, and for any $x \in \mathbb{R} \setminus (0, 1)$ we set $v_n^i(x) = d$, with d from (LJ2). With

$$v(x) = \begin{cases} xd & \text{for } x < 0, \\ u(x) & \text{for } x \in [0, 1], \\ \ell + (x - 1)d & \text{for } x > 1, \end{cases}$$

we have $v_n \rightarrow v$ in $L^1_{loc}(\mathbb{R})$. With the definitions above and (LJ2), we find

$$\begin{aligned} C &> \liminf_{n \rightarrow \infty} H_n^\ell(\omega, u_n) \\ &= \liminf_{n \rightarrow \infty} \left(\sum_{i=0}^{n-1} \lambda_n J_1 \left(\omega, i, \frac{u_n^{i+1} - u_n^i}{\lambda_n} \right) + \sum_{j=2}^K \sum_{i=0}^{n-j} \lambda_n J_j \left(\omega, i, \frac{u_n^{i+j} - u_n^i}{j\lambda_n} \right) \right) \\ &\geq \liminf_{n \rightarrow \infty} \left(\sum_{i=0}^{n-1} \lambda_n J_1 \left(\omega, i, \frac{u_n^{i+1} - u_n^i}{\lambda_n} \right) + \sum_{j=2}^K \sum_{i=0}^{n-j} \lambda_n (-d) \right) \\ &\geq \liminf_{n \rightarrow \infty} \left(\sum_{i=-n}^{2n-1} \lambda_n J_1 \left(\omega, i, \frac{v_n^{i+1} - v_n^i}{\lambda_n} \right) - \sum_{i=-n}^{-1} \lambda_n J_1(\omega, i, d) - \sum_{i=n}^{2n-1} \lambda_n J_1(\omega, i, d) - Kd \right). \end{aligned}$$

Since it holds true that $|J_1(\omega, i, d)| \leq b$ by (LJ2), we can continue the above estimate by using (3.3) from (LJ2) and get

$$\begin{aligned} C &> \liminf_{n \rightarrow \infty} H_n^\ell(\omega, u_n) \geq \liminf_{n \rightarrow \infty} \sum_{i=-n}^{2n-1} \lambda_n J_1 \left(\omega, i, \frac{v_n^{i+1} - v_n^i}{\lambda_n} \right) - 2b - Kd \\ &\geq \frac{1}{d} \liminf_{n \rightarrow \infty} F_n(v_n) - 3d - 2b - Kd \geq \frac{1}{d} F(v) - (K+3)d - 2b, \end{aligned}$$

where the last inequality is the liminf-inequality due to the Γ -convergence of F_n to F .

Thus, $F(v)$ is bounded and therefore the definition of $F(v)$ tells us $D^s v \geq 0$ in $I = (-1, 2)$. Note

that the restriction of $D^s v$ to $[0, 1]$ equals $D^s u$. Hence, we get that $D^s u \geq 0$ in $[0, 1]$. This concludes the proof of the liminf-inequality.

Step 3. Limsup inequality.

We need 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

$$\limsup_{n \rightarrow \infty} H_n^\ell(\omega, u_n) \leq H_{\text{hom}}^\ell(u). \quad (4.54)$$

By Proposition 2.8, it is sufficient to show (4.54) for $u \in W^{1,1}(0, 1)$, instead of $u \in BV(0, 1)$. This can be made clear as follows: From Proposition 2.8 it is known that the lower semicontinuous envelope of

$$\mathcal{E}(u) := \begin{cases} \int_0^1 J_{\text{hom}}(u'(x)) \, dx & \text{for } u \in W^{1,1}(0, 1), \\ +\infty & \text{else,} \end{cases}$$

is $H_{\text{hom}}^\ell(u)$, i.e. $\text{sc } \mathcal{E} \equiv H_{\text{hom}}^\ell$ with respect to the weak* convergence in $BV(0, 1)$. Further, we know that the lower semicontinuous envelope with respect to the strong convergence in $L^1(0, 1)$ can be even smaller, i.e. $\text{sc}_{L^1(0,1)} \mathcal{E} \leq \text{sc}_{BV(0,1)} \mathcal{E} \equiv H_{\text{hom}}^\ell$. Consequently, if we show (4.54) for \mathcal{E} , which means that we have

$$\Gamma\text{-lim sup}_{n \rightarrow \infty} H_n^\ell(\omega, u) \leq \mathcal{E}(u),$$

then, with the definition of the lower semicontinuous envelope as $\text{sc } f(x) := \sup\{g(x) : g \text{ l.s.c, } g \leq f\}$, we get

$$\Gamma\text{-lim sup}_{n \rightarrow \infty} H_n^\ell(\omega, u) \leq \text{sc}_{L^1(0,1)} \mathcal{E}(u) \leq \text{sc}_{BV(0,1)} \mathcal{E}(u) = H_{\text{hom}}^\ell(u).$$

This result holds true since the Γ -lim sup is always lower semicontinuous (see, e.g., [21, Prop. 1.28]). Therefore, (4.54) has to be shown only for $u \in W^{1,1}(0, 1)$. At first, we do not take boundary values into account in Steps A-C. They will be included and discussed in Step D. In order to indicate omitted boundary values, we drop the superscript ℓ .

Step A: Affine functions.

We start with constructing a recovery sequence for an affine function $u(x) := zx$ for $z \in \mathbb{R}$, that is $u'(x) = z$. We just consider $z \in (0, +\infty)$, since for $z \notin (0, +\infty)$, the limsup-inequality is trivial because then we have $H_{\text{hom}}(u) = \infty$, for $u(x) = zx$. With Proposition 4.10 and 4.13, we get the existence of an $\Omega' \subset \Omega$ with $\mathbb{P}(\Omega') = 1$ such that for all $z \in \mathbb{R}$ and all $A = [a, b)$, $a, b \in \mathbb{R}$ it holds true that

$$\lim_{n \rightarrow \infty} \frac{1}{|nA \cap \mathbb{Z}|} \inf \left\{ \sum_{j=1}^K \sum_{i=i_{\min}^A}^{i_{\max}^A+1-j} J_j \left(\omega, i, z + \frac{\phi^{i+j} - \phi^i}{j} \right), \phi_{\min}^{i_{\min}^A+s} = \phi_{\max}^{i_{\max}^A+1-s} = 0 \right. \\ \left. \text{for } s = 0, \dots, K-1 \right\} = J_{\text{hom}}(z), \quad (4.55)$$

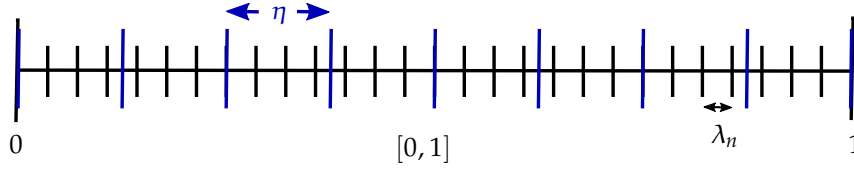


Figure 4.5 | The two length scales λ_n and η , involved in the proof of the limsup-inequality.

where, as before,

$$i_{\min}^A := \min\{i, i \in nA \cap \mathbb{Z}\} \quad \text{and} \quad i_{\max}^A := \max\{i, i \in nA \cap \mathbb{Z}\}.$$

Let $\eta > 0$ represent a coarser scale than λ_n . For simplicity, we assume $1/\eta \in \mathbb{N}$, such that the interval $[0, 1]$ can be split equidistantly. The partition of the interval is labelled by $I_k^\eta := [k\eta, (k+1)\eta)$ with $k = 0, \dots, \frac{1}{\eta} - 1$. An illustration of the two length scales, the finer one referring to λ_n and the coarser one referring to η , is shown in Figure 4.5.

Now, let η be fixed. Then, for every $n \in \mathbb{N}$ there exists a minimizer $\phi_{n, I_k^\eta} : \{i : i \in nI_k^\eta \cap \mathbb{Z}\} \rightarrow (-\infty, +\infty]$ of the minimum problem in (4.55) with $A = I_k^\eta$ for every $k = 0, \dots, \frac{1}{\eta} - 1$, which is interpolated to a piecewise affine function. Further, we define $\varphi_{n, I_k^\eta}(x) := \lambda_n \phi_{n, I_k^\eta}\left(\frac{x}{\lambda_n}\right)$ and

$$u_{n, \eta}(x) := zx + \sum_{k=0}^{\frac{1}{\eta}-1} \varphi_{n, I_k^\eta}(x) \chi_{I_k^\eta}(x),$$

where χ_I is the characteristic function of the interval I . This is not yet the recovery sequence. By definition, it holds $u_{n, \eta}(0) = 0$ and $u_{n, \eta}(1) = z := \ell$ for every $n \in \mathbb{N}$. First, we show

$$\limsup_{n \rightarrow \infty} H_n(\omega, u_{n, \eta}) \leq J_{\text{hom}}(z). \quad (4.56)$$

By the definition $H_n(\omega, u, I) := \sum_{j=1}^K \sum_{i=i_{\min}^I}^{i_{\max}^I+1-j} \lambda_n J_j\left(\omega, i, \frac{u^{i+j}-u^i}{j\lambda_n}\right)$ for shorthand, we obtain

$$\begin{aligned} H_n(\omega, u_{n, \eta}, I_k^\eta) &= \lambda_n \sum_{j=1}^K \sum_{i=i_{\min}^{I_k^\eta}}^{i_{\max}^{I_k^\eta}+1-j} J_j\left(\omega, i, z + \frac{\varphi_{n, I_k^\eta}((i+j)\lambda_n) - \varphi_{n, I_k^\eta}(i\lambda_n)}{j\lambda_n}\right) \\ &= \lambda_n \sum_{j=1}^K \sum_{i=i_{\min}^{I_k^\eta}}^{i_{\max}^{I_k^\eta}+1-j} J_j\left(\omega, i, z + \frac{\phi_{n, I_k^\eta}(i+j) - \phi_{n, I_k^\eta}(i)}{j}\right) \\ &\rightarrow |I_k^\eta| J_{\text{hom}}(z) \quad \text{as } n \rightarrow \infty, \end{aligned}$$

by (4.55). Since

$$H_n(\omega, u_{n, \eta}) = \sum_{k=0}^{\frac{1}{\eta}-1} H_n(\omega, u_{n, \eta}, I_k^\eta) + \sum_{k=0}^{\frac{1}{\eta}-2} \sum_{j=2}^K \sum_{s=0}^{j-2} \lambda_n J_j\left(\omega, i_{\max}^{I_k^\eta} - s, \frac{u_{n, \eta}^{i_{\max}^{I_k^\eta}-s+j} - u_{n, \eta}^{i_{\max}^{I_k^\eta}-s}}{j\lambda_n}\right),$$

by construction, we have for the first term

$$\lim_{n \rightarrow \infty} \sum_{k=0}^{\frac{1}{\eta}-1} H_n(\omega, u_{n,\eta}, I_k^\eta) = \sum_{k=0}^{\frac{1}{\eta}-1} |I_k^\eta| J_{\text{hom}}(z) = \sum_{k=0}^{\frac{1}{\eta}-1} \eta J_{\text{hom}}(z) = J_{\text{hom}}(z).$$

The second term yields, noting that $-s + j \leq K$ and $s \leq K - 1$,

$$\begin{aligned} & \sum_{k=0}^{\frac{1}{\eta}-2} \sum_{j=2}^K \sum_{s=0}^{j-2} \lambda_n J_j \left(\omega, i_{\max}^\eta - s, \frac{u_{n,\eta}^{i_{\max}^\eta - s + j} - u_{n,\eta}^{i_{\max}^\eta - s}}{j \lambda_n} \right) = \sum_{k=0}^{\frac{1}{\eta}-2} \sum_{j=2}^K \sum_{s=0}^{j-2} \lambda_n J_j \left(\omega, i_{\max}^\eta - s, z \right) \\ & \stackrel{(LJ2)}{\leq} \sum_{k=0}^{\frac{1}{\eta}-2} \sum_{j=2}^K \sum_{s=0}^{j-2} \lambda_n d \max\{\Psi(z), |z|\} \leq \lambda_n d \max\{\Psi(z), |z|\} \left(\frac{1}{\eta} - 1 \right) \frac{1}{2} (K+1) K \rightarrow 0 \quad \text{as } n \rightarrow \infty. \end{aligned}$$

Together, this shows (4.56). For later references, notice that this result is independent of η .

Next, we show

$$\lim_{\eta \rightarrow 0} \lim_{n \rightarrow \infty} \|u_{n,\eta} - u\|_{L^1(0,1)} = 0. \quad (4.57)$$

Since we know that the energy of $(u_{n,\eta})$ has to be equi-bounded, we get from the compactness result (4.43) for all $k \in \{0, \dots, \frac{1}{\eta} - 1\}$

$$\|u'_{n,\eta}\|_{L^1(I_k^\eta)} \leq |z| |I_k^\eta|, \quad (4.58)$$

because we have $u_{n,\eta}(b) - u_{n,\eta}(a) = z |I_k^\eta| + \varphi_{n,I_k^\eta}(b) - \varphi_{n,I_k^\eta}(a) = z |I_k^\eta| + 0$, where $a := \inf\{x : x \in I_k^\eta\}$ and $b := \sup\{x : x \in I_k^\eta\}$. It follows

$$\|\varphi'_{n,I_k^\eta}\|_{L^1(I_k^\eta)} \leq \tilde{C} \eta,$$

because of

$$\begin{aligned} \int_{I_k^\eta} |\varphi'_{n,I_k^\eta}(x)| \, dx &= \int_{I_k^\eta} |\varphi'_{n,I_k^\eta}(x) + z - z| \, dx \\ &\leq \int_{I_k^\eta} |u'_{n,\eta}(x)| \, dx + \int_{I_k^\eta} |z| \, dx \leq 2|z| |I_k^\eta| = \tilde{C} |I_k^\eta| = \tilde{C} \eta. \end{aligned}$$

Recall that $|I_k^\eta| = \eta$ by definition, which yields

$$\begin{aligned} \int_{I_k^\eta} |\varphi_{n,I_k^\eta}(x)| \, dx &= \int_{I_k^\eta} \left| \int_{k\eta}^x \varphi'_{n,I_k^\eta}(s) \, ds \right| \, dx \leq \int_{I_k^\eta} \int_{k\eta}^x |\varphi'_{n,I_k^\eta}(s)| \, ds \, dx \\ &\leq \int_{I_k^\eta} \int_{I_k^\eta} |\varphi'_{n,I_k^\eta}(s)| \, ds \, dx = |I_k^\eta| \int_{I_k^\eta} |\varphi'_{n,I_k^\eta}(s)| \, ds \leq \tilde{C} \eta^2. \end{aligned}$$

This leads us to

$$\|u_{n,\eta} - u\|_{L^1(0,1)} = \int_0^1 \left| \sum_{k=0}^{\frac{1}{\eta}-1} \varphi_{n,I_k^\eta}(x) \chi_{I_k^\eta}(x) \right| \, dx \leq \sum_{k=0}^{\frac{1}{\eta}-1} \int_{I_k^\eta} |\varphi_{n,I_k^\eta}(x)| \, dx \leq \sum_{k=0}^{\frac{1}{\eta}-1} \tilde{C} \eta^2 = \frac{1}{\eta} \tilde{C} \eta^2 = \tilde{C} \eta,$$

which proves (4.57) to be true. Since our aim is to construct a recovery sequence, which is only dependent on n , we have to pass to an appropriate subsequence. This is done with the help of the Attouch Lemma. Combined, the liminf-inequality, (4.56) and (4.57) yield that

$$\limsup_{\eta \rightarrow 0} \limsup_{n \rightarrow \infty} \left(|H_n(\omega, u_{n,\eta}) - J_{\text{hom}}(z)| + \|u_{n,\eta} - u\|_{L^1(0,1)} \right) = 0.$$

Using this result with the Attouch Lemma (Theorem 2.23), we therefore get the existence of a subsequence η_n with $\eta_n \rightarrow 0$ as $n \rightarrow \infty$ and

$$\begin{aligned} 0 &\leq \limsup_{n \rightarrow \infty} \left(|H_n(\omega, u_{n,\eta_n}) - J_{\text{hom}}(z)| + \|u_{n,\eta_n} - u\|_{L^1(0,1)} \right) \\ &\leq \limsup_{\eta \rightarrow 0} \limsup_{n \rightarrow \infty} \left(|H_n(\omega, u_{n,\eta}) - J_{\text{hom}}(z)| + \|u_{n,\eta} - u\|_{L^1(0,1)} \right) = 0. \end{aligned}$$

Finally, this shows that $H_n(\omega, u_{n,\eta_n}) \rightarrow J_{\text{hom}}(z)$ and $u_{n,\eta_n} \rightarrow u$ in $L^1(0,1)$ as $n \rightarrow \infty$. Therefore (u_{n,η_n}) is the recovery sequence for the affine function $u(x) = zx$ with $z \in \mathbb{R}$.

Moreover, we also have $u_{n,\eta_n} \rightarrow u$ weakly* in $BV(0,1)$, since (4.58) yields the boundedness of $\limsup_{n \rightarrow \infty} \|u'_{n,\eta_n}\|_{L^1(0,1)} < \infty$.

Note that the same construction can be applied on any interval (a,b) instead of $[0,1]$. This allows us to pass to the next step, namely the construction of a recovery sequence for piecewise affine functions.

Step B: Piecewise affine functions.

With this construction of a recovery sequence for affine functions, we can construct a recovery sequence for piecewise affine functions by dividing the interval $[0,1]$ into parts where the function is affine and repeating the above construction. The difficulty lies in gluing the different parts together. We show this by considering a function u with

$$u(x) := \begin{cases} z_1 x & \text{for } x \in [0, a), \\ z_1 a + z_2(x - a) & \text{for } x \in [a, 1], \end{cases}$$

for $0 < a < 1$. This function is piecewise affine with $u'(x) = z_1$ on $(0, a)$ and $u'(x) = z_2$ on $(a, 1)$. Let (u_n^1) be the recovery sequence for $u(x) = z_1 x$ on $(0, a)$ and (u_n^2) the recovery sequence for $u(x) = z_2 x$ on $(a, 1)$ constructed in Step A. Without relabelling it, we extend u_n^1 continuously with constant slope z_1 on $(i_{\max}^{[0,a]}, a)$, because it is not defined there yet. The same we do for u_n^2 on $(a, i_{\max}^{[a,1]})$ with slope z_2 . Then, we claim that

$$u_n(x) := u_n^1(x)\chi_{[0,a)} + \left(z_1 a + u_n^2(x - a) \right) \chi_{[a,1]}$$

is a recovery sequence for u . Indeed, it holds true that

$$\begin{aligned} u_n(x) &= u_n^1(x)\chi_{[0,a)} + \left(z_1 a + u_n^2(x - a) \right) \chi_{[a,1]} \\ &\rightarrow z_1 x \chi_{[0,a)} + (z_1 a + z_2(x - a)) \chi_{[a,1]} = u(x) \end{aligned}$$

in $L^1(0, 1)$ as $n \rightarrow \infty$, since both sequences are recovery sequences. Further, we get

$$\begin{aligned} H_n(\omega, u_n) &= H_n(\omega, u_n^1, [0, a]) + H_n(\omega, u_n^2, [a, 1]) \\ &+ \sum_{j=2}^K \sum_{s=0}^{j-2} \lambda_n J_j \left(\omega, i_{\max}^{[0,a]} - s, \frac{u_n^{i_{\max}^{[0,a]}-s+j} - u_n^{i_{\max}^{[0,a]}-s}}{j\lambda_n} \right). \end{aligned}$$

By construction, we have that

$$\begin{aligned} \lim_{n \rightarrow \infty} \left(H_n(\omega, u_n^1, [0, a]) + H_n(\omega, u_n^2, [a, 1]) \right) &= \int_0^a J_{\text{hom}}(z_1) \, dx + \int_a^1 J_{\text{hom}}(z_2) \, dx \\ &= \int_0^1 J_{\text{hom}}(u'(x)) \, dx. \end{aligned}$$

For the given values of s and j , we get

$$\begin{aligned} \frac{u_n^{i_{\max}^{[0,a]}-s+j} - u_n^{i_{\max}^{[0,a]}-s}}{j\lambda_n} &= \frac{z_1 a + z_2 \left(\left(i_{\max}^{[0,a]} - s + j \right) \lambda_n - a \right) - z_1 \left(i_{\max}^{[0,a]} - s \right) \lambda_n}{j\lambda_n} \\ &= (z_1 - z_2) \frac{a - \lambda_n \left(i_{\max}^{[0,a]} - s \right)}{j\lambda_n} + z_2 =: z_n. \end{aligned}$$

Since $\lambda_n i_{\max}^{[0,a]} \rightarrow a$, we obtain $\frac{a - \lambda_n \left(i_{\max}^{[0,a]} - s \right)}{j\lambda_n} \rightarrow \frac{s}{j} \leq 1$ as $n \rightarrow \infty$, and therefore it holds true that z_n is a convex combination of z_1 and z_2 for n large enough. This yields

$$\begin{aligned} \sum_{j=2}^K \sum_{s=0}^{j-2} \lambda_n J_j \left(\omega, i_{\max}^{[0,a]} - s, \frac{u_n^{i_{\max}^{[0,a]}-s+j} - u_n^{i_{\max}^{[0,a]}-s}}{j\lambda_n} \right) &= \sum_{j=2}^K \sum_{s=0}^{j-2} \lambda_n J_j \left(\omega, i_{\max}^{[0,a]} - s, z_n \right) \\ &\stackrel{(LJ2)}{\leq} \sum_{j=2}^K \sum_{s=0}^{j-2} \lambda_n d \max\{\Psi(z_n), |z_n|\} \leq \lambda_n d C \frac{1}{2} (K+1) K \rightarrow 0 \quad \text{as } n \rightarrow \infty. \end{aligned}$$

Altogether, this shows the limsup inequality

$$\limsup_{n \rightarrow \infty} H_n(\omega, u_n) \leq \int_0^1 J_{\text{hom}}(u'(x)) \, dx.$$

Step C: $W^{1,1}$ -functions.

Now, we provide arguments to pass to functions $u \in W^{1,1}$: For $u \in W^{1,1}(0, 1)$, consider the piecewise affine interpolation u_N of u with grid points t_N^j , which means $u_N \in C(0, 1)$ is affine on $[t_N^{j-1}, t_N^j]$ and it holds $u_N(t_N^j) = u(t_N^j)$ for all $j = 0, \dots, N$. This is well defined because we can

consider u as its absolute continuous representative. By the Jensen inequality, it holds true that

$$\begin{aligned}
 H_{\text{hom}}(u) &= \int_0^1 J_{\text{hom}}(u'(x)) \, dx = \sum_{j=1}^N \int_{t_N^{j-1}}^{t_N^j} J_{\text{hom}}(u'(x)) \, dx \\
 &\geq \sum_{j=1}^N (t_N^{j-1} - t_N^j) J_{\text{hom}} \left(\frac{1}{t_N^{j-1} - t_N^j} \int_{t_N^{j-1}}^{t_N^j} u'(x) \, dx \right) \\
 &= \sum_{j=1}^N (t_N^{j-1} - t_N^j) J_{\text{hom}} \left(\frac{1}{t_N^{j-1} - t_N^j} (u(t_N^j) - u(t_N^{j-1})) \right) \\
 &= \sum_{j=1}^N (t_N^{j-1} - t_N^j) J_{\text{hom}} \left(\frac{1}{t_N^{j-1} - t_N^j} (u_N(t_N^j) - u_N(t_N^{j-1})) \right) = \int_0^1 J_{\text{hom}}(u'_N(x)) \, dx.
 \end{aligned} \tag{4.59}$$

The Γ -lim sup is known to be lower semicontinuous. With the same line of arguments as in Step E of the liminf inequality, we get that $u_N \xrightarrow{*} u$ in $BV(0, 1)$. The Γ -lim sup of piecewise affine functions was already constructed in the previous steps. Thus we have

$$\begin{aligned}
 \Gamma\text{-lim sup}_{n \rightarrow \infty} H_n(\omega, u) &\stackrel{\text{l.s.c.}}{\leq} \liminf_{N \rightarrow \infty} \left\{ \Gamma\text{-lim sup}_{n \rightarrow \infty} H_n(\omega, u_N) \right\} \\
 &\leq \limsup_{N \rightarrow \infty} \int_0^1 J_{\text{hom}}(u'_N(x)) \, dx \stackrel{(4.59)}{\leq} \limsup_{N \rightarrow \infty} \int_0^1 J_{\text{hom}}(u'(x)) \, dx = H_{\text{hom}}(u),
 \end{aligned}$$

which yields the limsup-inequality for $W^{1,1}(0, 1)$. As argued in the beginning of the proof, this shows the limsup-inequality for the functional without boundary constraints.

Step D: Boundary values.

As a last step, we take boundary values into account. Following [26, Thm. 4.2], let $u \in BV^\ell(0, 1)$ be such that $H_{\text{hom}}(u) < +\infty$, $0 < u(0^+)$ and $u(1^-) < \ell$. We have shown in the previous steps that there exists a sequence (u_n) such that $u_n \rightarrow u$ in $L^1(0, 1)$ and

$$\limsup_{n \rightarrow \infty} \sum_{j=1}^K \sum_{i=0}^{n-j} \lambda_n J_j \left(\omega, i, \frac{u_n^{i+j} - u_n^i}{j\lambda_n} \right) \leq \int_0^1 J_{\text{hom}}(u'(x)) \, dx. \tag{4.60}$$

Note that the left-hand side does not equal $\limsup_{n \rightarrow \infty} H_n^\ell(\omega, u_n)$, because u_n possibly has not the correct boundary values, as well as that the right-hand side is not equal to $H_{\text{hom}}(u)$ for the same reason. The result above also holds true, if we pass to a subsequence of (u_n) which converges pointwise almost everywhere in $(0, 1)$. We fix two points α and β such that $0 < \alpha < \beta < \ell$, $\alpha \notin S_u$, $\beta \notin S_u$, $u_n(\alpha) \rightarrow u(\alpha)$ and $u_n(\beta) \rightarrow u(\beta)$. Further, let the sequences $(h_n^\alpha) \subset \mathbb{N}$ and $(h_n^\beta) \subset \mathbb{N}$ be such that $\alpha \in [h_n^\alpha, h_n^\alpha + 1)\lambda_n$ and $\beta \in [h_n^\beta, h_n^\beta + 1)\lambda_n$. First, we argue that it also holds true that

$$\limsup_{n \rightarrow \infty} \sum_{j=1}^K \sum_{i=h_n^\alpha+1}^{h_n^\beta-j-1} \lambda_n J_j \left(\omega, i, \frac{u_n^{i+j} - u_n^i}{j\lambda_n} \right) \leq \int_\alpha^\beta J_{\text{hom}}(u'(x)) \, dx, \tag{4.61}$$

which is the same as (4.60) but on the interval (α, β) . Note that the liminf-inequality also holds true for the interval (α, β) instead of $(0, 1)$ since J_j is uniformly bounded from below by d due to

(LJ2). Thus, this yields

$$\begin{aligned}
 & \limsup_{n \rightarrow \infty} \sum_{j=1}^K \sum_{i=h_n^{\alpha}+1}^{h_n^{\beta}-j-1} \lambda_n J_j \left(\omega, i, \frac{u_n^{i+j} - u_n^i}{j\lambda_n} \right) \\
 (4.60) \quad & \leq \int_0^1 J_{\text{hom}}(u'(x)) \, dx - \liminf_{n \rightarrow \infty} \sum_{j=1}^K \sum_{i=0}^{h_n^{\alpha}} \lambda_n J_j \left(\omega, i, \frac{u_n^{i+j} - u_n^i}{j\lambda_n} \right) \\
 & \quad - \liminf_{n \rightarrow \infty} \sum_{j=1}^K \sum_{i=h_n^{\beta}-j}^{n-j} \lambda_n J_j \left(\omega, i, \frac{u_n^{i+j} - u_n^i}{j\lambda_n} \right) \\
 & \leq \int_0^1 J_{\text{hom}}(u'(x)) \, dx - \int_0^{\alpha} J_{\text{hom}}(u'(x)) \, dx - \int_{\beta}^1 J_{\text{hom}}(u'(x)) \, dx = \int_{\alpha}^{\beta} J_{\text{hom}}(u'(x)) \, dx,
 \end{aligned}$$

which proves (4.61).

With the definitions from above and with d from (LJ2), we define $v_n \in \mathcal{A}_n(0, 1)$ by

$$v_n^i = \begin{cases} \lambda_n i d & \text{if } 0 \leq i < h_n^{\alpha}, \\ u_n(\alpha) - \frac{1}{2}\alpha & \text{if } i = h_n^{\alpha}, \\ u_n^i & \text{if } h_n^{\alpha} < i < h_n^{\beta}, \\ u_n(\beta) + \frac{1}{2}(1 - \beta) & \text{if } i = h_n^{\beta}, \\ \ell - \lambda_n(n - i)d & \text{if } h_n^{\beta} < i \leq n. \end{cases}$$

Note that v_n satisfies the boundary conditions $v_n(0) = 0$ and $v_n(1) = \ell$ by definition, and it holds true that $v_n \rightarrow u_{\alpha, \beta} := \bar{u}\chi_{(0, \alpha)} + u\chi_{(\alpha, \beta)} + (\bar{u} + \ell - d)\chi_{(\beta, 1)}$ in $L^1(0, 1)$ with $\bar{u}(x) = dx$, where $u_{\alpha, \beta}$ also satisfies the boundary conditions. That convergence holds true because of the pointwise convergence of u_n to u almost everywhere and the Vitali convergence theorem, where the equiintegrability holds true due to the boundedness of (v_n) in $L^\infty(0, 1)$. We want to show

$$\limsup_{n \rightarrow \infty} H_n^\ell(\omega, v_n) \leq \int_{\alpha}^{\beta} J_{\text{hom}}(u'(x)) \, dx + (\alpha + 1 - \beta)Kb, \quad (4.62)$$

with b from (LJ2). For this, we first discuss different terms showing up in the energy $H_n^\ell(\omega, v_n)$ separately, and combine all results in the end. First of all, we consider the terms containing $i = h_n^{\alpha}$. Since we have $u(0^+) > 0$ we get for α small enough $u(0^+)/2 < u(\alpha)$ due to $D^s u \geq 0$, and because of $u_n(\alpha) \rightarrow u(\alpha)$ it also holds true that $u(0^+)/2 < u_n(\alpha)$ for n large enough. Therefore, we obtain for α small enough and n large enough

$$\begin{aligned}
 \frac{v_n^{h_n^{\alpha}} - v_n^{h_n^{\alpha}-1}}{\lambda_n} &= \frac{u_n(\alpha) - \frac{1}{2}\alpha - \lambda_n(h_n^{\alpha} - 1)d}{\lambda_n} > \frac{u(0^+)/2 - \frac{1}{2}\alpha - \lambda_n(h_n^{\alpha} - 1)d}{\lambda_n} \\
 &\geq \frac{C}{\lambda_n} \rightarrow \infty \quad \text{as } n \rightarrow \infty,
 \end{aligned} \quad (4.63)$$

where we used that $\lambda_n h_n^{\alpha} \rightarrow \alpha$ as $n \rightarrow \infty$. Further, with $u_n(\alpha) = u_n^{h_n^{\alpha}} + \frac{\alpha - \lambda_n h_n^{\alpha}}{\lambda_n} (u_n^{h_n^{\alpha}+1} - u_n^{h_n^{\alpha}})$, we

have

$$\frac{v_n^{h_n^\alpha+1} - v_n^{h_n^\alpha}}{\lambda_n} = \frac{u_n^{h_n^\alpha+1} - u_n(\alpha) + \frac{1}{2}\alpha}{\lambda_n} = \frac{(u_n^{h_n^\alpha+1} - u_n^{h_n^\alpha}) \left(1 - \frac{\alpha - \lambda_n h_n^\alpha}{\lambda_n}\right) + \frac{1}{2}\alpha}{\lambda_n} \geq \frac{\frac{1}{2}\alpha}{\lambda_n}. \quad (4.64)$$

The last inequality can be explained as follows: Since it holds true that $\lambda_n h_n^\alpha \leq \alpha$ and $\alpha - \lambda_n h_n^\alpha \leq \lambda_n$, the second term in the second bracket is bounded by 1 and positive. Further, due to $\sup_n H_n(\omega, u_n) < \infty$, it holds true that $u_n^{i+1} - u_n^i \geq 0$ for every $i = 0, \dots, n-1$.

For the corresponding terms with h_n^β , the arguments are the same.

Now, we use the results (4.63) and (4.64) to consider the following terms of the energy

$$\limsup_{n \rightarrow \infty} \sum_{j=1}^K \sum_{i=h_n^\alpha-j}^{h_n^\alpha} \lambda_n J_j \left(\omega, i, \frac{v_n^{i+j} - v_n^i}{j\lambda_n} \right) \quad \text{and} \quad \limsup_{n \rightarrow \infty} \sum_{j=1}^K \sum_{i=h_n^\beta-j}^{h_n^\beta} \lambda_n J_j \left(\omega, i, \frac{v_n^{i+j} - v_n^i}{j\lambda_n} \right).$$

Again, we show the calculations for h_n^α and skip them for h_n^β , because the arguments are similar. In the given interval it holds true that, with $i = h_n^\alpha - j, \dots, h_n^\alpha$,

$$v_n^{i+j} - v_n^i = \sum_{k=0}^{j-1} (v_n^{i+k+1} - v_n^{i+k}).$$

At least one of the terms from (4.63) and (4.64) is always part of this telescopic sum. The other discrete differences from the telescopic sum are either $d > 0$ or $u_n^{i+1} - u_n^i$. Due to $\sup_n H_n^\ell(\omega, u_n) < \infty$, we have $\frac{u_n^{i+1} - u_n^i}{\lambda_n} \geq 0$ for every $i = 0, \dots, n-1$. Therefore, the remaining terms of the telescopic sum can be estimated from below by zero. Altogether, it holds true that $v_n^{i+j} - v_n^i \geq \hat{C}$ for some $\hat{C} > 0$, which yields $(v_n^{i+j} - v_n^i)/(j\lambda_n) \geq n\hat{C}/j = n\tilde{C} \geq d$ for n large enough (with d from (LJ2)). With that and (LJ2), we get for n large enough

$$\begin{aligned} \sum_{j=1}^K \sum_{i=h_n^\alpha-j}^{h_n^\alpha} \lambda_n J_j \left(\omega, i, \frac{v_n^{i+j} - v_n^i}{j\lambda_n} \right) &\leq \sum_{j=1}^K \sum_{i=h_n^\alpha-j}^{h_n^\alpha} \lambda_n b \leq \lambda_n K(K+1)b, \\ \sum_{j=1}^K \sum_{i=h_n^\beta-j}^{h_n^\beta} \lambda_n J_j \left(\omega, i, \frac{v_n^{i+j} - v_n^i}{j\lambda_n} \right) &\leq \sum_{j=1}^K \sum_{i=h_n^\beta-j}^{h_n^\beta} \lambda_n b \leq \lambda_n K(K+1)b. \end{aligned} \quad (4.65)$$

The last remaining terms of the energy are

$$\begin{aligned} \sum_{j=1}^K \sum_{i=0}^{h_n^\alpha-j-1} \lambda_n J_j \left(\omega, i, \frac{v_n^{i+j} - v_n^i}{j\lambda_n} \right) &= \sum_{j=1}^K \sum_{i=0}^{h_n^\alpha-j-1} \lambda_n J_j(\omega, i, d) \stackrel{(LJ2)}{\leq} \sum_{j=1}^K \sum_{i=0}^{h_n^\alpha-j-1} \lambda_n b \\ &= K(h_n^\alpha - j)\lambda_n b, \end{aligned} \quad (4.66)$$

as well as

$$\begin{aligned} \sum_{j=1}^K \sum_{i=h_n^\beta+1}^{n-j} \lambda_n J_j \left(\omega, i, \frac{v_n^{i+j} - v_n^i}{j\lambda_n} \right) &= \sum_{j=1}^K \sum_{i=h_n^\beta+1}^{n-j} \lambda_n J_j(\omega, i, d) \stackrel{(LJ2)}{\leq} \sum_{j=1}^K \sum_{i=h_n^\beta+1}^{n-j} \lambda_n b \\ &= K(n - j - h_n^\beta)\lambda_n b. \end{aligned} \quad (4.67)$$

Now, we combine the previous estimates and consider the energy. Using (4.65), (4.66), (4.67), we find

$$\begin{aligned}
 \limsup_{n \rightarrow \infty} H_n^\ell(\omega, v_n) &= \limsup_{n \rightarrow \infty} \sum_{j=1}^K \sum_{i=0}^{n-j} \lambda_n J_j \left(\omega, i, \frac{v_n^{i+j} - v_n^i}{j\lambda_n} \right) \\
 &\leq \limsup_{n \rightarrow \infty} \sum_{j=1}^K \sum_{i=h_n^\alpha+1}^{h_n^\beta-j-1} \lambda_n J_j \left(\omega, i, \frac{v_n^{i+j} - v_n^i}{j\lambda_n} \right) + \limsup_{n \rightarrow \infty} \sum_{j=1}^K \sum_{i=0}^{h_n^\alpha} \lambda_n J_j \left(\omega, i, \frac{v_n^{i+j} - v_n^i}{j\lambda_n} \right) \\
 &\quad + \limsup_{n \rightarrow \infty} \sum_{j=1}^K \sum_{i=h_n^\beta-j}^{n-j} \lambda_n J_j \left(\omega, i, \frac{v_n^{i+j} - v_n^i}{j\lambda_n} \right) \\
 &\stackrel{(4.61)}{\leq} \int_\alpha^\beta J_{\text{hom}}(u'(x)) \, dx + \limsup_{n \rightarrow \infty} K(h_n^\alpha - j)\lambda_n b + \limsup_{n \rightarrow \infty} \lambda_n K(K+1)b \\
 &\quad + \limsup_{n \rightarrow \infty} \lambda_n K(K+1)b + \limsup_{n \rightarrow \infty} K(n-j-h_n^\beta)\lambda_n b \\
 &\rightarrow \int_\alpha^\beta J_{\text{hom}}(u'(x)) \, dx + K\alpha b + K(1-\beta)b,
 \end{aligned}$$

as $n \rightarrow \infty$. This proves (4.62).

