Discrete-to-continuum limits for thin rods undergoing elastic deformation or brittle fracture

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Abstract:
Starting from a crystalline lattice with short-range interactions between particles, continuum models are derived for the bending, torsion or brittle fracture of inextensible rods moving in three-dimensional space.

In the derivation, limits of the rod thickness and interatomic distance simultaneously tending to zero are studied. If the two quantities are of the same order of magnitude, this leads to a novel theory for ultrathin rods composed of finitely many atomic fibres, which incorporates surface energy and new discrete terms in the limiting functional.

Further, in the elastic-brittle case, fracture energy in the Γ-limit is expressed by an implicit cell formula, which covers different modes of fracture, including (complete) cracks, folds and torsional cracks. In special cases, the cell formula can be significantly simplified. Our approach applies for example to atomistic systems with Lennard-Jones-type potentials and is motivated by the research of ceramic nanowires.

Keywords: discrete-to-continuum limits, dimension reduction, elastic rod theory, brittle materials, Γ-convergence, variational fracture, atomistic models, nanowires

This doctoral thesis was written during times of increasing concern about human-induced global climate change. If humanity fails to prevent the rise in global mean temperature to 2°C above pre-industrial levels, we can expect a significant increase in extreme weather events, harmful changes in ecosystems that we rely on, impactful reduction of crop yields, and negative consequences on people's health[1]. In our society, scientists should give a lead on taking conclusions of trustworthy research studies seriously. If you are reading these lines, consider supporting relevant NGOs or initiatives, such as the Alliance of World Scientists[2] or Scientists for Future[3].

[1] O. Hoegh-Guldberg et al. Impacts of 1.5°C Global Warming on Natural and Human Systems. In V. Masson-Delmotte et al., editors, *IPCC Special Report on Global Warming of 1.5°C*. Cambridge University Press, 2018.

[2] `https://scientistswarning.forestry.oregonstate.edu`

[3] `https://scientists4future.org`

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To the Creator of the universe,
who inspires our humble attempts
for scientific exploration and progress

Contents

1. Introduction and motivation

Without much doubt, nanotechnology ranked among paradigm-shifting and the fastest growing research areas of the last 30 years and influenced our lives in multiple different ways. To name one example, the versatility and high performance of latest smartphones derives from advanced computer chips, which contain billions of nanoscale transistors.

The mechanical response of engineered nanoworld objects differs so much from macroscopic bodies (e.g. because of size or structure effects) that new models and simulation methods are still being developed, to efficiently enhance the grasp gained by intricate laboratory measurements. In particular, there exist rod-like structures in nanoengineering which are long enough in one direction for continuum theories to be applicable, but in the perpendicular direction, they have a diameter on the scale of tens to hundreds (occasionally even units) of atoms.

This thesis tries to contribute to the subject of *mechanical modelling of nanowires*, benefiting from variational formulations of problems in elasticity theory. Passing from a discrete atomistic model to a continuum one by means of Γ-convergence seems to be a promising method for the derivation of phenomenological models which retain important physical features of the microscopic description, but also include all the mathematical precision needed for further mathematical analysis and/or the design of numerical schemes. For this intent, the thesis topic specifically draws inspiration from three paths of research in applied mathematical analysis which are:

(DR) rigorous derivation of elasticity theories for thin structures (often referred to as *dimension reduction*);

(D-C) discrete-to-continuum limits;

(F) fracture mechanics.

The purpose of the following sections of this introduction is to briefly survey research fields related to **(DR)**, **(D-C)** and **(F)**, in order to give the necessary background and motivation.

1.1 Γ-convergence

An important tool in all three branches **(DR)**, **(D-C)** and **(F)** is Γ-convergence (see [Bra02, Bra06] for an introduction). This mode of convergence was designed by De Giorgi in the 1970s for parametrized families of variational problems, i.e. if E_ε are functionals defined on some metric space X, we may consider the problems

$$\text{find } y \text{ such that } \min_{x\in X} E_\varepsilon(x) = E_\varepsilon(y)$$

depending on a parameter ε.

Definition 1.1.1. *Let* (X,d) *be a metric space. We say that the family* $(E_\varepsilon)_{\varepsilon>0}$, $E_\varepsilon\colon X \to \bar{\mathbb{R}} := \mathbb{R} \cup \{-\infty,+\infty\}$, Γ-converges *in* X *to* $E_0\colon X \to \bar{\mathbb{R}}$ *if for all* $y \in X$ *and all* $\varepsilon_k \to 0$ *we have*

(i) (lower bound) *for every sequence* (y_{ε_k}) *converging to* y

$$E_0(y) \le \liminf_{k\to\infty} E_{\varepsilon_k}(y_{\varepsilon_k});$$

(ii) (existence of a recovery sequence) *there exists a sequence* (y_{ε_k}) *converging to* y *such that*

$$E_0(y) = \lim_{k\to\infty} E_{\varepsilon_k}(y_{\varepsilon_k}).$$

The function E_0 *is called the* Γ*-limit of* (E_ε)*, and we write this fact as* $E_\varepsilon \xrightarrow{\Gamma} E_0$ *or* $E_0 = \Gamma\text{-}\lim_\varepsilon E_\varepsilon$.

In mechanics for instance, E_ε can have the meaning of elastic or interaction energy in a deformable solid or a particle system, respectively.

A distinctive property of Γ-convergence is that together with a *compactness condition*, it ensures the *convergence of* (approximative, global) *minimizers* of the parent problems as $\varepsilon \to 0$ to minimizers of the limiting problem. Thus certain important information is preserved in the effective problem and it can help us choose which minimizers of the limiting functional are the most reasonable from a modelling point of view, as they are related to the ones of the approximating problems. For illustration, a precise formulation of this convergence property is given in Corollary 3.6 using the example of our discrete-to-continuum limit from Section 3.3.

Advantageously, a Γ-limit is always lower semicontinuous, so the effective problem admits a solution if in addition, the limit has e.g. precompact sublevel sets so that the direct method of the calculus of variations can be applied. However, Γ-convergence also has certain 'exotic' properties – it is not induced by any topology on $\bar{\mathbb{R}}^X$, a constant sequence of functionals $E_k = E_0$ might not have the same functional as its Γ-limit (if E_0 is not lower semicontinuous), and Γ-limits are generally not stable under addition.

Γ-convergence has been successfully applied in many areas, while new ones still keep emerging (e.g. time-dependent problems [SS04, MMP21] or semi-supervised machine learning [RB22]). At the same time, tools for the treatment of local minimizers or stationary points are also under development. [Bra14]

1.2 Models of lower-dimensional objects in elasticity

Plate or rod models offer a useful approximation of three-dimensional elasticity theory. They allow efficient numerical simulations and are commonly used in civil and mechanical engineering. Their development witnesses a long history (see [Ant05, O'R17, Lov44] for an overview), as pioneering contributions were made by L. Euler and Jac. and D. Bernoulli in the 18th century, inspired by an earlier attempt by Galileo. Another milestone was marked in [Kir59] in

1859 and since then, Kirchhoff's theory has become the most widespread one for describing elastic rods moving in 3D space (although a reformulation in modern notation is now used). Some prominent lower-dimensional theories are listed below (for more details, see the three books mentioned above).

- Two-dimensional theories include *membranes* (in which *in-plane strain* is dominant), *Kirchhoff plates* (a theory for bending), *von-Kármán plates* (which model both bending and stretching, using specific assumptions), *Mindlin or Reissner plates* (used for thicker structures where shear strain becomes important) or *shells* (their reference state is not planar).

- One-dimensional theories focus on *strings* (which have no bending or torsion resistance), planar *Euler–Bernouilli beams*, *Kirchhoff rods* (presented in more detail in Chapter 2), or else the more refined *Timoshenko* or *Cosserat rods*.

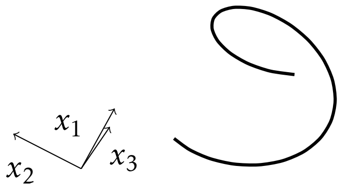


Figure 1.1: An elastic rod moving in 3D space.

(It should be noted, though, that different naming conventions for rod or plate theories exist and sometimes it is difficult to select researchers to which a theory should be correctly attributed.) Since this thesis is oriented to rod modelling, it is worth mentioning the wide applications of 1D elasticity theories: ranging from classical examples like beams, arches, bridges, pipes, or cables to more recent ones, such as lattice metamaterials [Gio21], soft robots [TAR19], collagen fibrils [BvdHH07], DNA molecules [MMK96], plant tendril perversion [MG02], or hair in computer graphics [USS14].

As Mora and Müller put it, nowadays there is a 'variety of lower dimensional theories which are often not consistent with each other'. [MM03] Hence it is useful to understand their foundations and explore mathematically how the lower-dimensional solutions are connected to 3D elasticity.[1] This is the aim in **(DR)**. Most mathematically rigorous derivations of lower-dimensional theories first appeared no sooner than in the 1990s. [ABP91, LDR93, ABP94] (Previous approaches based on some presumed form of the deformation or on formal asymptotic expansions are reviewed in [Cia21].) A decade later, the famous discovery of a *quantitative rigidity estimate* in [FJM02] brought forth an abundance of works on bending theories. [FJM02, FJM06, MM03] This nonlinear version of a corollary of Korn's inequality [Mü17, FJM06] also holds in L^p, $1 < p < \infty$, but for our purposes it suffices to cite its L^2 variant.

[1] To verify the validity of a particular theory, we should ascertain what 3D problem its solutions approximate and in what mathematical sense. An argument why this is important is given in [FJM02] – it turns out that a common ansatz that the out-of-plane displacement in a bent plate is linear leads to an incorrect constant λ instead of $\frac{\lambda\mu}{\mu+\lambda/2}$ in the elastic energy. This does not occur if the ansatz is abandoned and the Γ-limit of properly scaled energies is computed.

Theorem 1.1 ([FJM02]). *Let $n \geq 2$ and let $U \subset \mathbb{R}^n$ be a bounded Lipschitz domain. Then there exists a constant $C(U) > 0$ such that for every $v \in H^1(U;\mathbb{R}^n)$ there is a fixed rotation matrix $R \in \mathrm{SO}(3)$ satisfying*

$$\|\nabla v - R\|_{L^2(U;\mathbb{R}^{n\times n})} \leq C(U)\|\mathrm{dist}(\nabla v, \mathrm{SO}(n))\|_{L^2(U)}.$$

The constant $C(U)$ is invariant under scaling U.

In [MM03], a nonlinear bending-torsion theory for inextensible rods was rigorously derived from three-dimensional elasticity using Theorem 1.1 to locally approximate scaled deformation gradients by rotations in the Γ-liminf inequality. This rod theory, which was also independently obtained in [Pan02], embraces Kirchhoff rods as a special case. The reader is referred to [MM04, Sca06, FPPG15, EK21] for other results on mathematical derivation of dimensionally reduced theories in elasticity.