The argument above can be applied to every sequence $(\alpha_k) \subset (0, 1)$ and $(\beta_k) \subset (0, 1)$ fulfilling $\alpha_k \rightarrow 0$ and $\beta_k \rightarrow 1$ as $k \rightarrow \infty$. The lower semicontinuity of the Γ -lim sup, (4.62), and $u_{\alpha_k, \beta_k} \rightarrow u$ in $L^1(0, 1)$ as $k \rightarrow \infty$ provides

$$\begin{aligned}
 \Gamma\text{-lim sup}_{n \rightarrow \infty} H_n^\ell(\omega, u) &\leq \liminf_{k \rightarrow \infty} \left(\Gamma\text{-lim sup}_{n \rightarrow \infty} H_n^\ell(\omega, u_{\alpha_k, \beta_k}) \right) \\
 &\leq \limsup_{k \rightarrow \infty} \left(\int_{\alpha_k}^{\beta_k} J_{\text{hom}}(u'(x)) \, dx + (\alpha_k + 1 - \beta_k)Kb \right) = \int_0^1 J_{\text{hom}}(u'(x)) \, dx = H_{\text{hom}}^\ell(u).
 \end{aligned}$$

This proves the limsup inequality for $u \in BV^\ell(0, 1)$ with $0 < u(0^+)$ and $u(1^-) < \ell$.

The last step is to consider $u \in BV^\ell(0, 1)$ with $H_{\text{hom}}^\ell(u) < +\infty$ and $u(0^+) = 0$ and $u(1^-) = \ell$. Since $\ell > 0$, there exists a sequence (u_N) fulfilling $u_N \rightarrow u$ weakly* in $BV(0, 1)$ with

$$\int_0^1 J_{\text{hom}}(u'_N(x)) \, dx \rightarrow \int_0^1 J_{\text{hom}}(u'(x)) \, dx, \quad 0 < u_N(0^+), \quad u_N(1^-) < \ell, \quad D^s u_N \geq 0, \quad (4.68)$$

which can be easily constructed by some cut-off argument near the boundary, cf. [26, Thm 4.1].

With this construction of the recovery sequence, it holds true that $\Gamma\text{-lim sup}_{n \rightarrow \infty} H_n^\ell(\omega, u_N) \leq H_{\text{hom}}^\ell(u_N)$ for every N . Together with the lower semicontinuity of the Γ -lim sup, (4.68), and $u_N \rightarrow u$ in $L^1(0, 1)$ as $N \rightarrow \infty$, this provides

$$\Gamma\text{-lim sup}_{n \rightarrow \infty} H_n^\ell(\omega, u) \leq \liminf_{N \rightarrow \infty} \left(\Gamma\text{-lim sup}_{n \rightarrow \infty} H_n^\ell(\omega, u_N) \right) \leq \limsup_{N \rightarrow \infty} H_{\text{hom}}^\ell(u_N) \leq H_{\text{hom}}^\ell(u).$$

This proves the limsup inequality with boundary constraints.

Step 4. Convergence of minimum problems.

The convergence of minimum problems follows from the coercivity of $H_n^\ell(\omega, \cdot)$ and the fundamental theorem of Γ -convergence (see e.g. [21, Thm.1.21] and Theorem 2.22). Since J_{hom} is decreasing, we get from the Jensen inequality and from $D^s u \geq 0$

$$\min_u H_{\text{hom}}^\ell(u) \geq J_{\text{hom}} \left(\int_0^1 u'(x) \, dx \right) \geq J_{\text{hom}}(Du[0,1]) = J_{\text{hom}}(\ell).$$

Finally, we get the reverse inequality from testing with $u(x) = \ell x$.

□

5 Surface energies: rescaled model

In the previous chapter, we worked out the Γ -limit of our discrete model. Theorem 4.14 shows that this limit is finite for deformations $u \in BV^\ell(0,1)$ with only positive jumps, i.e. $D^s u \geq 0$. In particular, u is allowed to have jump points. The limiting energy reads

$$\int_0^1 J_{\text{hom}}(u'(x)),$$

which depends only on the absolute continuous part of the derivative and not on the discontinuity at all. Therefore, jumps do not cost any energy. It is energetically equivalent if the chain has a crack or not, and in particular the amount of cracks does not matter.

This observation is clearly not consistent with physical considerations. A jump, which corresponds to a crack in the chain, produces a surface on both sides of the broken material, and thus is expected to cost energy. In the limiting energy of Theorem 4.14, only the bulk part of the energy is present. Mathematically, this refers to a separation of scales between the bulk and the surface contribution of the energy, and was already discussed in, e.g., [109].

We are interested in obtaining information about jumps in the limit, the cost of energy that emerges together with a jump and the related minimizers of the limiting energy. Thus, we discuss here two approaches to overcome the separation of scales in the energy, which are both well established in the literature (see Chapter 1 for references). The first approach is to consider suitable rescaled energies, and the second one is the Γ -limit of first order.

The idea behind rescaling is to scale the energy in such a way that bulk and surface contributions are of the same order of magnitude. The limiting energy then consists of both contributions, bulk and surface, as none of them is subordinated. It turns out that in our case the so-called $\sqrt{\lambda_n}$ -scaling is the proper one for the energy (3.13). Establishing this rescaling and considering the Γ -limit of this rescaled energy are the main topics of this chapter and the content of Sections 5.1–5.4.

The Γ -limit of first order also contains surface contributions, cf., e.g., [24, 100]. It is part of the Γ -development of a function, which is an asymptotic expansion in terms of λ_n , introduced in [6]. The Γ -limit of zeroth order, i.e. the one of Theorem 4.14, is the first term of such a (formal) expansion, and the Γ -limit of first order is the second one, and therefore the term of order λ_n . The expansion also works for the minimizers, that is, minimizers of the first-order Γ -limit are the term of order λ_n in an asymptotic expansion of the minimizers of the functional. In Section 5.5 of this chapter we will show that the Γ -limit of first order neither exists in the periodic nor in the stochastic setting. Hence considering the rescaled energy is the method of choice for heterogeneous materials.

5.1 Rescaled energy

As discussed above, the problem of the energy of the system is the separation of scales, which becomes visible in the limiting energy of Theorem 4.14. There, the jumps of the deformation u

do not contribute to the energy. Thus, our method of choice consists in starting from a rescaled version of our energy functional, in which the bulk and the surface contributions are of the same order and can both contribute in the limit.

The rescaling involves two main steps. First, the deformation u is transferred into the displacement w , which means one does not consider the absolute position of the particles, but instead their deviation from the minimizer of the unconstrained problem. Second, the displacement w is rescaled properly into a new variable v . This was already established in [34]. Inspired by this preliminary work, and properly modified for our stochastic setting, we define a new piecewise affine function $w : \lambda_n \mathbb{Z} \cap [0, 1] \rightarrow \mathbb{R}$, being the displacement, as

$$w^i := u^i - u_{\min}^i = u^i - \sum_{k=0}^{i-1} \lambda_n \delta(\tau_k \omega),$$

with the global minimizer $u_{\min} : \lambda_n \mathbb{Z} \cap [0, 1] \rightarrow \mathbb{R}$ of the energy (3.13), which is given by $u_{\min}^i = \lambda_n \sum_{k=0}^{i-1} \delta(\tau_k \omega)$. This definition implies $(u^{i+1} - u^i)/\lambda_n - \delta(\tau_i \omega) = (w^{i+1} - w^i)/\lambda_n$. Next, the proper change of variables, for which one gets a non-trivial limit, was already identified in [34] and [37] as $w = \sqrt{\lambda_n} v$. It is called $\sqrt{\lambda_n}$ -scaling and provides our final rescaled variable

$$v^i := \frac{u^i - \sum_{k=0}^{i-1} \lambda_n \delta(\tau_k \omega)}{\sqrt{\lambda_n}} \quad \text{for all } i \in \{0, \dots, n\}. \quad (5.1)$$

In particular, note that

$$\frac{u^{i+1} - u^i}{\lambda_n} = \frac{v^{i+1} - v^i}{\sqrt{\lambda_n}} + \delta(\tau_i \omega).$$

So far, the rescaling shifts the minimizer of the potential $J(\omega, \cdot)$ to the position $v^i = 0$. The last step towards the final rescaled energy is adding a term independent of v to the potential. Note that the addition of a constant does not affect minimizers. This is done in such a way that it shifts the minimum of the resulting effective potential to the value 0. More precisely, the final energy in the surface scaling reads

$$E_n(\omega, v) := \sum_{i=0}^{n-1} \left(J \left(\tau_i \omega, \frac{v^{i+1} - v^i}{\sqrt{\lambda_n}} + \delta(\tau_i \omega) \right) - J(\tau_i \omega, \delta(\tau_i \omega)) \right). \quad (5.2)$$

We consider here the case of nearest-neighbour interactions, which is $K = 1$. Therefore, the index j of the potentials, which refers to the considered neighbour, is suppressed. We expect that analogous results hold true in the case $K \geq 2$, although the proofs would become more technical and would involve more cumbersome notation.

The Dirichlet boundary conditions of the energy in (3.13) read $u(0) = 0$ and $u(1) = \ell$. We consider a boundary value ℓ close to the threshold between the elastic and the fracture regime, where we expect the occurrence of fracture, i.e. $\ell = \mathbb{E}[\delta]$ due to Remark 4.15. Following the ideas of [101], adjusted to our stochastic setting, we focus on some sequence $(\ell_n) \subset \mathbb{R}$ with $\ell_n \rightarrow \mathbb{E}[\delta]$, satisfying $\ell_n > \mathbb{E}[\delta]$ for every $n \in \mathbb{N}$ and

$$\gamma_n := \frac{\ell_n - \sum_{k=0}^{n-1} \lambda_n \delta(\tau_k \omega)}{\sqrt{\lambda_n}} \rightarrow \gamma, \quad (5.3)$$

for some $\gamma \in \mathbb{R}$. This new boundary value γ_n which is a rescaled version of ℓ_n , is rescaled in the same way as the deformation u to the displacement v , and yields the new Dirichlet boundary condition $v(0) = 0$ and $v(1) = \gamma_n$. For simplification, we assume

$$\ell_n > \frac{1}{n} \sum_{i=0}^{n-1} \delta(\tau_i \omega) \quad \text{for every } n \in \mathbb{N}.$$

By definition, it holds true that $\gamma \geq 0$ as well as $\gamma_n > 0$ for all $n \in \mathbb{N}$. For every n , we set γ_n as the new boundary value for the displacement. If $u \in \mathcal{A}_n(0, 1)$, then the new variable v belongs to the space

$$\hat{\mathcal{A}}_n^{\gamma_n}(0, 1) := \{v \in \mathcal{A}_n(0, 1) : v(0) = 0, v(1) = \gamma_n\}.$$

Altogether, we get the rescaled energy functional $E_n^{\gamma_n} : \Omega \times L^1(0, 1) \rightarrow (-\infty, +\infty]$ with

$$E_n^{\gamma_n}(\omega, v) = \begin{cases} E_n(\omega, v) & \text{for } v \in \hat{\mathcal{A}}_n^{\gamma_n}(0, 1), \\ +\infty & \text{else.} \end{cases}$$

In what follows, we derive the Γ -limit of this energy.

5.2 Lennard-Jones type potentials: (LJ4) and (LJ5)

First we present additional assumptions on the interaction potentials needed in the derivation of the Γ -limit of the rescaled energy. These assure more regularity of the Lennard-Jones type potential than (LJ1)–(LJ3). The new assumptions are collected in the definition of $\mathcal{J}_{\text{reg}}(\alpha, b, c, d, \Psi, \eta) \subset \mathcal{J}(\alpha, b, d, \Psi)$ of Lennard-Jones type potentials. A list of all assumptions from the different chapters can be found at the end of the thesis.

Definition 5.1. Fix $\alpha \in (0, 1]$, $b > 0$, $d \in (1, +\infty)$ and a convex function $\Psi : \mathbb{R} \rightarrow [0, +\infty]$ as in Definition (3.1). Further, fix $\eta > 0$ and $c > 0$. We denote by $\mathcal{J}_{\text{reg}} = \mathcal{J}_{\text{reg}}(\alpha, b, c, d, \Psi, \eta)$ the class of functions $J : \mathbb{R} \rightarrow \mathbb{R} \cup \{+\infty\}$ which satisfy the properties (LJ1)–(LJ3) from Definition 3.1 and additionally the following properties:

(LJ4) (Regularity) It is $J \in C^3$ on its domain.

(LJ5) (Harmonic approximation near ground state) For $|z - \delta| < \eta$, it holds true that

$$J(z) - J(\delta) \geq \frac{1}{c}(z - \delta)^2.$$

Remark 5.2. This remark gives some comments on the new properties (LJ4) and (LJ5).

- (i) The regularity condition in (LJ4) is not sharp. In principle, it would suffice to demand $J \in C^2$. Due to the C^3 regularity, it is possible to use the Lagrange form of the remainder in a Taylor-expansion. This will be used in the proof of Theorem 5.8. Without a continuous third derivative, it is still possible to formulate the Taylor-expansion and use it in the proof. However, Hypothesis (H2) (see below) would be much more difficult to formulate, which is the reason for choosing $J \in C^3$.
- (ii) A harmonic approximation, like in (LJ5), of a function $f \in C^2$ at the minimum point x_0 is always possible as long as it holds true that $f''(x_0) > 0$. This can be seen as follows. Without loss of

generality, we set $x_0 = 0$ and consider the Taylor-expansion of $f(x)$, which reads

$$f(x) = f(0) + f'(0)x + \frac{1}{2}f''(0)x^2 + o(x^2) = f(0) + \frac{1}{2}f''(0)x^2 + o(x^2),$$

since 0 is a minimizer and therefore we get $f'(0) = 0$. Now, the question is under which assumptions one can find constants $c > 0$ and $\eta > 0$ such that

$$\begin{aligned} f(x) - f(0) &= \frac{1}{2}f''(0)x^2 + o(x^2) \geq \frac{1}{c}x^2 \\ \Leftrightarrow \left(\frac{1}{2}f''(0) - \frac{1}{c}\right)x^2 + o(x^2) &\geq 0 \end{aligned} \tag{5.4}$$

on $]-\eta, \eta[$, c.f. (LJ5). First of all, recall that 0 is a minimizer, from which we get $f''(0) \geq 0$. To show the initial assertion, we need to prove (a) that for $f''(0) = 0$ the estimate (5.4) can not be true, and (b) that for $f''(0) > 0$ one can always find $c > 0$ and $\eta > 0$ to fulfil (5.4). We start with (a). For $f''(0) = 0$, (5.4) reads

$$-\frac{1}{c}x^2 + o(x^2) = x^2 \left(-\frac{1}{c} + x^{-2}o(x^2)\right) \geq 0 \quad \Leftrightarrow \quad x^{-2}o(x^2) \geq \frac{1}{c},$$

which is a contradiction to the definition of the Landau-symbol. This shows (a). Now we discuss (b). With the definition $\tilde{C} := \frac{1}{2}f''(0) - \frac{1}{c}$, there always exists a $c > 0$ such that $\tilde{C} > 0$. With this specific $c > 0$, (5.4) reads

$$\tilde{C}x^2 + o(x^2) \geq 0 \quad \Leftrightarrow \quad \tilde{C} + x^{-2}o(x^2) \geq 0.$$

This inequality holds true for x small enough because of the convergence $x^{-2}o(x^2) \rightarrow 0$ for $x \rightarrow 0$ due to the definition of the Landau-symbol. This defines $\eta > 0$ and the assertion is proven.

(iii) With the definition

$$\alpha := \frac{1}{2} \frac{\partial^2 J(z)}{\partial z^2} \Big|_{z=\delta},$$

it follows from (LJ5) and (ii) that $\alpha > C_\alpha$ for a constant $C_\alpha > 0$ uniformly for all potentials in the class $\mathcal{J}_{\text{reg}}(\alpha, b, c, d, \Psi, \eta)$.

(iv) The assumption in (LJ5) contains a uniform bound to handle the situation of infinitely many potentials and is needed for the stochastic setting. For finitely many different potentials, (LJ5) is fulfilled automatically.

We consider the stochastic setting introduced in Section 3.2, with the random variable $J : \Omega \rightarrow \mathcal{J}_{\text{reg}}(\alpha, b, c, d, \Psi, \eta)$. We define some notation concerning the assumptions introduced above. We set for all $\omega \in \Omega$

$$\alpha(\omega) := \frac{1}{2} \frac{\partial^2 J(\omega, z)}{\partial z^2} \Big|_{z=\delta(\omega)},$$

and for $0 < \kappa < \frac{1}{d}$

$$C^\kappa(\omega) := \sup \left\{ \left| \frac{\partial^3 J}{\partial z^3}(\omega, z) \right| : z \in [\delta(\omega) - \kappa, \delta(\omega) + \kappa] \right\}.$$

Since $\frac{\partial^3 J}{\partial z^3}(\omega, \cdot)$ is continuous due to (LJ4), $C^\kappa(\omega) < \infty$ holds true for every $\omega \in \Omega$ and every $0 < \kappa < \frac{1}{d}$.

As in Section 3.2, we need further properties, coming along with the stochastic setting and the uncountability of the probability space. This new assumptions again are not phrased on the potentials themselves, but on the random variable J . They read:

(H2) (Third derivative near ground state) There exists $0 < \kappa^* < \frac{1}{d}$ such that $\mathbb{E}[C^{\kappa^*}] < \infty$. As a direct consequence, it also holds true that $\mathbb{E}[C^\kappa] < \infty$ for every $\kappa < \kappa^*$, by definition of C^κ .

(H3) (Uniform convergence of the asymptotic decay) It holds true that

$$\lim_{z \rightarrow \infty} \max_{\omega \in \Omega} |J(\omega, z)| = 0.$$

As already said, these conditions occur with respect to the infinite set of potentials. When dealing with finitely many different potentials, (H2) and (H3) are fulfilled automatically.

The stochastic setting of the chain with Lennard-Jones type interaction potentials in the rescaled setting is collected in the following assumption.

Assumption 5.3. Fix $\alpha \in (0, 1]$, $b > 0$, $c > 0$, $d \in (1, \infty)$, $\eta > 0$ and a convex function $\Psi : \mathbb{R} \rightarrow [0, \infty]$ satisfying (3.2). Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space and $(\tau_i)_{i \in \mathbb{Z}}$ be a family of stationary and ergodic group actions in the sense of Section 3.2. We suppose that the random variable $J : \Omega \rightarrow \mathcal{J}_{\text{reg}}(\alpha, b, c, d, \Psi, \eta)$ given as in Section 3.2 is measurable and (H2) as well as (H3) are satisfied, with $\mathcal{J}_{\text{reg}}(\alpha, b, c, d, \Psi, \eta)$ as in Definition 5.1.

Remark 5.4. Due to Remark 5.2 (iii), it holds true that $0 < (\alpha(\omega))^{-1} < C$ and this implies integrability of the random variable $(\alpha(\omega))^{-1}$. By definition of integrability, the expectation value of $(\alpha(\omega))^{-1}$ exists and is denote by $\mathbb{E}[\alpha^{-1}]$. Regarding the expectation value as an ensemble mean, we can also say something about the sample average. This connection is strongly related to ergodicity and is explained in the next proposition.

We define now functions, which represent sample averages of α^{-1} and C^κ and consider their limits in the next proposition. For arbitrary $N \in \mathbb{N}$ we set

$$\alpha^{-1, (N)}(\omega, A) := \frac{1}{|NA \cap \mathbb{Z}|} \sum_{i \in NA \cap \mathbb{Z}} \frac{1}{\alpha(\tau_i \omega)},$$

$$C^{\kappa, (N)}(\omega, A) := \frac{1}{|NA \cap \mathbb{Z}|} \sum_{i \in NA \cap \mathbb{Z}} C^\kappa(\tau_i \omega).$$

Proposition 5.5. Let Assumption 5.3 be satisfied. Then there exists an $\Omega' \subset \Omega$ with $\mathbb{P}(\Omega') = 1$ such that for all $\omega \in \Omega'$, all $j = 1, \dots, K$, all $\kappa < \kappa^*$ and for all $A = [a, b]$ with $a, b \in \mathbb{R}$ the limits

$$\mathbb{E}[\alpha^{-1}] = \lim_{N \rightarrow \infty} \alpha^{-1, (N)}(\omega, A),$$

$$\mathbb{E}[C^\kappa] = \lim_{N \rightarrow \infty} C^{\kappa, (N)}(\omega, A)$$

exist in $\overline{\mathbb{R}}$ and are independent of ω and the interval A .

Proof. The proof is fully analogous to the proof of Proposition 3.5, but with the following adaptations.

Integrability of the random variables is now guaranteed by Remark 5.4 and (H2).

The proof for $\alpha^{-1,(N)}(\omega, A)$ is done with the set $\Omega_{\alpha^{-1}}$. Note that $\alpha^{-1,(N)}(\omega, A)$ is bounded due to Remark 5.2 (iii), which is important for (3.12).

The proof for $C^{\kappa,(N)}(\omega, A)$ can be done analogously, with the set Ω_{C^κ} , but with a different estimate instead of (3.12). The new estimate can be derived, using $C^\kappa(\omega) > 0$, as follows:

$$\begin{aligned} C^{\kappa,(N)}(\omega, A) &= \frac{1}{|NA \cap \mathbb{Z}|} \sum_{i \in NA \cap \mathbb{Z}} C^\kappa(\tau_i \omega) \geq \frac{1}{|NA \cap \mathbb{Z}|} \sum_{i \in NB \cap \mathbb{Z}} C^\kappa(\tau_i \omega) \\ &= \frac{|NB \cup \mathbb{Z}|}{|NA \cup \mathbb{Z}|} C^{\kappa,(N)}(\omega, B). \end{aligned}$$

Defining $\Omega' := \Omega_{\alpha^{-1}} \cap \Omega_{C^\kappa}$ yields the assertion of the proposition. \square

5.3 Compactness

In the previous section, the new assumptions on the interaction potentials and the random variable were stated and discussed. With this, the Γ -limit of the rescaled energy and preliminary results can be considered. First, we want to state a compactness result for functions with equibounded energy, which will ensure the convergence of minimizers in the sense of the main theorem of Γ -convergence, Theorem 2.22.

Theorem 5.6. *Let Assumption 5.3 be satisfied. Let γ_n be such that (5.3) holds true. Let (v_n) be a sequence of functions such that*

$$\sup_n E_n^{\gamma_n}(\omega, v_n) < +\infty,$$

for every $\omega \in \Omega$. Then, there exist a subsequence (v_{n_k}) and $v \in SBV^\gamma(0, 1)$ such that $v_{n_k} \rightarrow v$ in $L^1(0, 1)$ holds true and

$$v' \in L^2(0, 1), \quad \#S_v < +\infty, \quad [v] \geq 0 \text{ in } [0, 1].$$

Moreover, there exists a finite set $S \subset [0, 1]$ such that $v_{n_k} \rightharpoonup v$ locally weakly in $H^1((0, 1) \setminus S)$.

The following proof is inspired by [34, 101]. Our assumptions of the Lennard-Jones type potentials are particularly developed in such a way that the proof of [34, 101] can be adopted easily. This mainly relies on the uniform harmonic approximation in (LJ5), that holds true for all $\omega \in \Omega$.

Proof. Let (v_n) be a sequence with $\sup_n E_n^{\gamma_n}(\omega, v_n) < +\infty$. Then, we have $v_n \in \hat{\mathcal{A}}_n^{\gamma_n}(0, 1)$. By (LJ5), there exist constants $K_1, K_2 > 0$ such that

$$\begin{aligned} E_n^{\gamma_n}(\omega, v_n) &= \sum_{i=0}^{n-1} \left(J \left(\tau_i \omega, \frac{v_n^{i+1} - v_n^i}{\sqrt{\lambda_n}} + \delta(\tau_i \omega) \right) - J(\tau_i \omega, \delta(\tau_i \omega)) \right) \\ &\geq \sum_{i=0}^{n-1} \left(K_1 \left(\frac{v_n^{i+1} - v_n^i}{\sqrt{\lambda_n}} \right)^2 \wedge K_2 \right) = \sum_{i=0}^{n-1} \left(\lambda_n K_1 \left(\frac{v_n^{i+1} - v_n^i}{\lambda_n} \right)^2 \wedge K_2 \right). \end{aligned} \tag{5.5}$$

We frequently make use of this inequality in the following. First of all, one can extract from (5.5) a bound for the gradients. The energy is equibounded and all terms in the sum are positive. Together

with the superlinear growth at zero due to (LJ1) this yields

$$\delta(\tau_i \omega) + \frac{v_n^{i+1} - v_n^i}{\sqrt{\lambda_n}} \geq 0,$$

for all $i \in \{0, \dots, n-1\}$ and for all $n \in \mathbb{N}$. Since we have $\delta(\tau_i \omega) \leq d$ for all $i \in \{0, \dots, n-1\}$ due to (LJ2), we have

$$\frac{v_n^{i+1} - v_n^i}{\lambda_n} \geq -\frac{d}{\sqrt{\lambda_n}}. \quad (5.6)$$

Step 1: We are going to show $\sup_n \|v_n\|_{W^{1,1}(0,1)} < +\infty$ and the existence of a subsequence v_{n_k} and $v \in BV^\gamma(0,1)$ such that $v_{n_k} \rightharpoonup^* v$ in $BV(0,1)$.

We define

$$I_n^- := \left\{ i \in \{0, \dots, n-1\} : v_n^{i+1} < v_n^i \right\},$$

$$I_n^{--} := \left\{ i \in I_n^- : \lambda_n K_1 \left(\frac{v_n^{i+1} - v_n^i}{\lambda_n} \right)^2 \geq K_2 \right\}.$$

Since all addends of the rescaled energy are positive, we have

$$E_n^{\gamma_n}(\omega, v_n) \geq \sum_{i \in I_n^-} \left(\lambda_n K_1 \left(\frac{v_n^{i+1} - v_n^i}{\lambda_n} \right)^2 \wedge K_2 \right) = \sum_{i \in I_n^- \setminus I_n^{--}} \left(\lambda_n K_1 \left(\frac{v_n^{i+1} - v_n^i}{\lambda_n} \right)^2 \right) + K_2 \# I_n^{--}$$

As the energy is equibounded and $K_2 > 0$ this shows $I^{--} := \sup_n \# I_n^{--} < +\infty$. Defining $(v_n')^- := -(v_n' \wedge 0)$, we get with the Hölder inequality

$$\begin{aligned} \|(v_n')^-\|_{L^1(0,1)} &= \sum_{i \in I_n^-} \lambda_n \left| \frac{v_n^{i+1} - v_n^i}{\lambda_n} \right| \stackrel{(5.6)}{\leq} \sum_{i \in I_n^- \setminus I_n^{--}} \lambda_n \left| \frac{v_n^{i+1} - v_n^i}{\lambda_n} \right| + \# I_n^{--} \lambda_n \left| \frac{d}{\sqrt{\lambda_n}} \right| \\ &\leq \left(\sum_{i \in I_n^- \setminus I_n^{--}} \lambda_n \left| \frac{v_n^{i+1} - v_n^i}{\lambda_n} \right|^2 \right)^{\frac{1}{2}} \cdot \left(\sum_{i \in I_n^- \setminus I_n^{--}} \lambda_n \right)^{\frac{1}{2}} + \# I_n^{--} \sqrt{\lambda_n} d \\ &\leq \left(\frac{1}{K_1} E_n^{\gamma_n}(\omega, v_n) \right)^{\frac{1}{2}} + I^{--} d \end{aligned}$$

Therefore, we have $\|(v_n')^-\|_{L^1(0,1)} < C$ for all $n \in \mathbb{N}$ and for a constant $C > 0$, because it was shown before that $I^{--} < \infty$ holds true. Together with the boundary data $v_n(0) = 0$ and $v_n(1) = \gamma_n$, this leads to

$$\int_{\{v_n' \geq 0\}} v_n'(x) \, dx = \gamma_n - \int_{\{v_n' < 0\}} v_n'(x) \, dx \leq \gamma_n + C.$$

From this, we get

$$\|v_n'\|_{L^1(0,1)} = \int_0^1 |v_n'(x)| \, dx \leq \gamma_n + 2C \leq \tilde{C},$$

as γ_n is converging and therefore bounded due to assumption (5.3). Since we have $v_n(0) = 0$, the Poincaré inequality (cf. [21, Thm. A.12]) now provides $\sup_n \|v_n\|_{W^{1,1}(0,1)} < +\infty$. The equiboundedness of the $W^{1,1}$ -norm then again yields the existence of a subsequence v_{n_k} and $v \in BV(0,1)$ such that $v_{n_k} \rightharpoonup^* v$ in $BV(0,1)$. By defining an extension of v_{n_k} as in (4.42) with an analogous argumentation, it also holds true that $v \in BV^\gamma(0,1)$.

Step 2: We show $v \in SBV^\gamma(0,1)$, $v' \in L^2(0,1)$ and $\#\mathcal{S}_v < +\infty$.

We define the set

$$I_n := \left\{ i \in \{0, \dots, n-1\} : \lambda_n K_1 \left(\frac{v_n^{i+1} - v_n^i}{\lambda_n} \right)^2 \geq K_2 \right\},$$

and $(\tilde{v}_n) \subset SBV(0,1)$ by $\tilde{v}_n(1) := \gamma_n$ and

$$\tilde{v}_n(x) := \begin{cases} v_n(x) & \text{if } x \in \lambda_n[i, i+1), i \notin I_n, \\ v_n(i\lambda_n) & \text{if } x \in \lambda_n[i, i+1), i \in I_n, |v_n(i\lambda_n)| < |v_n((i+1)\lambda_n)|, \\ v_n((i+1)\lambda_n) & \text{if } x \in \lambda_n[i, i+1), i \in I_n, |v_n(i\lambda_n)| \geq |v_n((i+1)\lambda_n)|. \end{cases}$$

The construction of \tilde{v}_n is done in such a way that we can show (i) $\lim_{n \rightarrow \infty} \|\tilde{v}_n - v_n\|_{L^1(0,1)} = 0$ and (ii) $\|\tilde{v}_n\|_{BV(0,1)} \leq C\|v_n\|_{W^{1,1}(0,1)}$ and therefore $\tilde{v}_n \rightharpoonup^* v$ in $BV(0,1)$ holds true up to the subsequence v_{n_k} , cf. Step 1 (not relabelled). We start with (i) and observe

$$\begin{aligned} \|\tilde{v}_n - v_n\|_{L^1(0,1)} &= \sum_{i \in I_n} \int_{i\lambda_n}^{(i+1)\lambda_n} |\tilde{v}_n(x) - v_n(x)| \, dx \\ &= \sum_{i \in I_n} \int_{i\lambda_n}^{(i+1)\lambda_n} \left| \tilde{v}_n(i\lambda_n) - v_n(i\lambda_n) + \int_{i\lambda_n}^x \tilde{v}_n'(y) - v_n'(y) \, dy \right| \, dx. \end{aligned} \tag{5.7}$$

We have to distinguish two cases, namely $|v_n(i\lambda_n)| < |v_n((i+1)\lambda_n)|$ and $|v_n(i\lambda_n)| \geq |v_n((i+1)\lambda_n)|$. For the first one, $\tilde{v}_n(i\lambda_n) = v_n(i\lambda_n)$ holds true as well as $\tilde{v}_n'(y) \equiv 0$ and therefore

$$\begin{aligned} \left| \tilde{v}_n(i\lambda_n) - v_n(i\lambda_n) + \int_{i\lambda_n}^x \tilde{v}_n'(y) - v_n'(y) \, dy \right| &= \left| \int_{i\lambda_n}^x -v_n'(y) \, dy \right| \\ &\leq \int_{i\lambda_n}^x |v_n'(y)| \, dy \leq \int_{i\lambda_n}^{(i+1)\lambda_n} |v_n'(y)| \, dy. \end{aligned}$$

For the second case $|v_n(i\lambda_n)| \geq |v_n((i+1)\lambda_n)|$, it holds true that $\tilde{v}_n(i\lambda_n) = v_n((i+1)\lambda_n)$ and $\tilde{v}_n'(y) \equiv 0$, thus we get

$$\begin{aligned} \left| \tilde{v}_n(i\lambda_n) - v_n(i\lambda_n) + \int_{i\lambda_n}^x \tilde{v}_n'(y) - v_n'(y) \, dy \right| &= \left| v_n((i+1)\lambda_n) - v_n(i\lambda_n) - \int_{i\lambda_n}^x v_n'(y) \, dy \right| \\ &= \left| \int_{i\lambda_n}^{(i+1)\lambda_n} v_n'(y) \, dy - \int_{i\lambda_n}^x v_n'(y) \, dy \right| = \left| \int_x^{(i+1)\lambda_n} v_n'(y) \, dy \right| \\ &\leq \int_x^{(i+1)\lambda_n} |v_n'(y)| \, dy \leq \int_{i\lambda_n}^{(i+1)\lambda_n} |v_n'(y)| \, dy, \end{aligned}$$

which is the same result as for the first case. Therefore, we continue with (5.7) as

$$\begin{aligned} \|\tilde{v}_n - v_n\|_{L^1(0,1)} &\leq \sum_{i \in I_n} \int_{i\lambda_n}^{(i+1)\lambda_n} \int_{i\lambda_n}^{(i+1)\lambda_n} \left| \frac{v_n^{i+1} - v_n^i}{\lambda_n} \right| dy dx \\ &= \lambda_n \int_0^1 \left| \frac{v_n^{i+1} - v_n^i}{\lambda_n} \right| dx = \lambda_n \|v_n'\|_{L^1(0,1)} \leq \lambda_n \tilde{C}, \end{aligned}$$

which shows (i) $\lim_{n \rightarrow \infty} \|\tilde{v}_n - v_n\|_{L^1(0,1)} = 0$. Next, we show (ii). It holds true that

$$\begin{aligned} \|\tilde{v}_n\|_{BV(0,1)} &= \int_0^1 |\tilde{v}_n(x)| dx + \int_0^1 |\tilde{v}_n'(x)| dx + \sum_{i \in I_n} |v_n((i+1)\lambda_n) - v_n(i\lambda_n)| \\ &\stackrel{(*)}{\leq} 2 \int_0^1 |v_n(x)| dx + \sum_{i \notin I_n} \lambda_n \left| \frac{v_n^{i+1} - v_n^i}{\lambda_n} \right| + \sum_{i \in I_n} \lambda_n \left| \frac{v_n^{i+1} - v_n^i}{\lambda_n} \right| \leq C \|v_n\|_{W^{1,1}(0,1)}. \end{aligned}$$

The estimate (*) can be seen as follows. For $i \notin I_n$, it holds true that $\tilde{v}_n(x) = v_n(x)$ and the estimate is obviously true. For $i \in I_n$, we have to distinguish between two cases, (a) $v_n(i\lambda_n)$ and $v_n((i+1)\lambda_n)$ have the same sign and (b) $v_n(i\lambda_n)$ and $v_n((i+1)\lambda_n)$ have different signs. For (a), it holds true $|\tilde{v}_n(x)| \leq |v_n(x)|$, by construction. For (b), $\int_{i\lambda_n}^{(i+1)\lambda_n} |\tilde{v}_n(x)| \leq 2 \int_{i\lambda_n}^{(i+1)\lambda_n} |v_n(x)|$ holds true, recalling that v_n is affine on the given interval. Altogether, this shows (ii) $\|\tilde{v}_n\|_{BV(0,1)} \leq C \|v_n\|_{W^{1,1}(0,1)}$.

Moreover, $\#\mathcal{S}_{\tilde{v}_n} = \#I_n$ holds true, by definition of \tilde{v}_n . From (5.5) and with $C > 0$, we get

$$C > E_n^{\gamma_n}(\omega, v_n) \geq \sum_{i \notin I_n} \left(\lambda_n K_1 \left(\frac{v_n^{i+1} - v_n^i}{\lambda_n} \right)^2 \right) + K_2 \#I_n \geq \min\{K_1, K_2\} \left(\int_0^1 |\tilde{v}_n'(x)|^2 dx + \#\mathcal{S}_{\tilde{v}_n} \right),$$

which yields $\sup_n \|\tilde{v}_n'\|_{L^2(0,1)} < +\infty$ and $\sup_n \#\mathcal{S}_{\tilde{v}_n} < +\infty$. Therefore, the closure theorem for SBV, see Theorem 2.10, provides $v \in SBV(0,1)$, $\tilde{v}_n' \rightharpoonup v'$ in $L^1(0,1)$, up to the subsequence v_{n_k} , cf. Step 1 (not relabelled), $D^j \tilde{v}_n \rightharpoonup^* D^j v$ in $(0,1)$ and $\#\mathcal{S}_v \leq \liminf_{n \rightarrow \infty} \#\mathcal{S}_{\tilde{v}_n} < \infty$. Further, $\sup_n \|\tilde{v}_n'\|_{L^2(0,1)} < +\infty$ yields $\tilde{v}_n' \rightharpoonup v'$ in $L^2(0,1)$ with $v' \in L^2(0,1)$. By Step 1, we have $v \in BV^\gamma(0,1)$, which also provides $v \in SBV^\gamma(0,1)$. This completes Step 2.

Step 3: We show that there exists a finite set $S \subset [0,1]$ such that $v_{n_k} \rightharpoonup v$ locally weakly in $H^1((0,1) \setminus S)$.