A mathematical approach for the derivation of rod equations different from Γ-convergence but worth mentioning is the centre manifold method. [Mie88] The approach is based on recasting the static problem as an ODE in a Banach space – the independent variable t does not have the meaning of time but a real parameter describing the longitudinal position within a long elastic body. In comparison with [MM03], not only bending and torsion are included, but also shear and extension; however, the centre-manifold approach only works for strains small in $C^{0,\lambda}$ and applied forces cannot be easily incorporated. [Mü17]

1.3 Derivation of continuum theories from atomic interactions

As for **(D-C)**, 'establishing the status of elasticity theory with respect to atomistic models' was listed by Ball among outstanding open problems in elasticity. [Bal02] Indeed, although variational formulation of elasticity has become standard, often an exact expression for the stored energy density is not available and it may be enlightening to explore the microscopic origins of this quantity. [BLL02] Research has been devoted to studying the so-called Cauchy–Born rule [FT02, EM07] (see Subsection 1.3.2), pointwise limits of interaction energies [BLL02] and their Γ-limits [AC04, Sch09, BS13], or to finding atomistic deformations approximating a given solution of the equations of elasticity [OT13, BS16, Bra17]. See also the recent articles [BBC20, ALP21] or [BLBL07] for a survey.

1.3.1 Mechanics of many-particle systems

Materials at the nanoscale are described by the laws of quantum mechanics, but for larger particle systems it is far out of reach to solve Schrödinger's equation, regardless whether numerically or analytically. Fortunately, a number of approximative theories are available.

- *Molecular dynamics* have been around since the 1950s and are based on integration of Newton's equations of motion for the n-particle system:

$$m_i \frac{\partial^2 y^{(i)}}{\partial t^2} = f^{(i)}, \quad i = 1, 2, \ldots, n,$$

where $y^{(i)}$ is the (time-dependent) position of i-th particle, whose mass is m_i and $f^{(i)}$ is the net force acting on this particle. For pair interactions[2], the forces can be derived from an interaction potential V, which depends on the distance between two particles:

$$f^{(i)} = -\sum_{\substack{j=1\\ i\neq j}}^{n} \nabla_{y^{(i)}} V\Big(|y^{(j)} - y^{(i)}|\Big) = -\sum_{\substack{j=1\\ i\neq j}}^{n} V'\Big(|y^{(j)} - y^{(i)}|\Big)\frac{y^{(i)} - y^{(j)}}{|y^{(i)} - y^{(j)}|}.$$

Generally, the force between two particles is *repulsive* if their distance is small and *attractive*, but decaying asymptotically if they are located further away. These two properties are combined into particular empirical potentials (Lennard–Jones, Morse. . .), which can look like in Figure 1.2. The discrete models in Chapters 3–4 are motivated by molecular dynamics with short-range interactions. As the complexity of the problem increases substantially otherwise, we work at zero temperature there. Questions of practical implementation of molecular dynamics simulations are treated e.g. in [FS02].

- *Monte Carlo methods* make use of random numbers generated by a computer to study equilibrium or non-equilibrium systems. A detailed exposition about these methods can be also found in [FS02].
- In the *Thomas–Fermi theory* and its later more complicated corrections, electron density is modelled separately, while the atomic nuclei are considered as classical charged particles. Blanc et al. [BLL02] achieved a discrete-to-continuum limit in this setting, relying on pointwise convergence of the energy functionals. A successor of Thomas–Fermi models in computational materials science and quantum chemistry is the *density functional theory*, which has become a popular method and a very active area of research.

Evidently, there is a multitude of relevant choices of the starting point for **(D-C)** and even in the realm of classical point-particle models, different results in the limit can be expected depending on the inclusion of longer-range or k-particle interactions, choice of the crystallographic structure etc. (see e.g. the references in [AC04]).

1.3.2 Cauchy–Born hypothesis

The Cauchy–Born rule is a method of relating a continuum deformation to displacements in a crystal lattice that constitutes the material. In our context it can formulated as follows[3]:

> Suppose that a crystalline solid is subject to an affine deformation φ on the boundary. Then the minimum interaction energy of atoms

[2] More complicated models also include interactions of k-tuples of particles with $k \geq 3$. This might model preferred angles between bonds, as we see in the *Stillinger–Weber potential*, used for semiconductors. [Phi01]

[3] The concept is nicely illustrated in [FT02, Fig. 2].

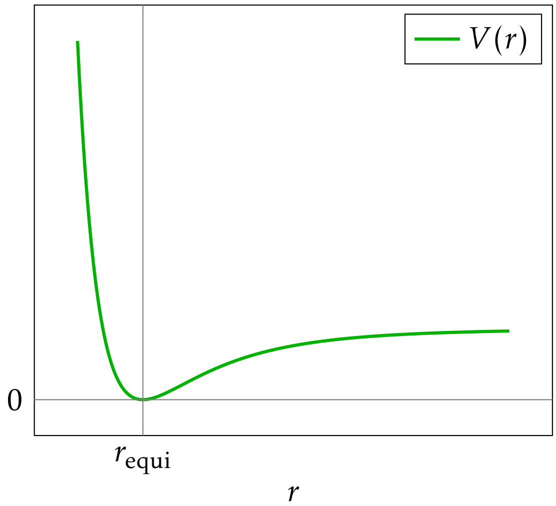


Figure 1.2: An interatomic potential with a minimum value at $r_{\text{equi}} > 0$.

in its crystal lattice is achieved when all the atoms follow the same affine deformation φ.

On the grounds of the Cauchy–Born hypothesis, we can define a macroscopic elastic energy density using the potential energy of a lattice given in a molecular model. [Zan96] Researchers have tried to determine the range of validity of this hypothesis. The study [FT02] contributes to the subject mathematically, investigating minimum-energy configurations in a 2D mass-spring lattice. It is proved there that for some values of the spring parameters, the Cauchy–Born rule holds and for other ones it does not. Conti et al. [CDKM06] generalized the result of [FT02] to higher dimensions.

In the discrete model of Chapter 3, the Cauchy–Born rule is not assumed directly, but assumptions from [CDKM06] about interatomic potentials are incorporated, which ensures that the hypothesis is valid for the crystalline material.

For a broader perspective on this topic, see e.g. the review [Eri08].

1.3.3 Models for thin films and nanowires

When it comes to modelling nanomaterials, elasticity theory has the advantage of condensing the complexity of a structure composed of many molecules (e.g. in [dFMGa05], Kirchhoff's rod theory was applied to nanowires for the purposes of identification of Young's modulus and Poisson's ratio). However, the natural question arises whether atomistic effects should not be part of continuum theories for bodies which only consist of a few atomic layers in their transversal direction. Bearing this in mind, Friesecke and James proposed in [FJ00] a method for deriving continuum models of 2D and 1D nanomaterials when in-plane strain is dominant (*membrane theory*) and the approach was implemented rigorously in [Sch08a] for thin films. The work [Sch06] focused on the bending of *Kirchhoff's plates* and introduced a continuum theory for thin films which comprise no more than several layers. A similar derivation of *von-Kármán's plate theory* has only been achieved recently [BS22].

Other approaches to nanowire mechanical modelling include adaptations of the Cauchy–Born rule [YE06, KKG16], the so-called *objective quasicontinuum method* [HTJ12], thermodynamically motivated constitutive relations using data from molecular dynamics [SIS15], and Eringen's nonlocal elasticity [KHH20]. Several works have also used couple-stress theories to account for size effects in Kirchhoff rods. [ZG19]

1.4 Fracture mechanics

There are different mechanisms of material failure, amply discussed in engineering textbooks. [And05] In *ductile fracture*, the gradually formed crack is preceded and surrounded by a plastically deformed zone, whereas *brittle fracture* propagates rapidly and on the microscopic level it often involves cleavage along specific planes. *Fatigue cracks* are also sudden and produced by cyclic loading – a common phenomenon in industrial metallic structures. Classical fracture formulations differ from *damage mechanics*, which applies to the formation and growth of microvoids that may lead to material softening, but the deformation of damaged material is still modelled as continuous in space.

The English engineer A. A. Griffith conceived a global criterion for brittle fracture propagation a hundred years ago, postulating that a crack may grow if the *elastic energy G released per unit area* of the rupture reaches the *fracture energy G_c* necessary to produce the crack.

The interest of mathematicians in **(F)** was particularly ignited after Francfort and Marigo [FM98] elaborated on Griffith's influential model, using modern variational methods (see e.g. [Fra21, BFM08] for further references). In variational models of fracture, be it *brittle* or *cohesive* [Bar62], we typically find functionals involving the sum of elastic and fracture energy:

$$\int_\Omega W(\nabla y(x))\mathrm{d}x + \int_{J_y} \kappa\,(y^+(x) - y^-(x), \nu(x))\,\mathrm{d}\mathcal{H}^{d-1}(x). \tag{1.1}$$

In the above, $W\colon \mathbb{R}^{3\times 3} \to [0,\infty)$ stands for the stored energy density of a material body $\Omega \subset \mathbb{R}^d$, $d \in \{2,3\}$, $y^+ - y^-$ is the jump of the deformation $y : \Omega \to \mathbb{R}^d$ across the crack set J_y, ν denotes the normal vector field to J_y, and $\kappa\colon (\mathbb{R}^d)^2 \to [0,\infty]$ is the fracture toughness.

Contemporary variational formulations of brittle fracture problems were also shaped by the study of the *Mumford–Shah functional* in image segmentation and by the related framework of *free-discontinuity problems* using *special functions of bounded variation* (SBV). [AFP00]

1.5 Nanomaterials

Nanotechnology is concerned with processing matter 1–100 nanometres in size (i.e. at the scale of atoms or molecules). [San18] Materials whose dimensions lie roughly in this range (or whose internal structure is based on such tiny building blocks) are called nanomaterials and can be classified as 0D, 1D, 2D, or 3D depending on their shape.

The most minute nanoobjects may have single nanometres in diameter and are therefore referred to as *zero-dimensional* (e.g. carbon fullerenes, quantum dots, or nanoparticles). [WHLW20]

One-dimensional nanomaterials like nanowires are the most relevant for the topic of this thesis, so they are described more thoroughly in the next subsection.

Examples of *2D nanomaterials* are various kinds of nanosheets, thin films, or even monatomic layers such as graphene or silicene. [BKF21]

Lastly, *3D nanomaterials* can be defined as those whose no dimension is confined to the nanoscale (graphite, nanowires organized in bundles, or other assemblies of lower-dimensional nanostructures etc.).

It should be noted that many sorts of nanoobjects are necessarily missing in this brief survey and can be found in the ever-growing specialized literature of this field.