In order to simplify notation, we omit the index k of the subsequence. Since $\sup_n \#\mathcal{S}_{\tilde{v}_n} < \infty$, there exist $m \in \mathbb{N}$ and $x_1^n, \dots, x_m^n \in [0,1]$ such that $\mathcal{S}_{\tilde{v}_n} \subset \{x_i^n : i \in \{1, \dots, m\}\}$. From $D^j \tilde{v}_n \rightharpoonup^* D^j v$ we get that $x_i^n \rightarrow x_i \in [0,1]$ for all $i \in \{1, \dots, m\}$ up to a subsequence. For a fixed $\eta > 0$, we define $S := \{x_1, \dots, x_m\}$ and $S_\eta := \bigcup_{i=1}^m (x_i - \eta, x_i + \eta)$. Due to the convergence of x_i^n , there exists $N \in \mathbb{N}$ such that $\mathcal{S}_{\tilde{v}_n} \subset S_\eta$ and therefore $v_n \equiv \tilde{v}_n$ on $(0,1) \setminus S_\eta$ for $n \geq N$ and $\sup_{n \geq N} \|v_n'\|_{L^2((0,1) \setminus S_\eta)} < +\infty$. Then, the Poincaré inequality on every connected subset A of $(0,1) \setminus S_\eta$ yields $\sup_n \|v_n\|_{L^2((0,1) \setminus S_\eta)} < \infty$, which can be shown as follows:

$$\begin{aligned} \int_A |v_n|^2 dx &\leq \int_A \left((v_n - \bar{v}_n)^2 + 2v_n \bar{v}_n \right) dx \leq C \|v_n'\|_{L^2(0,1)} + 2 \int_A v_n dx \cdot \bar{v}_n \\ &\leq C \|v_n'\|_{L^2(0,1)} + \frac{2}{|A|} \|v_n\|_{L^1(0,1)}^2, \end{aligned}$$

where $\bar{v}_n := \frac{1}{|A|} \int_A v_n(x) dx$. The right hand side is uniformly bounded, which was shown in Step 1 and Step 2. Altogether, we have $v_n \rightharpoonup v$ in $H^1((0, 1) \setminus S_\eta)$. Since η was chosen arbitrary, we get our final result by passing to the limit as $\eta \rightarrow 0$.

Step 4: We show $[v] \geq 0$ in $[0, 1]$, i.e. $[v](x) > 0$ for $x \in S_v$.

Inspired by [34, 101], there exist constants $D_1, D_2, D_3 > 0$, such that

$$E_n^{\gamma_n}(\omega, v_n) = \sum_{i=0}^{n-1} \left(J \left(\tau_i \omega, \frac{v_n^{i+1} - v_n^i}{\sqrt{\lambda_n}} + \delta(\tau_i \omega) \right) - J(\tau_i \omega, \delta(\tau_i \omega)) \right) \geq \sum_{i=0}^{n-1} \varphi \left(\frac{v_n^{i+1} - v_n^i}{\sqrt{\lambda_n}} \right) \quad (5.8)$$

with

$$\varphi(x) := \begin{cases} D_1 x^2 \wedge D_2 & \text{for } x > 0, \\ D_1 x^2 \wedge D_3 & \text{for } x \leq 0. \end{cases}$$

It is not restrictive to assume

$$D_3 > D_1 d^2, \quad (5.9)$$

because of the superlinear growth at $z \rightarrow 0^+$ of the potentials $J(\omega, z)$ and the asymptotic behaviour $\lim_{z \rightarrow +\infty} J(\omega, z) = 0 > J(\omega, \delta(\omega))$. We define

$$\begin{aligned} \tilde{I}_n^+ &:= \left\{ i \in \{0, \dots, n-1\} : v_n^{i+1} > v_n^i \text{ and } D_1 \left(\frac{v_n^{i+1} - v_n^i}{\sqrt{\lambda_n}} \right)^2 > D_2 \right\}, \\ \tilde{I}_n^- &:= \left\{ i \in \{0, \dots, n-1\} : v_n^{i+1} < v_n^i \text{ and } D_1 \left(\frac{v_n^{i+1} - v_n^i}{\sqrt{\lambda_n}} \right)^2 > D_3 \right\}. \end{aligned}$$

First of all, $\tilde{I}_n^- = \emptyset$ is valid, because

$$(v_n^{i+1} - v_n^i)^2 > \frac{\in \tilde{I}_n^-}{D_1} \frac{D_3}{\lambda_n} \stackrel{(5.9)}{>} \frac{D_1 d^2}{D_1} \lambda_n = d^2 \lambda_n \stackrel{\in \tilde{I}_n^- \text{ and } (5.6)}{\geq} (v_n^{i+1} - v_n^i)^2$$

is a contradiction. Since all summands in (5.8) are positive, we get

$$E_n^{\gamma_n}(\omega, v_n) \geq \sum_{i \notin \tilde{I}_n^\pm} \varphi \left(\frac{v_n^{i+1} - v_n^i}{\sqrt{\lambda_n}} \right) + \#\tilde{I}_n^+ D_2.$$

Thus, the equiboundedness of the energy implies $\sup_n \#\tilde{I}_n^+ < \infty$. We define $(\hat{v}_n) \subset SBV(0, 1)$ as

$$\hat{v}_n(x) := \begin{cases} v_n(x) & \text{for } x \in \lambda_n[i, i+1), i \notin \tilde{I}_n^+, \\ v_n(i\lambda_n) & \text{for } x \in \lambda_n[i, i+1), i \in \tilde{I}_n^+. \end{cases}$$

Similarly as in Step 2, we have $\hat{v}_n \rightharpoonup^* v$ in $BV(0, 1)$, up to a subsequence. By definition, $\hat{v}_n(x)$ has only positive jumps, i.e. $D^j \hat{v}_n \geq 0$ in $(0, 1)$. Now, we define the following auxiliary functions in

$SBV(a, b)$ for any $a < 0$ and $b > 1$.

$$w(x) := \begin{cases} 0 & \text{for } x \leq 0, \\ v(x) & \text{for } 0 < x < 1, \\ \gamma & \text{for } 1 \leq x, \end{cases} \quad w_n(x) := \begin{cases} 0 & \text{for } x \leq 0, \\ \hat{v}_n(x) & \text{for } 0 < x < 1, \\ \gamma_n & \text{for } 1 \leq x, \end{cases}$$

to capture also possible jumps at the boundary. With $\hat{v}_n \rightharpoonup^* v$ in $BV(0, 1)$, this also yields $w_n \rightharpoonup^* w$ in $BV(a, b)$ for any $a < 0$ and $1 < b$.

$$\begin{aligned} E_n^{\gamma_n}(w, v_n) &\geq \sum_{i=0}^{n-1} \varphi \left(\frac{v_n^{i+1} - v_n^i}{\sqrt{\lambda_n}} \right) = \sum_{i \notin \bar{I}_n^\pm} \lambda_n D_1 \left(\frac{\hat{v}_n^{i+1} - \hat{v}_n^i}{\lambda_n} \right)^2 + D_2 \# S_{\hat{v}_n} \\ &\geq D_1 \int_0^1 |\hat{v}_n'(x)|^2 dx + D_2 \# S_{\hat{v}_n} = D_1 \int_0^1 |w_n'(x)|^2 dx + D_2 \# S_{w_n}. \end{aligned}$$

Again due to Theorem 2.10, this provides $D^j w_n \rightharpoonup^* D^j w$ in (a, b) . By construction of w_n and by $D^j \hat{v}_n \geq 0$ in $(0, 1)$, we get $D^j w_n \geq 0$ in (a, b) . Altogether, this yields $D^j w \geq 0$ in (a, b) . And since $D^j v$ is the restriction of $D^j w$ to $[0, 1]$, we finally get $D^j v \geq 0$ in $[0, 1]$. \square

5.4 Γ -limit of the rescaled energy

Before we consider the Γ -limit itself, we first state a technical result which we need in the proof of this Γ -limit theorem. It shows an extension of the Birkhoff ergodic theorem (Theorem 2.12).

Proposition 5.7. *Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space and let $(\tau_i)_{i \in \mathbb{Z}}$ be the additive, stationary and ergodic group action introduced in Section 3.2. For $\epsilon > 0$ and $x \in \mathbb{R}$, let $I_x^\epsilon =]x - \epsilon, x + \epsilon[$ and let f be an integrable random variable. Then there exists an $\Omega' \subset \Omega$ with $\mathbb{P}(\Omega') = 1$ such that for every $x \in \mathbb{R}$ and every $k \in \mathbb{Q}$ we have*

$$\lim_{n \rightarrow \infty} \frac{1}{2\epsilon n} \sum_{i \in \mathbb{Z} \cap nI_x^\epsilon} \chi_{(f(\tau_i \omega) \leq k)} = \mathbb{E} [\chi_{f \leq k}].$$

Proof. From the Birkhoff ergodic theorem (Theorem 2.12), we get the existence of $\Omega_{x,k,\epsilon} \subset \Omega$ with $\mathbb{P}(\Omega_{x,k,\epsilon}) = 1$ such that

$$\lim_{n \rightarrow \infty} \frac{1}{2\epsilon n} \sum_{i \in \mathbb{Z} \cap nI_x^\epsilon} \chi_{(f(\tau_i \omega) \leq k)} = \mathbb{E} [\chi_{f \leq k}]$$

for a fixed $x \in \mathbb{Q}$, fixed $k \in \mathbb{Q}$ and a fixed $\epsilon \in \mathbb{Q}$. Since for $\tilde{\Omega} := \bigcap_{x \in \mathbb{Q}, k \in \mathbb{Q}, \epsilon \in \mathbb{Q}} \Omega_{x,k,\epsilon}$, we have $\mathbb{P}(\tilde{\Omega}) = 1$, the assertion of the theorem is already shown for every $x \in \mathbb{Q}$, $k \in \mathbb{Q}$ and $\epsilon \in \mathbb{Q}$. It is left to expand it to $\epsilon \in \mathbb{R}$ and $x \in \mathbb{R}$, which is done in two steps.

Step 1: We prove the assertion for $\epsilon \in \mathbb{R} \setminus \mathbb{Q}$. For this, notice that for every $\epsilon \in \mathbb{R} \setminus \mathbb{Q}$ there exist sequences $(\epsilon_N^1) \subset \mathbb{Q}$ and $(\epsilon_N^2) \subset \mathbb{Q}$ with $\epsilon_N^1 \rightarrow \epsilon$, $\epsilon_N^2 \rightarrow \epsilon$ and $\epsilon_N^1 \leq \epsilon \leq \epsilon_N^2$ for every $N \in \mathbb{N}$. The

definition implies $I_x^{\epsilon_N^1} \subset I_x^\epsilon \subset I_x^{\epsilon_N^2}$. Therefore, it holds true that

$$\frac{2\epsilon_N^1 n}{2\epsilon n} \frac{1}{2\epsilon_N^1 n} \sum_{i \in \mathbb{Z} \cap nI_x^{\epsilon_N^1}} \chi_{(f(\tau_i \omega) \leq k)} \leq \frac{1}{2\epsilon n} \sum_{i \in \mathbb{Z} \cap nI_x^\epsilon} \chi_{(f(\tau_i \omega) \leq k)} \leq \frac{2\epsilon_N^2 n}{2\epsilon n} \frac{1}{2\epsilon_N^2 n} \sum_{i \in \mathbb{Z} \cap nI_x^{\epsilon_N^2}} \chi_{(f(\tau_i \omega) \leq k)}.$$

Taking $\limsup_{n \rightarrow \infty}$, and recalling $x, k, \epsilon_N^1, \epsilon_N^2 \in \mathbb{Q}$, we get

$$\frac{\epsilon_N^1}{\epsilon} \mathbb{E}[\chi_{f \leq k}] \leq \limsup_{n \rightarrow \infty} \frac{1}{2\epsilon n} \sum_{i \in \mathbb{Z} \cap nI_x^\epsilon} \chi_{(f(\tau_i \omega) \leq k)} \leq \frac{\epsilon_N^2}{\epsilon} \mathbb{E}[\chi_{f \leq k}].$$

Passing subsequently to the limit as $N \rightarrow \infty$, we get the assertion by $\frac{\epsilon_N^{1,2}}{\epsilon} \rightarrow 1$.

Step 2: We prove the assertion for $x \in \mathbb{R} \setminus \mathbb{Q}$. For this, notice that for every $x_0 \in \mathbb{R} \setminus \mathbb{Q}$ there exist sequences $(x_N) \subset \mathbb{Q}$ and $(\epsilon_N) \subset \mathbb{R}$ with $x_N \rightarrow x_0$ and $\epsilon_N = \epsilon + |x_N - x_0|$ for every N . The definition implies $I_{x_0}^\epsilon \subset I_{x_N}^{\epsilon_N}$. Therefore, we get

$$\frac{1}{2\epsilon n} \sum_{i \in \mathbb{Z} \cap nI_{x_0}^\epsilon} \chi_{(f(\tau_i \omega) \leq k)} \leq \frac{2\epsilon_N n}{2\epsilon n} \frac{1}{2\epsilon_N n} \sum_{i \in \mathbb{Z} \cap nI_{x_N}^{\epsilon_N}} \chi_{(f(\tau_i \omega) \leq k)}.$$

Taking $\limsup_{n \rightarrow \infty}$, we get

$$\limsup_{n \rightarrow \infty} \frac{1}{2\epsilon n} \sum_{i \in \mathbb{Z} \cap nI_{x_0}^\epsilon} \chi_{(f(\tau_i \omega) \leq k)} \leq \frac{\epsilon_N}{\epsilon} \mathbb{E}[\chi_{f \leq k}],$$

because $x_N \in \mathbb{Q}$. Subsequently, we take the limit as N tends to infinity and get

$$\limsup_{n \rightarrow \infty} \frac{1}{2\epsilon n} \sum_{i \in \mathbb{Z} \cap nI_{x_0}^\epsilon} \chi_{(f(\tau_i \omega) \leq k)} \leq \mathbb{E}[\chi_{f \leq k}]. \quad (5.10)$$

Analogously, we prove

$$\liminf_{n \rightarrow \infty} \frac{1}{2\epsilon n} \sum_{i \in \mathbb{Z} \cap nI_{x_0}^\epsilon} \chi_{(f(\tau_i \omega) \leq k)} \geq \mathbb{E}[\chi_{f \leq k}], \quad (5.11)$$

if we replace the requirement $I_{x_0}^\epsilon \subset I_{x_N}^{\epsilon_N}$ by $I_{x_N}^{\epsilon_N} \subset I_{x_0}^\epsilon$ and $\epsilon_N = \epsilon + |x_N - x_0|$ by $\epsilon_N = \epsilon - |x_N - x_0|$. Then, (5.10) and (5.11) together yield

$$\lim_{n \rightarrow \infty} \frac{1}{2\epsilon n} \sum_{i \in \mathbb{Z} \cap nI_{x_0}^\epsilon} \chi_{(f(\tau_i \omega) \geq k)} = \mathbb{E}[\chi_{f \leq k}]$$

for $x_0 \in \mathbb{R} \setminus \mathbb{Q}$, which completes the proof. \square

In Theorem 5.6 we have stated and proven a compactness result preparing the upcoming Γ -convergence theorem. This compactness result shows properties of the limit v of a sequence of displacements v_n with equibounded energy. These properties are collected in the definition

$$SBV_c^\gamma(0, 1) := \left\{ v \in SBV^\gamma(0, 1) : v' \in L^2(0, 1), \#S_v < +\infty, [v] \geq 0 \text{ in } [0, 1] \right\},$$

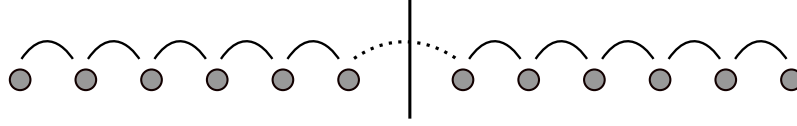


Figure 5.1 | Chain with a crack in the middle. The dotted line is the broken bond due to the crack and matches the term β in the energy functional, cf. Theorem 5.8.

which is used to simplify notation. Now, the theorem will be given. Remark 5.9 compares our result to previous work, for a more detailed overview, we refer to the introduction.

Theorem 5.8. *Let Assumption 5.3 be satisfied. Let γ_n be such that (5.3) holds true. Then, there exists an $\Omega' \subset \Omega$ with $\mathbb{P}(\Omega') = 1$ such that for all $\omega \in \Omega'$ the sequence $(E_n^{\gamma_n})$ Γ -converges with respect to the $L^1(0, 1)$ -topology to the functional E^γ given by*

$$E^\gamma(v) := \begin{cases} \underline{\alpha} \int_0^1 |v'(x)|^2 dx + \beta \#S_v & \text{if } v \in SBV_c^\gamma(0, 1), \\ +\infty & \text{otherwise,} \end{cases}$$

where $\underline{\alpha} := \left(\mathbb{E}\left[\frac{1}{\alpha}\right]\right)^{-1}$ and $\beta := \inf\{-J(\omega, \delta(\omega)) : \omega \in \Omega\}$, with $\alpha(\omega) := \frac{1}{2} \frac{\partial^2 J(\omega, z)}{\partial z^2} \Big|_{z=\delta(\omega)}$.

Moreover, for $\gamma > 0$ it holds true that

$$\liminf_{n \rightarrow \infty} \inf_v E_n^{\gamma_n}(\omega, v) = \min_v E^\gamma(v) = \min\{\underline{\alpha}\gamma^2, \beta\}.$$

Remark 5.9. (i) In our limiting energy, $\underline{\alpha}$ is the constant of the elastic part of the energy. This constant $\underline{\alpha}$ is the inverse of the expectation value of the inverted second term of the Taylor expansion of $J(\omega, \cdot)$. In the periodic setting, cf. Chapter 6, $\underline{\alpha}$ is given as the harmonic mean of $\alpha_i := \frac{1}{2} J_i''(\delta_i)$, i.e. the quadratic term in the Taylor expansion. In [30], where a periodic setting with truncated parabolas is considered, the prefactor of the quadratic energy replaces the coefficient α_i of the Taylor series. The elastic constant $\underline{\alpha}$ thus is also its harmonic mean. Therefore, our result, especially regarding the elastic constant, extends the periodic setting to the stochastic one in a natural way.

(ii) The constant β of the fracture part of the energy is not an expectation value, in contrast to $\underline{\alpha}$. Here, the infimum over all potentials is considered. This can be interpreted as the fact that if the chain breaks, it does so at its weakest point. The defining term of β can be seen as a boundary layer energy. The quantity which is infimized in the definition of β is $-J(\omega, \delta(\omega))$, which is exactly the bond of the chain which is broken or missing due to the crack, see Figure 5.1. In the case of more interacting neighbours, this term would take into account all bonds which are broken at the site of the crack. It is referred to as boundary layer term of the energy.

In the periodic setting, cf. Chapter 6, the infimum is replaced by a minimum. This is again in accordance with [30], where the constant of the fracture part of the limiting energy is the minimum over the truncation heights. This is the natural analogy to the value $-J(\omega, \delta(\omega))$, since both quantities represent the increase of energy from the minimum of the potential to $+\infty$.

Proof. First of all, the expectation value of α^{-1} exists due to Remark 5.4 and therefore $\underline{\alpha}$ is well defined. In the following, we use a Taylor expansion of $J(\tau_i \omega, x)$ several times, which reads

$$J(\tau_i \omega, \delta(\tau_i \omega) + x) = J(\tau_i \omega, \delta(\tau_i \omega)) + \alpha(\tau_i \omega) x^2 + \eta(\tau_i \omega, x), \quad (5.12)$$

with $\alpha(\tau_i \omega) := \frac{1}{2} J''(\tau_i \omega, \delta(\tau_i \omega))$ and

$$\frac{\eta(\tau_i \omega, x)}{|x|^2} \rightarrow 0 \quad \text{as } |x| \rightarrow 0.$$

Since $J \in C^3$ by (LJ4), we can use the Lagrange form of the remainder and get

$$\eta(\tau_i \omega, x) = \frac{1}{6} \frac{\partial^3 J(\tau_i \omega, y)}{\partial y^3} \Big|_{y=\xi} x^3 \quad \text{for some } \xi \text{ between } \delta(\tau_i \omega) \text{ and } \delta(\tau_i \omega) + x. \quad (5.13)$$

Step 1. Liminf inequality.

Let $v \in L^1(0, 1)$ and let $(v_n) \subset L^1(0, 1)$ be a sequence with $v_n \rightarrow v$ in $L^1(0, 1)$. We have to show

$$\liminf_{n \rightarrow \infty} E_n^{\gamma_n}(\omega, v_n) \geq \alpha \int_0^1 |v'(x)|^2 dx + \beta \# S_v. \quad (5.14)$$

It is sufficient to have a look at (sub-)sequences with equibounded energy, that means that it holds true $\sup_n E_n^{\gamma_n}(\omega, v_n) < \infty$, because the other case is trivial. For such a sequence, the compactness result from Theorem 5.6 provides $v \in SBV_c^\gamma(0, 1)$ and the existence of a finite set $S = \{x_1, \dots, x_N\}$ such that $v_n \rightharpoonup v$ locally weakly in $H^1((0, 1) \setminus S)$. Now, let $\rho > 0$ be such that $|x_i - x_j| > 2\rho$ for all $x_i, x_j \in S, i \neq j$. We define

$$\begin{aligned} S_\rho &:= \bigcup_{i=1}^N (x_i - \rho, x_i + \rho), \\ Q_n(\rho) &:= \{i \in \{0, \dots, n-1\} : (i, i+1)\lambda_n \subset (0, 1) \setminus S_\rho\}, \\ S_n(\rho) &:= \{i \in \{0, \dots, n-1\} : i \notin Q_n(\rho)\}. \end{aligned}$$

The sets $S_n(\rho)$ and $Q_n(\rho)$ separate indices close to a jump of v from those away from a jump. According to this, the energy can also be separated into

$$\begin{aligned} E_n^{\gamma_n}(\omega, v_n) &= \sum_{i \in Q_n(\rho)} \left(J \left(\tau_i \omega, \frac{v_n^{i+1} - v_n^i}{\sqrt{\lambda_n}} + \delta(\tau_i \omega) \right) - J(\tau_i \omega, \delta(\tau_i \omega)) \right) \\ &\quad + \sum_{i \in S_n(\rho)} \left(J \left(\tau_i \omega, \frac{v_n^{i+1} - v_n^i}{\sqrt{\lambda_n}} + \delta(\tau_i \omega) \right) - J(\tau_i \omega, \delta(\tau_i \omega)) \right). \end{aligned}$$

We now show that

$$\liminf_{n \rightarrow \infty} \sum_{i \in Q_n(\rho)} \left(J \left(\tau_i \omega, \frac{v_n^{i+1} - v_n^i}{\sqrt{\lambda_n}} + \delta(\tau_i \omega) \right) - J(\tau_i \omega, \delta(\tau_i \omega)) \right) \geq \alpha \int_{(0,1) \setminus S_\rho} |v'(x)|^2 dx \quad (5.15)$$

and

$$\liminf_{n \rightarrow \infty} \sum_{i \in S_n(\rho)} \left(J \left(\tau_i \omega, \frac{v_n^{i+1} - v_n^i}{\sqrt{\lambda_n}} + \delta(\tau_i \omega) \right) - J(\tau_i \omega, \delta(\tau_i \omega)) \right) \geq \beta \# S_v, \quad (5.16)$$

which provides (5.14) as $\rho \rightarrow 0$ and by using $v' \in L^2(0, 1)$.

Step A: Proof of the elastic part of the energy (5.15).

For $M \in \mathbb{N}$, which represents a coarser scale, we define

$$\begin{aligned} I_n &:= \left\{ i \in \{0, \dots, n-1\} : \left| \frac{v_n^{i+1} - v_n^i}{\lambda_n} \right| > \lambda_n^{-\frac{1}{8}} \right\}, \\ I_{n,M} &:= \{j \in \{0, \dots, n-1\} \cap M\mathbb{Z} : \{j, \dots, j+M-1\} \cap I_n \neq \emptyset\}, \\ \chi_n(x) &:= \begin{cases} 1 & \text{if } x \in [i, i+1)\lambda_n \text{ and } i \in \mathbb{Z} \setminus I_n, \\ 0 & \text{if } x \in [i, i+1)\lambda_n \text{ and } i \in I_n, \end{cases} \\ \chi_{n,M}(x) &:= \begin{cases} 1 & \text{if } x \in [j, j+M)\lambda_n \text{ and } j \in M\mathbb{Z} \setminus I_{n,M}, \\ 0 & \text{if } x \in [j, j+M)\lambda_n \text{ and } j \in I_{n,M}. \end{cases} \end{aligned}$$

The sets I_n and $I_{n,M}$ and the associated functions χ_n and $\chi_{n,M}$ are used in what follows. The choice of the exponent $-1/8$ is also of technical nature, fitting to the estimates in the following liminf and limsup estimates. First, we derive some properties of these functions. Since all summands are positive and with the help of (5.5), we can estimate for n large enough

$$\begin{aligned} E_n^{\gamma_n}(\omega, v_n) &\geq \sum_{i=0}^{n-1} \left(\lambda_n K_1 \left(\frac{v_n^{i+1} - v_n^i}{\lambda_n} \right)^2 \wedge K_2 \right) \geq \sum_{i \in I_n} \left(\lambda_n K_1 \left(\frac{v_n^{i+1} - v_n^i}{\lambda_n} \right)^2 \wedge K_2 \right) \\ &\geq \#I_n \lambda_n K_1 \left(\lambda_n^{-\frac{1}{8}} \right)^2 = \#I_n K_1 \lambda_n^{\frac{3}{4}}, \end{aligned}$$

which shows $\#I_n = \mathcal{O}(\lambda_n^{-\frac{3}{4}})$ due to the equiboundedness of the energy. Furthermore, we have

$$|\{x \in (0, 1) : \chi_n(x) \neq 1\}| \leq |\{x \in (0, 1) : \chi_{n,M}(x) \neq 1\}| \leq M \#I_n \cdot \lambda_n,$$

i.e. $\chi_n \rightarrow 1$ and $\chi_{n,M} \rightarrow 1$ bounded in measure in $(0, 1)$ as $n \rightarrow \infty$.

We set $\chi_n^i := \chi_n(i\lambda_n)$ and likewise for $\chi_{n,M}$. The energy then reads, with the help of the Taylor expansion (5.12),

$$\begin{aligned} &\sum_{i \in Q_n(\rho)} \left(J \left(\tau_i \omega, \frac{v_n^{i+1} - v_n^i}{\sqrt{\lambda_n}} + \delta(\tau_i \omega) \right) - J(\tau_i \omega, \delta(\tau_i \omega)) \right) \\ &= \sum_{i \in Q_n(\rho)} \left(\alpha(\tau_i \omega) \left(\frac{v_n^{i+1} - v_n^i}{\sqrt{\lambda_n}} \right)^2 + \eta \left(\tau_i \omega, \frac{v_n^{i+1} - v_n^i}{\sqrt{\lambda_n}} \right) \right) \\ &\geq \sum_{i \in Q_n(\rho)} \left(\chi_n^i \alpha(\tau_i \omega) \lambda_n \left(\frac{v_n^{i+1} - v_n^i}{\lambda_n} \right)^2 + \chi_n^i \eta \left(\tau_i \omega, \frac{v_n^{i+1} - v_n^i}{\sqrt{\lambda_n}} \right) \right). \end{aligned} \tag{5.17}$$

We consider both terms of the sum separately in the next two steps. This is possible, because the second term vanishes as $n \rightarrow \infty$ and we can use $\liminf_{n \rightarrow \infty} (a_n + b_n) = \liminf_{n \rightarrow \infty} (a_n) + b$ for $b_n \rightarrow b$.

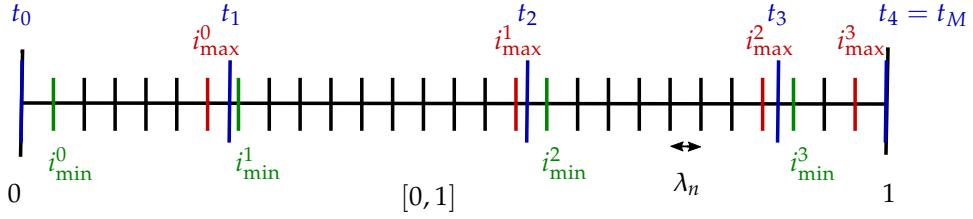


Figure 5.2 | The definitions of i_{\min}^m and i_{\max}^m for $M = 4$.

Step B: Proof of the elastic part of the energy (5.15) - Second addend of (5.17).

In order to show convergence to zero of the second term on the right-hand side of (5.17), we use the Lagrange form of the remainder from (5.13) and get, with ξ_i between $\delta(\tau_i\omega)$ and $\delta(\tau_i\omega) + \frac{v_n^{i+1} - v_n^i}{\sqrt{\lambda_n}}$,

$$\sum_{i \in Q_n(\rho)} \chi_n^i \eta \left(\tau_i \omega, \frac{v_n^{i+1} - v_n^i}{\sqrt{\lambda_n}} \right) = \sum_{i \in Q_n(\rho)} \chi_n^i \frac{1}{6} \left. \frac{\partial^3 J(\tau_i \omega, y)}{\partial y^3} \right|_{y=\xi_i} \left(\frac{v_n^{i+1} - v_n^i}{\sqrt{\lambda_n}} \right)^3.$$

For all $i \in Q_n(\rho)$ with $\chi_n^i(x) \neq 0$ we have $\left| \frac{v_n^{i+1} - v_n^i}{\lambda_n} \right| \leq \lambda_n^{-\frac{1}{8}}$ and equivalently it holds true that $\left| \frac{v_n^{i+1} - v_n^i}{\sqrt{\lambda_n}} \right| = \sqrt{\lambda_n} \left| \frac{v_n^{i+1} - v_n^i}{\lambda_n} \right| \leq \lambda_n^{\frac{3}{8}}$. Therefore, $\xi_i \in [\delta(\tau_i\omega), \delta(\tau_i\omega) + \kappa] \subset [\delta(\tau_i\omega) - \kappa, \delta(\tau_i\omega) + \kappa]$ for n large enough with $\kappa < \kappa^*$ from (H2). Thus, we can estimate for n large enough

$$\begin{aligned} \sum_{i \in Q_n(\rho)} \left| \chi_n^i \eta \left(\tau_i \omega, \frac{v_n^{i+1} - v_n^i}{\sqrt{\lambda_n}} \right) \right| &\leq \sum_{i \in Q_n(\rho)} \frac{1}{6} \left| \left. \frac{\partial^3 J(\tau_i \omega, y)}{\partial y^3} \right|_{y=\xi_i} \right| \left(\lambda_n^{\frac{3}{8}} \right)^3 \\ &\leq \frac{1}{6} \lambda_n^{\frac{1}{8}} \lambda_n \sum_{i=0}^{n-1} \sup_{x \in [\delta(\tau_i\omega) - \kappa, \delta(\tau_i\omega) + \kappa]} \left| \left. \frac{\partial^3 J(\tau_i \omega, y)}{\partial y^3} \right|_{y=x} \right| \leq C \lambda_n^{\frac{1}{8}}, \end{aligned}$$

where the last estimate is due to the convergence of the random variable C^κ to its expectation value, see Proposition 5.5. Therefore, the whole expression converges to zero as $n \rightarrow \infty$, which proves the assertion of convergence to zero of the second term to be correct.

Step C: Proof of the elastic part of the energy (5.15) - First addend of (5.17).

We continue with the first part of the sum in (5.17) and rearrange it. Following the construction in the proof of the liminf-inequality of Theorem 4.14, we define for $\delta > 0$ and $M \in \mathbb{N}$ the coarse grained grid $t_0, \dots, t_M \in [0, 1]$ with $t_0 = 0$, $t_M = 1$ and $\delta < t_{m+1} - t_m < 2\delta$ in such a way that it holds true that $v_n(t_m) \rightarrow v(t_m)$ pointwise as $n \rightarrow \infty$ and for every $m = 0, \dots, M$. For better readability, we define $I_m := [t_m, t_{m+1})$ for $m = 0, \dots, M$. Further, we set (pictured in Figure 5.2)

$$\begin{aligned} i_{\min}^m &:= \min \{ i : i \in \mathbb{Z} \cap nI_m \}, \\ i_{\max}^m &:= \max \{ i : i \in \mathbb{Z} \cap nI_m \}, \end{aligned}$$

for which it holds true by definition

$$\lambda_n i_{\min}^m \rightarrow t_m \quad \text{and} \quad \lambda_n i_{\max}^m \rightarrow t_{m+1} \quad \text{as} \quad n \rightarrow \infty.$$

The energy can be written as

$$\begin{aligned}
 & \sum_{i \in Q_n(\rho)} \lambda_n \chi_n^i \alpha(\tau_i \omega) \left(\frac{v_n^{i+1} - v_n^i}{\lambda_n} \right)^2 \geq \sum_{i \in Q_n(\rho)} \lambda_n \chi_{n,M}^i \alpha(\tau_i \omega) \left(\frac{v_n^{i+1} - v_n^i}{\lambda_n} \right)^2 \\
 & \geq \sum_{\substack{m=0 \\ (nI_m \cap \mathbb{Z}) \subset Q_n(\rho)}}^M \chi_{n,M}^m \sum_{i \in \mathbb{Z} \cap nI_m} \lambda_n \alpha(\tau_i \omega) \left(\frac{v_n^{i+1} - v_n^i}{\lambda_n} \right)^2 \\
 & \geq \sum_{\substack{m=0 \\ (nI_m \cap \mathbb{Z}) \subset Q_n(\rho)}}^M \chi_{n,M}^m \min \left\{ \sum_{i \in \mathbb{Z} \cap nI_m} \lambda_n \alpha(\tau_i \omega) \left(\frac{v_n^{i+1} - v_n^i}{\lambda_n} \right)^2 : \sum_{i \in \mathbb{Z} \cap nI_m} \frac{v_n^{i+1} - v_n^i}{\lambda_n} = n \left(v_n^{i_{\max}^m+1} - v_n^{i_{\min}^m} \right) \right\} \\
 & \stackrel{(*)}{=} \sum_{\substack{m=0 \\ (nI_m \cap \mathbb{Z}) \subset Q_n(\rho)}}^M \chi_{n,M}^m \lambda_n (i_{\max}^m - i_{\min}^m + 1) \left(\frac{1}{i_{\max}^m - i_{\min}^m + 1} \sum_{i \in \mathbb{Z} \cap nI_m} \frac{1}{\alpha(\tau_i \omega)} \right)^{-1} \left(\frac{v_n^{i_{\max}^m+1} - v_n^{i_{\min}^m}}{\lambda_n (i_{\max}^m - i_{\min}^m + 1)} \right)^2,
 \end{aligned}$$

where $(*)$ holds true due to Lemma 2.24. Now, we pass to the limit $\liminf_{n \rightarrow \infty}$. Therefore, note that it holds true that

$$\liminf_{n \rightarrow \infty} \left(\frac{1}{i_{\max}^m - i_{\min}^m + 1} \sum_{i \in \mathbb{Z} \cap nI_m} \frac{1}{\alpha(\tau_i \omega)} \right)^{-1} = \left(\mathbb{E}[\alpha^{-1}] \right)^{-1}.$$

This follows from Proposition 5.5, since $i_{\max}^m - i_{\min}^m + 1 = |\mathbb{Z} \cap nI_m|$. As a result, we get with $\liminf_n (a_n b_n) \geq \liminf_n (a_n) \cdot \liminf_n (b_n)$

$$\begin{aligned}
 & \liminf_{n \rightarrow \infty} \sum_{i \in Q_n(\rho)} \lambda_n \chi_n^i \alpha(\tau_i \omega) \left(\frac{v_n^{i+1} - v_n^i}{\lambda_n} \right)^2 \\
 & \geq \left(\mathbb{E}[\alpha^{-1}] \right)^{-1} \liminf_{n \rightarrow \infty} \sum_{\substack{m=0 \\ (nI_m \cap \mathbb{Z}) \subset Q_n(\rho)}}^M \chi_{n,M}^m \lambda_n (i_{\max}^m - i_{\min}^m + 1) \left(\frac{v_n^{i_{\max}^m+1} - v_n^{i_{\min}^m}}{\lambda_n (i_{\max}^m - i_{\min}^m + 1)} \right)^2.
 \end{aligned}$$

For the next term, since by construction it holds true that $\lambda_n (i_{\max}^m - i_{\min}^m + 1) \rightarrow (t_{m+1} - t_m)$, we can again follow the proof of the liminf-inequality of Theorem 4.14 and obtain pointwise convergence of

$$\frac{v_n^{i_{\max}^m+1} - v_n^{i_{\min}^m}}{\lambda_n (i_{\max}^m - i_{\min}^m + 1)} \rightarrow \frac{v_M(t_{m+1}) - v_M(t_m)}{t_{m+1} - t_m}, \quad (5.18)$$

since it holds true that $i_{\max}^m + 1 = i_{\min}^{m+1}$ and v_M is defined as the piecewise affine interpolation of v with grid points t_m . For writing the sum as an integral, we define

$$\begin{aligned}
 S_{\rho,M,n} & := \bigcup_{\substack{m=0 \\ I_m \cap S_n(\rho) \neq \emptyset}}^M I_m = \bigcup_{\substack{m=0 \\ I_m \cap S_n(\rho) \neq \emptyset}}^M [t_m, t_{m+1}), \\
 S_{\rho,M} & := \bigcup_{\substack{m=0 \\ I_m \cap S_\rho \neq \emptyset}}^M I_m = \bigcup_{\substack{m=0 \\ I_m \cap S_\rho \neq \emptyset}}^M [t_m, t_{m+1}),
 \end{aligned}$$

where, by definition, $S_{\rho,M,n} = S_{\rho,M}$ holds true as n large enough. Therefore, with the definition of

$v_{n,M}$ as the piecewise affine interpolation of v_n with respect to i_{\min}^m , we get

$$\begin{aligned} \liminf_{n \rightarrow \infty} \sum_{i \in Q_n(\rho)} \lambda_n \chi_n^i \alpha(\tau_i \omega) \left(\frac{v_n^{i+1} - v_n^i}{\lambda_n} \right)^2 &\geq \left(\mathbb{E}[\alpha^{-1}] \right)^{-1} \liminf_{n \rightarrow \infty} \int_{(0,1) \setminus S_{\rho,M,n}} \chi_{n,M} |v'_{n,M}|^2 dx \\ &\geq \left(\mathbb{E}[\alpha^{-1}] \right)^{-1} \int_{(0,1) \setminus S_{\rho,M}} |v'_M(x)|^2 dx, \end{aligned} \quad (5.19)$$

where the last inequality follows from the weak lower semicontinuity of the L^2 norm and because we have $\chi_{n,M} \rightarrow 1$ bounded in measure, $v'_{n,M} \rightarrow v'_M$ in L^2 (because of 5.18) and thus $\chi_{n,M} v'_{n,M} \rightharpoonup v'_M$ in L^2 .

It remains to perform the limit $\liminf_{M \rightarrow \infty}$. Since the left hand side of (5.19) is independent of M we only have to consider

$$\begin{aligned} \liminf_{M \rightarrow \infty} \int_{(0,1) \setminus S_{\rho,M}} |v'_M(x)|^2 dx \\ \geq \liminf_{M \rightarrow \infty} \int_{(0,1) \setminus S_\rho} |v'_M(x)|^2 dx - \limsup_{M \rightarrow \infty} \int_{S_{\rho,M} \setminus S_\rho} |v'_M(x)|^2 dx. \end{aligned} \quad (5.20)$$

Step E of the liminf-inequality in the proof of Theorem 4.14 shows that $v_M \rightharpoonup^* v$ in BV , and therefore $v_M \rightarrow v$ in $L^1(0,1)$. The compactness result in Theorem 5.6 further yields $v' \in L^2(0,1)$. For an interval $(a,b) \subset (0,1) \setminus S_\rho$ we define the coarser grid points as before, with $t_0 = a$ and $t_M = b$. Using the Hölder inequality, which is possible due to $v' = \nabla v$ on (a,b) , we get the uniform bound

$$\begin{aligned} \|v'_M\|_{L^2(a,b)}^2 &= \int_a^b |v'_M(x)|^2 dx = \sum_{m=0}^M (t_{m+1} - t_m) \left| \frac{v(t_{m+1}) - v(t_m)}{t_{m+1} - t_m} \right|^2 \\ &= \sum_{m=0}^M \frac{1}{t_{m+1} - t_m} \left| \int_{t_m}^{t_{m+1}} v'(x) dx \right|^2 \leq \sum_{m=0}^M \int_{t_m}^{t_{m+1}} |v'(x)|^2 dx = \|v'\|_{L^2(a,b)}^2, \end{aligned}$$

which yields $v'_M \rightarrow v'$ in $L^2(a,b)$ as $M \rightarrow \infty$. This result can be applied to $(0,1) \setminus S_\rho$ and reads $v'_M \rightarrow v'$ in $L^2((0,1) \setminus S_\rho)$ as $M \rightarrow \infty$. Since the integral functional is lower semicontinuous, we can estimate the first term of the right hand side of (5.20) by

$$\liminf_{M \rightarrow \infty} \int_{(0,1) \setminus S_\rho} |v'_M(x)|^2 dx \geq \int_{(0,1) \setminus S_\rho} |v'(x)|^2 dx.$$

The second part of (5.20) fulfils

$$\limsup_{M \rightarrow \infty} \int_{S_{\rho,M} \setminus S_\rho} |v'_M(x)|^2 dx = 0,$$

which can be seen as follows: We assume that S_ρ consists only of one interval (which corresponds to $S = \{x_1\}$) and note that the proof for finitely many intervals is analogous. By construction, there exist sequences k_M and ℓ_M such that

$$S_{\rho,M} \setminus S_\rho \subset \left([t_{k_M}, t_{k_M+1}] \cup [t_{\ell_M}, t_{\ell_M+1}] \right)$$

and

$$\begin{aligned} t_{k_M} &\rightarrow x_i - \rho, & t_{k_{M+1}} &\rightarrow x_i - \rho, \\ t_{\ell_M} &\rightarrow x_i + \rho, & t_{\ell_{M+1}} &\rightarrow x_i + \rho \quad \text{as } M \rightarrow \infty. \end{aligned} \quad (5.21)$$

Therefore, it holds true that

$$\int_{S_{\rho,M} \setminus S_\rho} |v'_M(x)|^2 dx \leq \int_{t_{k_M}}^{t_{k_{M+1}}} |v'_M(x)|^2 dx + \int_{t_{\ell_M}}^{t_{\ell_{M+1}}} |v'_M(x)|^2 dx.$$

We are going to consider only one of these two terms, because they have basically the same structure, and show that it converges to zero. Observing that the integration area is contained in $(0,1) \setminus S$ for $M \gg \rho$ (in fact, for $2\delta < \rho$) and therefore v can be assumed as the absolutely continuous representative, we get with the Hölder inequality

$$\begin{aligned} \int_{t_{k_M}}^{t_{k_{M+1}}} |v'_M(x)|^2 dx &= (t_{k_{M+1}} - t_{k_M}) \left| \frac{v(t_{k_{M+1}}) - v(t_{k_M})}{t_{k_{M+1}} - t_{k_M}} \right|^2 = \frac{|v(t_{k_{M+1}}) - v(t_{k_M})|^2}{t_{k_{M+1}} - t_{k_M}} \\ &= \frac{1}{t_{k_{M+1}} - t_{k_M}} \left| \int_{t_{k_M}}^{t_{k_{M+1}}} v'(x) dx \right|^2 \leq \frac{1}{t_{k_{M+1}} - t_{k_M}} \left(\int_{t_{k_M}}^{t_{k_{M+1}}} |v'(x)| dx \right)^2 \\ &\leq \frac{1}{t_{k_{M+1}} - t_{k_M}} \left[\left(\int_{t_{k_M}}^{t_{k_{M+1}}} |v'(x)|^2 dx \right)^{\frac{1}{2}} (t_{k_{M+1}} - t_{k_M})^{\frac{1}{2}} \right]^2 = \int_{t_{k_M}}^{t_{k_{M+1}}} |v'(x)|^2 dx. \end{aligned}$$

Since v is absolutely continuous, the integral functional is continuous with respect to its integral bounds due to the fundamental theorem of calculus. Together with (5.21), this shows

$$\limsup_{M \rightarrow \infty} \int_{t_{k_M}}^{t_{k_{M+1}}} |v'(x)|^2 dx = \lim_{M \rightarrow \infty} \int_{t_{k_M}}^{t_{k_{M+1}}} |v'(x)|^2 dx = 0.$$

Together, Step A–C show (5.15).

Step D: Proof of the jump part of the energy (5.16).

It is left to show

$$\liminf_{n \rightarrow \infty} \sum_{i \in S_n(\rho)} \left(J \left(\tau_i \omega, \frac{v_n^{i+1} - v_n^i}{\sqrt{\lambda_n}} + \delta(\tau_i \omega) \right) - J(\tau_i \omega, \delta(\tau_i \omega)) \right) \geq \beta \# S_v.$$

According to [34, (117)], one can find a sequence $(h_n^t) \subset \mathbb{N}$ for every $t \in S_v$ with $\lambda_n h_n^t \rightarrow t$ as $n \rightarrow \infty$ such that

$$\lim_{n \rightarrow \infty} \frac{v_n^{h_n^t+1} - v_n^{h_n^t}}{\sqrt{\lambda_n}} = +\infty. \quad (5.22)$$

Especially, $h_n^t \notin Q_n(\rho)$ holds true for n large enough. The existence of such a sequence can be seen by a contradiction argument: If this did not exist, we would get $v_n' < C/\sqrt{\lambda_n}$ in a neighbourhood $(t - \xi, t + \xi)$ of t . Following Step 1 of the proof of Theorem 5.6, this would imply $\int_{t-\xi}^{t+\xi} |v_n'|^2 dt \leq CE_n^{\gamma_n}(\omega, v_n)$, and therefore v_n would be equibounded in $H^1(0,1)$ in a

neighbourhood of t . Therefore, we get

$$\begin{aligned}
 & \sum_{i \in S_n(\rho)} \left(J \left(\tau_i \omega, \frac{v_n^{i+1} - v_n^i}{\sqrt{\lambda_n}} + \delta(\tau_i \omega) \right) - J(\tau_i \omega, \delta(\tau_i \omega)) \right) \\
 & \geq \sum_{t \in S_v} \left(J \left(\tau_{h_n^t} \omega, \frac{v_n^{h_n^t+1} - v_n^{h_n^t}}{\sqrt{\lambda_n}} + \delta(\tau_{h_n^t} \omega) \right) - J(\tau_{h_n^t} \omega, \delta(\tau_{h_n^t} \omega)) \right) \\
 & \geq \sum_{t \in S_v} J \left(\tau_{h_n^t} \omega, \frac{v_n^{h_n^t+1} - v_n^{h_n^t}}{\sqrt{\lambda_n}} + \delta(\tau_{h_n^t} \omega) \right) + \sum_{t \in S_v} \inf \{ -J(\omega, \delta(\omega)) : \omega \in \Omega \} \\
 & = \sum_{t \in S_v} J \left(\tau_{h_n^t} \omega, \frac{v_n^{h_n^t+1} - v_n^{h_n^t}}{\sqrt{\lambda_n}} + \delta(\tau_{h_n^t} \omega) \right) + \beta \#S_v.
 \end{aligned}$$

By taking $\liminf_{n \rightarrow \infty}$, the first term vanishes because of (5.22) and (H3) which says that every Lennard-Jones type potential uniformly converges to 0 as $z \rightarrow \infty$.

Step 2. Limsup inequality.

We have to show that for every $v \in SBV_c^\gamma$ there exists a sequence v_n with $v_n \rightarrow v$ in $L^1(0, 1)$ such that

$$\limsup_{n \rightarrow \infty} E_n^{\gamma_n}(\omega, v_n) \leq E^\gamma(v).$$

Without loss of generality, we consider $\#S_v = 1$ to keep the notation simple. The extension to the case $\#S_v > 1$ can easily be proven since we construct the recovery sequence step by step, starting from affine functions and glueing them together to a piecewise affine function. The case $\#S_v = 0$ is included by setting the jump height to zero which simplifies the subsequent calculations.

We already know from the compactness result in Theorem 5.6 that v is piecewise $H^1(0, 1)$. Therefore, we can write $v = v_c + v_j$, where $v_c \in H^1(0, 1)$ and v_j is a piecewise constant function. By a density argument, see [21, Rem. 1.29], we can assume $v_c \in C^2[0, 1]$. Note that this approximation can be chosen in such a way, that it keeps the boundary values, see e.g. [39, Section 2.4, Cor. 3]. We construct explicitly a recovery sequence for affine functions with a single jump and extend it afterwards to the general case.

Step A: Affine function.

We construct a recovery sequence for an affine function v with slope z , a jump in 0 and constant near the jump. That is, for $z \in \text{dom}J_j$ and a small $\rho > 0$, we have

$$v(x) = \begin{cases} 0 & \text{for } x = 0, \\ v(0^+) & \text{for } x \in (0, \rho), \\ v(0^+) + (x - \rho)z & \text{for } x \in [\rho, 1], \end{cases}$$

with $v(0^+) > 0$ defined such that

$$v(1) = v(0^+) + (1 - \rho)z = \gamma, \tag{5.23}$$

in order to fulfil the boundary constraint as well as the assumption $\#S_v = 1$ and $[v] \geq 0$ from the compactness result in Theorem 5.6. Without loss of generality, the jump is at 0. A jump at 1 can be constructed analogously, with small changes. Wherever in the proof it is important where exactly the jump lies (which will be in (5.29)), we highlight it and proof it in a general way.

There exists a unique sequence T_n such that $\rho \in [T_n, T_n + 1)\lambda_n$. First, we consider $\epsilon > 0$ fixed such that $\epsilon < \rho$ and $\epsilon < T_n\lambda_n$ and define

$$h_n^\epsilon := \operatorname{argmin}_{0 \leq i \leq n-1} \{-J(\tau_i \omega, \delta(\tau_i \omega)) : |i\lambda_n - \rho| < \epsilon\}.$$

Let $(\mu_k)_{k \in \mathbb{N}} > 0$ be a sequence in \mathbb{R} with $\mu_k = \frac{1-\rho}{k}$ for all $k \in \mathbb{N}$. We define a partition of the interval $(\rho, 1]$ by $I_j^{\mu_k} := (\rho + j\mu_k, \rho + (j+1)\mu_k]$ with $j = 0, \dots, \frac{1-\rho}{\mu_k} - 1$. Hence, the set

$$\left\{ I_j^{\mu_k} : \mu_k = \frac{1-\rho}{k}, j = 0, \dots, k-1, k \in \mathbb{N} \right\}$$

is a countable set of sets. Thus, for all $I = I_j^{\mu_k}$ with $\mu_k = \frac{1}{k}, k \in \mathbb{N}$ and $j = 0, \dots, k-1$, we can pass to the limit in the sense of Tempel'man's ergodic theorem, cf. Theorem 2.14. Thereby, the set Ω' , for which the ergodic result holds true, is the intersection of countably many sets Ω_I . In the following, we leave out the index k and just refer to the sequence μ_k by μ .

From now on, let μ be fixed. We define for $j = 0, \dots, (1-\rho)/\mu - 1 =: j_{\max}$

$$\begin{aligned} I_j^\mu &:= (\rho + j\mu, \rho + (j+1)\mu], \\ I_{j,n}^\mu &:= \mathbb{Z} \cap nI_j^\mu, \\ i_{\min}^{j,n} &:= \min\{i : i \in \mathbb{Z} \cap nI_j^\mu\}, \\ i_{\max}^{j,n} &:= \max\{i : i \in \mathbb{Z} \cap nI_j^\mu\}, \\ I_{j,n}^{\mu*} &:= I_{j,n}^\mu \cup \{i_{\min}^{j,n} - 1\} \setminus \{i_{\max}^{j,n}\}. \end{aligned}$$

Note that $\bigcup_{j=0}^{j_{\max}} I_{j,n}^{\mu*} = \{T_n, \dots, n-1\}$ holds true. With this notation, we define two sequences of piecewise affine functions, (φ_n) and (ϕ_n) , which together (almost) form the recovery sequence (v_n) , defined by

$$v_n := \varphi_n + \phi_n.$$

To be precise, the sequence v_n has to be a sequence $v_{n,\mu}$, depending on μ . Since this does not affect most of the calculations, we drop the subscript μ whenever it is not relevant. In the last step of the proof, we get from the Attouch-Lemma, see Theorem 2.23, the existence of a sequence μ_n , such that (v_{n,μ_n}) finally is the recovery sequence. We first define (φ_n) , which accounts for the jump and the boundary conditions, by

$$\varphi_n^i := \begin{cases} v(0^-) = 0 & \text{for } 0 \leq i \leq h_n^\epsilon, \\ v(0^+) + \gamma_n - \gamma & \text{for } h_n^\epsilon < i \leq n. \end{cases}$$

Since later we extend this construction to piecewise affine functions, we have to take care of the boundary values γ_n and γ . They have to be understood as the boundary data of the considered

interval. That is, for an interval which does not contain $x = 0$ or $x = 1$, it holds true that $\gamma_n = \gamma$ and therefore the term $\gamma_n - \gamma$ cancels out.

The sequence (ϕ_n) optimizes the elastic energy and is given by

$$\phi_n^i := \begin{cases} 0 & \text{for } 0 \leq i \leq h_n^\epsilon, \\ z(T_n \lambda_n - \rho) & \text{for } h_n^\epsilon < i \leq T_n, \\ z\left((i_{\min}^{j,n} - 1)\lambda_n - \rho\right) + \left(\frac{1}{|I_{j,n}^{\mu*}|} \sum_{k \in I_{j,n}^{\mu*}} \frac{1}{\alpha(\tau_k \omega)}\right)^{-1} \lambda_n z \sum_{k=i_{\min}^{j,n}-1}^{i-1} \frac{1}{\alpha(\tau_k \omega)} & \text{for } i \in I_{j,n}^\mu. \end{cases}$$

Note that the definition provides for every $j = 0, \dots, (1 - \rho)/\mu - 1$

$$\begin{aligned} v_n^{i_{\max}^{j,n}} &= \varphi_n^{i_{\max}^{j,n}} + \phi_n^{i_{\max}^{j,n}} \\ &= v(0^+) + \gamma_n - \gamma + z\left((i_{\min}^{j,n} - 1)\lambda_n - \rho\right) + \left(\frac{1}{|I_{j,n}^{\mu*}|} \sum_{k \in I_{j,n}^{\mu*}} \frac{1}{\alpha(\tau_k \omega)}\right)^{-1} \lambda_n z \sum_{k=i_{\min}^{j,n}-1}^{i_{\max}^{j,n}-1} \frac{1}{\alpha(\tau_k \omega)} \\ &= v(0^+) + \gamma_n - \gamma + z\left((i_{\min}^{j,n} - 1)\lambda_n - \rho\right) + \lambda_n z |I_{j,n}^{\mu*}| \\ &= v(0^+) + \gamma_n - \gamma + z\left((i_{\min}^{j,n} - 1)\lambda_n - \rho\right) + \lambda_n z (i_{\max}^{j,n} - i_{\min}^{j,n} + 1) \\ &= v(0^+) + \gamma_n - \gamma + z\left((i_{\max}^{j,n})\lambda_n - \rho\right) = v^{i_{\max}^{j,n}} + \gamma_n - \gamma. \end{aligned} \tag{5.24}$$

Therefore, v_n and v coincide at the value $i_{\max}^{j,n}$ up to their boundary conditions. Together, the sequence (v_{n,μ_n}) of piecewise affine functions $v_n \in \hat{\mathcal{A}}_n^{\gamma_n}(0, 1)$, with $v_n := \varphi_n + \phi_n$, is the recovery sequence for a well-chosen μ_n . To prove this, we have to show that (a) v_n fulfils the boundary conditions, (b) the limsup inequality is fulfilled and (c) $v_n \rightarrow v$ in $L^1(0, 1)$.

(a) We consider the point $i = n$ because $v(1) = v_n^n$. Since $n = i_{\max}^{j,n}$, by (5.24) we get $v_n^n = v_n^{i_{\max}^{j,n}} = v(0^+) + z(n\lambda_n - \rho) + \gamma_n - \gamma \stackrel{(5.23)}{=} \gamma_n$. Thus, the boundary condition is fulfilled.

(b) We have

$$\begin{aligned} E_n^{\gamma_n}(\omega, v_n) &= \sum_{i=0}^{n-1} \left(J\left(\tau_i \omega, \frac{v_n^{i+1} - v_n^i}{\sqrt{\lambda_n}} + \delta(\tau_i \omega)\right) - J(\tau_i \omega, \delta(\tau_i \omega)) \right) \\ &= \sum_{i=0}^{h_n^\epsilon-1} \left(J\left(\tau_i \omega, \frac{v_n^{i+1} - v_n^i}{\sqrt{\lambda_n}} + \delta(\tau_i \omega)\right) - J(\tau_i \omega, \delta(\tau_i \omega)) \right) \\ &\quad + \sum_{i=h_n^\epsilon+1}^{T_n-1} \left(J\left(\tau_i \omega, \frac{v_n^{i+1} - v_n^i}{\sqrt{\lambda_n}} + \delta(\tau_i \omega)\right) - J(\tau_i \omega, \delta(\tau_i \omega)) \right) \\ &\quad + \sum_{i=T_n}^{n-1} \left(\lambda_n \alpha(\tau_i \omega) \left(\frac{v_n^{i+1} - v_n^i}{\lambda_n}\right)^2 + \eta\left(\tau_i \omega, \frac{v_n^{i+1} - v_n^i}{\sqrt{\lambda_n}}\right) \right) \\ &\quad + J\left(\tau_{h_n^\epsilon} \omega, \frac{v_n^{h_n^\epsilon+1} - v_n^{h_n^\epsilon}}{\sqrt{\lambda_n}} + \delta(\tau_{h_n^\epsilon} \omega)\right) - J(\tau_{h_n^\epsilon} \omega, \delta(\tau_{h_n^\epsilon} \omega)). \end{aligned}$$

This energy has four parts. The first two parts (from zero to $h_n^\epsilon - 1$ and from $h_n^\epsilon + 1$ to $T_n - 1$) are identically zero by definition of v_n . To get the limsup-inequality, we have to show the two inequalities

$$\limsup_{n \rightarrow \infty} \sum_{i=T_n}^{n-1} \left(\lambda_n \alpha(\tau_i \omega) \left(\frac{v_n^{i+1} - v_n^i}{\lambda_n} \right)^2 + \eta \left(\tau_i \omega, \frac{v_n^{i+1} - v_n^i}{\sqrt{\lambda_n}} \right) \right) \leq \underline{\alpha} \int_0^1 |v'(x)|^2, \quad (5.25)$$

and

$$\limsup_{n \rightarrow \infty} \left(J \left(\tau_{h_n^\epsilon} \omega, \frac{v_n^{h_n^\epsilon+1} - v_n^{h_n^\epsilon}}{\sqrt{\lambda_n}} + \delta(\tau_{h_n^\epsilon} \omega) \right) - J(\tau_{h_n^\epsilon} \omega, \delta(\tau_{h_n^\epsilon} \omega)) \right) \leq \beta, \quad (5.26)$$

where the first one is the elastic part and the second one is the jump part of the limiting energy.

Proof of Equation (5.25), elastic part.

We start with rearranging the sum, i.e.

$$\begin{aligned} & \sum_{i=T_n}^{n-1} \left(\lambda_n \alpha(\tau_i \omega) \left(\frac{v_n^{i+1} - v_n^i}{\lambda_n} \right)^2 + \eta \left(\tau_i \omega, \frac{v_n^{i+1} - v_n^i}{\sqrt{\lambda_n}} \right) \right) \\ &= \sum_{j=0}^{j_{\max}} \sum_{i \in I_{j,n}^{\mu^*}} \lambda_n \alpha(\tau_i \omega) \left(\frac{v_n^{i+1} - v_n^i}{\lambda_n} \right)^2 + \sum_{j=0}^{j_{\max}} \sum_{i \in I_{j,n}^{\mu^*}} \eta \left(\tau_i \omega, \frac{v_n^{i+1} - v_n^i}{\sqrt{\lambda_n}} \right). \end{aligned}$$

By the definition of v_n , we get

$$\begin{aligned} \sum_{i \in I_{j,n}^{\mu^*}} \lambda_n \alpha(\tau_i \omega) \left(\frac{v_n^{i+1} - v_n^i}{\lambda_n} \right)^2 &= \sum_{i \in I_{j,n}^{\mu^*}} \lambda_n \frac{1}{\alpha(\tau_i \omega)} \left(\frac{1}{|I_{j,n}^{\mu^*}|} \sum_{k \in I_{j,n}^{\mu^*}} \frac{1}{\alpha(\tau_k \omega)} \right)^{-2} z^2 \\ &= \lambda_n |I_{j,n}^{\mu^*}| z^2 \left(\frac{1}{|I_{j,n}^{\mu^*}|} \sum_{k \in I_{j,n}^{\mu^*}} \frac{1}{\alpha(\tau_k \omega)} \right)^{-1}. \end{aligned}$$

Plugging this in, we obtain

$$\begin{aligned} & \sum_{i=T_n}^{n-1} \left(\lambda_n \alpha(\tau_i \omega) \left(\frac{v_n^{i+1} - v_n^i}{\lambda_n} \right)^2 + \eta \left(\tau_i \omega, \frac{v_n^{i+1} - v_n^i}{\sqrt{\lambda_n}} \right) \right) \\ &= \sum_{j=0}^{j_{\max}} \lambda_n |I_{j,n}^{\mu^*}| z^2 \left(\frac{1}{|I_{j,n}^{\mu^*}|} \sum_{k \in I_{j,n}^{\mu^*}} \frac{1}{\alpha(\tau_k \omega)} \right)^{-1} \\ & \quad + \sum_{j=0}^{j_{\max}} \sum_{i \in I_{j,n}^{\mu^*}} \eta \left(\tau_i \omega, \sqrt{\lambda_n} \left(\frac{1}{|I_{j,n}^{\mu^*}|} \sum_{k \in I_{j,n}^{\mu^*}} \frac{1}{\alpha(\tau_k \omega)} \right)^{-1} z \frac{1}{\alpha(\tau_i \omega)} \right). \end{aligned} \quad (5.27)$$

Now we consider $\limsup_{n \rightarrow \infty}$ of (5.27). The two parts of the sum are discussed separately in (i) and (ii) below. The first one becomes the elastic part of the energy and the second one vanishes.

(i) The first part of (5.27) is

$$\sum_{j=0}^{j_{\max}} \lambda_n |I_{j,n}^{\mu^*}| z^2 \left(\frac{1}{|I_{j,n}^{\mu^*}|} \sum_{k \in I_{j,n}^{\mu^*}} \frac{1}{\alpha(\tau_k \omega)} \right)^{-1}.$$

We take lim sup of this equation, and with Proposition 5.5 and $\lambda_n |I_{j,n}^{\mu^*}| \rightarrow \mu$ we obtain

$$\begin{aligned} & \limsup_{n \rightarrow \infty} \sum_{j=0}^{j_{\max}} \lambda_n |I_{j,n}^{\mu^*}| z^2 \left(\frac{1}{|I_{j,n}^{\mu^*}|} \sum_{k \in I_{j,n}^{\mu^*}} \frac{1}{\alpha(\tau_k \omega)} \right)^{-1} \\ & \leq \sum_{j=0}^{j_{\max}} \left(\limsup_{n \rightarrow \infty} \lambda_n |I_{j,n}^{\mu^*}| \right) z^2 \limsup_{n \rightarrow \infty} \left(\frac{1}{|I_{j,n}^{\mu^*}|} \sum_{k \in I_{j,n}^{\mu^*}} \frac{1}{\alpha(\tau_k \omega)} \right)^{-1} \\ & = \frac{1-\rho}{\mu} \mu z^2 \left(\mathbb{E} [\alpha^{-1}] \right)^{-1} = (1-\rho) z^2 \left(\mathbb{E} [\alpha^{-1}] \right)^{-1} = \underline{\alpha} \int_{\rho}^1 z^2 dx = \underline{\alpha} \int_0^1 |v'(x)|^2 dx, \end{aligned}$$

\mathbb{P} -almost everywhere. This is exactly the result we expected in order to get (5.25). We now show that the remaining part of (5.27) vanishes, which will conclude the proof of (5.25).

(ii) The second part of (5.27) is

$$\sum_{j=0}^{j_{\max}} \sum_{i \in I_{j,n}^{\mu^*}} \eta \left(\tau_i \omega, \sqrt{\lambda_n} \left(\frac{1}{|I_{j,n}^{\mu^*}|} \sum_{i \in I_{j,n}^{\mu^*}} \frac{1}{\alpha(\tau_i \omega)} \right)^{-1} z \frac{1}{\alpha(\tau_i \omega)} \right).$$

Before continuing with the estimate, we have a closer look at the argument of $\eta(\tau_i \omega)$. Since $\alpha(\omega)$ is bounded from below due to Remark 5.2 (iii), we get

$$\sqrt{\lambda_n} \left(\frac{1}{|I_{j,n}^{\mu^*}|} \sum_{i \in I_{j,n}^{\mu^*}} \frac{1}{\alpha(\tau_i \omega)} \right)^{-1} |z| \frac{1}{\alpha(\tau_i \omega)} \leq \sqrt{\lambda_n} C,$$

because of the convergence of the sum to $\mathbb{E} [\alpha^{-1}]$, due to Proposition 5.5. As before, we use the Lagrange form of the remainder from (5.13) and get with $\xi_i \in [\delta(\tau_i \omega) - \sqrt{\lambda_n} C, \delta(\tau_i \omega) + \sqrt{\lambda_n} C]$

$$\begin{aligned} & \sum_{j=0}^{j_{\max}} \sum_{i \in I_{j,n}^{\mu^*}} \eta \left(\tau_i \omega, \sqrt{\lambda_n} \left(\frac{1}{|I_{j,n}^{\mu^*}|} \sum_{i \in I_{j,n}^{\mu^*}} \frac{1}{\alpha(\tau_i \omega)} \right)^{-1} z \frac{1}{\alpha(\tau_i \omega)} \right) \\ & = \sum_{j=0}^{j_{\max}} \sum_{i \in I_{j,n}^{\mu^*}} \frac{1}{6} \frac{\partial^3 J(\tau_i \omega, y)}{\partial y^3} \Big|_{y=\xi_i} \left(\sqrt{\lambda_n} \left(\frac{1}{|I_{j,n}^{\mu^*}|} \sum_{i \in I_{j,n}^{\mu^*}} \frac{1}{\alpha(\tau_i \omega)} \right)^{-1} z \frac{1}{\alpha(\tau_i \omega)} \right)^3. \end{aligned}$$

We can again use the estimate from above and get with $\kappa < \kappa^*$ from (H2) for n large enough

$$\begin{aligned} & \sum_{j=0}^{j_{\max}} \sum_{i \in I_{j,n}^{\mu^*}} \frac{1}{6} \left| \frac{\partial^3 J(\tau_i \omega, y)}{\partial y^3} \right|_{y=\xi_i} \left| \left(\sqrt{\lambda_n} \left(\frac{1}{|I_{j,n}^{\mu^*}|} \sum_{i \in I_{j,n}^{\mu^*}} \frac{1}{\alpha(\tau_i \omega)} \right) - |z| \frac{1}{\alpha(\tau_i \omega)} \right) \right|^3 \\ & \leq \sum_{i=0}^{n-1} \frac{1}{6} \left| \frac{\partial^3 J(\tau_i \omega, y)}{\partial y^3} \right|_{y=\xi_i} \left| (\sqrt{\lambda_n} C)^3 \right| \\ & \leq \frac{1}{6} C^3 \lambda_n^{\frac{1}{2}} \lambda_n \sum_{i=0}^{n-1} \sup_{x \in [\delta(\tau_i \omega) - \kappa, \delta(\tau_i \omega) + \kappa]} \left| \frac{\partial^3 J(\tau_i \omega, y)}{\partial y^3} \right|_{y=x} \leq \hat{C} \lambda_n^{\frac{1}{2}}, \end{aligned}$$

where the last estimate is due to the convergence of the random variable C^κ to its expectation value, see Proposition 5.5. Therefore, the whole expression converges to zero, which concludes the proof of Equation (5.25).

Proof of Equation (5.26), jump part.

The last remaining part of the energy is the limsup of

$$J \left(\tau_{h_n^\epsilon} \omega, \frac{v_{h_n^\epsilon}^{h_n^\epsilon+1} - v_{h_n^\epsilon}^{h_n^\epsilon}}{\sqrt{\lambda_n}} + \delta(\tau_{h_n^\epsilon} \omega) \right) - J(\tau_{h_n^\epsilon} \omega, \delta(\tau_{h_n^\epsilon} \omega)).$$

We get

$$\frac{v_{h_n^\epsilon}^{h_n^\epsilon+1} - v_{h_n^\epsilon}^{h_n^\epsilon}}{\sqrt{\lambda_n}} = \frac{v(0^+) + \gamma_n - \gamma + z(T_n \lambda_n - \rho)}{\sqrt{\lambda_n}} \rightarrow \infty$$

as $n \rightarrow \infty$ since $\gamma_n - \gamma \rightarrow 0$, $T_n \lambda_n \rightarrow \rho$ and $v(0^+) > 0$. Therefore, we obtain

$$J \left(\tau_{h_n^\epsilon} \omega, \frac{v_{h_n^\epsilon}^{h_n^\epsilon+1} - v_{h_n^\epsilon}^{h_n^\epsilon}}{\sqrt{\lambda_n}} + \delta(\tau_{h_n^\epsilon} \omega) \right) \rightarrow 0$$

due to (H3). By definition of h_n^ϵ it holds true that

$$-J(\tau_{h_n^\epsilon} \omega, \delta(\tau_{h_n^\epsilon} \omega)) = \inf_{0 \leq i \leq n-1} \{-J(\tau_i \omega, \delta(\tau_i \omega)) : |i\lambda_n - 0| < \epsilon\}.$$

For further reference in the proof of Theorem 7.11, Step 1, we define

$$\beta_n(\omega, x, \epsilon) := \inf_{0 \leq i \leq n-1} \{-J(\tau_i \omega, \delta(\tau_i \omega)) : |i\lambda_n - x| < \epsilon\}. \quad (5.28)$$

In our case, the jump is at $x = 0$. Since we are going to extend this construction to piecewise affine functions, the jump needs also to be allowed to be placed at any point in the interval $[0, 1]$. Therefore, we have to show that the results also work for an arbitrary x .

For the result of equation (5.26), it is now left to show that for every $\omega \in \Omega'$ and every $x \in [0, 1]$ and every $\epsilon > 0$ it holds true that

$$\lim_{n \rightarrow \infty} \beta_n(\omega, x, \epsilon) = \lim_{n \rightarrow \infty} \inf_{0 \leq i \leq n-1} \{-J(\tau_i \omega, \delta(\tau_i \omega)) : |i\lambda_n - 0| < \epsilon\} = \beta.$$

Since $\beta_n(\omega, x, \epsilon) \geq \beta$ holds true for every ω, n, x and ϵ by definition, we only need to prove

$$\lim_{n \rightarrow \infty} \beta_n(\omega, x, \epsilon) = \lim_{n \rightarrow \infty} \inf_{0 \leq i \leq n-1} \{-J(\tau_i \omega, \delta(\tau_i \omega)) : |i\lambda_n - 0| < \epsilon\} \leq \beta. \quad (5.29)$$

First, notice that $\beta_n(\omega, x, \epsilon)$ is bounded, because of the boundedness of J by Ψ due to (LJ2). Let $\beta_n(\omega, x, \epsilon)$ be an arbitrary subsequence (not relabelled). Then, there exists a further subsequence (again not relabelled) which is convergent due to Bolzano-Weierstraß. If we can show, that every subsequence of that type converges to the same limit independent of ω and x , we get convergence of the whole sequence, since then every subsequence has a further subsequence with the same limit. This is what we are going to prove in the following. It holds true, with $I_x^\epsilon :=]x - \epsilon, x + \epsilon[$ and $k \in \mathbb{R}$, that

$$\begin{aligned} & \inf_{0 \leq i \leq n-1} \{-J(\tau_i \omega, \delta(\tau_i \omega)) : |i\lambda_n - x| < \epsilon\} \cdot \frac{1}{2\epsilon n} \sum_{i \in \mathbb{Z} \cap nI_x^\epsilon} \chi_{(-J(\tau_i \omega, \delta(\tau_i \omega)) \leq k)} \\ & \leq \frac{1}{2\epsilon n} \sum_{i \in \mathbb{Z} \cap nI_x^\epsilon} (-J(\tau_i \omega, \delta(\tau_i \omega))) \chi_{(-J(\tau_i \omega, \delta(\tau_i \omega)) \leq k)} \\ & \leq k \cdot \frac{1}{2\epsilon n} \sum_{i \in \mathbb{Z} \cap nI_x^\epsilon} \chi_{(-J(\tau_i \omega, \delta(\tau_i \omega)) \leq k)}. \end{aligned} \quad (5.30)$$

From Proposition 5.7, we get for $k \in \mathbb{Q}$ and all $x \in \mathbb{R}$

$$\frac{1}{2\epsilon n} \sum_{i \in \mathbb{Z} \cap nI_x^\epsilon} \chi_{(-J(\tau_i \omega, \delta(\tau_i \omega)) \leq k)} \rightarrow \mathbb{E} \left[\chi_{(-J(\delta) \leq k)} \right] \quad \text{as } n \rightarrow \infty,$$

independent of x and ω , where $J(\delta)$ represents the random variable $\omega \mapsto J(\omega, \delta(\omega))$. Since we consider a convergent subsequence of $\beta_n(\omega, x, \epsilon)$, passing to the limit $n \rightarrow \infty$ in (5.30) yields for $k \in \mathbb{Q}$

$$\lim_{n \rightarrow \infty} \inf_{0 \leq i \leq n-1} \{-J(\tau_i \omega, \delta(\tau_i \omega)) : |i\lambda_n - x| < \epsilon\} \cdot \mathbb{E} \left[\chi_{(-J(\delta) \leq k)} \right] \leq k \cdot \mathbb{E} \left[\chi_{(-J(\delta) \leq k)} \right]. \quad (5.31)$$

For $k > \inf \{-J(\omega, \delta(\omega)) : \omega \in \Omega\} = \beta$, it holds true that

$$\mathbb{E} \left[\chi_{(-J(\delta) \leq k)} \right] = \mathbb{P}(\{-J(\delta) \leq k\}) > 0.$$

Therefore, we divide by the expectation value in (5.31) and obtain for $k > \beta, k \in \mathbb{Q}$

$$\lim_{n \rightarrow \infty} \beta_n(\omega, x, \epsilon) = \lim_{n \rightarrow \infty} \inf_{0 \leq i \leq n-1} \{-J(\tau_i \omega, \delta(\tau_i \omega)) : |i\lambda_n - x| < \epsilon\} \leq k.$$

Further, we get for $k \in \mathbb{Q}$

$$\begin{aligned} \lim_{n \rightarrow \infty} \beta_n(\omega, x, \epsilon) &= \lim_{n \rightarrow \infty} \inf_{0 \leq i \leq n-1} \{-J(\tau_i \omega, \delta(\tau_i \omega)) : |i\lambda_n - x| < \epsilon\} \\ &= \liminf_{k \searrow \beta} \lim_{n \rightarrow \infty} \inf_{0 \leq i \leq n-1} \{-J(\tau_i \omega, \delta(\tau_i \omega)) : |i\lambda_n - x| < \epsilon\} \leq \lim_{k \searrow \beta} k = \beta, \end{aligned}$$

which finishes the prove of (5.29) and therefore the proof of (5.26).