1.5.1 Nanowires and nanotubes

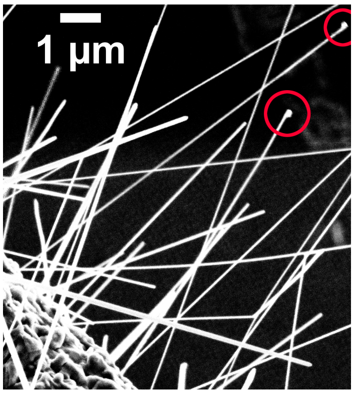


Figure 1.3: ZnO nanowires (US National Institute of Standards and Technology (NIST), `https://commons.wikimedia.org/wiki/File:Nanowires_(5884868572).jpg`, 2008. Accessed: 3. 1. 2023).

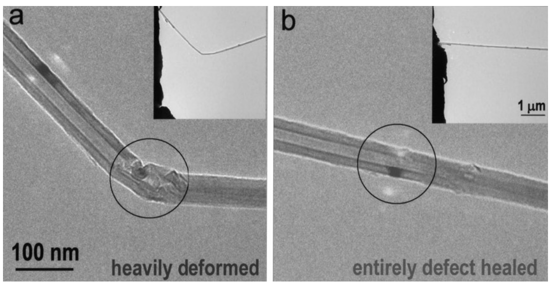


Figure 1.4: Bent boron nitride nanotube (licensed under CC BY 4.0, `https://commons.wikimedia.org/wiki/File:Recovery_of_bent_BN_nanotube.jpg`, Accessed: 3. 1. 2023). Originally published in [GCMB09].

Since the first boom in research on carbon nanotubes in the 1990s, we have been experiencing discoveries of a wide variety of 1D nanomaterials. These include nanowires, nanorods[4], nanopillars, and nanowhiskers [Eva20, BJ21], which find applications in electronics, photonics [San18, HGB18], sensor design [ML20, ASL+13], or biomedicine [Cof21, AIP+21]. Another important category is nanofibres. [KL17]

As such thin structures only have tens of nanometres in diameter, they exhibit unusual deformation behaviour under external loads, different from that of bulk materials (e.g. great flexibility, anisotropy, structure dependence, or surface effects).

The model in Chapter 4 is particularly motivated by ceramic and semiconductor nanowires (composed of Si, SiC, Si_3N_4, TiO_2, or ZnO etc.) which, apart from large deflections, also show brittle or ductile fracture under loading. [CL16] In practice, fracture and defects are common in 1D nanomaterials [KKG16] and may considerably alter the structure's properties.

1.6 Overlaps of the previous research fields

Given the myriads of physical situations that emerge in modern materials science, it seems natural that researchers have made efforts to bridge some of the gaps between **(DR)**, **(D-C)** and **(F)**.

Combining **(DR)** and **(D-C)** is motivated by the need of accurate models for thin structures in nanoengineering, such as thin films or nanotubes, as mentioned before. [FJ00, Sch08a, Sch08b, ABC08] Interestingly, when the thickness h of the reference crystalline body is very small (i.e. comparable to the interatomic distance ε), the simultaneous Γ-limit as $\varepsilon \to 0+$, $h \to 0+$ gives rise to new *ultrathin plate* or *rod theories* which could not be obtained by **(DR)** in the purely continuum setting. [Sch06, BS22] (This is observed in the models in Chapters 3–4 too.)

Atomistic effects also lie at the core of crack formation and propagation. [BHO20, BKG15] However, up to now combinations of **(D-C)** and **(F)** have only been explored in specific situations such as one-dimensional chains of atoms [BC07, SSZ11, JKST21], scalar-valued models [BG02], or cleavage in crystals [FS14, FS15a, FS15b].

Similarly, despite the recent progress, theories uniting **(DR)** and **(F)** are still under development. In linearized elasticity, models for brittle plates [BH16, AT23, FPZ10, LBBB+14], beams [GG23] or shells [ABMP21] have been derived mostly using a weak formulation in SBD or $GSBD$ function spaces [ACDM97, DM13]. The nonlinear setting of membranes as in [BF01, Bab06] or [ARS23], on the other hand, employs the more regular spaces SBV and $GSBV$. [AFP00] As for nonlinear bending theories, the lack of a piecewise quantitative rigidity estimate in 3D presents an obstacle, so the result of [Sch17] with a dimension reduction from 2D to 1D seems rather isolated; we also refer to [FKZ21, SS23] for materials with voids.

[4] Some authors use the term nanorod for objects with a smaller aspect ratio than a nanowire has, hence here the term nanorod is avoided in the sequel.

1.7 Outline and a summary of results

Continuing with the introductory matter, Chapter 2 is devoted to a presentation of Kirchhoff's rod theory and to showing its connections with the variational formulation in [MM03]. Thus, it also allows a comparison with the effective rod models in subsequent chapters, where crystalline structure or brittleness of the rod is additionally considered.

1.7.1 Purely elastic models

The presentation of the thesis' results begins in Chapter 3, where two continuum theories for the bending and torsion of inextensible rods are established as Γ-limits of 3D atomistic models. Simultaneous limits of vanishing rod thickness h and interatomic distance ε are studied in the derivation. First, a novel theory is set up for *ultrathin rods* with a fixed number of atoms within their cross section ($\varepsilon \sim h$), where surface energy and new discrete terms are included in the effective functional. This can be thought of as a contribution to the mechanical modelling of nanowires. Second, the case where $\varepsilon \ll h$ is treated and the nonlinear rod model from [MM03] is recovered. The findings are also presented in the preprint [SZ23a].

1.7.2 Model with brittle fracture

To set off on a path towards elastic-fractural modelling of nanowires, in Chapter 4 (see also [SZ23b]) we extend the ultrathin purely elastic model from Chapter 3 considerably by adding liability of the material to develop brittle cracks.

Thus the chapter approaches a problem that falls into all three branches **(DR)**, **(D-C)** and **(F)**. The main Theorem 4.3 provides the Γ-limit of atomic interaction energies defined on cubic crystalline lattices in the shape of a slender rod. Unlike in the purely elastic model from Chapter 3, the interaction potentials (expressed by a cell energy function W_{cell} like in e.g. [FT02, CDKM06, Sch06]) are replaced there with a sequence $(W_{\mathrm{cell}}^{(k)})_{k=1}^{\infty}$ of cell energies to ensure that elastic deformations (bending and torsion) are comparably favourable in terms of energy as cracks. This is specifically expressed in condition (W5) for the constants $(\bar{c}_1^{(k)})_{k=1}^{\infty}$, which give a lower bound on the cost of placing atoms far away from each other (see Subsection 4.1.3). Physically we can interpret this as considering a sequence of materials that are mutually similar but are characterized by different values of material parameters. The limiting strain energy has, just like in (1.1):

1. A bulk part that coincides with its counterpart in Chapter 3 and features an *ultrathin correction* and *atomic surface layer terms*, neither of which appears in the corresponding rod theory [MM03] derived by **(DR)** without **(D-C)**. These traits might make a model better-suited for the description of nanostructures.

2. A fracture part which turns out to be a weighted sum over the singular set of a limiting deformation. The weights are given by an implicit cell

formula $\varphi = \varphi(y^+ - y^-, (R^-)^{-1}R^+)$, where $y^+ - y^- \in \mathbb{R}^3$ denotes the jump of the deformation mapping at a specified crack point and $(R^-)^{-1}R^+ \in \mathrm{SO}(3)$ is related to kinks/folds or torsional rupture.

Implicit cell formulas arise in Γ-convergence problems in homogenization [Bra06] or phase transitions [CS06, KLR17, CFL02].

To comment on some important aspects of the proofs, in the *liminf inequality* we first derive a preliminary cell formula by a blowup technique reminiscent of [FM92, AFP00] and then relate it to a more simple asymptotic formula which uses rigid boundary values (cf. [FKS21]). The atomistic setting allows us to circumvent the unavailability of a 3D piecewise rigidity theorem in SBV (in fact, it is enough to work with piecewise Sobolev functions here). The main challenge of the analysis is, however, to provide a matching *limsup inequality*. Due to the k-dependency of the interaction potential $W_{\mathrm{cell}}^{(k)}$, it is a priori not clear how to construct a global recovery sequence $(y^{(k)})$ that not only works for a specific subsequence. We resolve this difficulty by establishing a localization of cracks on the atomic length scale, which appears to be of some independent interest. More precisely, it is argued that an approximative minimizing sequence $(\mathcal{Y}^{(k)})$ for φ can be chosen with cracks confined to a fixed number of atomic slices (Lemma 4.6), which lets us transfer $\mathcal{Y}^{(k)}$ to a lattice with different interatomic distances (Proposition 4.7) and thus define $(y^{(k)})$ for every $k \in \mathbb{N}$. Γ-convergence problems involving brittle fracture often have to deal with pieces of the deformed body escaping to ∞. As our limiting theory is one-dimensional we can sidestep working on $GSBV$-type spaces and instead obtain a limiting functional on piecewise H^2 functions. By an explicit construction using assumption (W9) in Lemma 4.8 it is shown that L^∞ (or weaker) bounds could be imposed energetically so as to ensure matching compactness properties of low-energy sequences.

The short conclusion at the end of this thesis gives some hints on possible future research.

1.8 Basic notation

If $S \subset \mathbb{R}^n$, we write $\operatorname{Int} S$ for the interior of S, $\overline{S}$ for the closure of S, $\operatorname{diam} S = \sup_{x,y\in S} |x-y|$, and, if S is Lebesgue measurable, $|S|$ for the n-dimensional Lebesgue measure of S. The integral average over S of an integrable function f defined in S is then $\fint_S f \,\mathrm{d}x = \frac{1}{|S|}\int_S f\,\mathrm{d}x$ (if $|S| > 0$). In the whole text, we reserve the letter C for a generic positive constant whose value may vary from line to line, but is independent of the quantities involved in a limit passage. We use standard notation for function spaces: namely the Lebesgue spaces $L^p(\Omega;\mathbb{R}^n)$, $p \in [1,\infty]$, Sobolev spaces $H^m(\Omega;\mathbb{R}^n) = W^{m,2}(\Omega;\mathbb{R}^n)$, $m \in \mathbb{N}$, and weak convergence ($f_k \rightharpoonup f$; see [Eva98, ACM18]). Further, $A_{\bullet j}$ denotes the j-th column vector of a matrix $A \in \mathbb{R}^{m\times n}$; $\mathbb{R}^{3\times 3}_{\mathrm{skew}} = \{A \in \mathbb{R}^{3\times 3};\ A = -A^\top\}$ stands for the space of all 3-by-3 skew-symmetric matrices; $e_i = \mathrm{Id}_{\bullet i}$, $1 \le i \le 3$, are the standard basis vectors in $\mathbb{R}^3$, and $|u|$ and $|A| = \sqrt{\operatorname{Tr} A^\top A}$ denote the Euclidean and Frobenius norms of $u \in \mathbb{R}^n$ and $A \in \mathbb{R}^{m\times n}$, respectively. The orthogonal group is $\mathrm{O}(n) = \{R \in \mathbb{R}^{n\times n};\ R^\top R = RR^\top = \mathrm{Id},\ \det R = 1\}$ and the special orthogonal group $\mathrm{SO}(n) = \{R \in \mathrm{O}(n);\ \det R = 1\}$. All vectors, unless otherwise specified, are treated as column vectors. For an open set $\Omega \subset \mathbb{R}^n$ we write $\Omega' \subset\subset \Omega$ if $\bar{\Omega}' \subset \Omega$ and $\bar{\Omega}'$ is compact. Besides, $V^\perp$ is the orthogonal complement of a subspace V in an inner product space X.