Altogether, we have shown (b), namely

$$\limsup_{n \rightarrow \infty} E_n^{\gamma_n}(\omega, v_n) \leq \alpha \int_0^1 |v'(x)|^2 dx + \beta = E^\gamma(v). \quad (5.32)$$

(c) It is left to show $v_n \rightarrow v$ in $L^1(0, 1)$. For this, we split the integral as

$$\begin{aligned} \|v_n - v\|_{L^1(0,1)} &= \int_0^1 |v_n(x) - v(x)| dx \\ &= \int_0^{h_n^\epsilon \lambda_n} |v_n(x) - v(x)| dx + \int_{h_n^\epsilon \lambda_n}^{T_n \lambda_n} |v_n(x) - v(x)| dx + \int_{T_n \lambda_n}^1 |v_n(x) - v(x)| dx \end{aligned} \quad (5.33)$$

and consider each interval separately, in Part (i) to (iii) below. Later, in Part (iv), we combine the results from (i) to (iii) with the Attouch-Lemma, see Lemma 2.23.

(i) For the first integral in (5.33), we get

$$\begin{aligned} \int_0^{h_n^\epsilon \lambda_n} |v_n(x) - v(x)| dx &= \int_0^{h_n^\epsilon \lambda_n} |v(0^-) - v(0^+)| dx \\ &= |v(0^-) - v(0^+)| h_n^\epsilon \lambda_n \leq |v(0^-) - v(0^+)| \epsilon. \end{aligned}$$

(ii) For the second integral in (5.33), we get

$$\begin{aligned} &\int_{h_n^\epsilon \lambda_n}^{T_n \lambda_n} |v_n(x) - v(x)| dx \\ &= \int_{(h_n^\epsilon + 1)\lambda_n}^{T_n \lambda_n} |v(0^+) + \gamma_n - \gamma + z(T_n \lambda_n - \rho) - v(0^+)| dx \\ &\quad + \int_{h_n^\epsilon \lambda_n}^{(h_n^\epsilon + 1)\lambda_n} \left| \frac{v(0^+) + \gamma_n - \gamma + z(T_n \lambda_n - \rho)}{\lambda_n} (x - h_n^\epsilon \lambda_n) - v(0^+) \right| dx \\ &= |\gamma_n - \gamma + z(T_n \lambda_n - \rho)| (T_n - h_n^\epsilon - 1) \lambda_n \\ &\quad + |v(0^+) + \gamma_n - \gamma + z(T_n \lambda_n - \rho)| \left(2\lambda_n h_n^\epsilon + \frac{1}{2}\lambda_n \right) - \lambda_n v(0^+) \\ &\leq |\gamma_n - \gamma + z(T_n \lambda_n - \rho)| (T_n - h_n^\epsilon - 1) \lambda_n \\ &\quad + |v(0^+) + \gamma_n - \gamma + z(T_n \lambda_n - \rho)| \left(2\epsilon + \frac{1}{2}\lambda_n \right) - \lambda_n v(0^+) \\ &\rightarrow 2v(0^+) \epsilon \quad \text{as } n \rightarrow \infty, \end{aligned}$$

since $h_n^\epsilon \lambda_n$ is bounded by ϵ , $\gamma_n \rightarrow \gamma$ and $T_n \lambda_n \rightarrow \rho$.

(iii) The last integral in (5.33),

$$\int_{T_n \lambda_n}^1 |v_n(x) - v(x)| dx,$$

is the most interesting one. With $\epsilon_{j,0} = 1$ for $j = 0$ and $\epsilon_{j,0} = 0$ for $j > 0$, we get

$$\begin{aligned}
 \int_{T_n \lambda_n}^1 |v_n(x) - v(x)| dx &= \sum_{j=0}^{j_{\max}} \int_{(i_{\min}^{j,n}-1)\lambda_n}^{i_{\max}^{j,n}\lambda_n} |v_n(x) - v(x)| dx \\
 &= \sum_{j=0}^{j_{\max}} \int_{(i_{\min}^{j,n}-1)\lambda_n}^{i_{\max}^{j,n}\lambda_n} \left| \gamma_n - \gamma + z(T_n \lambda_n - \rho) \epsilon_{j,0} + \int_{(i_{\min}^{j,n}-1)\lambda_n}^x v'_n(y) - v'(y) dy \right| dx \\
 &\leq \sum_{j=0}^{j_{\max}} \int_{(i_{\min}^{j,n}-1)\lambda_n}^{i_{\max}^{j,n}\lambda_n} \int_{(i_{\min}^{j,n}-1)\lambda_n}^{i_{\max}^{j,n}\lambda_n} |v'_n(y) - v'(y)| dy dx + \sum_{j=0}^{j_{\max}} \int_{(i_{\min}^{j,n}-1)\lambda_n}^{i_{\max}^{j,n}\lambda_n} |\gamma_n - \gamma + z(T_n \lambda_n - \rho) \epsilon_{j,0}| dx \\
 &\leq \sum_{j=0}^{j_{\max}} (i_{\max}^{j,n} - i_{\min}^{j,n} + 1) \lambda_n \int_{(i_{\min}^{j,n}-1)\lambda_n}^{i_{\max}^{j,n}\lambda_n} |v'_n(x) - v'(x)| dx + \frac{1-\rho}{\mu} (\mu + \lambda_n) (|\gamma_n - \gamma| + z\lambda_n) \\
 &\leq \sum_{j=0}^{j_{\max}} (\mu + \lambda_n) \int_{(i_{\min}^{j,n}-1)\lambda_n}^{i_{\max}^{j,n}\lambda_n} |v'_n(x) - v'(x)| dx + \frac{1-\rho}{\mu} (|\gamma_n - \gamma| + z\lambda_n),
 \end{aligned} \tag{5.34}$$

because we have $\rho - T_n \lambda_n \leq \lambda_n$ and $\lambda_n (i_{\max}^{j,n} - i_{\min}^{j,n} + 1) \leq \mu + \lambda_n$. The integral in the last row of (5.34) has to be considered separately. For $j > 0$, it is $v'(x) = z$ and therefore we get

$$\begin{aligned}
 &\int_{(i_{\min}^{j,n}-1)\lambda_n}^{i_{\max}^{j,n}\lambda_n} |v'_n(x) - v'(x)| dx \\
 &= \sum_{i \in I_{j,n}^{\mu^*}} \int_{i\lambda_n}^{(i+1)\lambda_n} |v'_n(x) - v'(x)| dx = \sum_{i \in I_{j,n}^{\mu^*}} \lambda_n \left| \left(\frac{1}{|I_{j,n}^{\mu^*}|} \sum_{k \in I_{j,n}^{\mu^*}} \frac{1}{\alpha(\tau_k \omega)} \right)^{-1} z \frac{1}{\alpha(\tau_i \omega)} - z \right| \\
 &\leq \lambda_n |z| \sum_{i \in I_{j,n}^{\mu^*}} \left(\left(\frac{1}{|I_{j,n}^{\mu^*}|} \sum_{k \in I_{j,n}^{\mu^*}} \frac{1}{\alpha(\tau_k \omega)} \right)^{-1} \frac{1}{\alpha(\tau_i \omega)} + 1 \right) \\
 &\leq \lambda_n |z| \left(\left(\frac{1}{|I_{j,n}^{\mu^*}|} \sum_{k \in I_{j,n}^{\mu^*}} \frac{1}{\alpha(\tau_k \omega)} \right)^{-1} \cdot \left(\sum_{i \in I_{j,n}^{\mu^*}} \frac{1}{\alpha(\tau_i \omega)} \right) + \sum_{i \in I_{j,n}^{\mu^*}} 1 \right) \\
 &= 2|z| \lambda_n |I_{j,n}^{\mu^*}| \leq C \cdot (\mu + \lambda_n),
 \end{aligned} \tag{5.35}$$

since it holds true that $\lambda_n |I_{j,n}^{\mu^*}| = \lambda_n (i_{\max}^{j,n} - i_{\min}^{j,n} + 1) \leq \mu + \lambda_n$. Now that we have determined the integral in the last row of (5.34) for $j > 0$, we calculate it for $j = 0$ by

$$\begin{aligned}
 &\int_{T_n \lambda_n}^{i_{\max}^{0,n}\lambda_n} |v'_n(x) - v'(x)| dx \\
 &= \int_{T_n \lambda_n}^{\rho} |v'_n(x) - v'(x)| dx + \int_{\rho}^{(T_n+1)\lambda_n} |v'_n(x) - v'(x)| dx + \int_{(T_n+1)\lambda_n}^{i_{\max}^{0,n}\lambda_n} |v'_n(x) - v'(x)| dx.
 \end{aligned} \tag{5.36}$$

The first addend of (5.36) is

$$\begin{aligned} \int_{T_n \lambda_n}^{\rho} |v'_n(x) - v'(x)| \, dx &= \int_{T_n \lambda_n}^{\rho} \left| \left(\frac{1}{|I_{j,n}^{\mu^*}|} \sum_{k \in I_{j,n}^{\mu^*}} \frac{1}{\alpha(\tau_k \omega)} \right)^{-1} z \frac{1}{\alpha(\tau_{T_n} \omega)} - 0 \right| \, dx \\ &= (\rho - T_n \lambda_n) \left(\frac{1}{|I_{j,n}^{\mu^*}|} \sum_{k \in I_{j,n}^{\mu^*}} \frac{1}{\alpha(\tau_k \omega)} \right)^{-1} |z| \frac{1}{\alpha(\tau_{T_n} \omega)}, \end{aligned}$$

which converges to zero as $n \rightarrow \infty$ because of the convergence $T_n \lambda_n \rightarrow \rho$, Proposition 5.5 and the boundedness of $\alpha^{-1}(\omega)$ due to Remark 5.4. The second addend of (5.36) is

$$\begin{aligned} \int_{\rho}^{(T_n+1)\lambda_n} |v'_n(x) - v'(x)| \, dx &= \int_{\rho}^{(T_n+1)\lambda_n} \left| \left(\frac{1}{|I_{j,n}^{\mu^*}|} \sum_{k \in I_{j,n}^{\mu^*}} \frac{1}{\alpha(\tau_k \omega)} \right)^{-1} z \frac{1}{\alpha(\tau_{T_n} \omega)} - z \right| \, dx \\ &= ((T_n + 1)\lambda_n - \rho) |z| \left| \left(\frac{1}{|I_{j,n}^{\mu^*}|} \sum_{k \in I_{j,n}^{\mu^*}} \frac{1}{\alpha(\tau_k \omega)} \right)^{-1} \frac{1}{\alpha(\tau_{T_n} \omega)} - 1 \right|, \end{aligned}$$

which again converges to zero as $n \rightarrow \infty$ because of the convergence $(T_n + 1)\lambda_n \rightarrow \rho$, Proposition 5.5 and the boundedness of $\alpha^{-1}(\omega)$ due to Remark 5.4. For the last addend of (5.36), we reuse the calculations from (5.35) and get

$$\begin{aligned} \int_{(T_n+1)\lambda_n}^{i_{\max}^{0,n}\lambda_n} |v'_n(x) - v'(x)| \, dx &= \sum_{i \in I_{j,n}^{\mu^*} \setminus \{T_n\}} \int_{i\lambda_n}^{(i+1)\lambda_n} |v'_n(x) - v'(x)| \, dx \\ &= \sum_{i \in I_{j,n}^{\mu^*}} \lambda_n \left| \left(\frac{1}{|I_{j,n}^{\mu^*}|} \sum_{k \in I_{j,n}^{\mu^*}} \frac{1}{\alpha(\tau_k \omega)} \right)^{-1} z \frac{1}{\alpha(\tau_i \omega)} - z \right| - \lambda_n \left| \left(\frac{1}{|I_{j,n}^{\mu^*}|} \sum_{k \in I_{j,n}^{\mu^*}} \frac{1}{\alpha(\tau_k \omega)} \right)^{-1} z \frac{1}{\alpha(\tau_{T_n} \omega)} - z \right| \\ &\leq 2|z|\lambda_n |I_{j,n}^{\mu^*}| + \hat{C}\lambda_n \leq C(\mu + \lambda_n), \end{aligned}$$

where the bound \hat{C} is due to the boundedness of $\alpha^{-1}(\omega)$ by Remark 5.4 and the convergence of the sum according to Proposition 5.5. Altogether, this yields, for (5.36) and for n large enough,

$$\int_{T_n \lambda_n}^{i_{\max}^{0,n}\lambda_n} |v'_n(x) - v'(x)| \, dx \leq C(\mu + \lambda_n). \quad (5.37)$$

Combined, (5.34), (5.35) and (5.37) lead to

$$\begin{aligned} \int_{T_n \lambda_n}^1 |v_n(x) - v(x)| \, dx &\leq \sum_{j=0}^{j_{\max}} (\mu + \lambda_n) C(\mu + \lambda_n) + \frac{1-\rho}{\mu} (|\gamma_n - \gamma| + z\lambda_n) \\ &= \frac{1-\rho}{\mu} (\mu + \lambda_n) C(\mu + \lambda_n) + \frac{1-\rho}{\mu} (|\gamma_n - \gamma| + z\lambda_n) \\ &\leq \tilde{C} \left(\mu + 2\lambda_n + \frac{\lambda_n^2}{\mu} \right) + \frac{1-\rho}{\mu} (|\gamma_n - \gamma| + z\lambda_n) \rightarrow \tilde{C}\mu \quad \text{as } n \rightarrow \infty. \end{aligned}$$

(iv) Altogether, we have shown in the steps i)-iii), that

$$\limsup_{n \rightarrow \infty} \|v_n - v\|_{L^1(0,1)} \leq \hat{C}\epsilon + \tilde{C}\mu. \quad (5.38)$$

Now, by setting $\epsilon = \mu$, we combine the results from (5.32) and (5.38) and get (recall that v_n strictly accurate is $v_{n,\mu}$)

$$\limsup_{\mu \rightarrow 0} \limsup_{n \rightarrow \infty} \left(|E_n^{\gamma_n}(\omega, v_{n,\mu}) - E^\gamma(v)| + \|v_{n,\mu} - v\|_{L^1(0,1)} \right) = 0.$$

From the Attouch-Lemma in Theorem 2.23, we therefore get the existence of a subsequence μ_n with $\mu_n \rightarrow 0$ as $n \rightarrow \infty$ and

$$\begin{aligned} 0 &\leq \limsup_{n \rightarrow \infty} \left(|E_n^{\gamma_n}(\omega, v_{n,\mu_n}) - E^\gamma(v)| + \|v_{n,\mu_n} - v\|_{L^1(0,1)} \right) \\ &\leq \limsup_{\mu \rightarrow 0} \limsup_{n \rightarrow \infty} \left(|E_n^{\gamma_n}(\omega, v_{n,\mu}) - E^\gamma(v)| + \|v_{n,\mu} - v\|_{L^1(0,1)} \right) = 0. \end{aligned}$$

Finally, this proves $\|v_{n,\mu_n} - v\|_{L^1(0,1)} \rightarrow 0$ as $n \rightarrow \infty$, which concludes (c). Altogether, (v_{n,μ_n}) is the recovery sequence for the affine function $v(x) = zx$, which was the goal of Step A.

This construction of a recovery sequence for affine functions with a jump can easily be extended to piecewise affine functions with jumps by dividing the interval $[0, 1]$ into parts where the function is affine.

Step B: Smooth functions, constant near the jump.

We have constructed a recovery sequence for piecewise affine functions with jumps. With this result, we get a recovery sequence for every $v \in C^2([0, 1] \setminus S_v)$ where v is constant on $x \in [x_0 - \eta, x_0 + \eta]$ with $S_v = \{x_0\}$ and $\eta > 0$ small enough. The justification is as follows: on $x \in [x_0 - \eta, x_0 + \eta]$, v is already affine. On $[0, x_0 - \eta]$ and $[x_0 + \eta, 1]$, we take, for $\delta > 0$, the piecewise affine interpolation v_N of v with grid points $(t_j^N)_{j=0, \dots, a_N, b_N, \dots, j_N}$ with $t_0 = 0, t_{a_N} = x_0 - \eta, t_{b_N} = x_0 + \eta, t_{j_N} = 1$ and $\delta < t_{j+1}^N - t_j^N < 2\delta$ for $j = 0, \dots, a_N - 1, b_N, \dots, j_N$. Note that for $\delta \rightarrow 0$ we also get $N \rightarrow \infty$, which is the reason why we use both equivalently. Then, we get by using the Jensen inequality

$$\begin{aligned} E^\gamma(v) &= \underline{\alpha} \int_0^1 |v'(x)|^2 dx + \beta \\ &= \underline{\alpha} \sum_{j=0}^N (t_j^N - t_{j-1}^N) \frac{1}{t_j^N - t_{j-1}^N} \int_{t_{j-1}^N}^{t_j^N} |v'(x)|^2 dx + \beta \\ &\geq \underline{\alpha} \sum_{j=0}^N (t_j^N - t_{j-1}^N) \left| \frac{1}{t_j^N - t_{j-1}^N} \int_{t_{j-1}^N}^{t_j^N} v'(x) dx \right|^2 + \beta \\ &= \underline{\alpha} \sum_{j=0}^N (t_j^N - t_{j-1}^N) \left| \frac{v(t_j^N) - v(t_{j-1}^N)}{t_j^N - t_{j-1}^N} \right|^2 + \beta \\ &= \underline{\alpha} \sum_{j=0}^N \int_{t_{j-1}^N}^{t_j^N} |v'_N(x)|^2 dx + \beta = \underline{\alpha} \int_0^1 |v'_N(x)|^2 dx + \beta = E^\gamma(v_N). \end{aligned} \quad (5.39)$$

We argue as in Step E of the proof of the liminf inequality from Theorem 4.14 to get $v_N \rightarrow v$ in $L^1(0, 1)$. Further, the Γ -lim sup is lower semicontinuous. Therefore, we get

$$\Gamma\text{-lim sup}_{n \rightarrow \infty} E_n^{\gamma_n}(\omega, v) \stackrel{\text{l.s.c.}}{\leq} \liminf_{N \rightarrow \infty} \left(\Gamma\text{-lim sup}_{n \rightarrow \infty} E_n^{\gamma_n}(\omega, v_N) \right) \stackrel{(*)}{\leq} \liminf_{N \rightarrow \infty} E^\gamma(v_N) \stackrel{(5.39)}{\leq} E^\gamma(v),$$

where $(*)$ follows from the construction of the recovery sequence for piecewise affine functions in Step A, which keeps the boundary values, see [39, Section 2.4, Corollary 3].

Step C: Smooth functions.

Now that we have a recovery sequence for $v \in C^2([0, 1] \setminus S_v)$ where v is constant on $x \in [x_0 - \eta, x_0 + \eta]$, we can extend it to functions $v = v_c + v_j$ with $v_c \in C^2[0, 1]$ and v_j is piecewise constant, which concludes the limsup-inequality. Without loss of generality, we set $S_v = \{x_0\}$. Now, we define, for $\eta > 0$ small enough, an approximation v_c^η with

$$v_c^\eta(x) := \begin{cases} v_c(x) & \text{for } x < x_0 - \eta, \\ v_c(x_0 - \eta) & \text{for } x \in [x_0 - \eta, x_0 + \eta], \\ v_c(x) - v_c(x_0 + \eta) + v_c(x_0 - \eta) & \text{for } x > x_0 + \eta. \end{cases}$$

Then, $v^\eta = v_c^\eta + v_j$ has two properties, namely (a) $v^\eta \rightarrow v$ in $L^1(0, 1)$ for $\eta \rightarrow 0$ and (b) $\int_0^1 |v_c^{\eta'}(x)|^2 dx \rightarrow \int_0^1 |v_c'(x)|^2 dx$ for $\eta \rightarrow 0$, which can be seen as follows.

(a) We prove $v^\eta \rightarrow v$ in $L^1(0, 1)$ for $\eta \rightarrow 0$:

$$\begin{aligned} \int_0^1 |v^\eta(x) - v(x)| dx &= \int_{x_0 - \eta}^{x_0 + \eta} |v_c(x_0 - \eta) - v_c(x)| dx + \int_{x_0 + \eta}^1 |v_c(x_0 - \eta) - v_c(x_0 + \eta)| dx \\ &\leq 2\eta |v_c(x_0 - \eta)| + \int_{x_0 - \eta}^{x_0 + \eta} |v_c(x)| dx + (1 - x_0 - \eta) |v_c(x_0 - \eta) - v_c(x_0 + \eta)| \\ &\rightarrow 2 \cdot 0 \cdot |v_c(x_0)| + 0 + (1 - x_0) \cdot |v_c(x_0) - v_c(x_0)| = 0 \quad \text{for } \eta \rightarrow 0. \end{aligned}$$

Recall that we have $v_c \in C^2[0, 1]$.

(b) We prove $\int_0^1 |v_c^{\eta'}(x)|^2 dx \rightarrow \int_0^1 |v_c'(x)|^2 dx$ for $\eta \rightarrow 0$:

$$\int_0^1 |v_c^{\eta'}(x)|^2 dx = \int_0^{x_0 - \eta} |v_c'(x)|^2 dx + \int_{x_0 + \eta}^1 |v_c'(x)|^2 dx \rightarrow \int_0^1 |v_c'(x)|^2 dx \quad \text{for } \eta \rightarrow 0.$$

Similarly to the density argument of [21], we get with the properties (a) and (b)

$$\Gamma\text{-lim sup}_{n \rightarrow \infty} E_n^{\gamma_n}(\omega, v) \stackrel{(a)+\text{l.s.c.}}{\leq} \liminf_{\eta \rightarrow 0} \left(\Gamma\text{-lim sup}_{n \rightarrow \infty} E_n^{\gamma_n}(\omega, v^\eta) \right) \stackrel{(*)}{\leq} \liminf_{\eta \rightarrow 0} E^\gamma(v^\eta) \stackrel{(b)}{\leq} E^\gamma(v),$$

where $(*)$ follows from the construction of the recovery sequence from Step B. Note that this construction also keeps the boundary values. Since the conclusion to an arbitrary $v \in SBV_c^\gamma$ was already discussed in the beginning of the limsup-part, the construction of the recovery sequence is completed.

Step 3. Convergence of minimum problems.

The convergence of minimum problems follows from the coerciveness of $E_n^{\gamma_n}$ and the Γ -convergence result due to the main theorem of Γ -convergence, cf. Theorem 2.22. It is left to show

$$\min_v E^\gamma(v) = \min\{\underline{\alpha}\gamma^2, \beta\}. \quad (5.40)$$

This is done analogously to [101]. For $\gamma > 0$ fixed and v with boundary conditions $v(0) = 0$ and $v(1) = \gamma$ and fulfilling $[v] > 0$ on S_v we have to distinguish two cases: First, let $S_v = \emptyset$, then we have $v \in W^{1,1}(0,1)$ and with the Jensen-inequality we get

$$\underline{\alpha} \int_0^1 |v'(x)|^2 dx \geq \underline{\alpha} \left| \int_0^1 v'(x) dx \right|^2 = \underline{\alpha}\gamma^2$$

and therefore with the minimizer $v(x) = \gamma x$

$$\min_v E^\gamma(v) = \min_v \left\{ \underline{\alpha} \int_0^1 |v'(x)|^2 dx \right\} = \underline{\alpha}\gamma^2.$$

Second, for $S_v \neq \emptyset$, we get because of $\underline{\alpha} > 0$

$$\min_v E^\gamma(v) = \min_v \left\{ \underline{\alpha} \int_0^1 |v'(x)|^2 dx + \beta \#S_v \right\} = \beta$$

where the minimizer has one jump point $S_v = \{t\}$ and is given by

$$v(x) = \begin{cases} 0 & \text{if } x \in [0, t), \\ \gamma & \text{if } x \in [t, 1]. \end{cases}$$

This shows (5.40). □

5.5 Comment on the Γ -limit of first order

The Γ -limit of first order of a functional E_n is defined as the Γ -limit of the rescaled functional

$$E_{1,n}(u) := \frac{E_n(u) - \inf_u E(u)}{\lambda_n},$$

where $E(u) = \Gamma\text{-lim } E_n(u)$.

In the heterogeneous, periodic setting, this first order Γ -limit does not exist. We show this in the following. This is in line with [37], where the authors consider a periodic integral energy functional and its homogenized limit and conclude that the Γ -limit of first order does not exist.

In our case, the Γ -limit E_{hom}^ℓ of $E_n^\ell(\omega, u)$ is derived in Theorem 4.14, as well as $\min_u E_{\text{hom}}^\ell(u) =$

$J_{\text{hom}}(\ell)$. Therefore, the Γ -limit of first order is the Γ -limit of

$$\begin{aligned} E_{1,n}^\ell(\omega, u) &= \frac{\sum_{i=0}^{n-1} \lambda_n J\left(\tau_i \omega, \frac{u^{i+1} - u^i}{\lambda_n}\right) - \min_u E^\ell(u)}{\lambda_n} \\ &= \sum_{i=0}^{n-1} \left(J\left(\tau_i \omega, \frac{u^{i+1} - u^i}{\lambda_n}\right) - J(\tau_i \omega, \delta(\tau_i \omega)) \right) + \sum_{i=0}^{n-1} (J(\tau_i \omega, \delta(\tau_i \omega)) - J_{\text{hom}}(\ell)). \end{aligned} \quad (5.41)$$

The first term is exactly the rescaled energy (5.2) of Section 5.1. From Theorem 5.8, we know that its Γ -limit exists. The second term

$$\sum_{i=0}^{n-1} (J(\tau_i \omega, \delta(\tau_i \omega)) - J_{\text{hom}}(\ell)) \quad (5.42)$$

is independent of u . If its limit $n \rightarrow \infty$ existed, it could be treated as a continuous perturbation, see Remark 2.20. Then, the Γ -limit of (5.41) would be the sum of the rescaled Γ -limit and the limit of (5.42).

However, we now show for the periodic case that the sum in (5.42) is not convergent. For this, $J_i(z)$ is used for the interaction potential between atom i and $i + 1$ and the expectation value is replaced by the arithmetic mean. For details on the special case of periodicity and the related definitions and results, we refer to Chapter 6. For simplicity, assume $\delta_i = \delta$ for all $i \in \mathbb{Z}$ and $\ell = \delta$. Then, Proposition 4.13 yields

$$J_{\text{hom}}(\ell) = J_{\text{hom}}(\delta) = J_{\text{hom}}(\bar{\delta}) = \overline{J(\delta)}.$$

We can assume to have at least two different potentials (otherwise we are in the homogeneous case), and without loss of generality we set $J_0(\delta) \neq \overline{J(\delta)}$. With $M \in \mathbb{N}$ being the periodicity length, (5.42) reads

$$\sum_{i=0}^{n-1} (J_i(\delta) - \overline{J(\delta)}) = \begin{cases} 0 & \text{if } n = kM \text{ for some } k \in \mathbb{N}, \\ J_0(\delta) - \overline{J(\delta)} \neq 0 & \text{if } n = kM + 1 \text{ for some } k \in \mathbb{N}. \end{cases}$$

This shows that in the periodic case, (5.42) has at least two different accumulation points. For every accumulation point, (5.42) is a continuous perturbation to the already known Γ -limit of the rescaled energy, and leads to a different Γ -limit of first order in each case. Thus, the Γ -limit of first order depends on the subsequence chosen and therefore does not exist.

In the stochastic case, the (non-)convergence of (5.42) is difficult to handle. We note that (5.42) can be reformulated as

$$n \left(\frac{1}{n} \sum_{i=0}^{n-1} J(\tau_i \omega, \delta(\tau_i \omega)) - J_{\text{hom}}(\ell) \right),$$

and is thus related to the topic of convergence rates in the field of ergodic theorems, with $\frac{1}{n} \sum_{i=0}^{n-1} J(\tau_i \omega, \delta(\tau_i \omega)) \rightarrow J_{\text{hom}}(\ell)$. This is addressed in various papers. For an overview, see, e.g., [79, p.14–15]. In [76], the author states that it is not possible to obtain an estimate on the convergence rate that only depends on J . A fundamental step towards this statement is the work

in [68] and [79]. There, the authors prove theorems stating that for any given ergodic group action, one can choose indicator functions with arbitrarily high and arbitrarily low rate of convergence in the ergodic theorem. Especially, this indicates that (5.42) does not converge in our general setting, and thus is a strong hint that the Γ -limit does not exist. It remains an open problem whether convergence of (5.42) can be obtained in some special cases.

6 Periodic setting

This chapter is devoted to the periodic setting, i.e., compared to the previous model, we replace the stochastic dependence of the Lennard-Jones interaction potentials by a periodic dependence. This is in some sense a simplification or specification of the stochastic setting, since the proofs of the Γ -convergence theorems are mainly the same but much simpler. However, the results show interesting new features, especially regarding the homogenization formula.

The theorems of this chapter are chronologically the first results of the doctoral thesis. The stochastic case was then built on the periodic case, which served as a foundation. I published the results of the periodic setting, that are presented in this chapter, in [82], jointly with M. Schäffner and A. Schlömerkemper.

The motivation and the approach is completely analogous to that of Chapter 3–5. Therefore, we here highlight only the differences in setting and assumptions to the stochastic case and state the corresponding results for the theorems and propositions. The proofs are only given in that cases where they differ considerably or show new and interesting features. We refer for the remaining proofs and further details to [82].

6.1 Discrete model and Lennard-Jones type assumptions

The discrete model of the one-dimensional chain of atoms with reference configuration equidistributed in $[0, 1]$ is the same as in Chapter 3. As in [82], we consider the case of nearest neighbour interactions, i.e. $K = 1$. Instead of the random distribution of the interaction potentials, we assume a periodic setting with periodicity length $M \in \mathbb{N}$. Therefore, we redefine the interaction potential of particle i and $i + 1$ by

$$J(i, z) := J_i(z) \quad \text{for every } i \in \mathbb{Z},$$

where the variable ω is not needed any more because there is no random variable. Periodicity now means that we have

$$J_i = J_{i+M} \quad \text{for every } i \in \mathbb{Z}.$$

Fig. 6.1 shows an example of a periodic chain with periodicity length $M = 3$ and two different types of atoms, grey and white, where the interaction potential of two atoms of the same type is assumed to be different from the interaction between different types of atoms.

In the following, we frequently make use of the abbreviations for the averages

$$\bar{\delta} := \frac{1}{M} \sum_{i=0}^{M-1} \delta_i \quad \text{and} \quad \overline{J(\delta)} := \frac{1}{M} \sum_{i=0}^{M-1} J_i(\delta_i). \quad (6.1)$$

These mean values substitute the expectation values from the stochastic setting. Since they

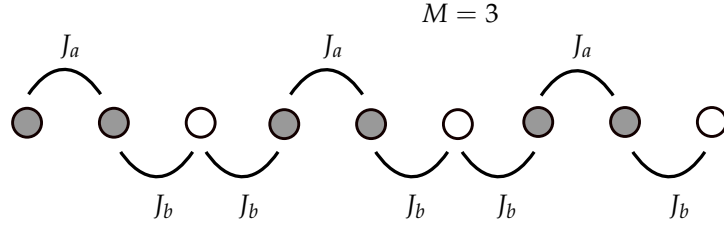


Figure 6.1 | Chain of atoms with periodicity $M = 3$ and two different types of atoms (grey and white). The interaction potential J_a between two grey atoms is different to the interaction J_b between a white and a grey atom.

can simply be computed without any limiting process, we do not need results like those in Propositions 3.5 or 5.5.

Next, we introduce the Lennard-Jones type potentials that are allowed in the periodic case. We first state the assumptions and then discuss the differences to the earlier class of Lennard-Jones type potentials. They are slightly modified compared to [82]. We say that the interaction potentials J_i are of Lennard-Jones type if they fulfil the following conditions:

(LJ1*) For any $i \in \{0, \dots, M-1\}$, the function $J_i : \mathbb{R} \rightarrow (-\infty, +\infty]$ is lower semicontinuous and in $C_{\text{loc}}^{0,\alpha}$, $0 < \alpha \leq 1$ on its domain $\text{dom} J_i = \{z \in \mathbb{R} : J_i(z) < +\infty\}$. Further, we assume that the domain is an open set and independent of i , i.e. $\text{dom} J_i = (z_{\text{dom}}, +\infty) =: \text{dom} J$, with $z_{\text{dom}} \leq 0$, and that

$$\lim_{z \rightarrow +\infty} J_i(z) = 0.$$

(LJ2*) There exists a convex function $\Psi : \mathbb{R} \rightarrow [0, +\infty]$ and constants d_1, d_2 such that

$$\lim_{z \rightarrow -\infty} \frac{\Psi(z)}{|z|} = +\infty \quad \text{and}$$

$$d_1(\Psi(z) - 1) \leq J_i(z) \leq d_2 \max\{\Psi(z), |z|\} \quad \text{for all } z \in \mathbb{R}, i \in \{0, \dots, M-1\}.$$

Further, J_i has a unique minimum point δ_i with $J_i(\delta_i) < 0$ and it is strictly convex in $(-\infty, \delta_i)$ on its domain.

(LJ3*) The functions $J_i, i \in \{0, \dots, M-1\}$ are C^2 on their domain.

(LJ4*) There exist $\mu > 0$ and $C > 0$ such that for all $i \in \{0, \dots, M-1\}$

$$J_i(x) - J_i(\delta_i) \geq C(x - \delta_i)^2$$

for $|x - \delta_i| < \mu$.

The assumptions (LJ1*)–(LJ2*) are applied in the proof of Theorem 6.3 regarding the Γ -limit of the energy H_n , defined in (6.2). Theorem 6.4 deals with the rescaled version of that energy and is based on the assumptions (LJ1*)–(LJ4*).

The main difference of (LJ1*)–(LJ4*) to the original Lennard-Jones type assumptions (LJ1)–(LJ5) together with (H1)–(H3) is that most assumptions that deal with common lower or upper bounds are not needed any more. This is due to the fact that in the periodic case we only consider M different functions as interaction potentials, while in the stochastic case uncountably many potentials are allowed. Therefore, the assumptions with common bounds are fulfilled automatically.

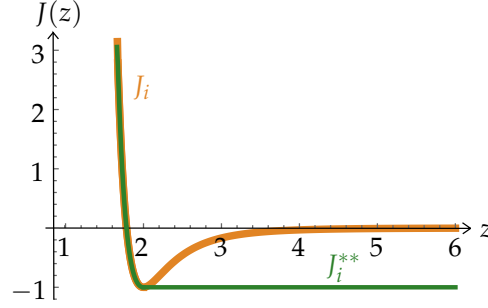


Figure 6.2 | A potential J_i and its convex, lower semicontinuous envelope J_i^{**} .

In contrast, the bounds in (LJ2*) and (LJ4*) are retained, since those estimates deal not only with common bounds by constants but instead with a common bound by a convex function or a quadratic estimate, respectively. These bounds are also required in the homogeneous case, cf. [24, 100, 101]. In particular, the following assumptions are not needed any more:

- The bound on the minimizers from (LJ2), i.e. $\delta \in (\frac{1}{d}, d)$.
- The bound for large values of z from (LJ2), i.e. $\|J\|_{L^\infty(\delta, \infty)} < b$.
- The regularity in (LJ3*) is of the type C^2 , instead of C^3 in (LJ4), which also refers to a common bound of the remainder in the Taylor approximation, which is formulated in (H2).
- The expectation value of the Hölder coefficient in (H1) and the uniform convergence in (H3).

A further difference concerns the domain of the function J . In the periodic case, the domain can even be $(-\infty, +\infty)$. This is ruled out by (LJ1) in the stochastic setting, where we assume $(0, \infty)$ to be the domain and allow for shifting it. That is the reason for the slight changes in the definition of the blow up of the function Ψ at $-\infty$ or 0^+ respectively, and of the function J at 0^+ .