We write $\mathrm{dist}(B_1, B_2) := \inf\{|x^{(1)} - x^{(2)}|;\ x^{(1)} \in B_1,\ x^{(2)} \in B_2\}$ for $B_1, B_2 \subset \mathbb{R}^3$. Whenever the symbol $\pm$ appears in an equation, we mean that the equation holds both in the version with + in all occurrences *and* in the version with −. One-sided limits are written as $f(\sigma\pm) = \lim_{x\to\sigma\pm} f(x)$. Further, $\mathcal{H}^n$ is the n-dimensional Hausdorff measure. The restriction $\mu \llcorner K$ of a measure μ to the measurable set K is defined by $\mu \llcorner K(U) = \mu(U \cap K)$. Given a finite set B, we denote by $\sharp B$ the number of its elements.

2. Mechanics of Kirchhoff rods

'Wir werden uns jetzt mit dem Gleichgewicht und der Bewegung von Körpern beschäftigen, deren Dimensionen theilweise unendlich klein sind; dünne Stäbe und Platten können näherungsweise als solche angesehen werden.'

Kirchhoff's Vorlesungen über Mechanik, 1897 (28^{th} lecture)

The nonlinear bending-torsion theory of thin rods introduced by Kirchhoff [Kir59] was reformulated and further expanded by Clebsch [Cle62] and Love [Lov44]. Reviewing the theory in this chapter is aimed at making a connection with readers having an engineering background and presenting further mechanical insight into the rod model in [MM03] that mathematicians can find useful. Thus, a highest possible level of mathematical precision is not a priority here.

The presentation follows a review article by Dill [Dil92]. Modelling assumptions and notation are adapted here to facilitate the comparison with [MM03] and later chapters. For the same reason, only straight (i.e. not initially curved) rods are treated in this exposition. To avoid conflicts of notation, points $\boldsymbol{x} \in \mathbb{R}^3$, vectors ($\boldsymbol{n}$, $\boldsymbol{\nu}\dots$), and matrices ($\boldsymbol{R}$, $\boldsymbol{E}$, $\boldsymbol{I} = (\boldsymbol{e}_1|\boldsymbol{e}_2|\boldsymbol{e}_3)\dots$) are typeset in boldface.

2.1 Kinematics

We consider a three-dimensional rod-like body that occupies a fixed reference configuration $\Omega = (0, L) \times S$ before the deformation. For convenience, the cross section $S \subset \mathbb{R}^2$ is assumed to be a simply connected domain with sufficiently smooth boundary. The rod's thickness $h = \frac{1}{2}\operatorname{diam} S$ is significantly smaller than the length L of the rod. We choose the reference coordinate system, without loss of generality, in such a way that

$$\int_S x_2 x_3 \mathrm{d}x_2 \mathrm{d}x_3 = \int_S x_2 \mathrm{d}x_2 \mathrm{d}x_3 = \int_S x_3 \mathrm{d}x_2 \mathrm{d}x_3 = 0$$

so that the line segment $(0, L) \times \{(0, 0)\}$ can be called the rod's *axis* (also known as the *base curve* or *centreline*).

In general, the idea of modern rod theories is to approximate the slender body's deformation by the motion of its axis and by a set of vectors, called *directors*, assigned to each point $x_1 \in (0, L)$ – this leads to the notion of a *directed curve*.

Specifically, when the rod is deformed, the axis becomes a curve parametrized by $x_1 \mapsto \boldsymbol{y}(x_1, t)$ for every time $t \in (0, t_*)$, $t_* > 0$. (At the beginning of the loading process, i.e. for $t = 0$, the rod is situated in its reference configuration.) Contrarily to some treatments of Kirchhoff's theory [Lov44, Dil92], we regard the rod as inextensible, hence the tangent vector $\boldsymbol{d}_1(x_1,t) := \partial_{x_1}\boldsymbol{y}(x_1,t)$ is assumed to have unit length. To further characterize rotations of the material cross section, we introduce vector-valued functions $\boldsymbol{d}_2 = \boldsymbol{d}_2(x_1,t)$ and $\boldsymbol{d}_3 = \boldsymbol{d}_3(x_1,t)$ such that $(\boldsymbol{d}_i(x_1,t))_{i=1}^3$ is a right-handed orthonormal frame, associated with each point of the axis. We call $\boldsymbol{d}_2$ and $\boldsymbol{d}_3$ directors[1]. Note that in [Ant05, O'R17] a different definition of $\boldsymbol{d}_1$ is employed: $\boldsymbol{d}_2$ and $\boldsymbol{d}_3$ may not be perpendicular to $\partial_{x_1}\boldsymbol{y}$ there and $\boldsymbol{d}_1 = \boldsymbol{d}_2 \times \boldsymbol{d}_3$; we follow the convention of [MM03], though. Introducing the rotation matrix $\boldsymbol{R} = (\boldsymbol{d}_1|\boldsymbol{d}_2|\boldsymbol{d}_3) \in \mathrm{SO}(3)$, we have

$$\frac{\partial \boldsymbol{R}}{\partial x_1} = \boldsymbol{R}\left(\boldsymbol{R}^\top \frac{\partial \boldsymbol{R}}{\partial x_1}\right) \quad \text{in } (0,L)\times(0,t_*). \tag{2.1}$$

To obtain some useful interpretation of the previous equation, let $\kappa_2 = \frac{\partial^2 \boldsymbol{y}}{\partial x_1^2}\cdot \boldsymbol{d}_2$, $\kappa_3 = \frac{\partial^2 \boldsymbol{y}}{\partial x_1^2}\cdot \boldsymbol{d}_3$, and $\tau = \frac{\partial \boldsymbol{d}_2}{\partial x_1}\cdot \boldsymbol{d}_3$ in $(0,L)\times(0,t_*)$ so that the columns in (2.1) become

$$\frac{\partial^2 \boldsymbol{y}}{\partial x_1^2} = \kappa_2 \boldsymbol{d}_2 + \kappa_3 \boldsymbol{d}_3 \qquad \frac{\partial \boldsymbol{d}_2}{\partial x_1} = -\kappa_2 \frac{\partial \boldsymbol{y}}{\partial x_1} + \tau \boldsymbol{d}_3 \tag{2.2a}$$

$$\frac{\partial \boldsymbol{d}_3}{\partial x_1} = -\kappa_3 \frac{\partial \boldsymbol{y}}{\partial x_1} - \tau \boldsymbol{d}_2 \tag{2.2b}$$

by noting that $\boldsymbol{R}^\top \partial_{x_1}\boldsymbol{R}$ is skew-symmetric[2]. In (2.2) we see how the scalars κ_2, κ_3, and τ express the rate of change of $\partial_{x_1}\boldsymbol{y}$, $\boldsymbol{d}_2$ or $\boldsymbol{d}_3$ projected into the direction of another vector in this triad. Thus the strain variables κ_2 and κ_3 are referred to as *curvatures* and τ is called the *torsion* of the rod. (None of the three should be confused with curvature or torsion as defined in geometry.) In accord with the reasoning of Kirchhoff and Love, we express the position of a rod particle in the present (i.e. deformed) configuration as

$$\boldsymbol{y}_{3\mathrm{D}}(\boldsymbol{x},t) = \boldsymbol{y}(x_1,t) + x_2\boldsymbol{d}_2(x_1,t) + x_3\boldsymbol{d}_3(x_1,t) + \boldsymbol{R}(x_1,t)\boldsymbol{\alpha}(\boldsymbol{x},t), \quad (\boldsymbol{x},t) \in \Omega \times (0,t_*),$$

where $\boldsymbol{\alpha}$ is such that $\boldsymbol{\alpha}(x_1,0,0,t) = 0$. The term $\boldsymbol{\alpha}$ is connected with secondary effects, namely warping the cross section (in torsion, the section does not, in general, stay planar) and its lateral contraction in flexure. It is worth mentioning that in [MM03], no ansatz on the form of the deformation is imposed; only a suitable strain energy scaling is assumed.

The initial conditions for $t = 0$ are given by $\boldsymbol{R}(x_1,0) = \boldsymbol{I}$ and $\boldsymbol{\alpha}(\boldsymbol{x},0) = \boldsymbol{0}$.

Let us find formulas[3] for $\boldsymbol{\alpha}$, connecting it with κ_2, κ_3, and τ. For this we need several approximating assumptions. In fact, we limit ourselves to motions of the rod during which neither of the functions $|\kappa_2|$, $|\kappa_3|$, and $|\tau|$ exceeds $1/a$ (at any point (x_1,t)), where a is a chosen positive number. Moreover, let

[1] Certain more general rod theories remove some of the constraints on the directors. For instance, in the *special Cosserat theory of rods*, $\boldsymbol{d}_2$ and $\boldsymbol{d}_3$ may not be orthogonal to the tangent $\partial_{x_1}\boldsymbol{y}$ so that transverse shear can be modelled and the tangent may not be a unit vector so that dilatation of the rod can be described. *General Cosserat theories* even drop the orthonormality of $\boldsymbol{d}_2$ and $\boldsymbol{d}_3$ or use more than two directors. [Ant05]

[2] Dill [Dil92] uses the matrix $\partial_{x_1}\boldsymbol{R}\boldsymbol{R}^\top$, which gives the formula $\partial_{x_1}\boldsymbol{R} = (\partial_{x_1}\boldsymbol{R}\boldsymbol{R}^\top)\boldsymbol{R}$ instead. The two matrices are related by a similarity transformation: $\boldsymbol{R}^\top\partial_{x_1}\boldsymbol{R} = \boldsymbol{R}^\top(\partial_{x_1}\boldsymbol{R}\boldsymbol{R}^\top)\boldsymbol{R}$.

[3] This was an important contribution of Kirchhoff. Yet, it is not uncommon in the literature to call theories with the more restrictive ansatz $\boldsymbol{y}_{3\mathrm{D}} = \boldsymbol{y} + \sum_{s=2}^3 x_s\boldsymbol{d}_s$ 'Kirchhoff rods'.

δ be the larger of the ratios $\frac{h}{L}$ and $\frac{h}{a}$. We suppose that the rod's dimensions and deformations considered imply that δ is a small quantity (compared to 1). Hopefully, the deficiency of this approach in mathematical rigour will be compensated by the gain of better physical understanding of Kirchhoff's rod model. Kirchhoff did not content himself with requiring that $\alpha_k = 0$, he just assumed that these additional displacements are small. More precisely, the theory applies to motions such that

$$\frac{\alpha_k}{h} = O(\delta), \quad \frac{\partial \alpha_k}{\partial x_s} = O(\delta), \quad \frac{\partial \alpha_k}{\partial x_1} = O(\delta^2), \quad s = 2,3, \quad k = 1,2,3. \tag{2.3}$$

Later it will be seen from (2.9) that the third assumption above with $k = 2,3$ holds if $La\frac{\partial \kappa_s}{\partial x_1} = O(1)$ – a condition that precludes crumpling the rod, as the rate of change of curvature along the axis is limited.

By (2.3), the deformation gradient of $\boldsymbol{y}_{3\mathrm{D}}$ is

$$\begin{aligned}\nabla \boldsymbol{y}_{3\mathrm{D}} = (\boldsymbol{d}_1 + x_2\partial_{x_1}\boldsymbol{d}_2 + x_3\partial_{x_1}\boldsymbol{d}_3 + \partial_{x_1}\boldsymbol{R}\boldsymbol{\alpha} + \boldsymbol{R}\partial_{x_1}\boldsymbol{\alpha} \,|\, \boldsymbol{d}_2 + \boldsymbol{R}\partial_{x_2}\boldsymbol{\alpha} \,|\, \boldsymbol{d}_3 + \boldsymbol{R}\partial_{x_3}\boldsymbol{\alpha})\\ = \boldsymbol{R}\Big(\boldsymbol{I} + \boldsymbol{f} + O(\delta^2)\Big) = \boldsymbol{R} + O(\delta),\end{aligned}$$

where we have set

$$\boldsymbol{f} := \left(\boldsymbol{R}^\top \frac{\partial \boldsymbol{R}}{\partial x_1}\begin{pmatrix}0\\x_2\\x_3\end{pmatrix} \Bigg| \frac{\partial \boldsymbol{\alpha}}{\partial x_2} \Bigg| \frac{\partial \boldsymbol{\alpha}}{\partial x_3}\right) = O(\delta).$$

From this we compute the Green–St. Venant strain tensor (see [GFA09])

$$\boldsymbol{E} = \frac{1}{2}((\nabla \boldsymbol{y}_{3\mathrm{D}})^\top \nabla \boldsymbol{y}_{3\mathrm{D}} - \boldsymbol{I}) = \frac{1}{2}(\boldsymbol{f} + \boldsymbol{f}^\top) + O(\delta^2)$$

and define $\boldsymbol{e} = \frac{1}{2}(\boldsymbol{f} + \boldsymbol{f}^\top)$.

For the sake of illustration, we use the isotropic St. Venant–Kirchhoff constitutive relation[4], so the second Piola–Kirchhoff stress tensor $\boldsymbol{T}^{(2)}$, related to the Cauchy stress $\boldsymbol{T}$ by $\boldsymbol{T}^{(2)} = \det \nabla \boldsymbol{y}_{3\mathrm{D}} (\nabla \boldsymbol{y}_{3\mathrm{D}})^{-1} [\boldsymbol{T}(\nabla \boldsymbol{y}_{3\mathrm{D}})^{-1}]^\top$, is given by

$$\boldsymbol{T}^{(2)} = 2\mu \boldsymbol{E} + \lambda(\operatorname{Tr} \boldsymbol{E})\boldsymbol{I} = 2\mu \boldsymbol{e} + \lambda(\operatorname{Tr} \boldsymbol{e})\boldsymbol{I} + O(\delta^2),$$

where λ, μ are Lamé's parameters. Hence, if we set $\boldsymbol{\sigma} := 2\mu \boldsymbol{e} + \lambda(\operatorname{Tr} \boldsymbol{e})\boldsymbol{I}$, the first Piola–Kirchhoff stress tensor reads

$$\boldsymbol{T}^{(1)} = \nabla \boldsymbol{y}_{3\mathrm{D}} \boldsymbol{T}^{(2)} = \boldsymbol{R}\boldsymbol{\sigma} + O(\delta^2). \tag{2.4}$$

2.2 Consequences of the balance of momentum

As it is known in continuum mechanics, the balance of momentum can be globally expressed in the reference configuration by

$$\int_{\partial\Omega} \boldsymbol{T}^{(1)} \boldsymbol{n}\, \mathrm{dS} + \int_\Omega \rho_0 \boldsymbol{b}\, \mathrm{d}\boldsymbol{x} = \int_\Omega \rho_0 \frac{\partial^2 \boldsymbol{y}_{3\mathrm{D}}}{\partial t^2} \mathrm{d}\boldsymbol{x} \tag{2.5}$$

[4]Other material models can also be applied in rod theories. Mora and Müller [MM03] start their derivation from a general anisotropic hyperelastic material assumption, which, however, only enters the effective rod model by the quadratic form of linearized elasticity.

and locally by

$$\operatorname{div} \boldsymbol{T}^{(1)} + \rho_0 \boldsymbol{b} = \rho_0 \frac{\partial^2 \boldsymbol{y}_{3\mathrm{D}}}{\partial t^2},$$

where $\boldsymbol{n}$ is the unit outer normal vector field to Ω, ρ_0 stands for the initial density of the material, and $\boldsymbol{b}$ is the density of applied body force. Kirchhoff's intuition about the distribution of stress inside the loaded rod led him to the following condition, derived from the local momentum balance:

$$\frac{\partial \boldsymbol{T}^{(1)}}{\partial x_2}\boldsymbol{e}_2 + \frac{\partial \boldsymbol{T}^{(1)}}{\partial x_3}\boldsymbol{e}_3 = \boldsymbol{0},$$

which gave rise to a debate in the subsequent literature. Without attempting to review the outcomes of this debate, let us bear in mind that the theory is limited to situations in which the above relation holds. Substituting (2.4) into the equation and neglecting the second order terms, we get

$$\Big(\frac{\partial \sigma_{12}}{\partial x_2} + \frac{\partial \sigma_{13}}{\partial x_3}\Big)\boldsymbol{d}_1 + \Big(\frac{\partial \sigma_{22}}{\partial x_2} + \frac{\partial \sigma_{23}}{\partial x_3}\Big)\boldsymbol{d}_2 + \Big(\frac{\partial \sigma_{32}}{\partial x_2} + \frac{\partial \sigma_{33}}{\partial x_3}\Big)\boldsymbol{d}_3 = \boldsymbol{0}, \tag{2.6}$$

which can only be true if the individual coefficients of the linear combination vanish, as $\boldsymbol{d}_k$ are orthonormal.

Concerning the boundary conditions for $\boldsymbol{\sigma}$, it is assumed that tractions on the sides of the rod are small, namely of the order $O(\delta^2)$. By formula (2.4) for $\boldsymbol{T}^{(1)}$, these tractions equal $\boldsymbol{T}^{(1)}(0,\boldsymbol{\nu})^\top = \boldsymbol{R}(\boldsymbol{\sigma}_{\bullet 2}\nu_2 + \boldsymbol{\sigma}_{\bullet 3}\nu_3) + O(\delta^2)$, where $\boldsymbol{\nu} = \boldsymbol{\nu}(x_2, x_3)$ is the unit outward normal to the cross section S at the point $(x_2, x_3) \in \partial S$. Upon neglecting the $O(\delta^2)$ terms, this yields the boundary condition

$$\sigma_{k2}\nu_2 + \sigma_{k3}\nu_3 = 0, \quad k = 1, 2, 3. \tag{2.7}$$

Fix $t \in (0, t_*)$. The partial differential equations originating from (2.6) together with boundary conditions (2.7) now have to be solved for α_k. In the solution procedure, bending and torsion effects can be discerned.

2.2.1 Torsion

First let us focus on the set of equations

$$\begin{gathered}
\frac{\partial \sigma_{12}}{\partial x_2} + \frac{\partial \sigma_{13}}{\partial x_3} = 0, \\
\sigma_{1s} = 2\mu e_{1s}, \quad \alpha_1(x_1, 0, 0, t) = 0, \\
e_{1s} = \frac{1}{2}\Big(\frac{\partial \alpha_1}{\partial x_s} + x_2 \boldsymbol{d}_s \cdot \partial_{x_1}\boldsymbol{d}_2 + x_3 \boldsymbol{d}_s \cdot \partial_{x_1}\boldsymbol{d}_3\Big), \quad s \in \{2,3\}, \quad \text{in } S, \\
\sigma_{12}\nu_2 + \sigma_{13}\nu_3 = 0 \quad \text{on } \partial S.
\end{gathered}$$

Combining the equations, we easily check that

$$\alpha_1(\boldsymbol{x}, t) = \tau(x_1, t)\phi(x_2, x_3) \tag{2.8}$$

is the (unique) solution, where the so-called *warping function* ϕ (also called *torsion function*) satisfies

$$\frac{\partial^2\phi}{\partial x_2^2} + \frac{\partial^2\phi}{\partial x_3^2} = 0 \quad \text{in } S, \quad \phi(0,0) = 0,$$
$$\Big(\frac{\partial\phi}{\partial x_2} - x_3\Big)\nu_2 + \Big(\frac{\partial\phi}{\partial x_3} + x_2\Big)\nu_3 = 0 \quad \text{on } \partial S.$$

The warping function is a property of the cross section (if S is radially symmetric, then $\phi = 0$). In fact, out-of-plane deformations of the cross section do not have an analogue in plate or shell theories, as for bending it is meaningful to assume that plane sections remain plane after deformation (this can be demonstrated by bending a soft foam bar with stripes marked perpendicularly to the centreline).

See [Sad09] for methods of finding solutions to the torsion problem analytically as well as technical differences in case S is multiply connected.

2.2.2 Bending

Next we examine the other set of equations, related to bending:

$$\frac{\partial\sigma_{s2}}{\partial x_2} + \frac{\partial\sigma_{s3}}{\partial x_3} = 0,$$
$$\sigma_{rs} = 2\mu e_{rs} + \lambda(e_{11} + e_{22} + e_{33})\delta_{rs},$$
$$e_{rs} = \frac{1}{2}\Big(\frac{\partial\alpha_r}{\partial x_s} + \frac{\partial\alpha_s}{\partial x_r}\Big), \quad \alpha_s(x_1, 0, 0, t) = 0, \quad r, s \in \{2, 3\},$$
$$\sigma_{s2}\nu_2 + \sigma_{s3}\nu_3 = 0 \quad \text{on } \partial S, \quad s \in \{2, 3\}.$$

The classical solution of this boundary value problem is:

$$\alpha_2 = -\frac{\lambda}{2(\lambda+\mu)}\Big[-\kappa_3 x_2 x_3 - \frac{1}{2}\kappa_2(x_2^2 - x_3^2)\Big], \tag{2.9a}$$
$$\alpha_3 = -\frac{\lambda}{2(\lambda+\mu)}\Big[-\kappa_2 x_2 x_3 + \frac{1}{2}\kappa_3(x_2^2 - x_3^2)\Big]. \tag{2.9b}$$

We recall that $\frac{\lambda}{2(\lambda+\mu)}$ is Poisson's ratio, commonly denoted by ν. Another common material constant, Young's modulus $E = \frac{\mu(3\lambda+2\mu)}{\lambda+\mu}$, will appear in the sequel.