Remark 6.1. Notice that a consequence of (LJ1*) and (LJ2*) is that the convex, lower semicontinuous envelope J_i^{**} of J_i is given for each $i \in \{0, \dots, M-1\}$ by

$$J_i^{**}(z) = \begin{cases} J_i(z) & \text{if } z \leq \delta_i, \\ J_i(\delta_i) & \text{else.} \end{cases}$$

An illustration of the convex, lower semicontinuous envelope J_i^{**} can be found in Figure 6.2. With the deformation of the particles denoted by $u : \lambda_n \mathbb{Z} \cap [0, 1] \rightarrow \mathbb{R}$ and the abbreviation $u(x_n^i) = u^i$, as before, we can again identify the discrete deformations u with their piecewise affine interpolations, i.e. $u \in \mathcal{A}_n$ with

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

The energy in the periodic case reads

$$H_n(u) := \sum_{i=1}^n \lambda_n J_i \left(\frac{u^{i+1} - u^i}{\lambda_n} \right), \quad (6.2)$$

and we impose the same Dirichlet boundary conditions $u(0) = 0$ and $u(1) = \ell$ for some given

$\ell > 0$ as before. Altogether, this yields the functional $H_n^\ell : L^1(0, 1) \rightarrow (-\infty, +\infty]$ defined by

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

The rescaling here is similar to that of Section 5.1 and reads

$$v^i := \frac{u^i - \sum_{k=0}^{i-1} \lambda_n \delta_k}{\sqrt{\lambda_n}} \quad \text{for all } i \in \{0, \dots, n\},$$

cf. (5.1). Since this definition yields

$$\frac{u^{i+1} - u^i}{\lambda_n} = \delta_i + \frac{v^{i+1} - v^i}{\sqrt{\lambda_n}},$$

we get the following rescaled energy

$$E_n(v) := \frac{H_n(u_{\min} + \sqrt{\lambda_n}v) - \min_u H_n(u)}{\lambda_n} = \sum_{i=0}^{n-1} \left(J_i \left(\frac{v^{i+1} - v^i}{\sqrt{\lambda_n}} + \delta_i \right) - J_i(\delta_i) \right).$$

We also have to rescale the boundary data. Theorem 6.3 and Lemma 6.2, which we state below, show that the threshold between the regime of elasticity and that of fracture is given by $\ell = \bar{\delta}$. In the stochastic setting, this threshold is the expectation value of the minimizers. Now, it is the mean value. As in [82], we follow again the ideas of [101] and consider the energy E_n for some sequence $(\ell_n) \subset \mathbb{R}$ with $\ell_n \rightarrow \bar{\delta}$, satisfying

$$\eta_n := \frac{\ell_n - \sum_{k=0}^{n-1} \lambda_n \delta_k}{\sqrt{\lambda_n}} \rightarrow \eta \quad (6.3)$$

and $\ell_n > \bar{\delta}$ for every $n \in \mathbb{N}$. For simplicity, we assume

$$\ell_n > \frac{1}{n} \sum_{k=0}^{n-1} \delta_k \quad \text{for every } n \in \mathbb{N}.$$

By definition, it holds $\eta \geq 0$ as well as $\eta_n > 0$ for all $n \in \mathbb{N}$. They serve as boundary values of the new variable v , and therefore, for $u \in \mathcal{A}_n(0, 1)$, the new variables v belong to the space

$$\hat{\mathcal{A}}_n^{\eta_n} := \{v \in \mathcal{A}_n(0, 1) : v^0 = 0, v^n = \eta_n\}.$$

Altogether, we get the rescaled functional $E_n^{\eta_n} : L^1(0, 1) \rightarrow (-\infty, +\infty]$ with

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

6.2 Homogenization formula and Γ -convergence results

The biggest difference between the stochastic and the periodic case is the representation of the homogenized energy density. In the stochastic case, J_{hom} was given by an asymptotic homog-

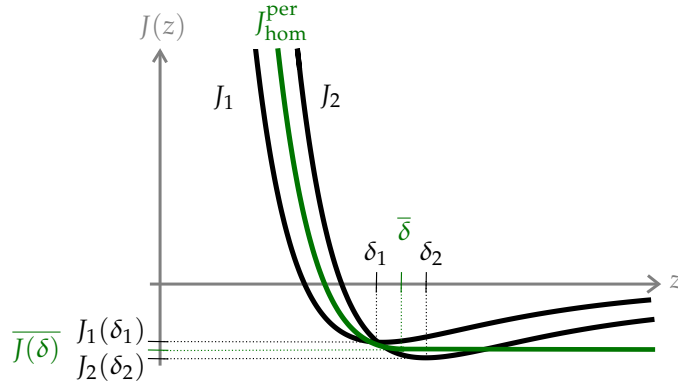


Figure 6.3 | The function $J_{\text{hom}}^{\text{per}}$ together with the two interaction potentials J_1 and J_2 in the case $M = 2$.

enization formula. In the periodic case, it reduces to a cell-problem formula. It is defined as $J_{\text{hom}}^{\text{per}} : \mathbb{R} \rightarrow (-\infty, \infty]$ and given by

$$J_{\text{hom}}^{\text{per}}(z) := \min \left\{ \frac{1}{M} \sum_{i=0}^{M-1} J_i^{**}(z_i) : \sum_{i=0}^{M-1} z_i = Mz \right\}, \quad (6.4)$$

which is well-defined since the minimum exists. The validity of the cell-problem formula (6.4) crucially relies on the fact that we use only nearest-neighbour interactions. Indeed, even in the case of homogeneous interactions and a setting beyond nearest neighbours with $K \geq 3$, the effective energy density is in general given by an asymptotic cell formula, see, e.g., [32]. Further, for $K \geq 2$, it was recently shown in [103] that in the case of homogeneous Lennard-Jones type interactions with finite range the effective energy density can be computed explicitly, due to the specific convex-concave shape of the interaction potentials.

We now state a lemma, which is the counterpart to the results in Proposition 4.12. In order to highlight the main differences between the stochastic and the periodic setting, we present the proof, which has already been published in [82]. It is essentially copied from the published version in [82]. A sketch of $J_{\text{hom}}^{\text{per}}$, relying on the results of the next Lemma and in particular on the cell-problem formula, is shown in Figure 6.3.

Lemma 6.2. *Suppose that the hypotheses (LJ1*) and (LJ2*) hold true. Then, the function $J_{\text{hom}}^{\text{per}}$, defined in (6.4), is convex, monotone decreasing, and it holds*

$$J_{\text{hom}}^{\text{per}}(z) = \begin{cases} f(z) & \text{if } z \leq \bar{\delta} \\ \overline{J(\delta)} & \text{if } z \geq \bar{\delta}, \end{cases} \quad (6.5)$$

where

$$f(z) := \min \left\{ \frac{1}{M} \sum_{i=0}^{M-1} J_i(z_i) : \sum_{i=0}^{M-1} z_i = Mz \right\}$$

and $\overline{J(\delta)}$ is defined in (6.1). Moreover, it holds

$$\lim_{z \rightarrow -\infty} \frac{J_{\text{hom}}^{\text{per}}(z)}{|z|} = +\infty. \quad (6.6)$$

Proof. **Step 1.** Convexity.

Let $z^{(1)}, z^{(2)} \in \mathbb{R}$ and $t \in [0, 1]$ be given and consider $z = tz^{(1)} + (1-t)z^{(2)}$. According to the definition of $J_{\text{hom}}^{\text{per}}$ in (6.4), there exist $Z^{(1)}, Z^{(2)} \in \mathbb{R}^M$ satisfying $\frac{1}{M} \sum_{i=0}^{M-1} Z_i^{(j)} = z^{(j)}$ for $j = 1, 2$ such that

$$J_{\text{hom}}^{\text{per}}(z^{(j)}) = \frac{1}{M} \sum_{i=0}^{M-1} J_i^{**}(Z_i^{(j)}), \quad j = 1, 2.$$

Note that $\frac{1}{M} \sum_{i=0}^{M-1} (tZ_i^{(1)} + (1-t)Z_i^{(2)}) = z$ and thus

$$\begin{aligned} tJ_{\text{hom}}^{\text{per}}(z^{(1)}) + (1-t)J_{\text{hom}}^{\text{per}}(z^{(2)}) &= \frac{1}{M} \sum_{i=0}^{M-1} (tJ_i^{**}(Z_i^{(1)}) + (1-t)J_i^{**}(Z_i^{(2)})) \\ &\geq \frac{1}{M} \sum_{i=0}^{M-1} J_i^{**}(tZ_i^{(1)} + (1-t)Z_i^{(2)}) \geq J_{\text{hom}}^{\text{per}}(z), \end{aligned}$$

which proves the claim.

Step 2. Monotonicity.

Since J_i^{**} is monotone decreasing for $i = 0, \dots, M-1$, cf. (LJ1*), (LJ2*) and Remark 6.1, we obtain the monotonicity of $J_{\text{hom}}^{\text{per}}$.

Step 3. The identity (6.5).

First, we notice that (LJ1*) and (LJ2*) imply that

$$\overline{J(\delta)} \leq J_{\text{hom}}^{\text{per}}(z) \leq f(z) \quad \text{for all } z \in \mathbb{R}.$$

For given $z \geq \bar{\delta}$, we find $Z \in \mathbb{R}^M$ satisfying $\frac{1}{M} \sum_{i=0}^{M-1} Z_i = z$ and $Z_i \geq \delta_i$ and thus the definition of $J_{\text{hom}}^{\text{per}}$ in (6.4) and Remark 6.1 yield $J_{\text{hom}}^{\text{per}}(z) = \overline{J(\delta)}$.

Hence, it is left to show (6.5) for $z \leq \bar{\delta}$. Let $z \leq \bar{\delta}$ be given and let $Z \in \mathbb{R}^M$ be such that

$$J_{\text{hom}}^{\text{per}}(z) = \frac{1}{M} \sum_{i=0}^{M-1} J_i^{**}(Z_i) \quad \text{and} \quad \frac{1}{M} \sum_{i=0}^{M-1} Z_i = z. \quad (6.7)$$

We claim that $Z_i \leq \delta_i$ for every $i \in \{0, \dots, M-1\}$. Indeed, assume that there exists $i' \in \{0, \dots, M-1\}$ such that $Z_{i'} > \delta_{i'}$. By (6.7), $z \leq \bar{\delta}$ and the definition of $\bar{\delta}$ (cf. (6.1)), we find $i'' \in \{0, \dots, M-1\}$ such that $Z_{i''} < \delta_{i''}$. Set $q = \min\{Z_{i'} - \delta_{i'}, \delta_{i''} - Z_{i''}\} > 0$ and consider $\tilde{Z} \in \mathbb{R}^M$ given by $\tilde{Z}_i = Z_i$ if $i \in \{0, \dots, M-1\} \setminus \{i', i''\}$ and $\tilde{Z}_{i'} = Z_{i'} - q$, $\tilde{Z}_{i''} = Z_{i''} + q$. The construction of \tilde{Z} implies $\frac{1}{M} \sum_{i=0}^{M-1} \tilde{Z}_i = z$, $\delta_{i'} \leq \tilde{Z}_{i'} \leq Z_{i'}$ and $Z_{i''} < \tilde{Z}_{i''} \leq \delta_{i''}$. From Assumption (LJ2*) and Remark 6.1 it follows that J_i^{**} is strictly decreasing on $\text{dom } J_i \cap (-\infty, \delta_i)$ and $J_i^{**}(z) = J_i^{**}(\delta_i)$ for $z > \delta_i$ for every $i = 0, \dots, M-1$. Hence, we obtain

$$J_{\text{hom}}^{\text{per}}(z) \leq \frac{1}{M} \sum_{i=0}^{M-1} J_i^{**}(\tilde{Z}_i) < \frac{1}{M} \sum_{i=0}^{M-1} J_i^{**}(Z_i) = J_{\text{hom}}^{\text{per}}(z),$$

which is absurd.

The existence of $Z \in \mathbb{R}^M$ satisfying (6.7) is straightforward and it holds $J_i^{**}(z) = J_i(z)$ for $z \leq \delta_i$, cf. Remark 6.1. Thus, we obtain $f(z) \leq J_{\text{hom}}^{\text{per}}(z) \leq f(z)$ and thus $f(z) = J_{\text{hom}}^{\text{per}}(z)$ for all $z \leq \bar{\delta}$.

Step 4. The limit (6.6).

A combination of the lower bound in (LJ2*) and Jensen's inequality yields for every $z \in \mathbb{R}^d$

$$J_{\text{hom}}^{\text{per}}(z) \geq \min \left\{ d_1 \frac{1}{M} \sum_{i=1}^M \Psi(z_i) - d_1 : \sum_{i=1}^M z_i = Mz \right\} \geq d_1 \Psi(z) - d_1.$$

Thus, the superlinear growth of $J_{\text{hom}}^{\text{per}}$ at $-\infty$, i.e. (6.6), is a direct consequence of the superlinear growth of Ψ at $-\infty$, cf. (LJ2*). \square

In the limit $n \rightarrow \infty$, which means that the number of lattice points tends to infinity, we get the following Γ -convergence results in the periodic setting. The first theorem gives the Γ -limit of zeroth order, similar to that of Chapter 4, and uses the homogenization formula $J_{\text{hom}}^{\text{per}}$, which we have discussed in Lemma 6.2.

Theorem 6.3. *Let $\ell > 0$ and let (LJ1*)–(LJ2*) hold true. Then, the Γ -limit of H_n^ℓ with respect to the $L^1(0, 1)$ -topology is $H^\ell : L^1(0, 1) \rightarrow (-\infty, +\infty]$, given by*

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

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

$$\lim_{n \rightarrow \infty} \inf_u H_n^\ell(u) = \min_u H^\ell(u) = f_{\text{hom}}(\ell).$$

The second theorem states the Γ -limit of the rescaled functional, corresponding to the stochastic results in Chapter 5.

Theorem 6.4. *Let $\eta_n \rightarrow \eta$ be such that (6.3) holds. Let (LJ1*)–(LJ4*) hold true. Then, the sequence $(E_n^{\eta_n})$ Γ -converges with respect to the $L^1(0, 1)$ -topology to the functional E^η given by*

$$E^\eta(v) := \begin{cases} \underline{\alpha} \int_0^1 |v'(x)|^2 \, dx + \beta \#S_v & \text{if } v \in SBV^\eta(0, 1), \\ +\infty & \text{else,} \end{cases}$$

$$\text{where } \underline{\alpha} := \left(\frac{1}{M} \sum_{i=1}^M \frac{1}{\alpha_i} \right)^{-1} \text{ and } \beta := \min_{i \in \{1, \dots, M\}} (-J_i(\delta_i)), \text{ with } \alpha_i := \frac{1}{2} J_i''(\delta_i).$$

Moreover, for $\eta > 0$ it holds true that

$$\lim_{n \rightarrow \infty} \inf_v E_n^{\eta_n}(v) = \min_u E^\eta(v) = \min\{\underline{\alpha}\eta^2, \beta\}.$$

The proofs of both theorems are similar to the corresponding ones from the stochastic setting but simpler. One of the main differences is that the mesoscale, introduced in the proofs, is not needed because the periodicity length M operates as a mesoscale. Further, no ergodic theorems are needed. Instead, the calculation of mean values and an approximation of the remainder is sufficient. We refer for details and for the proofs to [82].

7 Fracture on the discrete scale

In the previous chapters, we investigated the discrete model by means of Γ -convergence. We obtained that the chain of atoms, subjected to the boundary conditions $u(0) = 0$ and $u(1) = \ell$, can show fracture in the limit. The threshold where the elastic behaviour of the chain changes into fracture is given by a certain value of the boundary constraint ℓ . The continuum limit is given in the framework of BV functions. There, a jump is defined as the discontinuity point of the good representative of u .

The discrete model only provides the values of the deformation for the lattice points. The deformation on the whole interval $[0, 1]$ is considered as a piecewise affine function, by interpolation. Thus, by definition, the deformation is continuous and does not show jumps at all. The aim of this chapter is to provide a suitable definition for a jump point in the discrete setting, and according to this, a definition of a threshold separating the elastic and jump regime. Section 7.1 contains these new definitions as well as a number of preliminary results. The new definitions come along with further properties on the class of Lennard-Jones type potentials. They are phrased and discussed in Section 7.2.

In Section 7.3, we consider the limiting behaviour of the newly established jump threshold as $n \rightarrow \infty$. This is done first for the special case of a fixed minimizer of the random potentials. This restriction allows to consider also the rescaled version of the jump threshold. Later, the assumption on the minimizer is dropped and the non-rescaled version of the theorem can be proved. The chapter is completed by Section 7.4, where the results are compared to those of Chapter 4 and Chapter 5 employing Γ -convergence analysis.

7.1 Jump threshold

A jump in the continuum regime is defined as a discontinuity point in the setting of BV -functions. Since in the discrete setting the deformation is given as a piecewise affine function, there are no discontinuity points, by definition. Therefore, we need a new definition for a jump in the discrete picture. This is done by defining a threshold z_{frac} for a given potential. We then say that the chain has a jump at a given site, if the slope at this site is larger than the threshold.

Definition 7.1. For a Lennard-Jones type potential $J \in \mathcal{J}_{\text{reg}}(\alpha, b, c, d, \Psi, \eta)$, cf. Definition 5.1, we define a jump or fracture point by

$$z_{\text{frac}} := \sup \left\{ a : \frac{\partial^2 J(z)}{\partial z^2} > 0 \text{ on } [\delta, a] \right\}.$$

Then, we say that a jump occurs at position i^* of the chain of particles if and only if the discrete gradient fulfils $z^{i^*} := \frac{u^{i^*+1} - u^{i^*}}{\lambda_n} > z_{\text{frac}}$.

Especially for the classical Lennard-Jones potential, z_{frac} is the inflection point, see Figure 7.1.

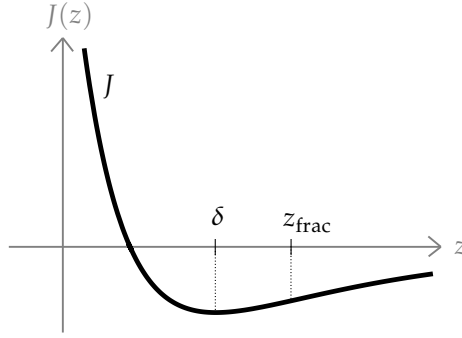


Figure 7.1 | Jump threshold. For a classical Lennard-Jones potential J , where z_{frac} is the inflection point.

Similar definitions and constructions are well known, e.g., from image processing or numerical simulations, where an edge or a shock, respectively, is characterized as a given quantity being larger than a presumed value. The new idea here is to take the (generalized version of the) inflection point of the Lennard-Jones type potential as the threshold for the jump regime.

The threshold from Definition 7.1 is well defined. Indeed, by (LJ5) and Remark 5.2 (iii), we know that $\frac{\partial^2 J(z)}{\partial z^2} \Big|_{z=\delta} > C$ for some constant $C > 0$. Together with (LJ4), which ensures that $J \in C^3$, we know that for all Lennard-Jones type potentials there exists an $a > 0$ with $\frac{\partial^2 J(z)}{\partial z^2} > 0$ on $[\delta, a]$.

Before we continue with further definitions concerning the threshold of fracture we highlight some technical properties of the Lennard-Jones type potentials, corresponding to the newly defined jump point. These properties follow from (LJ1)–(LJ5).

Proposition 7.2. *Let Assumption 5.3 be satisfied. Then the following statements hold true for all $J \in \mathcal{J}_{\text{reg}}(\alpha, b, c, d, \Psi, \eta)$:*

- (i) J is strictly convex on $(0, z_{\text{frac}})$, i.e. $\frac{\partial^2 J(z)}{\partial z^2} > 0$ for $z \in (0, z_{\text{frac}})$.
- (ii) $\frac{\partial J}{\partial z}$ is increasing and positive on $(\delta, z_{\text{frac}})$.
- (iii) There exists $z_{\text{frac}}^{\text{sup}} \in \mathbb{R}$ with $\sup\{z_{\text{frac}} : J \in \mathcal{J}_{\text{reg}}(\alpha, b, c, d, \Psi, \eta)\} = z_{\text{frac}}^{\text{sup}}$.

Proof. **Step 1.** Proof of (i) and (ii).

Since we know from (LJ2) that J is strictly convex on $(0, \delta)$, we get $\frac{\partial^2 J(z)}{\partial z^2} > 0$ on $(0, \delta]$. Together with Definition 7.1, this yields $\frac{\partial^2 J(z)}{\partial z^2} > 0$ on $(0, z_{\text{frac}})$ or rather that J is strictly convex on $(-\infty, z_{\text{frac}})$, which proves (i). Therefore, it also holds true that $\frac{\partial J}{\partial z}$ is increasing on $(\delta, z_{\text{frac}})$, which proves the first part of claim (ii).

A Taylor expansion yields

$$\frac{\partial J}{\partial z}(z) = \frac{\partial J}{\partial z}(\delta) + \frac{\partial^2 J}{\partial z^2}(\xi)(z - \delta) \quad \text{for some } \xi \in [\delta, z].$$

Together with $\frac{\partial J}{\partial z}$ being increasing and δ being the minimizer of J , i.e. $\frac{\partial J}{\partial z}(\delta) = 0$ due to (LJ2), we

get for $z \in (\delta, z_{\text{frac}})$

$$\frac{\partial J}{\partial z}(z) = \frac{\partial^2 J}{\partial z^2}(\xi)(z - \delta) > 0,$$

which proves the second claim of (ii).

Step 2. Proof of (iii).

By claim (i), it holds true that $\frac{\partial J}{\partial z}$ is increasing on $(\delta, z_{\text{frac}})$. Convexity further yields, for all $\epsilon \leq \eta$,

$$J(\delta + \epsilon) - J(\delta) \leq \frac{\partial J}{\partial z}(\delta + \epsilon)\epsilon.$$

Using (LJ5), we then get

$$\frac{1}{c}\epsilon^2 \stackrel{\text{(LJ5)}}{\leq} J(\delta + \epsilon) - J(\delta) \leq \frac{\partial J}{\partial z}(\delta + \epsilon)\epsilon,$$

which yields

$$\frac{1}{c}\epsilon \leq \frac{\partial J}{\partial z}(\delta + \epsilon). \quad (7.1)$$

Further with (LJ4), we can calculate

$$\begin{aligned} J(z_{\text{frac}}) &= J(\delta + \epsilon) + \int_{\delta + \epsilon}^{z_{\text{frac}}} \frac{\partial J}{\partial z}(x) dx \\ &\stackrel{(*)}{\geq} -d + \frac{1}{c}\epsilon(z_{\text{frac}} - \delta - \epsilon) \geq -d + \frac{1}{c}\epsilon(z_{\text{frac}} - d - \epsilon), \end{aligned} \quad (7.2)$$

where in (*) we used (LJ2), (7.1) and claim (ii) (the first derivative is increasing and therefore minimal at $\delta + \epsilon$ on the integration area).

Assume, as a contradiction argument, that for one J we have $z_{\text{frac}} > \max\left\{d, \frac{(b+d)c}{\epsilon} + d + \epsilon\right\} = \frac{(b+d)c}{\epsilon} + d + \epsilon$. We then get

$$J(z_{\text{frac}}) \stackrel{(7.2)}{\geq} -d + \frac{1}{c}\epsilon(z_{\text{frac}} - d - \epsilon) > b \quad \text{and} \quad z_{\text{frac}} > d,$$

which is a contradiction to (LJ2). Therefore, it holds true that $z_{\text{frac}} \leq \hat{C}$, and we can define $z_{\text{frac}}^{\text{sup}} := \sup\{z_{\text{frac}} : J \in \mathcal{J}_{\text{reg}}(\alpha, b, c, d, \Psi, \eta)\}$.

□

Recall the stochastic setting of our model of Chapter 3. For the fracture point, we set for $\omega \in \Omega$

$$z_{\text{frac}}(\omega) := \sup\left\{a : \frac{\partial^2 J(\omega, z)}{\partial z^2} > 0 \text{ on } [\delta(\omega), a]\right\}.$$

After the definition of the jump point for the interaction potentials, we now define the threshold of fracture, separating the elastic and the jump regime. This is done by means of the energy. First,

the minimal energy of our chain of atoms is defined as

$$M_n(\omega, z) = \min \left\{ \sum_{i=0}^{n-1} \lambda_n J \left(\tau_i \omega, \frac{u^{i+1} - u^i}{\lambda_n} \right) : u \in \mathcal{A}_n(0, 1), u(0) = 0, u(1) = z \right\}.$$

In the following, we switch to a different notation for better readability. That is, we use the change of variables $z_n^i := \frac{u^{i+1} - u^i}{\lambda_n}$ and accordingly the adapted boundary condition $\sum_{i=0}^{n-1} z_n^i = nz$.

We are interested in energy minimization together with the question whether a jump occurs or not. The jump is only preferable if the energy of the chain with jump is smaller than any energy without a jump. Therefore we define a minimal elastic energy

$$M_n^{\text{el}}(\omega, z) := \begin{cases} \min \left\{ \sum_{i=0}^{n-1} \lambda_n J \left(\tau_i \omega, z_n^i \right) : \sum_{i=0}^{n-1} z_n^i = nz, z_n^i \leq z_{\text{frac}}(\tau_i \omega) \forall i \in \{0, \dots, n-1\} \right\} \\ \text{if } z \leq \lambda_n \sum_{i=0}^{n-1} z_{\text{frac}}(\tau_i \omega), \\ +\infty \text{ otherwise.} \end{cases}$$

The definition of M_n^{el} takes into account the fact that, for large values of z , it is not possible to fulfil $\sum_{i=0}^{n-1} z_n^i = nz$ and $z_n^i \leq z_{\text{frac}}(\tau_i \omega)$ for all $i \in \{0, \dots, n-1\}$ simultaneously. Further, we define a minimal fracture energy

$$M_n^{\text{frac}}(\omega, z) := \inf \left\{ \sum_{i=0}^{n-1} \lambda_n J(\tau_i \omega, z_n^i) : \sum_{i=0}^{n-1} z_n^i = nz, \exists \hat{i} \in \{0, \dots, n-1\} \text{ with } z_n^{\hat{i}} \geq z_{\text{frac}}(\tau_{\hat{i}} \omega) \right\}.$$

Note that if the minimizer of $M_n(\omega, z)$ fulfils $z_n^i \leq z_{\text{frac}}(\tau_i \omega)$ for all $i \in \{0, \dots, n-1\}$, then we get $M_n^{\text{el}}(\omega, z) = M_n(\omega, z)$. On the other hand, if the minimizer of $M_n(\omega, z)$ consists at least of one $\hat{i} \in \{0, \dots, n-1\}$ such that $z_n^{\hat{i}} \geq z_{\text{frac}}(\tau_{\hat{i}} \omega)$, then $M_n^{\text{frac}}(\omega, z) = M_n(\omega, z)$ holds true.

With the definitions of the minimal elastic and fracture energy, we define the threshold for a jump in the discrete picture as

$$\ell_n^*(\omega) := \sup \left\{ \ell \in \mathbb{R} : M_n^{\text{el}}(\omega, \ell) \leq M_n^{\text{frac}}(\omega, \ell) \right\}.$$

The limiting behaviour and the convergence rate of this variable is the topic of the next sections. For preparing the convergence analysis, we first prove that ℓ_n^* is bounded.

Proposition 7.3. *Let Assumption 5.3 be fulfilled. Then, it holds true that $\frac{1}{d} \leq \ell_n^*(\omega) \leq z_{\text{frac}}^{\text{sup}}$ for every $n \in \mathbb{N}$ and for every $\omega \in \Omega$, with the constant d from (LJ2).*

Proof. **Step 1.** Upper bound.

The upper bound is given by $z_{\text{frac}}^{\text{sup}}$ from Proposition 7.2 (iii). This follows from the definition of M_n^{el} and $\ell_n^*(\omega)$, since we have $\ell_n^*(\omega) \leq \lambda_n \sum_{i=0}^{n-1} z_{\text{frac}}(\tau_i \omega) \leq \lambda_n \sum_{i=0}^{n-1} z_{\text{frac}}^{\text{sup}} = z_{\text{frac}}^{\text{sup}}$.

Step 2. Lower bound.

To prove that $\ell_n^*(\omega) \geq \frac{1}{d}$, we have to show that $M_n^{\text{el}}(\omega, z) \leq M_n^{\text{frac}}(\omega, z)$ for all $z \leq \frac{1}{d}$. We drop for a moment ω in the formulae for better readability. Thus, assume z_n^i to be a minimizer of $M_n^{\text{frac}}(z)$ for $z \leq \frac{1}{d}$, i.e. to fulfill the constraint $\sum_{i=0}^{n-1} z_n^i = nz$ and define the set $\hat{I}_n := \{i \in \{0, \dots, n-1\}, z_n^i \geq z_{\text{frac}}(\tau_i \omega)\}$. \hat{I}_n is not empty, by definition of M_n^{frac} .

Now, we introduce $\gamma_i \geq 0$ such that the following conditions are satisfied:

- (i) $z_n^i + \gamma_i \leq \delta_i$ if $z_n^i \leq \delta_i$,
- (ii) $\gamma_i = 0$ if $z_n^i > \delta_i$,
- (iii) $\sum_{i=0}^{n-1} \gamma_i = \sum_{i \in \hat{I}_n} (z_n^i - \delta_i)$.

Especially, this definition yields $\gamma_i = 0$ for $i \in \hat{I}_n$. The well-posedness of the conditions for γ_i can be proven by showing that (ii) and (iii) allow for (i). Set $\check{I}_n := \{i \in \{0, \dots, n-1\} : z_n^i \leq \delta_i\}$. By definition, we get

$$\frac{1}{n} \sum_{i=0}^{n-1} \delta_i \geq \frac{1}{d} \geq z = \frac{1}{n} \sum_{i=0}^{n-1} z_n^i.$$

and with this

$$\sum_{i \in \check{I}_n} (\delta_i - z_n^i) \geq \sum_{i \in \hat{I}_n} (z_n^i - \delta_i) + \sum_{i \notin (\hat{I}_n \cup \check{I}_n)} (z_n^i - \delta_i) \geq \sum_{i \in \hat{I}_n} (z_n^i - \delta_i) \stackrel{(iii)}{=} \sum_{i=0}^{n-1} \gamma_i \stackrel{(ii)}{\geq} \sum_{i \in \check{I}_n} \gamma_i,$$

since $z_n^i - \delta_i > 0$ for $i \notin (\hat{I}_n \cup \check{I}_n)$. This shows (i) and therefore γ_i with the required properties exist. With this, we now define

$$\bar{z}_n^i := \begin{cases} \delta_i & \text{for } i \in \hat{I}_n, \\ z_n^i + \gamma_i & \text{else.} \end{cases}$$

The constraint is still fulfilled, since $\gamma_i = 0$ for $i \in \hat{I}_n$ by definition and thus

$$\begin{aligned} \frac{1}{n} \sum_{i=0}^{n-1} \bar{z}_n^i &= \frac{1}{n} \left(\sum_{i \in \hat{I}_n} \delta_i + \sum_{i \notin \hat{I}_n} (z_n^i + \gamma_i) \right) = \frac{1}{n} \sum_{i \in \hat{I}_n} \delta_i + \frac{1}{n} \sum_{i=0}^{n-1} (z_n^i + \gamma_i) - \frac{1}{n} \sum_{i \in \hat{I}_n} z_n^i \\ &= \frac{1}{n} \sum_{i \in \hat{I}_n} (\delta_i - z_n^i) + \frac{1}{n} \sum_{i=0}^{n-1} \gamma_i + z = z, \end{aligned}$$

and it holds true that

$$\lambda_n \sum_{i=0}^{n-1} J_i(z_n^i) > \lambda_n \sum_{i=0}^{n-1} J_i(\bar{z}_n^i),$$

since J_i is strictly decreasing on $(0, \delta_i]$ due to (LJ2). By construction, it holds true that $\bar{z}_n^i \leq z_{\text{frac}}(\tau_i \omega)$ for all $i = 0, \dots, n-1$ and therefore we have

$$M_n^{\text{frac}}(z) = \lambda_n \sum_{i=0}^{n-1} J_i(z_n^i) > \lambda_n \sum_{i=0}^{n-1} J_i(\bar{z}_n^i) \geq M_n^{\text{el}}(z).$$

This shows

$$M_n^{\text{frac}}(z) - M_n^{\text{el}}(z) > 0,$$

which proves the assertion. \square

7.2 Lennard-Jones type potentials: (LJ6)–(LJ9)

We list the assumptions which we need for the following proofs and theorems. They deal with the jump threshold and, related to this, with the second derivative and the curvature. For notational convenience, we introduce for all $J \in \mathcal{J}_{\text{reg}}(\alpha, b, c, d, \Psi, \eta)$

$$m_{\text{frac}} := \min \{J(z) : z \in [z_{\text{frac}}, +\infty)\},$$

and the related definition for the stochastic setting for all $\omega \in \Omega$

$$m_{\text{frac}}(\omega) := \min \{J(\omega, z) : z \in [z_{\text{frac}}(\omega), +\infty)\},$$

which is the minimum value of J or $J(\omega, z)$, respectively, in the regime beyond the jump threshold. Indeed, this is well defined because of (LJ2) and (LJ3) together with the continuity of J due to (LJ1). The next two definitions introduce the class of Lennard-Jones type potentials $\tilde{\mathcal{J}}_{\text{curv}}(\alpha, b, c, d, \Psi, \eta)$ and $\mathcal{J}_{\text{curv}}(\alpha, b, c, d, \Psi, \eta)$, respectively. They are subclasses of $\mathcal{J}_{\text{reg}}(\alpha, b, c, d, \Psi, \eta)$ and are used for the results in this section. A list of all assumptions from the different chapters can be found at the end of the thesis.

Definition 7.4. Fix $\alpha \in (0, 1]$, $b > 0$, $c > 0$, $d \in (1, +\infty)$, $\eta > 0$, and a convex function $\Psi : \mathbb{R} \rightarrow [0, +\infty]$ satisfying (3.2), as in Definition 5.1. We denote by $\tilde{\mathcal{J}}_{\text{curv}} = \tilde{\mathcal{J}}_{\text{curv}}(\alpha, b, c, d, \Psi, \eta)$ the class of functions $J : \mathbb{R} \rightarrow \mathbb{R} \cup \{+\infty\}$ which satisfy the properties (LJ1)–(LJ5) from Definitions 3.1 and 5.1, and additionally the following properties:

(LJ6) It holds true that $z_{\text{frac}} - \delta \geq \frac{1}{b}$.

(LJ7) It holds true that $m_{\text{frac}} - J(\delta) \geq \frac{1}{b}$.

(LJ8) It holds true that

$$\inf \left\{ \frac{\partial^2 J(z)}{\partial z^2} : z \in [\delta, \delta + \eta] \right\} \geq \frac{1}{c}.$$

(LJ9) It holds true that

$$\sup \left\{ \frac{\partial^2 J(z)}{\partial z^2} : z \in [\delta, \delta + \eta] \right\} \leq c.$$

Remark 7.5. (i) In the case of finitely many potentials, (LJ6)–(LJ9) are trivially fulfilled.

(ii) Due to the uniqueness of the minimum, cf. (LJ2), it holds true that $m_{\text{frac}} > J(\delta)$ for all $J \in \mathcal{J}(\alpha, b, d, \Psi)$. (LJ7) additionally asks for a common lower bound of the difference between the unique minimum and the other local minima.

(iii) (LJ9) can be replaced by a weaker assumption:

(H4) Fix $0 \leq \theta < \frac{1}{6}$. Then it holds true that

$$\sup \left\{ \frac{\partial^2 J}{\partial z^2}(\tau_i \omega, z) : z \in [\delta(\tau_i \omega), \delta(\tau_i \omega) + \eta], \omega \in \Omega, i \in \{0, \dots, n-1\} \right\} \leq cn^\theta.$$

This is no longer a property of the class of Lennard-Jones type potentials, but instead an assumption on the random variable $J(\omega, \cdot)$. Consequently, we phrase this in an additional hypothesis (H4). We will give all of

the following proofs with this weaker assumption (H4) instead of (LJ9). Indeed,

$$\begin{aligned} & \sup \left\{ \frac{\partial^2 J}{\partial z^2}(\tau_i \omega, z) : z \in [\delta(\tau_i \omega), \delta(\tau_i \omega) + \eta], \omega \in \Omega, i \in \{0, \dots, n-1\} \right\} \\ & \leq \sup_{J \in \tilde{\mathcal{J}}_{\text{curv}}} \sup \left\{ \frac{\partial^2 J(z)}{\partial z^2} : z \in [\delta, \delta + \eta] \right\} \stackrel{(LJ9)}{\leq} c \leq cn^\theta. \end{aligned}$$

(iv) In the case $\delta(\omega) = 1$ for all $\omega \in \Omega$, (LJ6) reduces to $\inf\{z_{\text{frac}}(\omega) : \omega \in \Omega\} > 1$.

Since we want to replace assumption (LJ9) by (H4), we need a modified definition of the Lennard-Jones type potentials $\tilde{\mathcal{J}}_{\text{curv}}(\alpha, b, c, d, \Psi, \eta)$, without assumption (LJ9).

Definition 7.6. Fix $\alpha \in (0, 1]$, $b > 0$, $c > 0$, $d \in (1, +\infty)$, $\eta > 0$ and a convex function $\Psi : \mathbb{R} \rightarrow [0, +\infty]$ satisfying (3.2), as in Definition 5.1. We denote by $\mathcal{J}_{\text{curv}} = \mathcal{J}_{\text{curv}}(\alpha, b, c, d, \Psi, \eta)$ the class of functions $J : \mathbb{R} \rightarrow \mathbb{R} \cup \{+\infty\}$ which satisfy the properties (LJ1)–(LJ8) from Definitions 3.1, 5.1 and 7.4.

The stochastic setting of the chain with Lennard-Jones type interaction potentials in the discrete fracture setting is collected in the following assumption.

Assumption 7.7. Fix $\alpha \in (0, 1]$, $b > 0$, $c > 0$, $d \in (1, \infty)$, $\eta > 0$, $0 \leq \theta < \frac{1}{6}$ and a convex function $\Psi : \mathbb{R} \rightarrow [0, \infty]$ satisfying (3.2). Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space and $(\tau_i)_{i \in \mathbb{Z}}$ be a family of stationary and ergodic group actions in the sense of Section 3.2. We suppose that the random variable $J : \Omega \rightarrow \mathcal{J}_{\text{curv}}(a, b, c, d, \Psi, \eta)$ given as in Section 3.2 is measurable and (H2), (H3) as well as (H4) are satisfied, with $\mathcal{J}_{\text{curv}}(a, b, c, d, \Psi, \eta)$ as in Definition 7.6.

7.3 Convergence results

We are now in the position to consider convergence of the quantity ℓ_n^* in the limit $n \rightarrow \infty$. This is separated in two subsections. The difference between Section 7.3.1 and Section 7.3.2 is that in the first one additionally $\delta(\omega) = 1$ for all $\omega \in \Omega$ is assumed, while in the second one, the fully random potentials are considered. The additional assumption allows to consider also the limit of the rescaled threshold γ_n^* , arising from ℓ_n^* by the $\sqrt{\lambda_n}$ -rescaling, as in Chapter 5.

7.3.1 Random potentials with fixed minimizers

In this section, we set $\delta(\omega) = 1$ for all $\omega \in \Omega$.

First, we give preliminary results. The next proposition is dealing with minimizers of the minimal elastic and fracture energies.