Determination of the extra displacements α_k, $k = 1, 2, 3$, is also an integral part of the variationally formulated model in [MM03]. By restricting their model to an isotropic material, Mora and Müller recover, in fact, formulas (2.8)–(2.9). In the ultrathin model for nanowires (see Chapter 3), $\boldsymbol{\alpha}$ has a discrete nature, since the cross section consists of a finite number of particles.

2.3 Bending and torsional rigidity

With the formulas for α_k it is now straightforward to express $\boldsymbol{e}$, $\boldsymbol{\sigma}$, and the $O(\delta)$ part of $\boldsymbol{T}^{(1)}$ in terms of κ_2, κ_3, τ, and ϕ. The resultant moment $\boldsymbol{M} = \boldsymbol{M}(x_1, t)$

about a point $\boldsymbol{y}(x_1,t)$ on the deformed axis of the stress vector $\boldsymbol{T}^{(1)}\boldsymbol{e}_1$ onto the cross section is

$$\boldsymbol{M} = \int_S (x_2\boldsymbol{d}_2 + x_3\boldsymbol{d}_3 + \boldsymbol{R}\alpha) \times \boldsymbol{T}^{(1)}\boldsymbol{e}_1 \mathrm{d}x_2\mathrm{d}x_3.$$

We write $\boldsymbol{M} = \boldsymbol{R}(\mathcal{M}_1, \mathcal{M}_2, \mathcal{M}_3)^\top$ and further assume[5] that $\frac{1}{h^2}\phi(x_2,x_3) = \phi(\frac{x_2}{h},\frac{x_3}{h}) = O(\delta^0)$ and $\frac{1}{h}\frac{\partial\phi}{\partial x_s}(x_2,x_3) = \frac{\partial\phi}{\partial x_s}(\frac{x_2}{h},\frac{x_3}{h}) = O(\delta^0)$ for $s = 2,3$. Using the expression for $\boldsymbol{T}^{(1)}$ and the choice of referential coordinate system, up to terms of order $O(\delta)$ we obtain

$$\begin{aligned} \mathcal{M}_1 &= \mu J\tau, \\ \mathcal{M}_2 &= -EI_3\kappa_3, \\ \mathcal{M}_3 &= EI_2\kappa_2, \end{aligned} \tag{2.10}$$

where the *second moments of area* are $I_s = \int_S x_s^2 \mathrm{d}x_2\mathrm{d}x_3$ with $s = 2$ or $s = 3$ and the *torsional rigidity*, calculated for the particular shape of a cross section, is defined as

$$J = \int_S x_2^2 + x_3^2 + x_2\frac{\partial\phi}{\partial x_3} - x_3\frac{\partial\phi}{\partial x_2}\mathrm{d}x_2\mathrm{d}x_3$$

(cf. [MM03, p. 298]). The products EI_2 and EI_2 are known as *bending stiffnesses*. (In this context the shear modulus μ is often denoted by G.)

2.4 Balance of angular momentum

Restricting the balance of linear momentum (2.5) to a segment of the form $(x_1-\eta, x_1+\eta)\times S$, dividing it by $\eta > 0$, and then letting $\eta \to 0+$, we find

$$\frac{\partial}{\partial x_1}\int_S \boldsymbol{T}^{(1)}\boldsymbol{e}_1\mathrm{d}x_2\mathrm{d}x_3 + \int_S \rho_0\boldsymbol{b}\mathrm{d}x_2\mathrm{d}x_3 = \int_S \rho_0\frac{\partial^2\boldsymbol{y}_{3\mathrm{D}}}{\partial t^2}\mathrm{d}x_2\mathrm{d}x_3 \text{ in } (0,L), \tag{2.11}$$

neglecting the $O(\delta^2)$ contribution from tractions on the lateral surface. Further, the balance of angular momentum for the rod can be expressed as

$$\int_{\partial\Omega} \boldsymbol{y}_{3\mathrm{D}} \times \boldsymbol{T}^{(1)}\boldsymbol{n}\,\mathrm{dS} + \int_\Omega \rho_0\boldsymbol{y}_{3\mathrm{D}}\times\boldsymbol{b}\mathrm{d}\boldsymbol{x} = \frac{\partial}{\partial t}\int_\Omega \rho_0\boldsymbol{y}_{3\mathrm{D}}\times\frac{\partial\boldsymbol{y}_{3\mathrm{D}}}{\partial t}\mathrm{d}\boldsymbol{x}.$$

In analogy to the previous step, we consider the above equation for an η-segment and in the limit $\eta \to 0+$ we get

$$\frac{\partial\boldsymbol{M}}{\partial x_1} + \frac{\partial}{\partial x_1}\int_S \boldsymbol{y}\times\boldsymbol{T}^{(1)}\boldsymbol{e}_1\,\mathrm{d}x_2\mathrm{d}x_3 + \int_S \rho_0\boldsymbol{y}_{3\mathrm{D}}\times\boldsymbol{b}\mathrm{d}x_2\mathrm{d}x_3 = \int_S \rho_0\boldsymbol{y}_{3\mathrm{D}}\times\frac{\partial^2\boldsymbol{y}_{3\mathrm{D}}}{\partial t^2}\mathrm{d}x_2\mathrm{d}x_3, \tag{2.12}$$

again leaving out the $O(\delta^2)$ lateral tractions. In a static equilibrium, combining (2.12) with (2.11) gives

$$\frac{\partial\boldsymbol{M}}{\partial x_1} + \frac{\partial\boldsymbol{y}}{\partial x_1} \times \int_S \boldsymbol{T}^{(1)}\boldsymbol{e}_1\mathrm{d}x_2\mathrm{d}x_3 + \int_S \rho_0\Big(\sum_{s=2}^{3} x_s\boldsymbol{d}_s + \boldsymbol{R}\boldsymbol{\alpha}\Big) \times \boldsymbol{b}\mathrm{d}x_2\mathrm{d}x_3 = \boldsymbol{0}.$$

[5] Dill [Dil92] proceeds by making strong assumptions on ϕ, probably motivated by the analytical solution $\phi_{\mathrm{e}}(x_2,x_3) = cx_2x_3$ for an elliptic cross section.

By formula (2.10) for the moments and by grouping the coefficients in front of each $\boldsymbol{d}_k$, this implies the following nonlinear system of ordinary differential equations:

$$\begin{aligned}
EI_2\kappa_2' + \kappa_3\tau(\mu J - EI_3) &= \int_S \rho_0\Big[\alpha_1 \boldsymbol{b}\cdot\boldsymbol{d}_2 - (x_2+\alpha_2)\boldsymbol{b}\cdot\boldsymbol{d}_1 - \boldsymbol{g}\cdot\boldsymbol{d}_2\Big]\mathrm{d}x_2\mathrm{d}x_3\\
EI_3\kappa_3' - \kappa_2\tau(\mu J - EI_2) &= \int_S \rho_0\Big[\alpha_1 \boldsymbol{b}\cdot\boldsymbol{d}_3 - (x_3+\alpha_3)\boldsymbol{b}\cdot\boldsymbol{d}_1 - \boldsymbol{g}\cdot\boldsymbol{d}_3\Big]\mathrm{d}x_2\mathrm{d}x_3\\
\mu J\tau' + \kappa_2\kappa_3(EI_3 - EI_2) &= \int_S \rho_0\Big[(x_2+\alpha_2)\boldsymbol{b}\cdot\boldsymbol{d}_3 - (x_3+\alpha_3)\boldsymbol{b}\cdot\boldsymbol{d}_2\Big]\mathrm{d}x_2\mathrm{d}x_3,
\end{aligned}$$

where f' denotes $\partial_{x_1} f$ for f depending on x_1 and $\boldsymbol{g} := \int_S \boldsymbol{T}^{(1)} e_1 \mathrm{d}x_2\mathrm{d}x_3$. An analogous system can be found in [MM08] on page 878, where it arises as the Euler–Lagrange equations of the elastic energy functional, which for an isotropic material takes the form

$$\mathcal{E}(\boldsymbol{y},\boldsymbol{d}_2,\boldsymbol{d}_3) := \int_0^L \tfrac{1}{2}\Big[E(I_2\kappa_2^2 + I_3\kappa_3^2) + \mu J\tau^2\Big]\mathrm{d}x_1 - \int_0^L \bar{\boldsymbol{g}}\cdot\boldsymbol{y}\,\mathrm{d}x_1$$

with $\bar{\boldsymbol{g}}\colon (0,L)\to\mathbb{R}^3$ being a forcing term. The first integrand also reminds of a classical expression for the stored energy density of a Kirchhoff rod (cf. [O'R17, Equation (5.64)]).

3. A bending-torsion theory for thin and ultrathin rods as a Γ-limit of atomistic models

'However, as is always the case for intuition-based models, an all-important experimental confirmation does not replace for a rigorous *justification*, that is, validation as a convincing approximation of an accepted parent theory.'

L. Falach, R. Paroni, and P. Podio-Guidugli [FPPG15]

3.1 Introduction

In this chapter, we treat continuum limits of discrete energies of the type

$$E^{(k)}(y^{(k)}) = \sum_{x \in \Lambda'_{\varepsilon_k}} W_{\text{cell}}\Big(\vec{y}^{(k)}(x)\Big) + \text{surface terms},$$

where Λ'_{ε_k} is an ε_k-fine cubic crystalline lattice in the shape of a thin rod, $y^{(k)}$ its deformation and the matrix $\vec{y}^{(k)}(x)$ describes the deformation of an atomic cube around the point x. Such cell energies W_{cell} cover the case of nearest neighbour and next-to-nearest neighbour interactions and appeared previously e.g. in [FT02, CDKM06, Sch06, SZ23a].

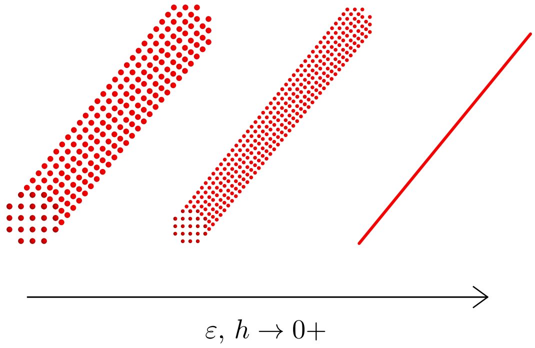
Section 2 sets up basic notation and introduces model assumptions that are common for the rest of this chapter. A compactness theorem is also formulated that complements theorems on Γ-convergence in the following sections. Having appeared in [MM03], the result needs only minor adjustments in our discrete framework.