Proposition 7.8. Let Assumption 7.7 be satisfied. Let $C > 0$ be such that $C^2 > cb$, with b, c being the constants from the class of Lennard-Jones type potentials. Then, the following statements hold true for all $\omega \in \Omega$.

(i) Any minimizer $\bar{z}_n \in \mathbb{R}^n$ of $M_n^{\text{el}}(\omega, 1 + \sqrt{\lambda_n}C)$ or $M_n^{\text{frac}}(\omega, 1 + \sqrt{\lambda_n}C)$, respectively, satisfies, for n large enough,

$$0 \leq \frac{\partial J}{\partial z}(\omega, \bar{z}_n^i) \leq cCn^{\theta - \frac{1}{2}} \quad \text{for all } i \in \{0, \dots, n-1\}. \quad (7.3)$$

(ii) For a minimizer $\bar{z}_n \in \mathbb{R}^n$ of $M_n^{\text{el}}(\omega, 1 + \sqrt{\lambda_n}C)$ it holds true that, for n large enough,

$$1 \leq \bar{z}_n^i \leq 1 + c^2 C n^{\theta - \frac{1}{2}}, \quad (7.4)$$

for all $i \in \{0, \dots, n-1\}$, which especially yields $\bar{z}_n^i \rightarrow 1$ uniformly as $n \rightarrow \infty$.

(iii) Any minimizer $\bar{z}_n \in \mathbb{R}^n$ of $M_n^{\text{frac}}(\omega, 1 + \sqrt{\lambda_n}C)$ satisfies: If the subsequence (\bar{z}_{n_k}) fulfils $\bar{z}_{n_k}^i \leq z_{\text{frac}}^i(\tau_i \omega)$ for all $i = 0, \dots, n-1$, we have

$$1 \leq \bar{z}_{n_k}^i \leq 1 + c^2 C n_k^{\theta - \frac{1}{2}}, \quad (7.5)$$

for k large enough, which especially yields $\bar{z}_{n_k}^i \rightarrow 1$ uniformly as $k \rightarrow \infty$.

Further, there exists at least one subsequence (\bar{z}_{n_k}) and for every n_k a corresponding index i_{n_k} with

$$\bar{z}_{n_k}^{i_{n_k}} \rightarrow \infty \quad \text{as } k \rightarrow \infty.$$

Remark 7.9. When using (LJ9) instead of (H4), the corresponding inequalities read

$$(7.3): 0 \leq \frac{\partial J}{\partial z}(\omega, \bar{z}_n^i) \leq c C n^{-\frac{1}{2}},$$

$$(7.4): 1 \leq \bar{z}_n^i \leq 1 + c^2 C n^{-\frac{1}{2}},$$

$$(7.5): 1 \leq \bar{z}_{n_k}^i \leq 1 + c^2 C n_k^{-\frac{1}{2}}.$$

Proof. We drop here the dependence of ω for a better readability and define $z_{\text{frac}}^i := z_{\text{frac}}^i(\tau_i \omega)$, $J_i(z) := J(\tau_i \omega, z)$ and $m_{\text{frac}}^i := m_{\text{frac}}^i(\tau_i \omega)$. Then, we can use the short form J'_i and J''_i for the first and second derivative of J with respect to z .

Step 1. Proof of (i).

Let \bar{z}_n be a minimizer of $M_n^{\text{el}}(1 + \sqrt{\lambda_n}C)$ or $M_n^{\text{frac}}(1 + \sqrt{\lambda_n}C)$, respectively. Then, there exists i_1 such that $\bar{z}_n^{i_1} \geq 1 + \sqrt{\lambda_n}C$ and i_2 such that $\bar{z}_n^{i_2} \leq 1 + \sqrt{\lambda_n}C$. By (LJ6), we have $z_{\text{frac}} - 1 \geq \frac{1}{b}$ and hence

$$1 \leq 1 + \sqrt{\lambda_n}C \leq \bar{z}_n^{i_1}, \quad (7.6)$$

$$\bar{z}_n^{i_2} \leq 1 + \sqrt{\lambda_n}C < z_{\text{frac}}^{i_2}, \quad (7.7)$$

for sufficiently large n . Due to the method of Lagrange multipliers, it holds true that, for $i = 0, \dots, n-1$ and for n large enough such that $\sqrt{\lambda_n}C < \eta$,

$$\begin{aligned} 0 &\stackrel{(7.6)}{\leq} J'_{i_1}(\bar{z}_n^{i_1}) = J'_i(\bar{z}_n^i) = J'_{i_2}(\bar{z}_n^{i_2}) \stackrel{(7.7)}{\leq} J'_{i_2}(1 + \sqrt{\lambda_n}C) = J'_{i_2}(1) + J''_{i_2}(\xi) \sqrt{\lambda_n}C \\ &\stackrel{(H4)}{\leq} C c n^\theta \sqrt{\lambda_n} = c C n^{\theta - \frac{1}{2}} \quad \text{with } \xi \in [1, 1 + \sqrt{\lambda_n}C], \end{aligned}$$

where we used that for every i the function J'_i is increasing for $z \leq z_{\text{frac}}^i$ (Proposition 7.2 (i)) and positive for $z \geq 1$ (Proposition 7.2 (ii)). This proves for all $i \in \{0, \dots, n-1\}$

$$0 \leq J'_i(\bar{z}_n^i) \leq c C n^{\theta - \frac{1}{2}}.$$

Step 2. Proof of (ii) and the first part of (iii).

We can now use (7.1) and (7.3) for all $\epsilon \leq \eta$ and n large enough ($0 \leq \theta < \frac{1}{6}$ by definition), and get

$$J'_i(1) = 0 \leq J'_i(\bar{z}_n^i) \stackrel{(7.3)}{\leq} cCn^{\theta-\frac{1}{2}} < \frac{1}{c}\epsilon \stackrel{(7.1)}{\leq} J'(1+\epsilon).$$

Therefore, for a minimizer of $M_n^{\text{el}}(1 + \sqrt{\lambda_n}C)$ the following holds true, due to (LJ6): by definition, we have $\bar{z}_n^i \leq z_{\text{frac}}^i$ for all $i = 0, \dots, n-1$. Further, for all $\epsilon < \frac{1}{b} \leq z_{\text{frac}}^i - 1$ and since J'_i is strictly increasing on $(-\infty, z_{\text{frac}}^i]$ due to Proposition 7.2 (i) and (ii), this yields $1 \leq \bar{z}_n^i < 1 + \epsilon$. This especially holds true for all $\epsilon < \min\left\{\frac{1}{b}, \eta\right\}$. Thus, with $\xi_i \in [1, \bar{z}_n^i] \subset [1, 1 + \epsilon]$ and n large enough, we can use the mean value theorem to obtain

$$cCn^{\theta-\frac{1}{2}} \stackrel{(7.3)}{\geq} J'_i(\bar{z}_n^i) = J''_i(\xi_i)(\bar{z}_n^i - 1) \stackrel{(LJ8)}{\geq} \frac{1}{c}(\bar{z}_n^i - 1),$$

which yields

$$1 \leq \bar{z}_n^i \leq 1 + c^2Cn^{\theta-\frac{1}{2}},$$

and hence a uniform convergence $\bar{z}_n^i \rightarrow 1$ as $n \rightarrow \infty$, since $0 \leq \theta < \frac{1}{6}$ by assumption.

The corresponding estimate holds true for every subsequence $(\bar{z}_{n_k}^i)$ with $\bar{z}_{n_k}^i \leq z_{\text{frac}}^i$ of a minimizer of the minimal fracture energy $M_n^{\text{frac}}(1 + \sqrt{\lambda_n}C)$.

Step 3. Technical interlude.

In order to prepare the proof of (iii), we first study the following assertion: Let \bar{z}_n be a minimizer of $M_n^{\text{frac}}(1 + \sqrt{\lambda_n}C)$ and define

$$I_n^w := \left\{ i \in \{0, \dots, n-1\} : \bar{z}_n^i \geq z_{\text{frac}}^i \right\}.$$

Then, it holds true that

$$\frac{|I_n^w|}{\sqrt{n}} \rightarrow 0 \quad \text{as } n \rightarrow \infty. \quad (7.8)$$

The proof of this assertion is given in the following. Assume that $\frac{|I_n^w|}{\sqrt{n}}$ does not converge to zero. Then, there exists an $\epsilon > 0$ such that for a subsequence (not relabelled) it holds true that

$$\frac{|I_n^w|}{\sqrt{n}} \geq \epsilon \quad (7.9)$$

We want to compare the minimizer \bar{z}_n with another competitor \hat{z}_n fulfilling also the boundary constraints of $M_n^{\text{frac}}(1 + \sqrt{\lambda_n}C)$. We set $i_{\text{min}}^w := \min\{i : i \in I_n^w\}$ and set

$$\hat{z}_n^i := \begin{cases} \sqrt{n}C + 1 & \text{for } i = i_{\text{min}}^w, \\ 1 & \text{otherwise.} \end{cases} \quad (7.10)$$

which is well defined, since $|I_n^w| \geq 1$ holds true due to the definition of M_n^{frac} . Consequently, we

get with the minimizer \bar{z}_n

$$M_n^{\text{frac}} \left(1 + \sqrt{\lambda_n} C\right) = \lambda_n \sum_{i=0}^{n-1} J_i(\bar{z}_n^i) = \lambda_n \sum_{i \neq i_{\min}^w} J_i(\bar{z}_n^i) + \lambda_n J_{i_{\min}^w}(\bar{z}_n^{i_{\min}^w}), \quad (7.11)$$

and with the new competitor \hat{z}_n

$$M_n^{\text{frac}} \left(1 + \sqrt{\lambda_n} C\right) \leq \lambda_n \sum_{i=0}^{n-1} J_i(\hat{z}_n^i) = \lambda_n \sum_{i \neq i_{\min}^w} J_i(1) + \lambda_n J_{i_{\min}^w}(C\sqrt{n} + 1). \quad (7.12)$$

We now calculate the difference of (7.11) and (7.12) and show that this difference is strictly positive, which is a contradiction to the minimality of \bar{z}_n . Indeed for n large enough, it holds true that

$$\begin{aligned} & \lambda_n \sum_{i \neq i_{\min}^w} \left(J_i(\bar{z}_n^i) - J_i(1) \right) + \lambda_n \left(J_{i_{\min}^w}(\bar{z}_n^{i_{\min}^w}) - J_{i_{\min}^w}(C\sqrt{n} + 1) \right) \\ & \stackrel{\text{(LJ2)}}{\geq} \lambda_n \sum_{\substack{i \in I_n^w \\ i \neq i_{\min}^w}} \left(J_i(\bar{z}_n^i) - J_i(1) \right) + \lambda_n \left(-b - J_{i_{\min}^w}(C\sqrt{n} + 1) \right) \\ & \geq \lambda_n \sum_{\substack{i \in I_n^w \\ i \neq i_{\min}^w}} \left(m_{\text{frac}}^i - J_i(1) \right) + \lambda_n \left(-b - J_{i_{\min}^w}(C\sqrt{n} + 1) \right) \\ & \stackrel{\text{(LJ7)}}{\geq} \frac{|I_n^w| - 1}{n} \frac{1}{b} + \frac{1}{n} \left(-b - J_{i_{\min}^w}(C\sqrt{n} + 1) \right) \\ & \stackrel{\text{(7.9)}}{\geq} \frac{1}{n} \left((\sqrt{n}\epsilon - 1) \frac{1}{b} - b - J_{i_{\min}^w}(C\sqrt{n} + 1) \right) > 0. \end{aligned}$$

The lower bound by zero follows from (H3) for n large enough. Thus, this is the desired contradiction and therefore (7.9) is wrong and (7.8) is proven.

Step 4. Proof of the second part of (iii).

Assume \bar{z}_n to be a minimizer of $M_n^{\text{frac}}(1 + \sqrt{\lambda_n} C)$ which is uniformly bounded, i.e. $\bar{z}_n^i \leq A$ holds true for all n and for all $i = 0, \dots, n-1$.

With the boundary condition of $M_n^{\text{frac}}(1 + \sqrt{\lambda_n} C)$, we get by the uniform bound of the minimizer

$$\sqrt{\lambda_n} C = \frac{1}{n} \sum_{i \notin I_n^w} (\bar{z}_n^i - 1) + \frac{1}{n} \sum_{i \in I_n^w} (\bar{z}_n^i - 1) \leq \frac{1}{n} \sum_{i \notin I_n^w} (\bar{z}_n^i - 1) + \frac{|I_n^w|}{n} (A - 1),$$

thus

$$0 \leq \sqrt{\lambda_n} \left(C - \frac{|I_n^w|}{\sqrt{n}} (A - 1) \right) \leq \frac{1}{n} \sum_{i \notin I_n^w} (\bar{z}_n^i - 1), \quad (7.13)$$

for n large enough. The lower bound by zero follows from (7.8).

We use once again \hat{z}_n from (7.10) as a competitor for the minimum problem of the minimal

fracture energy $M_n^{\text{frac}}(1 + \sqrt{\lambda_n}C)$, fulfilling also the boundary constraint. Thus, the difference of (7.11) to (7.12) is calculated and it is shown that this difference is strictly positive. Therefore, this is a contradiction to the minimality of \bar{z}_n . Indeed, it holds true for n large enough that

$$\begin{aligned} & \lambda_n \sum_{i \neq i_{\min}^w} J_i(\bar{z}_n^i) + \lambda_n J_{i_{\min}^w}(\bar{z}_n^{i_{\min}^w}) - \lambda_n \sum_{i \neq i_{\min}^w} J_i(1) - \lambda_n J_{i_{\min}^w}(C\sqrt{n} + 1) \\ & \stackrel{\text{(LJ2)}}{\geq} \lambda_n \sum_{i \notin I_n^w} \left(J_i(\bar{z}_n^i) - J_i(1) \right) + \lambda_n \left(-b - J_{i_{\min}^w}(C\sqrt{n} + 1) \right) \\ & \stackrel{\text{(LJ5)}}{\geq} \lambda_n \frac{1}{c} \sum_{i \notin I_n^w} \left(\bar{z}_n^i - 1 \right)^2 + \lambda_n \left(-b - J_{i_{\min}^w}(C\sqrt{n} + 1) \right), \end{aligned}$$

and continuing with the Hölder-inequality

$$\begin{aligned} & \geq \frac{1}{c} \frac{n}{n - |I_n^w|} \left(\frac{1}{n} \sum_{i \notin I_n^w} \left(\bar{z}_n^i - 1 \right) \right)^2 + \frac{1}{n} \left(-b - J_{i_{\min}^w}(C\sqrt{n} + 1) \right) \\ & \stackrel{\text{(7.13)}}{\geq} \frac{1}{c} \left(\sqrt{\frac{1}{n}} \left(C - \frac{|I_n^w|}{\sqrt{n}}(A - 1) \right) \right)^2 + \frac{1}{n} \left(-b - J_{i_{\min}^w}(C\sqrt{n} + 1) \right) \\ & = \frac{1}{n} \left(\frac{1}{c} \left(C - \frac{|I_n^w|}{\sqrt{n}}(A - 1) \right)^2 - b - J_{i_{\min}^w}(C\sqrt{n} + 1) \right) > 0, \end{aligned}$$

for n large enough. The last inequality, i.e. the strict lower bound by zero, is due to (H3) and (7.8), from which we have $J_{i_{\min}^w}(C\sqrt{n} + 1) \rightarrow 0$ and $|I_n^w|/\sqrt{n} \rightarrow 0$, and from the assumption $C^2 > cb$ of the proposition.

Thus, this is the desired contradiction and therefore the claim of the uniform bound of the minimizer \bar{z}_n is wrong. This shows assertion (iii). \square

The next proposition is a refinement of Proposition 7.3, that asserts boundedness of ℓ_n^* . Now, we derive a sharper upper bound.

Proposition 7.10. *Let Assumption 7.7 be fulfilled. Let $C > 0$ be such that $C^2 > cb$, with b, c being the constants of the class of Lennard-Jones type potentials. Then, it holds true that $\ell_n^*(\omega) \leq 1 + \sqrt{\lambda_n}C$ for all $\omega \in \Omega$ and for $n \in \mathbb{N}$ large enough.*

Proof. We drop here the dependence of ω for better readability and define $J_i(z) := J(\tau_i \omega, z)$. We show in the following that for a fixed $C > 0$ with $C^2 > cb$ there exists $n_0 \in \mathbb{N}$ such that for all $x \in [1 + \sqrt{\lambda_n}C, +\infty)$ and $n \geq n_0$ it holds true that $M_n^{\text{el}}(x) > M_n^{\text{frac}}(x)$, which then yields the assertion.

Step 1: Proof of $M_n^{\text{frac}}(1 + \sqrt{\lambda_n}C) < M_n^{\text{el}}(1 + \sqrt{\lambda_n}C)$ for large n .

Fix $C > 0$ with $C^2 > cb$. Let z_n be a minimizer of $M_n^{\text{el}}(1 + \sqrt{\lambda_n}C)$. Since (7.4) shows that $z_n^i \rightarrow 1$ uniformly for all i , we get from (LJ5), because $z_n^i \leq 1 + \eta$ for all $n > n_1$ with $n_1 \in \mathbb{N}$, and together

with Jensen's inequality

$$\begin{aligned} M_n^{\text{el}} \left(1 + \sqrt{\lambda_n C} \right) &\geq \lambda_n \sum_{i=0}^{n-1} \left(J_i(1) + \frac{1}{c} (z_n^i - 1)^2 \right) \\ &\geq \lambda_n \sum_{i=0}^{n-1} J_i(1) + \frac{1}{c} \left(\lambda_n \sum_{i=0}^{n-1} (z_n^i - 1) \right)^2 = \lambda_n \sum_{i=0}^{n-1} J_i(1) + \frac{1}{c} C^2 \lambda_n. \end{aligned} \quad (7.14)$$

On the other hand, for n large enough, the competitor $z_n^i := 1$ for $i \geq 1$ and $z_n^0 := \sqrt{n}C + 1 > z_{\text{frac}}$ satisfies the boundary constraint $\sum_{i=0}^{n-1} z_n^i = n(1 + \sqrt{\lambda_n C})$ and thus we have

$$\begin{aligned} M_n^{\text{frac}} \left(1 + \sqrt{\lambda_n C} \right) &\leq \lambda_n \sum_{i=1}^{n-1} J_i(1) + \lambda_n J_0(\sqrt{n}C + 1) \\ &= \lambda_n \sum_{i=0}^{n-1} J_i(1) + \lambda_n (J_0(\sqrt{n}C + 1) - J_0(1)). \end{aligned} \quad (7.15)$$

Since $C^2 > cb$ by assumption, there exists $\epsilon > 0$ with $C^2 = cb + \epsilon$. Due to (H3), there also exists $n_2 \in \mathbb{N}$ such that $|J_0(\sqrt{n}C + 1)| \leq \frac{\epsilon}{2c}$ for all $n \geq n_2$. Thus, we define $n_0 = \max\{n_1, n_2\}$ and get for all $n > n_0$ by (7.14) and (7.15)

$$\begin{aligned} M_n^{\text{el}} \left(1 + \sqrt{\lambda_n C} \right) - M_n^{\text{frac}} \left(1 + \sqrt{\lambda_n C} \right) &\geq \lambda_n \left(\frac{1}{c} C^2 - J_0(\sqrt{n}C + 1) + J_0(1) \right) \\ &\stackrel{(LJ2)}{>} \lambda_n \left(b + \frac{\epsilon}{c} - J_0(\sqrt{n}C + 1) - b \right) = \lambda_n \left(\frac{\epsilon}{c} - J_0(\sqrt{n}C + 1) \right) \geq \lambda_n \frac{\epsilon}{2c} > 0. \end{aligned} \quad (7.16)$$

This yields for all $n > n_0$

$$M_n^{\text{frac}} \left(1 + \sqrt{\lambda_n C} \right) < M_n^{\text{el}} \left(1 + \sqrt{\lambda_n C} \right),$$

which concludes Step 1.

Step 2: Proof of $M_n^{\text{frac}} \left(1 + \sqrt{\lambda_n C^*} \right) < M_n^{\text{el}} \left(1 + \sqrt{\lambda_n C} \right)$ for large n .

Now, consider $C^* > C$. Analogously to (7.15) we obtain

$$M_n^{\text{frac}} \left(1 + \sqrt{\lambda_n C^*} \right) \leq \lambda_n \sum_{i=0}^{n-1} J_i(1) + \lambda_n (J_0(\sqrt{n}C^* + 1) - J_0(1)).$$

Due to (H3), it holds true that $|J_0(\sqrt{n}C^* + 1)| \leq \frac{\epsilon}{2c}$ for all $n \geq n_2$ with the same index n_2 as before, since $\sqrt{n}C + 1 < \sqrt{n}C^* + 1$. Thus, with an analogous calculation as in (7.16) we get for all $n > n_0$

$$M_n^{\text{el}} \left(1 + \sqrt{\lambda_n C} \right) - M_n^{\text{frac}} \left(1 + \sqrt{\lambda_n C^*} \right) > \lambda_n \frac{\epsilon}{2c} > 0,$$

which yields

$$M_n^{\text{frac}} \left(1 + \sqrt{\lambda_n C^*} \right) < M_n^{\text{el}} \left(1 + \sqrt{\lambda_n C} \right),$$

which concludes Step 2.

Step 3: Proof of $M_n^{\text{el}}(1 + \sqrt{\lambda_n}C) < M_n^{\text{el}}(1 + \sqrt{\lambda_n}C^*)$ for large n .

Let z_n be a minimizer of $M_n^{\text{el}}(1 + \sqrt{\lambda_n}C^*)$. Due to the boundary constraint, which reads $\sum_{i=0}^{n-1} z_n^i = n(1 + \sqrt{\lambda_n}C^*)$, it holds true

$$\sum_{i=0}^{n-1} (z_n^i - 1) = \sqrt{n}C^* > \sqrt{n}(C^* - C).$$

Thus, there exists $\beta_n^i \geq 0$ with $\sum_{i=0}^{n-1} \beta_n^i = \sqrt{n}(C^* - C)$ such that $z_n^i - \beta_n^i \geq 1$. We define a competitor \bar{z}_n for the minimum problem of $M_n^{\text{el}}(1 + \sqrt{\lambda_n}C)$ by

$$\bar{z}_n^i := z_n^i - \beta_n^i$$

for all $i \in \{0, \dots, n-1\}$. Indeed, \bar{z}_n fulfils the boundary constraint, since

$$\sum_{i=0}^{n-1} \bar{z}_n^i = \sum_{i=0}^{n-1} z_n^i - \sum_{i=0}^{n-1} \beta_n^i = n(1 + \sqrt{\lambda_n}C^*) - \sqrt{n}(C^* - C) = n(1 + \sqrt{\lambda_n}C).$$

For all $i = 0, \dots, n-1$, it holds true that $z_n^i \leq z_{\text{frac}}^i$ by definition of the minimal elastic energy, and due to Proposition 7.8 it is $z_n^i \geq 1$. The definition of β_n further yields $\bar{z}_n^i \leq z_{\text{frac}}^i$ and $\bar{z}_n^i \geq 1$ and $\bar{z}_n^i \leq z_n^i$. Since Proposition 7.2 shows that J_i' is positive on $(1, z_{\text{frac}}^i)$, we get $J_i(\bar{z}_n^i) \leq J_i(z_n^i)$, which gives

$$M_n^{\text{el}}(1 + \sqrt{\lambda_n}C) \leq M_n^{\text{el}}(1 + \sqrt{\lambda_n}C^*). \quad (7.17)$$

This includes also the trivial case of C^* being large, where $M_n^{\text{el}}(1 + \sqrt{\lambda_n}C^*) = +\infty$. Thus, Step 3 is proven.

Step 4: Conclusion.

The result of Step 2, together with (7.17), yields

$$M_n^{\text{frac}}(1 + \sqrt{\lambda_n}C^*) < M_n^{\text{el}}(1 + \sqrt{\lambda_n}C^*),$$

for every $C^* \geq C$. Since C^* can be chosen arbitrarily large, this yields for all $n > n_0$

$$M_n^{\text{frac}}(x) < M_n^{\text{el}}(x)$$

for all $x \in [1 + \sqrt{\lambda_n}C, +\infty)$. Therefore, by definition of ℓ_n^* , we get $\ell_n^* \leq 1 + \sqrt{\lambda_n}C$, which proves the assertion of the proposition. \square

As announced earlier, we consider here not only the threshold ℓ_n^* but also its rescaled version γ_n^* . The rescaling is done in the same way as in Chapter 5, i.e. we switch from the boundary data ℓ_n^* of the deformation to the boundary value γ_n^* of the displacement and additionally scale it with $\sqrt{\lambda_n}$. Together, this reads

$$\gamma_n^*(\omega) := \frac{\ell_n^*(\omega) - 1}{\sqrt{\lambda_n}}.$$

The following theorem gives the limiting behaviour of both, the threshold ℓ_n^* and its rescaled version γ_n^* .

Theorem 7.11. *Let Assumption 7.7 be satisfied. Then, there exists an $\Omega' \subset \Omega$ with $\mathbb{P}(\Omega') = 1$ such that for all $\omega \in \Omega'$ it holds true that*

$$\lim_{n \rightarrow \infty} \gamma_n^*(\omega) = \lim_{n \rightarrow \infty} \frac{\ell_n^*(\omega) - 1}{\sqrt{\lambda_n}} = \sqrt{\frac{\beta}{\underline{\alpha}'}}$$

where $\underline{\alpha}' := \left(\mathbb{E}\left[\frac{1}{\alpha}\right]\right)^{-1}$ and $\beta := \inf\{-J(\omega, \delta(\omega)) : \omega \in \Omega\} = \inf\{-J(\omega, 1) : \omega \in \Omega\}$, with $\alpha(\omega) := \frac{1}{2} \frac{\partial^2 J(\omega, z)}{(\partial z)^2} \Big|_{z=\delta(\omega)}$. Particularly, this yields

$$\lim_{n \rightarrow \infty} \ell_n^*(\omega) = 1.$$

Proof. We drop here the dependence on ω for better readability and define $z_{\text{frac}}^i := z_{\text{frac}}(\tau_i \omega)$ and $J_i(z) := J(\tau_i \omega, z)$. Then, the first, second and third derivative with respect to z are written J_i' , J_i'' and J_i''' in short.

From Propositions 7.3 and 7.10, we get

$$\frac{1}{d} - 1 \leq \gamma_n^* = \frac{\ell_n^* - 1}{\sqrt{\lambda_n}} \leq C,$$

with $C^2 > cb$. This shows that every subsequence of γ_n^* has a convergent subsequence. We define A as its limit and prove the limit to be equal to $\sqrt{\frac{\beta}{\underline{\alpha}'}}$ and thus independent of the subsequence.

Step 1. Proof of $A \leq \sqrt{\frac{\beta}{\underline{\alpha}'}}$.

We prove this by a contradiction argument. Assume that $A > \sqrt{\frac{\beta}{\underline{\alpha}'}}$. Then, for every $\epsilon > 0$ (small enough) there exists $\bar{N} \in \mathbb{N}$ such that

$$\gamma_n^* > \sqrt{\frac{\beta}{\underline{\alpha}'}} + \epsilon \quad \text{for } n > \bar{N}. \quad (7.18)$$

Let $\sigma_n \geq 0$ be such that $\sigma_n < \lambda_n \sqrt{\frac{\beta}{\underline{\alpha}'}} < \sqrt{\lambda_n} \sqrt{\frac{\beta}{\underline{\alpha}'}} < \sqrt{\lambda_n} \sqrt{\frac{\beta}{\underline{\alpha}'}} + \epsilon < \sqrt{\lambda_n} \gamma_n^*$. Then, we obtain

$$\sqrt{\lambda_n} \gamma_n^* - \sigma_n > \sqrt{\lambda_n} \left(\sqrt{\frac{\beta}{\underline{\alpha}'}} + \epsilon - \sqrt{\frac{\beta}{\underline{\alpha}'}} \right) = \sqrt{\lambda_n} \frac{\epsilon}{\sqrt{\frac{\beta}{\underline{\alpha}'}} + \epsilon + \sqrt{\frac{\beta}{\underline{\alpha}'}}} \geq \sqrt{\lambda_n} \frac{\epsilon}{2\sqrt{\frac{\beta}{\underline{\alpha}'}} + \epsilon} \geq \sqrt{\lambda_n} \epsilon C_\epsilon, \quad (7.19)$$

with $C_\epsilon > 0$. Together with Proposition 7.10, this yields

$$1 + \sqrt{\lambda_n} \epsilon C_\epsilon \leq \ell_n^* - \sigma_n \leq 1 + \sqrt{\lambda_n} \bar{C}, \quad (7.20)$$

with a fixed constant $\bar{C} > 0$ fulfilling $\bar{C}^2 > cb$. Let z_n be a minimizer of $M_n^{\text{el}}(\ell_n^* - \sigma_n)$, i.e. $\sum_{i=0}^{n-1} z_n^i = n(\ell_n^* - \sigma_n)$. Further, we define $\bar{z}_n^i := \frac{z_n^i - 1}{\sqrt{\lambda_n}}$, or equivalently $z_n^i = 1 + \sqrt{\lambda_n} \bar{z}_n^i$. Note that this

definition yields $\lambda_n \sum_{i=0}^{n-1} \bar{z}_n^i = \frac{1}{\sqrt{\lambda_n}} (\ell_n^* - \sigma_n - 1) = \gamma_n^* - \sqrt{n}\sigma_n$. Now, we get

$$\begin{aligned} M_n^{\text{el}}(\ell_n^* - \sigma_n) &= \lambda_n \sum_{i=0}^{n-1} J_i \left(1 + \sqrt{\frac{1}{n}} \bar{z}_n^i \right) \\ &= \lambda_n \sum_{i=0}^{n-1} J_i(1) + \lambda_n \sum_{i=0}^{n-1} \frac{1}{2} J_i''(1) \lambda_n (\bar{z}_n^i)^2 + \lambda_n \sum_{i=0}^{n-1} \frac{1}{6} J_i'''(\xi_i) \frac{1}{n^{3/2}} (\bar{z}_n^i)^3 \\ &\stackrel{(*)}{\geq} \lambda_n \sum_{i=0}^{n-1} J_i(1) + \lambda_n \left(\lambda_n \sum_{i=0}^{n-1} \frac{1}{\alpha_i} \right)^{-1} (\gamma_n^* - \sqrt{n}\sigma_n)^2 + \lambda_n \sum_{i=0}^{n-1} \frac{1}{6} J_i'''(\xi_i) \frac{1}{n^{3/2}} (\bar{z}_n^i)^3, \end{aligned} \quad (7.21)$$

with $\xi_i \in [1, 1 + \sqrt{\lambda_n} \bar{z}_n^i]$ and $(*)$ from Lemma 2.24.

Since (7.20) holds true, we can apply Proposition 7.8 (i) with $C = C(n)$ and $\epsilon C_\epsilon \leq C(n) \leq \bar{C}$. We can derive from (7.3) with $\xi_i \in [1, 1 + \sqrt{\lambda_n} \bar{z}_n^i]$

$$c\bar{C}n^{\theta-\frac{1}{2}} \geq J_i' \left(1 + \sqrt{\lambda_n} \bar{z}_n^i \right) \stackrel{(7.1)}{\geq} \frac{1}{c} \sqrt{\lambda_n} \bar{z}_n^i,$$

since $\sqrt{\lambda_n} \bar{z}_n^i \leq \eta$ for n large enough because of the uniform convergence $1 + \sqrt{\lambda_n} \bar{z}_n^i \rightarrow 1$ due to (7.4) in Proposition 7.8 (ii). It follows that

$$\bar{z}_n^i \leq c^2 \bar{C} n^\theta$$

holds true and therefore, with $\kappa_M := c^2 \bar{C} M^{\theta-\frac{1}{2}}$ and $M < n$,

$$\begin{aligned} \lambda_n \sum_{i=0}^{n-1} \frac{1}{6} J_i'''(\xi_i) \frac{1}{n^{3/2}} (\bar{z}_n^i)^3 &\leq \frac{1}{n^{3/2}} \frac{1}{6} (c^2 \bar{C})^3 n^{3\theta} \lambda_n \sum_{i=0}^{n-1} J_i'''(\xi_i) \\ &\leq n^{3\theta-\frac{3}{2}} \frac{1}{6} (c^2 \bar{C})^3 \lambda_n \sum_{i=0}^{n-1} \sup \left\{ |J_i'''(x)|, x \in [1 - \kappa_M, 1 + \kappa_M] \right\} = n^{3\theta-\frac{3}{2}} \frac{1}{6} (c^2 \bar{C})^3 \lambda_n \sum_{i=0}^{n-1} C_i^{\kappa_M}, \end{aligned}$$

with $C_i^{\kappa_M}$ from (H2). From Proposition 5.5 and (H2), we get, for n large enough, the existence of an M^* such that $\lambda_n \sum_{i=0}^{n-1} C_i^{\kappa_{M^*}} \rightarrow \mathbb{E}[C^{\kappa_{M^*}}] < \infty$ as $n \rightarrow \infty$, and thus the sum is also bounded by a constant $\tilde{C} > 0$. Altogether, (7.21) yields, for n large enough,

$$M_n^{\text{el}}(\ell_n^* - \sigma_n) \geq \lambda_n \sum_{i=0}^{n-1} J_i(1) + \lambda_n \left(\lambda_n \sum_{i=0}^{n-1} \frac{1}{\alpha_i} \right)^{-1} (\gamma_n^* - \sqrt{n}\sigma_n)^2 - n^{3\theta-\frac{3}{2}} \frac{1}{6} (c^2 \bar{C})^3 \tilde{C}. \quad (7.22)$$

On the other hand, for n large enough, the competitor $z_n^i := 1$ for $i \geq 1$ and $z_n^0 := n(\sqrt{\lambda_n} \gamma_n^* - \sigma_n) + 1 > z_{\text{frac}}$ satisfies the boundary constraint $\sum_{i=0}^{n-1} z_n^i = n(\ell_n^* - \sigma_n)$ and thus we have

$$\begin{aligned} M_n^{\text{frac}}(\ell_n^* - \sigma_n) &\leq \lambda_n \sum_{i=1}^{n-1} J_i(1) + \lambda_n J_{\hat{I}_n} \left(n(\sqrt{\lambda_n} \gamma_n^* - \sigma_n) + 1 \right) \\ &= \lambda_n \sum_{i=0}^{n-1} J_i(1) + \lambda_n \left(J_{\hat{I}_n} \left(n(\sqrt{\lambda_n} \gamma_n^* - \sigma_n) + 1 \right) - J_{\hat{I}_n}(1) \right) \\ &\leq \lambda_n \sum_{i=0}^{n-1} J_i(1) + \lambda_n \left(\max_{i \in \{0, \dots, n-1\}} |J_i(x_n)| - J_{\hat{I}_n}(1) \right), \end{aligned} \quad (7.23)$$

with $x_n := n(\sqrt{\lambda_n}\gamma_n^* - \sigma_n) + 1 \geq \sqrt{n}C_\epsilon\epsilon$ due to (7.19) and with $\hat{I}_n := \operatorname{argmin}\{-J_i(1) : 0 \leq i \leq n-1\}$.

We combine the results of (7.18), (7.22), (7.23) and $0 < \sigma_n < \lambda_n\sqrt{\frac{\beta}{\alpha}}$ with the fact that γ_n^* is bounded by $C_f > 0$, since it is convergent. This yields for n large enough, together with the definitions $\alpha_n := \left(\lambda_n \sum_{i=0}^{n-1} \frac{1}{\alpha_i}\right)^{-1}$ and $\beta_n := \min\{-J_i(1) : 0 \leq i \leq n-1\}$,

$$\begin{aligned}
& M_n^{\text{el}}(\ell_n^* - \sigma_n) - M_n^{\text{frac}}(\ell_n^* - \sigma_n) \\
& \geq \lambda_n \left(\alpha_n \left((\gamma_n^*)^2 - 2\sqrt{n}\sigma_n\gamma_n^* + n\sigma_n^2 \right) - \frac{1}{6}n^{3\theta-\frac{1}{2}} \left(c^2\bar{C} \right)^3 \tilde{C} - \left(\max_{i \in \{0, \dots, n-1\}} |J_i(x_n)| - J_{\hat{I}_n}(1) \right) \right) \\
& \geq \lambda_n \left(\alpha_n \left(\frac{\beta}{\alpha} + \epsilon \right) - \alpha_n 2\sqrt{n}\lambda_n \sqrt{\frac{\beta}{\alpha}} C_f - \frac{1}{6}n^{3\theta-\frac{1}{2}} \left(c^2\bar{C} \right)^3 \tilde{C} - \beta_n - \max_{i \in \{0, \dots, n-1\}} |J_i(x_n)| \right) \\
& \geq \lambda_n \left(\left(\frac{\alpha_n}{\alpha} - 1 \right) \beta + (\beta - \beta_n) + \alpha_n \epsilon - \frac{2\alpha_n}{\sqrt{n}} \sqrt{\frac{\beta}{\alpha}} C_f - \frac{n^{3\theta-\frac{1}{2}}}{6} \left(c^2\bar{C} \right)^3 \tilde{C} - \max_{i \in \{0, \dots, n-1\}} |J_i(x_n)| \right).
\end{aligned} \tag{7.24}$$

The definition implies $\beta_n(\omega) \leq \beta_n(\omega, x, \epsilon)$, with $\beta_n(\omega, x, \epsilon)$ from (5.28), for every $x \in [0, 1]$. In (5.29), we proved for $\omega \in \Omega'$ that we have $\lim_{n \rightarrow \infty} \beta_n(\omega, x, \epsilon) \leq \beta$. Further, $\beta_n \geq \beta$ also holds true by definition. Together, this yields $\beta_n \rightarrow \beta$ as $n \rightarrow \infty$. Since (H3) yields $\max_{i \in \{0, \dots, n-1\}} |J_i(x_n)| \rightarrow 0$, and it holds true that $3\theta - \frac{1}{2} < 0$ and $\alpha_n \rightarrow \alpha$ by Proposition 5.5 as $N \rightarrow \infty$, we get from (7.24) for n large enough

$$M_n^{\text{el}}(\ell_n^* - \sigma_n) - M_n^{\text{frac}}(\ell_n^* - \sigma_n) > 0,$$

because $\alpha_n \rightarrow \alpha > 0$ and $\epsilon > 0$. This holds true for every $0 \leq \sigma_n < \lambda_n\sqrt{\frac{\beta}{\alpha}}$, and therefore we get $M_n^{\text{el}}(x) > M_n^{\text{frac}}(x)$ for all $x \in \left(\ell_n^* - \lambda_n\sqrt{\frac{\beta}{\alpha}}, \ell_n^*\right]$. This is a contradiction to the definition of ℓ_n^* .