We seek a limiting energy functional E_{lim} for the continuum model. To get a nontrivial limit with $k \to \infty$, we multiply the energy $E^{(k)}$ by the volume element ε_k^3 and divide it by the fourth power of the rod thickness h_k, which is the energy scaling corresponding to bending and torsion without extending the rod, cf. [MM03].

We are interested in two possible limit processes, which yield different effective models in the end (see Figure 3.1 for an illustration).

1. To model an *ultrathin rod* composed of a small number of atomic fibres, we let the interatomic distance $\varepsilon_k \to 0$ and keep h_k/ε_k fixed. This is the content of Section 3.3, which includes the Γ-convergence Theorem 3.5 – the main contribution in this chapter. Remarkably, even though this new *bending/torsion theory for ultrathin rods* thus derived can be related to the

Figure 3.1: An illustration of the simultaneous dimension reduction and discrete-to-continuum limit.



findings in [MM03], our elastic energy functional features a so-called *ultrathin correction* and surface terms, none of which would be present in a limiting theory based on the Cauchy-Born rule. Moreover, in the limiting functional we identify a discrete minimization formula accounting for warping the rod's cross section – a more complex ingredient than in plate theories from [Sch06] and [BS22]. With these traits, the author believes that the proposed effective model might describe very thin 1D nanostructures more accurately than would conventional elasticity.

2. When the numbers of atoms in the rod in the directions x_1, x_2, x_3 are large, we speak of a *thin rod* and study the simultaneous limit with $\varepsilon_k \to 0$ and $h_k \to 0$ in such a way that $\frac{h_k}{\varepsilon_k} \to \infty$. In this regime, which is investigated in Section 3.4, all discreteness fades away and we recover the continuum functional from [MM03] (see Theorem 3.8).

For ease of notation, we only consider $\varepsilon_k := 1/k$ in the following, but it would be possible to work with arbitrary interatomic distances too, see [BS22].

3.2 Notation, common model assumptions

3.2.1 Discrete model

Our starting point is an atomistic interaction model for an elastic rod. We consider a cubic atomic lattice Λ_k, given by

$$\Lambda_k = \left([0,L] \times \frac{1}{k}\overline{S_k}\right) \cap \frac{1}{k}\mathbb{Z}^3,$$

where $\frac{1}{k}$ is the interatomic spacing and $L > 0$ denotes the length of the rod. Its cross section is the polygonal set $\emptyset \neq S_k \subset \mathbb{R}^2$ (possibly not simply connected) determining a cross-sectional lattice $\mathcal{L}_k := \overline{S_k} \cap \mathbb{Z}^2$ and for which there is a set $\mathcal{L}'_k \subset (\frac{1}{2} + \mathbb{Z})^2$ such that

$$S_k = \operatorname{Int} \bigcup_{x' \in \mathcal{L}'_k} \left(x' + \left[-\frac{1}{2}, \frac{1}{2}\right]^2\right). \tag{3.1}$$

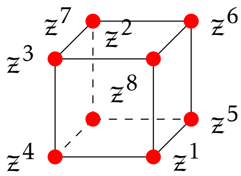
(It is assumed that $x' \in \mathcal{L}'_k$ whenever $x' + \{-\frac{1}{2}, \frac{1}{2}\}^2 \subset \mathcal{L}_k$ – like this we avoid holes that are too narrow to be interaction-free.) If $S_k = S$ is a fixed cross section that does not depend on k we will speak of an *ultrathin* rod. The rod's thickness is then comparable to the typical interatomic spacing. By contrast, in a *thin* rod the scaled cross section $\frac{1}{k} S_k$ eventually exhausts a domain of diameter h, where $\frac{1}{k} \ll h \ll 1$. We use the symbol Λ'_k for the lattice of midpoints of open cubes with sidelength $1/k$ and corners in Λ_k.

These set-ups may be described simultaneously by our fixing a positive null sequence (h_k) with $h_k \geq 1/k$ that we choose as equal to $1/k$ in the ultrathin case and for which we suppose $kh_k \to \infty$ for merely thin rods. We then assume that there exists a fixed bounded Lipschitz domain $S \subset \mathbb{R}^2$ such that the above S_k is the unique largest (in terms of cardinality) connected set of the form (3.1) that is contained in $kh_k S$.

The lattice Λ_k corresponds to an undeformed reference configuration that is subject to a static deformation $y^{(k)} \colon \Lambda_k \to \mathbb{R}^3$, which stores elastic energy into the rod. As the energy originates from interactions of nearby atoms we introduce a rescaling to atomic units by passing to a rescaled lattice with unit distances between atoms.

Points in this lattice are distinguished using the hat diacritic – here for a point $x = (x_1, x_2, x_3) \in \mathbb{R}^3$ we write $\hat{x}_1 := kx_1$, $\hat{x}' = (\hat{x}_2, \hat{x}_3) := kx' = k(x_2, x_3)$ and $\hat{y}^{(k)}(\hat{x}_1, \hat{x}_2, \hat{x}_3) := ky^{(k)}(\frac{1}{k}\hat{x}_1, \frac{1}{k}\hat{x}')$ so that $\hat{y}^{(k)} \colon k\Lambda_k \to \mathbb{R}^3$. Then $\hat{\Lambda}_k$, $\hat{\Lambda}'_k$ stand for the sets of all $\hat{x} = (\hat{x}_1, \hat{x}_2, \hat{x}_3)$ such that the corresponding downscaled points x lie in the lattices Λ_k, Λ'_k, respectively. We introduce eight direction vectors $\mathfrak{z}^1, \ldots, \mathfrak{z}^8$:

$$
\begin{aligned}
\mathfrak{z}^1 &= \tfrac{1}{2}(-1,-1,-1)^\top, & \mathfrak{z}^5 &= \tfrac{1}{2}(+1,-1,-1)^\top,\\
\mathfrak{z}^2 &= \tfrac{1}{2}(-1,-1,+1)^\top, & \mathfrak{z}^6 &= \tfrac{1}{2}(+1,-1,+1)^\top,\\
\mathfrak{z}^3 &= \tfrac{1}{2}(-1,+1,+1)^\top, & \mathfrak{z}^7 &= \tfrac{1}{2}(+1,+1,+1)^\top,\\
\mathfrak{z}^4 &= \tfrac{1}{2}(-1,+1,-1)^\top, & \mathfrak{z}^8 &= \tfrac{1}{2}(+1,+1,-1)^\top.
\end{aligned}
$$



This allows us to collect into a matrix the information about the deformation of a unit cell $\hat{x} + \{-\frac{1}{2}, \frac{1}{2}\}^3$, $\hat{x} \in \hat{\Lambda}'_k$:

$$
\vec{y}^{(k)}(\hat{x}) = (\hat{y}^{(k)}(\hat{x} + \mathfrak{z}^1) | \cdots | \hat{y}^{(k)}(\hat{x} + \mathfrak{z}^8)) \in \mathbb{R}^{3 \times 8}.
$$

With $\langle \hat{y}^{(k)}(\hat{x}) \rangle = \frac{1}{8} \sum_{i=1}^{8} \hat{y}^{(k)}(\hat{x} + \mathfrak{z}^i)$, $\hat{x} \in \hat{\Lambda}'_k$, we further define the discrete gradient

$$
\bar{\nabla} \hat{y}^{(k)}(\hat{x}) = \vec{y}^{(k)}(\hat{x}) - \langle \hat{y}^{(k)}(\hat{x}) \rangle (1, \ldots, 1) \in \mathbb{R}^{3 \times 8}.
$$

Then the matrix $\bar{\mathrm{Id}} = (\mathfrak{z}^1 | \cdots | \mathfrak{z}^8) \in \mathbb{R}^{3 \times 8}$ is the discrete gradient of $\hat{y}^{(k)} = \mathrm{id}$. Note that a discrete gradient has the sum of columns equal to 0.

There are two more important subsets of $\mathbb{R}^{3 \times 8}$, used for characterizing rigid motions:

$$
\bar{\mathrm{SO}}(3) := \{R \bar{\mathrm{Id}};\ R \in \mathrm{SO}(3)\}, \qquad V_0 := \{(c | \cdots | c) \in \mathbb{R}^{3 \times 8};\ c \in \mathbb{R}^3\}.
$$

3.2.2 Rescaling, interpolation and extension

It is desirable to have the deformations defined on a common domain $\Omega := (0,L)\times S$, independent of k, in order to handle their convergence. Given a positive null sequence (h_k) such that $h_k \geq 1/k$ (and $h_k = 1/k$ in the ultrathin case) set $\tilde{y}^{(k)}(x_1,x_2,x_3) := y^{(k)}(x_1,h_k x')$ for $(x_1,h_k x')\in\Lambda_k$. Furthermore, we introduce an interpolation of $\tilde{y}^{(k)}$ so that it is also defined outside lattice points.

Let $\tilde{z}^i = (\frac{1}{k}z_1^i, \frac{1}{kh_k}z_2^i, \frac{1}{kh_k}z_3^i)$ and $\tilde{\Lambda}_k' = \{\xi\in\mathbb{R}^3;\ (k\xi_1, kh_k\xi')\in\hat{\Lambda}_k'\}$. We split every block $\tilde{Q}(\bar{x}) = \bar{x} + [-\frac{1}{2k},\frac{1}{2k}]\times[-\frac{1}{2kh_k},\frac{1}{2kh_k}]^2$, $\bar{x}\in\tilde{\Lambda}_k'$, into 24 simplices as in [Sch06, BS22] and get a piecewise affine interpolation of $\tilde{y}^{(k)}$, which we denote again by $\tilde{y}^{(k)}$. More precisely, set $\tilde{y}^{(k)}(\bar{x}) := \frac{1}{8}\sum_{i=1}^{8}\tilde{y}^{(k)}(\bar{x}+\tilde{z}^i)$ and for each face $\tilde{F}$ of the block $\tilde{Q}(\bar{x})$ and the corresponding centre $x_{\tilde{F}}$ of the face $\tilde{F}$, define $\tilde{y}^{(k)}(x_{\tilde{F}}) := \frac{1}{4}\sum_j \tilde{y}^{(k)}(\bar{x}+\tilde{z}^j)$, where we sum over all j such that $\bar{x}+\tilde{z}^j$ is a corner of $\tilde{F}$. In fact, a face can be labelled as $\tilde{F}_{ij}$ if it has $\bar{x}+\tilde{z}^i$ and $\bar{x}+\tilde{z}^j$ such that $|z^i - z^j| = 1$ as vertices; the ambiguity in this notation can be resolved by using the order of indices. Then, let $\tilde{y}^{(k)}$ be interpolated in an affine way on every simplex $\tilde{T}_{ij} = \mathrm{conv}\{\bar{x},\bar{x}+\tilde{z}^i,\bar{x}+\tilde{z}^j,x^{ij}\}$ with x^{ij} being the centre of the face $\tilde{F}_{ij}$, so that $\tilde{y}^{(k)}$ is everywhere continuous.