Therefore, the claim is wrong and we obtain $A \leq \sqrt{\frac{\beta}{\alpha}}$.

Step 2. Proof of $A \geq \sqrt{\frac{\beta}{\alpha}}$.

We proof this by a contradiction argument. Assume that $A < \sqrt{\frac{\beta}{\alpha}}$. Then, for every $\epsilon > 0$ (small enough) there exists an $\bar{N} \in \mathbb{N}$ such that

$$\gamma_n^* < \sqrt{\frac{\beta}{\alpha} - \epsilon} \quad \text{for } n > \bar{N},$$

and therefore

$$\ell_n^* < \sqrt{\lambda_n} \sqrt{\frac{\beta}{\alpha} - \epsilon} + 1 =: k_n \quad \text{for } n > \bar{N}. \tag{7.25}$$

Since $\hat{z}_n^i := \sqrt{\frac{\beta}{\alpha} - \epsilon} \left(\lambda_n \sum_{i=0}^{n-1} \frac{1}{\alpha_i} \right)^{-1} \frac{1}{\alpha_i}$ fulfils the boundary condition $\sum_{i=0}^{n-1} \hat{z}_n^i = n\sqrt{\frac{\beta}{\alpha} - \epsilon}$, we get

with $\xi_i \in [1, 1 + \sqrt{\lambda_n \hat{z}_n^i}]$

$$\begin{aligned}
M_n^{\text{el}}(k_n) &\leq \lambda_n \sum_{i=0}^{n-1} J_i \left(1 + \sqrt{\lambda_n \hat{z}_n^i}\right) \\
&= \lambda_n \sum_{i=0}^{n-1} J_i(1) + \lambda_n \sum_{i=0}^{n-1} \frac{1}{2} J_i''(1) \lambda_n \left(\hat{z}_n^i\right)^2 + \lambda_n \sum_{i=0}^{n-1} \frac{1}{6} J_i'''(\xi_i) \frac{1}{n^{3/2}} \left(\hat{z}_n^i\right)^3 \\
&= \lambda_n \sum_{i=0}^{n-1} J_i(1) + \lambda_n \left(\frac{\beta}{\alpha} - \epsilon\right) \alpha_n + \lambda_n \frac{\sqrt{\left(\frac{\beta}{\alpha} - \epsilon\right)^3 \alpha_n^3}}{6} \frac{1}{n^{3/2}} \sum_{i=0}^{n-1} J_i'''(\xi_i) \frac{1}{\alpha_i^3}.
\end{aligned}$$

We already know that $\alpha_n \rightarrow \alpha$ as $n \rightarrow \infty$ for $\omega \in \Omega'$, which yields that α_n is bounded. Further, $\alpha_i^{-1} \leq \hat{C}_\alpha$ for all i by Remark 5.2 (iii). Thus, $\hat{z}_n^i = \sqrt{\frac{\beta}{\alpha} - \epsilon} \alpha_n \frac{1}{\alpha_i}$ is also bounded and therefore $\xi_i \in [1, 1 + \sqrt{\lambda_n C}]$. Using these results, we get, with $\kappa_M := \sqrt{\frac{1}{M} C}$ and $M < n$, that

$$\begin{aligned}
&\lambda_n \frac{\sqrt{\left(\frac{\beta}{\alpha} - \epsilon\right)^3 \alpha_n^3}}{6} \frac{1}{n^{3/2}} \sum_{i=0}^{n-1} J_i'''(\xi_i) \frac{1}{\alpha_i^3} \leq \frac{1}{n^{3/2}} \hat{C} \lambda_n \sum_{i=0}^{n-1} J_i'''(\xi_i) \\
&\leq \frac{1}{n^{3/2}} \hat{C} \lambda_n \sum_{i=0}^{n-1} \sup \{ |J_i'''(x)| : x \in [1 - \kappa_M, 1 + \kappa_M] \} = \frac{1}{n^{3/2}} \hat{C} \lambda_n \sum_{i=0}^{n-1} C_i^{\kappa_M}.
\end{aligned}$$

with $C_i^{\kappa_M}$ from (H2). Again from (H2), we get the existence of an M^* for which it holds true that, together with Proposition 5.5, $\lambda_n \sum_{i=0}^{n-1} C_i^{\kappa_{M^*}} \rightarrow \mathbb{E}[C^{\kappa_{M^*}}] < \infty$. Therefore the sum is also bounded by a constant $\check{C} > 0$. Altogether, this yields for n large enough

$$M_n^{\text{el}}(k_n) \leq \lambda_n \sum_{i=0}^{n-1} J_i(1) + \lambda_n \left(\frac{\beta}{\alpha} - \epsilon\right) \alpha_n + \frac{1}{n^{3/2}} \check{C}. \quad (7.26)$$

On the other hand, we take a minimizer \hat{z}_n^i of $M_n^{\text{frac}}(k_n)$. From Proposition 7.8 (iii), we get the existence of a subsequence (not relabelled) and for every n a corresponding index i_n with

$$\bar{z}_n^{i_n} \rightarrow \infty \quad \text{as } n \rightarrow \infty. \quad (7.27)$$

We define \hat{I}_n as the index i_N for which $\bar{z}_n^{\hat{I}_n} > z_{\text{frac}}^i$. Then, we get

$$\begin{aligned}
M_n^{\text{frac}}(k_n) &= \lambda_n \sum_{i=0}^{n-1} J_i \left(\hat{z}_n^i\right) = \lambda_n \sum_{\substack{i=0 \\ i \neq \hat{I}_n}}^{n-1} J_i \left(\hat{z}_n^i\right) + \lambda_n J_{\hat{I}_n} \left(\hat{z}_n^{\hat{I}_n}\right) \\
&\geq \lambda_n \sum_{\substack{i=0 \\ i \neq \hat{I}_n}}^{n-1} J_i(1) + \lambda_n J_{\hat{I}_n} \left(\hat{z}_n^{\hat{I}_n}\right) = \lambda_n \sum_{i=0}^{n-1} J_i(1) + \lambda_n \left(J_{\hat{I}_n} \left(\hat{z}_n^{\hat{I}_n}\right) - J_{\hat{I}_n}(1) \right).
\end{aligned} \quad (7.28)$$

Altogether, (7.26) and (7.28) yield

$$\begin{aligned}
M_n^{\text{frac}}(k_n) - M_n^{\text{el}}(k_n) &\geq \lambda_n \left(J_{\hat{I}_n}(\bar{z}_n^{\hat{I}_n}) - J_{\hat{I}_n}(1) - \left(\frac{\beta}{\underline{\alpha}} - \epsilon \right) \alpha_n - \frac{1}{n^{1/2}} \tilde{C} \right) \\
&\geq \lambda_n \left(J_{\hat{I}_n}(\bar{z}_n^{\hat{I}_n}) + \beta_n - \left(\frac{\beta}{\underline{\alpha}} - \epsilon \right) \alpha_n - \frac{1}{n^{1/2}} \tilde{C} \right) \\
&= \lambda_n \left(J_{\hat{I}_n}(\bar{z}_n^{\hat{I}_n}) + (\beta_n - \beta) + \left(1 - \frac{\alpha_n}{\underline{\alpha}} \right) \beta + \epsilon \alpha_n - \frac{1}{n^{1/2}} \tilde{C} \right).
\end{aligned} \tag{7.29}$$

Assumption (H3) together with (7.27) yields $J_{\hat{I}_n}(\bar{z}_n^{\hat{I}_n}) \rightarrow 0$. Since $\alpha_n \rightarrow \underline{\alpha} > 0$ and $\beta_n \rightarrow \beta$ as $n \rightarrow \infty$ for $\omega \in \Omega'$ (c.f. Step 1), we get from (7.29) for n large enough

$$M_n^{\text{frac}}(k_n) - M_n^{\text{el}}(k_n) > 0.$$

This is a contradiction to the definition of ℓ_n^* , because we know from (7.25) that $k_n > \ell_n^*$ and therefore ℓ_n^* is not the supremum. Therefore, the claim is wrong and we obtain $A \geq \sqrt{\frac{\beta}{\underline{\alpha}}}$.

Step 3. Conclusion.

All in all, we have shown that for each subsequence there is a convergent subsequence (not relabelled) such that

$$\gamma_n^* := \frac{\ell_n^* - 1}{\sqrt{\lambda_n}} \rightarrow \sqrt{\frac{\beta}{\underline{\alpha}}} \quad \text{as } n \rightarrow \infty.$$

Since the limit is independent of the chosen subsequence, the hole sequence converges. This especially yields

$$\ell_n^* \rightarrow 1 \quad \text{as } n \rightarrow \infty.$$

□

7.3.2 Fully random potentials

From now on, we drop the assumption $\delta(\omega) = 1$ for all $\omega \in \Omega$ and allow for arbitrary values of $\delta(\omega)$. In this case, we cannot recover the full Theorem 7.11, but part of it. The next theorems shows us the limiting behaviour of the jump threshold ℓ_n^* .

Theorem 7.12. *Let Assumption 7.7 be fulfilled. Then, there exists an $\Omega' \subset \Omega$ with $\mathbb{P}(\Omega') = 1$ such that for all $\omega \in \Omega'$ it holds true that*

$$\lim_{n \rightarrow \infty} \ell_n^*(\omega) = \mathbb{E}[\delta].$$

Proof. We drop here the dependence on ω for a better readability and define $z_{\text{frac}}^i := z_{\text{frac}}(\tau_i \omega)$ and $J_i(z) := J(\tau_i \omega, z)$. Then, we can use the short form J_i' , J_i'' and J_i''' for the first, second and third derivative with respect to z .

Due to Proposition 7.3, ℓ_n^* is bounded and therefore every subsequence of ℓ_n^* has a convergent subsequence (not relabelled). We define A as its limit and prove the limit to be equal to $\mathbb{E}[\delta]$ and thus independent of the subsequence.

Step 1. Proof of $A \leq \mathbb{E}[\delta]$.

We proof this by a contradiction argument. Assume that $A > \mathbb{E}[\delta]$. Then, for every $\epsilon > 0$ (small enough) there exists $\hat{N} \in \mathbb{N}$ such that

$$\ell_n^* > \mathbb{E}[\delta] + 2\epsilon \quad \text{for } n > \hat{N}.$$

Further, we know that $\lambda_n \sum_{i=0}^{n-1} \delta_i \rightarrow \mathbb{E}[\delta]$ and therefore there exists for every $\epsilon > 0$ (small enough) an $\tilde{N} \in \mathbb{N}$ such that

$$\left| \lambda_n \sum_{i=0}^{n-1} \delta_i - \mathbb{E}[\delta] \right| < \epsilon \quad \text{for } n > \tilde{N}.$$

Together, this yields for $\bar{N} := \max\{\hat{N}, \tilde{N}\}$

$$\ell_n^* > \lambda_n \sum_{i=0}^{n-1} \delta_i + \epsilon \quad \text{for } n > \bar{N}. \quad (7.30)$$

Let $\sigma \geq 0$ with $\sigma < \epsilon$. Let z_n be a minimizer of $M_n^{\text{el}}(\ell_n^* - \sigma)$. We set

$$I_n := \left\{ i \in \{0, \dots, n-1\} : z_n^i > \delta_i + \epsilon \right\}.$$

It is $0 \leq \#I_n \leq n$ and therefore $0 \leq \#I_n/n \leq 1$. Further, it holds true that $\#I_n/n \rightarrow \Lambda$ as $n \rightarrow \infty$, for some $\Lambda > 0$. This can be seen by a contradiction argument. Assume $\#I_n/n \rightarrow 0$. Then the upper bound of the fracture points by $z_{\text{frac}}^{\text{sup}}$ from Proposition 7.2 (iii) yields

$$\begin{aligned} \mathbb{E}[\delta] + 2\epsilon - \sigma < \ell_n^* - \sigma &= \frac{1}{n} \sum_{i=0}^{n-1} z_n^i = \frac{1}{n} \sum_{i \in I_n} z_n^i + \frac{1}{n} \sum_{i \notin I_n} z_n^i \\ &\leq \frac{1}{n} \#I_n z_{\text{frac}}^{\text{sup}} + \frac{1}{n} \sum_{i \notin I_n} (\delta_i + \epsilon) = \frac{1}{n} \#I_n z_{\text{frac}}^{\text{sup}} + \frac{1}{n} \sum_{i \notin I_n} \delta_i + \left(1 - \frac{\#I_n}{n}\right) \epsilon. \end{aligned} \quad (7.31)$$

We further have

$$\frac{1}{n} \sum_{i \notin I_n} \delta_i = \frac{1}{n} \sum_{i=0}^{n-1} \delta_i - \frac{1}{n} \sum_{i \in I_n} \delta_i \rightarrow \mathbb{E}[\delta] + 0,$$

because of the boundedness of δ_i and the assertion $\#I_n/n \rightarrow 0$. With this, we get from (7.31), as $n \rightarrow \infty$,

$$\mathbb{E}[\delta] + 2\epsilon - \sigma \leq 0 + \mathbb{E}[\delta] + \epsilon,$$

which is a contradiction to $\sigma < \epsilon$, and therefore $\#I_n/n \rightarrow \Lambda > 0$ as $N \rightarrow \infty$ holds true.

Now, we can estimate, with J'_i being positive on $[\delta_i, z_{\text{frac}}^i]$ (see Proposition 7.2 (ii)) and with $\xi_i \in [\delta_i, \delta_i + \epsilon]$,

$$M_n^{\text{el}}(\ell_n^* - \sigma) = \lambda_n \sum_{i \in I_n} J_i(z_n^i) + \lambda_n \sum_{i \notin I_n} J_i(z_n^i) \geq \lambda_n \sum_{i \in I_n} J_i(\delta_i + \epsilon) + \lambda_n \sum_{i \notin I_n} J_i(\delta_i)$$

$$\begin{aligned}
&= \lambda_n \sum_{i \in I_n} \left(J_i(\delta_i) + \alpha_i \epsilon^2 + \frac{J_i'''(\xi_i)}{6} \epsilon^3 \right) + \lambda_n \sum_{i \notin I_n} J_i(\delta_i) \\
&\stackrel{(*)}{\geq} \lambda_n \sum_{i=0}^{n-1} J_i(\delta_i) + \hat{C} C_\alpha \epsilon^2 - \lambda_n \sum_{i=0}^{n-1} \frac{|J_i'''(\xi_i)|}{6} \epsilon^3 \stackrel{(H2)}{\geq} \lambda_n \sum_{i=0}^{n-1} J_i(\delta_i) + \hat{C} C_\alpha \epsilon^2 - \lambda_n \sum_{i=0}^{n-1} \frac{C_i^\epsilon}{6} \epsilon^3,
\end{aligned}$$

where in $(*)$ we used $\alpha_i \geq C_\alpha$ from Remark 5.2 (iii) and $\#I_n/n \geq \hat{C} > 0$, for n large enough and with $\hat{C} < \Lambda$, because of $\#I_n/n \rightarrow \Lambda > 0$. Due to (H2), we have $\lambda_n \sum_{i=0}^{n-1} C_i^\epsilon \rightarrow \mathbb{E}[C^{\epsilon^*}] \leq \tilde{C}$ for some ϵ^* small enough. This yields, for all $\omega \in \Omega'$,

$$\begin{aligned}
M_n^{\text{el}}(\ell_n^* - \sigma) &\geq \lambda_n \sum_{i=0}^{n-1} J_i(\delta_i) + \hat{C} C_\alpha \epsilon^2 - \lambda_n \sum_{i=0}^{n-1} \frac{C_i^\epsilon}{6} \epsilon^3 \\
&\rightarrow \mathbb{E}[J(\delta)] + \hat{C} C_\alpha \epsilon^2 - \frac{\tilde{C}}{6} \epsilon^3 = \mathbb{E}[J(\delta)] + \epsilon^2 \left(\hat{C} C_\alpha - \frac{\tilde{C}}{6} \epsilon \right) \geq \mathbb{E}[J(\delta)] + \epsilon^2 C,
\end{aligned}$$

for $C > 0$ and ϵ small enough.

On the other hand, for n large enough, the competitor $z_n^i := \delta_i$ for $i \geq 1$ and $z_n^0 := n(\ell_n^* - \sigma) - \left(\sum_{i=0}^{n-1} \delta_i \right) + \delta_0$ satisfies the boundary constraint $\sum_{i=0}^{n-1} z_n^i = n(\ell_n^* - \sigma)$ and thus we have

$$\begin{aligned}
M_n^{\text{frac}}(\ell_n^* - \sigma) &\leq \lambda_n \sum_{i=1}^{n-1} J_i(\delta_i) + \lambda_n J_0 \left(n(\ell_n^* - \sigma) - \left(\sum_{i=0}^{n-1} \delta_i \right) + \delta_0 \right) \\
&= \lambda_n \sum_{i=0}^{n-1} J_i(\delta_i) + \lambda_n \left(J_0 \left(n(\ell_n^* - \sigma) - \left(\sum_{i=0}^{n-1} \delta_i \right) + \delta_0 \right) - J_0(\delta_0) \right) \\
&\rightarrow \mathbb{E}[J(\delta)] + 0,
\end{aligned}$$

since we have $n \left(\ell_n^* - \sigma - \lambda_n \sum_{i=0}^{n-1} \delta_i \right) \geq n(\epsilon - \sigma)$ for n sufficiently large, due to (7.30), combined with (LJ3). Together, this shows that for n large enough,

$$M_n^{\text{frac}}(\ell_n^* - \sigma) < M_n^{\text{el}}(\ell_n^* - \sigma),$$

for every $0 \leq \sigma < \epsilon$, and therefore we obtain $M_n^{\text{el}}(x) > M_n^{\text{frac}}(x)$ for all $x \in (\ell_n^* - \epsilon, \ell_n^*]$. This is a contradiction to the definition of ℓ_n^* . Therefore, the claim is wrong and the assertion $A \leq \mathbb{E}[\delta]$ is proven.

Step 2. Proof of $A \geq \mathbb{E}[\delta]$.

We prove this by a contradiction argument. Assume that $A < \mathbb{E}[\delta]$. Then, for every $\epsilon > 0$ (small enough) there exists an $\hat{N} \in \mathbb{N}$ such that for all $n > \hat{N}$

$$\ell_n^* < \lambda_n \sum_{i=0}^{n-1} \delta_i - \epsilon =: k_n. \quad (7.32)$$

Assume z_n^i to be a minimizer of $M_n^{\text{frac}}(k_n)$ fulfilling the constraint $\sum_{i=0}^{n-1} z_n^i = nk_n$ and define the set $\hat{I}_n := \{i \in \{0, \dots, n-1\} : z_n^i > z_{\text{frac}}^i\}$. By definition of M_n^{frac} , the set \hat{I}_n is not empty. Now, we introduce $\gamma_i \geq 0$ such that the following conditions are satisfied:

- (i) $z_n^i + \gamma_i \leq \delta_i$ if $z_n^i \leq \delta_i$,

(ii) $\gamma_i = 0$ if $z_n^i > \delta_i$,

(iii) $\sum_{i=0}^{n-1} \gamma_i = \sum_{i \in \hat{I}_n} (z_n^i - \delta_i)$.

Especially, this definition yields $\gamma_i = 0$ for $i \in \hat{I}_n$. The well-posedness of the conditions for γ_i can be proven by showing that (ii) and (iii) allow for (i). Set $\check{I}_n := \{i \in \{0, \dots, n-1\} : z_n^i \leq \delta_i\}$. From (7.32), we get

$$\frac{1}{n} \sum_{i=0}^{n-1} \delta_i - \epsilon = k_n = \frac{1}{n} \sum_{i=0}^{n-1} z_n^i \Leftrightarrow \frac{1}{n} \sum_{i=0}^{n-1} (\delta_i - z_n^i) = \epsilon,$$

and with this

$$\begin{aligned} \frac{1}{n} \sum_{i \in \check{I}_n} (\delta_i - z_n^i) &= \frac{1}{n} \sum_{i \in \hat{I}_n} (z_n^i - \delta_i) + \frac{1}{n} \sum_{i \notin (\hat{I}_n \cup \check{I}_n)} (z_n^i - \delta_i) + \epsilon \geq \frac{1}{n} \sum_{i \in \hat{I}_n} (z_n^i - \delta_i) \\ &\stackrel{(iii)}{=} \frac{1}{n} \sum_{i=0}^{n-1} \gamma_i \stackrel{(ii)}{\geq} \frac{1}{n} \sum_{i \in \hat{I}_n} \gamma_i, \end{aligned}$$

since $\epsilon > 0$ and $z_n^i - \delta_i > 0$ for $i \notin (\hat{I}_n \cup \check{I}_n)$. This shows (i) and therefore γ_i with the required properties exist. With this, we now define

$$\bar{z}_n^i := \begin{cases} \delta_i & \text{for } i \in \hat{I}_n, \\ z_n^i + \gamma_i & \text{else.} \end{cases}$$

The constraint is still fulfilled, since

$$\begin{aligned} \frac{1}{n} \sum_{i=0}^{n-1} \bar{z}_n^i &= \frac{1}{n} \left(\sum_{i \in \hat{I}_n} \delta_i + \sum_{i \notin \hat{I}_n} (z_n^i + \gamma_i) \right) = \frac{1}{n} \sum_{i \in \hat{I}_n} \delta_i + \frac{1}{n} \sum_{i=0}^{n-1} (z_n^i + \gamma_i) - \frac{1}{n} \sum_{i \in \hat{I}_n} z_n^i \\ &= \frac{1}{n} \sum_{i \in \hat{I}_n} (\delta_i - z_n^i) + \frac{1}{n} \sum_{i=0}^{n-1} \gamma_i + k_n = k_n, \end{aligned}$$

and it holds true that

$$\lambda_n \sum_{i=0}^{n-1} J_i(z_n^i) > \lambda_n \sum_{i=0}^{n-1} J_i(\bar{z}_n^i),$$

since J_i is strictly decreasing on $(z_{\text{dom}}, \delta_i]$ due to (LJ2). By construction, it holds true that $\bar{z}_n^i \leq z_{\text{frac}}^i$ for all $i = 0, \dots, n-1$ and therefore we have

$$M_n^{\text{frac}}(k_n) = \lambda_n \sum_{i=0}^{n-1} J_i(z_n^i) > \lambda_n \sum_{i=0}^{n-1} J_i(\bar{z}_n^i) \geq M_n^{\text{el}}(k_n).$$

This shows

$$M_n^{\text{frac}}(k_n) - M_n^{\text{el}}(k_n) > 0,$$

which is a contradiction to the definition of ℓ_n^* , because we know from (7.32) that $k_n > \ell_n^*$ holds true and therefore ℓ_n^* is not the supremum. Therefore, the claim is wrong and we have $A \geq \mathbb{E}[\delta]$.

Step 3. Conclusion.

All in all, we have shown that for each subsequence there is a convergent subsequence (not relabelled) such that

$$\ell_n^* \rightarrow \mathbb{E}[\delta] \quad \text{as } n \rightarrow \infty.$$

Since the limit is independent of the chosen subsequence, the whole sequence converges to $\mathbb{E}[\delta]$. \square

7.4 Comparison to Γ -convergence results

In the previous sections, we have established the limit of the jump threshold in Theorem 7.12 and 7.11. The results are only valid under stricter assumptions than those imposed for the Γ -limit in Theorem 4.14 and 5.8. In particular, the stronger assumptions are (LJ6)–(LJ9), and in Theorem 7.11 the additional assumption is $\delta(\omega) = 1$ for all $\omega \in \Omega$. Nevertheless, we compare here the results of the discrete fracture jump threshold with the results of the Γ -limits of zeroth order and of the rescaled case.

The Γ -limit of zeroth order, Theorem 4.14, is finite for $u \in BV^\ell(0, 1)$ with $D^s u \geq 0$ and reads

$$E_{\text{hom}}^\ell(u) = \int_0^1 J_{\text{hom}}(u'(x)) \, dx.$$

Moreover, the theorem yields us information about the minimum values. They can be calculated as

$$\min_u E_{\text{hom}}^\ell(u) = J_{\text{hom}}(\ell) = \begin{cases} J_{\text{hom}}(\ell) & \text{for } \ell < \mathbb{E}[\delta], \\ J_{\text{hom}}(\mathbb{E}[\delta]) & \text{for } \ell \geq \mathbb{E}[\delta]. \end{cases}$$

According to this, the threshold where the elastic and the jump regimes are separated is $\mathbb{E}[\delta]$. This exactly corresponds to the result of Theorem 7.12, which says that the fracture threshold ℓ_n^* converges to the same value, i.e.

$$\ell_n^*(\omega) \rightarrow \mathbb{E}[\delta] \quad \text{as } n \rightarrow \infty.$$

Even in the rescaled case, the results are in good compliance. The Γ -limit of the rescaled energy in the $\sqrt{\lambda_n}$ -scaling is given in Theorem 5.8. The energy is finite for $v \in SBV_c^\gamma(0, 1)$ and reads

$$E^\gamma(v) = \alpha \int_0^1 |v'(x)|^2 \, dx + \beta \#S_v.$$

Again, the theorem gives the minima of the energy. For $\gamma > 0$, they are given by

$$\min_v E^\gamma(v) = \min\{\alpha\gamma^2, \beta\} = \begin{cases} \alpha\gamma^2 & \text{if } \gamma < \sqrt{\frac{\beta}{\alpha}}, \\ \beta & \text{if } \gamma \geq \sqrt{\frac{\beta}{\alpha}}. \end{cases}$$

This shows us the threshold between elasticity and fracture in the rescaled case. In fact, the value $\sqrt{\frac{\beta}{\alpha}}$ divides the region into elastic behaviour and the regime where cracks occur. The rescaled

fracture threshold γ_n^* , which arises from ℓ_n^* by the same $\sqrt{\lambda_n}$ -rescaling in the same way than the rescaled energy, provides the same information. Theorem 7.11 shows that

$$\gamma_n^*(\omega) = \frac{\ell_n^*(\omega) - 1}{\sqrt{\lambda_n}} \rightarrow \sqrt{\frac{\beta}{\underline{\alpha}}} \quad \text{as } n \rightarrow \infty.$$

The techniques, by which the results for the threshold are calculated, are completely different. While the Γ -limits from Chapter 4 and Chapter 5 are derived within the variational framework of Γ -convergence, the theorems in this chapter are based only on convergence in the real numbers. Nevertheless, they yield the same threshold that divides the elastic and the fracture regime of the chain.

The Γ -limit of course specifies the limiting energy functional and gives information about the minimizers. None of this is so far achieved in the framework of this chapter. It remains an open problem whether it is possible to recover the same results as those of the Γ -limits.

8 Outlook

As closing remarks we outline some ideas of possible extensions of the results of this thesis. The most obvious generalisation is to consider higher dimensions. All results in this thesis are stated and proven in the one-dimensional setting. Difficulties in dimensions higher than one are a proper definition of K interacting particles and even more technical estimates. Most likely the properties of the interaction potentials have to be adjusted in order to achieve compactness, cf. [35, page 3].

Furthermore, one can think of extending the K -interacting neighbours to interactions where each particle interacts with each other particle. This could be done by an additional limiting procedure, where K tends to infinity, which is an open problem even in the homogeneous case. Another possible reformulation would be considering other approaches to the random setting, like working with stochastic lattices, cf. [4], instead of the stochastic interaction potentials that we have chosen. It would be interesting to analyse whether the results in the continuum limit coincide.

In the variational limit of the energy in Chapter 4, the energy density of the limiting functional is given by the asymptotic homogenization formula J_{hom} . In Proposition 4.13, some additional properties of this function have been worked out, but only in the case $K = 1$. It would be interesting to study, whether one can derive similar results in the case $K > 1$. This will make the proof even more technical and would supposedly be only possible by imposing further assumptions on the Lennard-Jones type potentials.

In Chapter 5, the rescaled energy is discussed in the case of only nearest neighbour interactions, i.e. $K = 1$. In the case of $K > 1$, surface terms are a part of the limiting energy. To this end one has to choose carefully the right amount of boundary data of the discrete energy, because this influences the exact representation of the jump and the boundary layer energies in the limit, see, e.g., [34, 101] for corresponding work in the homogeneous setting. Further, it would be of interest to search for special cases which yield existence of the first order Γ -limit and would allow to understand its limitations in more detail, cf. the end of Chapter 5.

Chapter 7 deals with the new ansatz for fracture in the discrete setting, where the fracture point z_{frac} of a potential is defined in such a way that values of the discrete gradient of the deformation above z_{frac} are considered as jumps. The limiting analysis of the fracture threshold ℓ_n^* as well as of the rescaled fracture threshold γ_n^* is so far restricted to the case $K = 1$. An extension to K interacting neighbours, with $K > 1$, would be desirable. Moreover, the rescaled fracture threshold was only derived under the assumption that all potentials have the same minimizer. It would be interesting to see, whether the same result holds true without this condition. We established the fracture point z_{frac} by means of the second derivative and showed that, with this choice, ℓ_n^* leads to a threshold between the elastic and fracture regime in the continuum that is identical to the one obtained by Γ -convergence. An immediate question would be if also other definitions and choices of such a fracture point yield comparable or even identical results. In the stochastic setting, another task is to derive convergence rates and fluctuation of the fracture threshold, especially regarding probabilities for fracture in the discrete problem. Furthermore, it is also of interest, to consider pointwise convergence of the energy minimization problems, involving the fracture point, and to see whether the outcome is related to the Γ -limit results.

List of assumptions

Assumptions for the variational limit.

Assumption on the Lennard-Jones type potentials, page 27.

Fix $\alpha \in (0, 1]$, $b > 0$, $d \in [1, +\infty)$ and a convex function $\Psi : \mathbb{R} \rightarrow [0, +\infty]$ satisfying

$$\lim_{z \rightarrow 0^+} \Psi(z) = +\infty.$$

We denote by $\mathcal{J} = \mathcal{J}(\alpha, b, d, \Psi)$ the class of functions $J : \mathbb{R} \rightarrow \mathbb{R} \cup \{+\infty\}$ which satisfies the following properties:

(LJ1) (Regularity and asymptotic decay) The function J is lower semicontinuous, $J \in C_{loc}^{0,\alpha}(0, \infty)$ and

$$\lim_{z \rightarrow 0^+} J(z) = \infty \quad \text{as well as} \quad J(z) = \infty \quad \text{for } z \leq 0.$$

(LJ2) (Convex bound, minimum and minimizer) J has a unique minimizer δ with $\delta \in (\frac{1}{d}, d)$ and $J(\delta) < 0$, and J is strictly convex on $(0, \delta)$. Moreover, $\|J\|_{L^\infty(\delta, \infty)} < b$ and it holds

$$\frac{1}{d}\Psi(z) - d \leq J(z) \leq d \max\{\Psi(z), |z|\} \quad \text{for all } z \in (0, +\infty).$$

(LJ3) (Asymptotic behaviour) It holds

$$\lim_{z \rightarrow \infty} J(z) = 0.$$

Assumption on the random variable, page 30.

(H1) (Hölder coefficient) For every $j = 1, \dots, K$ it holds true that $\mathbb{E} \left[[J_j]_{C^{0,\alpha}(\delta_j, +\infty)} \right] < \infty$.

Assumptions for the rescaled model.

Assumption on the Lennard-Jones type potentials, page 87.

Fix $\alpha \in (0, 1]$, $b > 0$, $d \in [1, +\infty)$ and a convex function $\Psi : \mathbb{R} \rightarrow [0, +\infty]$ as above. Further, fix $\eta > 0$ and $c > 0$. We denote by $\mathcal{J}_{\text{reg}} = \mathcal{J}_{\text{reg}}(\alpha, b, c, d, \Psi, \eta)$ the class of functions $J : \mathbb{R} \rightarrow \mathbb{R} \cup \{+\infty\}$ which satisfy the properties (LJ1)–(LJ3) and additionally the following properties:

(LJ4) (Regularity) It is $J \in C^3$ on its domain.

(LJ5) (Harmonic approximation near ground state) For $|z - \delta| < \eta$, it holds true that

$$J(z) - J(\delta) \geq \frac{1}{c}(z - \delta)^2.$$

Assumption on the random variable, page 89.

(H2) (Third derivative near ground state) It exists $0 < \kappa^* < \frac{1}{d} - z_{\text{dom}}$ such that $\mathbb{E}[C^{\kappa^*}] < \infty$. As a direct consequence, it also holds true that $\mathbb{E}[C^\kappa] < \infty$ for every $\kappa < \kappa^*$, by definition of C^κ .

(H3) (Uniform convergence of the asymptotic decay) It holds true that

$$\lim_{z \rightarrow \infty} \max_{\omega \in \Omega} |J(\omega, z)| = 0.$$

Assumptions for fracture in the discrete.

Assumption on the Lennard-Jones type potentials, page 132.

Fix $\alpha \in (0, 1]$, $b > 0$, $c > 0$, $d \in [1, +\infty)$, $\eta > 0$, and a convex function $\Psi : \mathbb{R} \rightarrow [0, +\infty]$ as above. We denote by $\tilde{\mathcal{J}}_{\text{curv}} = \tilde{\mathcal{J}}_{\text{curv}}(\alpha, b, c, d, \Psi, \eta)$ the class of functions $J : \mathbb{R} \rightarrow \mathbb{R} \cup \{+\infty\}$ which satisfy the properties (LJ1)–(LJ5), and additionally the following properties:

(LJ6) It holds true that $z_{\text{frac}} - \delta \geq \frac{1}{b}$.

(LJ7) It holds true that $m_{\text{frac}} - J(\delta) \geq \frac{1}{b}$.

(LJ8) It holds true that

$$\inf \left\{ \frac{\partial^2 J(z)}{\partial z^2} : z \in [\delta, \delta + \eta] \right\} \geq \frac{1}{c}.$$

(LJ9) It holds true that

$$\sup \left\{ \frac{\partial^2 J(z)}{\partial z^2} : z \in [\delta, \delta + \eta] \right\} \leq c.$$

The class $\mathcal{J}_{\text{curv}} = \mathcal{J}_{\text{curv}}(\alpha, b, c, d, \Psi, \eta)$ is defined in the same way as $\tilde{\mathcal{J}}_{\text{curv}}(\alpha, b, c, d, \Psi, \eta)$, but without assumption (LJ9).

Assumption on the random variable, page 132.

(H4) Fix $0 \leq \theta < \frac{1}{6}$. Then it holds true that

$$\sup \left\{ \frac{\partial^2 J}{(\partial z)^2}(\tau_i \omega, z) : z \in [\delta(\tau_i \omega), \delta(\tau_i \omega) + \eta], \omega \in \Omega, i \in \{0, \dots, n-1\} \right\} \leq cn^\theta.$$

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Acknowledgement

First of all, I would like to express my gratitude to my supervisor **Anja Schlömerkemper**. I really liked to be part of her team and join in this interesting field of mathematics. I appreciate all the fruitful discussions with her, scientifically as well as advisory. In addition, I really value her support and her care. I want to say thank you for this great opportunity.

Further, I want to thank my collaborators and co-authors **Stefan Neukamm** and **Mathias Schäffner**. During my research stays at TU Dresden I joined the working group of Stefan Neukamm and had the chance for stimulating discussions with his team members, Mathias Schäffner and himself. Especially, I am very grateful for several invitations and the kind hospitality of Stefan Neukamm to the TU Dresden.

I also want to say thank you to **Martin Kružík** for his invitation to the Academy of Sciences of the Czech Republic. I really enjoyed my time there, from his hospitality and the scientific discussions to his cultural recommendations in this great city.

It was a pleasure for me to visit **Barbara Zwicknagl** at the Humboldt-Universität zu Berlin. I am very grateful for the opportunity to present my work in the Langenbach seminar. Moreover, I appreciated her great hospitality and her guided tour to enjoyable and extraordinary places.

I would like to express my special thanks to my friend and colleague **Joshua Kortum**, who was the best office partner one could wish for. He was not only offering constantly support in scientific questions and helpful discussions, but also he understood the importance of coffee in the morning and unicorns in the office.

Moreover, I enjoyed the time together with my colleagues and friends of the working group. Not only during office time, but also in the evenings, you have been a great community. Especially, I really liked the enjoyable coffee breaks and the visits of Hasenstall together with **Martin Kalousek**. Furthermore, I appreciated the companionship of **Francesco De Anna** to various Marvel and DC movies (I know, you are not going to watch another one), and of course, his cheesecake.

I am very grateful to all of my colleagues and friends, who have spent time for proofreading my thesis: **Joshua Kortum, Martin Kalousek, Jan Scherz, Manuel Schrauth** and **Julian Schrauth**.

Of course, I also want to say thank you to all of my friends and colleagues at the Institute of Mathematics. I had a great time there and this would not have been the case without you. Especially I enjoyed the ongoing and timeless contributions of **Sandra Warnecke** and **Lukas Berberich** to the Word of the Week committee, the support of **Jonas Berberich** with coffee and scientific, computing, teaching and entertaining news, and last but not least, **Marc Herrmann** for his contributions to a pleasant atmosphere by joint and enjoyable coffee breaks and the pink (and not so pretty) unicorn.