We thus obtain $\tilde{y}^{(k)}\colon [0,L_k]\times\bar{S}_k\to\mathbb{R}^3$, where we have abbreviated $L_k := \lfloor kL\rfloor/k$. It satisfies

$$\tilde{y}^{(k)}(x_{\tilde{F}}) = \fint_{\tilde{F}} \tilde{y}^{(k)}\,\mathrm{d}\mathcal{H}^2, \quad \tilde{y}^{(k)}(\bar{x}) = \fint_{\tilde{Q}(x)} \tilde{y}^{(k)}(\xi)\,\mathrm{d}\xi \tag{3.2}$$

for any face $\tilde{F}$ of $\tilde{Q}(x)$ with face centre $x_{\tilde{F}}$.

Setting $\nabla_k\tilde{y}^{(k)} := \left(\frac{\partial\tilde{y}^{(k)}}{\partial x_1}\,\middle|\, h_k^{-1}\frac{\partial\tilde{y}^{(k)}}{\partial x_2}\,\middle|\, h_k^{-1}\frac{\partial\tilde{y}^{(k)}}{\partial x_3}\right)$, we proceed with an auxiliary result.

Lemma 3.1. *There are $c, C > 0$ such that for any $k\in\mathbb{N}$, $h_k > 0$ and lattice block $\tilde{Q}(\bar{x}) = \bar{x} + [-\frac{1}{2k},\frac{1}{2k}]\times[-\frac{1}{2kh_k},\frac{1}{2kh_k}]^2$ with centre $\bar{x}\in\tilde{\Lambda}_k'$ and corresponding $\hat{x} = (k\bar{x}_1, kh_k\bar{x}')\in\hat{\Lambda}_k'$,*

$$c|\bar{\nabla}\hat{y}^{(k)}(\hat{x})|^2 \leq k^3h_k^2\int_{\tilde{Q}(\bar{x})}|\nabla_k\tilde{y}^{(k)}|^2\mathrm{d}\xi \leq C|\bar{\nabla}\hat{y}^{(k)}(\hat{x})|^2. \tag{3.3}$$

Proof. The statement is contained in [Sch09, Lemma 3.5]. □

In a tubular neighbourhood of the rod we now construct an extension to 'ghost atoms' whose rigidity is controlled by the original atom positions. For $m\in\mathbb{N}$ set

$$\begin{aligned}
\mathcal{L}_k^{\mathrm{ext}} &= \mathcal{L}_k + \{-m,\dots,m\}^2, & \Lambda_k^{\mathrm{ext}} &= \{-\tfrac{1}{k},0,\dots,L_k+\tfrac{1}{k}\}\times\tfrac{1}{k}\mathcal{L}_k^{\mathrm{ext}},\\
\mathcal{L}_k^{\prime,\mathrm{ext}} &= \mathcal{L}_k' + \{-m,\dots,m\}^2 & \Lambda_k^{\prime,\mathrm{ext}} &= \{-\tfrac{1}{2k},\tfrac{1}{2k},\dots,L_k+\tfrac{1}{2k}\}\times\tfrac{1}{k}\mathcal{L}^{\prime,\mathrm{ext}}\\
S_k^{\mathrm{ext}} &= S_k + (-m,m)^2, & \Omega_k^{\mathrm{ext}} &= (-\tfrac{1}{k},L_k+\tfrac{1}{k})\times\frac{1}{kh_k}S_k^{\mathrm{ext}}.
\end{aligned}$$

We suppress m, which will be a fixed constant, from our notation. It will be equal to 1 for ultrathin rods and ≥ 1 such that $S_k^{\mathrm{ext}}\supset kh_kS$ for thin rods. We also consider the lattices $\tilde{\Lambda}_k^{\mathrm{ext}}$ and $\tilde{\Lambda}_k^{\prime,\mathrm{ext}}$ that are related to their unrescaled versions Λ_k^{ext} and $\Lambda_k^{\prime,\mathrm{ext}}$ like we saw it for $\tilde{\Lambda}_k'$ above.

Our extension follows a scheme from [Sch09, Section 3.1], see in particular [Sch09, Lemmas 3.1, 3.2 and 3.4] and cf. also [BS22, Lemma 3.1]. Notice that for our choice of S_k as the largest connected set of the form (3.1) that is contained in kh_kS for a bounded Lipschitz domain $S \subset \mathbb{R}^2$ in particular guarantees that there is a constant $C > 0$, independent of k, such that for any two points $\hat{x}', \hat{y}' \in \mathcal{L}_k'$

$$\mathrm{dist}_{\mathcal{L}_k'}(\hat{x}', \hat{y}') \le C|\hat{x}' - \hat{y}'|,$$

where

$$\mathrm{dist}_{\mathcal{L}_k'}(\hat{x}', \hat{y}') = \min\Big\{N \in \mathbb{N}_0 : \\ \exists\, \hat{x}' = \hat{x}_0', \dots, \hat{x}_N' = \hat{y}' \in \mathcal{L}_k' \text{ with } |\hat{x}_{n+1} - \hat{x}_n| = 1\, \forall\, n < N\Big\}$$

denotes the lattice geodesic distance of two elements $\hat{x}', \hat{y}' \in \mathcal{L}_k'$.

Lemma 3.2. *There are extensions $y^{(k)} \colon \Lambda_k^{\mathrm{ext}} \to \mathbb{R}^3$ such that their interpolations $\tilde{y}^{(k)}$ satisfy*

$$\operatorname{ess\,sup}_{\Omega_k^{\mathrm{ext}}} \mathrm{dist}^2(\nabla_k \tilde{y}^{(k)}, \mathrm{SO}(3)) \le C \operatorname{ess\,sup}_{(0,L_k)\times \frac{1}{kh_k}S_k} \mathrm{dist}^2(\nabla_k \tilde{y}^{(k)}, \mathrm{SO}(3))$$

and

$$\int_{\Omega_k^{\mathrm{ext}}} \mathrm{dist}^2(\nabla_k \tilde{y}^{(k)}, \mathrm{SO}(3))\mathrm{d}x \le C \int_{(0,L_k)\times \frac{1}{kh_k}S_k} \mathrm{dist}^2(\nabla_k \tilde{y}^{(k)}, \mathrm{SO}(3))\mathrm{d}x.$$

Proof. Let $y^{(k)} \colon \Lambda_k \to \mathbb{R}^3$ be a lattice deformation. We partition $\Lambda_k^{\prime,\mathrm{ext}} \setminus \Lambda_k'$ into the 8 sublattices $\Lambda_{k,i}' = (\Lambda_k^{\prime,\mathrm{ext}} \setminus \Lambda_k') \cap \frac{1}{k}(z^i + 2\mathbb{Z}^3)$ and apply the following extension procedure consecutively for $i = 1, \dots, 8$:

If $x \in \Lambda_{k,i}'$ we write $\mathcal{B}_R(x)$ for the set of those $z \in \Lambda_k^{\prime,\mathrm{ext}}$ with $|z - x| \le R/k$ for which $y^{(k)}(z + \frac{1}{k}z^j)$ is defined already for all j with $1 \le j \le 8$. Now if $\mathcal{B}_1(x) \neq \emptyset$, extend $y^{(k)}$ to all $z + \frac{1}{k}z^j$, $1 \le j \le 8$, by choosing an extension such that $\mathrm{dist}^2(\bar{\nabla}\hat{y}^{(k)}(\hat{x}), \mathrm{SO}(3)\bar{\mathrm{Id}})$ is minimal.

Due to [Sch09, Lemma 3.1] and the property of lattice geodesics within $\mathcal{L}_k'$, this distance will then be controlled by

$$C \sum_{z \in \mathcal{B}_R(x)} \mathrm{dist}^2(\bar{\nabla}\hat{y}^{(k)}(\hat{z}), \bar{\mathrm{SO}}(3)),$$

for some uniformly bounded R. We repeat this extension step $8m$ times. $\square$

Remark 3.1. The construction implies that for ultrathin rods, the following local estimate holds: For any $x \in \Lambda_k^{\prime,\mathrm{ext}}$, defining $\mathcal{U}(x) = \Big(\{x_1 - \frac{1}{k}, x_1, x_1 + \frac{1}{k}\} \times \frac{1}{k}\mathcal{L}_k'\Big) \cap \Lambda_k'$ we have

$$\mathrm{dist}^2(\bar{\nabla}\hat{y}^{(k)}(\hat{x}), \bar{\mathrm{SO}}(3)) \le C \sum_{\xi \in k\mathcal{U}(x)} \mathrm{dist}^2(\bar{\nabla}\hat{y}^{(k)}(\xi), \bar{\mathrm{SO}}(3)).$$

3.2.3 Elastic energy

In the expression for total elastic energy, we group contributions from individual atomic cells (cf. [CDKM06, Sch06]).

Definition 3.2.1. *We say that* $W\colon \mathbb{R}^{3\times 8} \to [0,\infty)$ *is a* full cell energy function *if the following assertions hold true:*

(E1) Frame-indifference: $W(R\vec{y} + (c|\cdots|c)) = W(\vec{y})$, $R \in \mathrm{SO}(3)$, $\vec{y} \in \mathbb{R}^{3\times 8}$, $c \in \mathbb{R}^3$,

(E2) W attains its minimum (equal to 0) at and only at all rigid deformations, i.e. deformations $\vec{y} = (\hat{y}_1|\cdots|\hat{y}_8)$ *with* $\hat{y}_i = Rz^i + c$ *for all* $i \in \{1,\dots,8\}$ *and some* $R \in \mathrm{SO}(3)$, $c \in \mathbb{R}^3$,

(E3) W is everywhere Borel measurable and of class $\mathcal{C}^2$ *in a neighbourhood of* $\bar{\mathrm{SO}}(3)$ *and the quadratic form associated with* $\nabla^2 W(\bar{\mathrm{Id}})$ *is positive definite when restricted to* $\mathrm{span}\{V_0 \cup \mathbb{R}^{3\times 3}_{\mathrm{skew}}\bar{\mathrm{Id}}\}^\perp$,

(E4) $\liminf_{\substack{|\vec{y}|\to\infty,\\ \vec{y}\in V_0^\perp}} \frac{W(\vec{y})}{|\vec{y}|^2} > 0.$

We say that $W\colon \mathbb{R}^{3\times 8} \to [0,\infty)$ *is a* partial cell energy function *if it fulfils (E1) together with*

(E2') W equals zero for all rigid deformations,

(E3') W is everywhere Borel measurable and of class $\mathcal{C}^2$ *in a neighbourhood of* $\bar{\mathrm{SO}}(3)$.

Trivially, we see that $W \equiv 0$ is a partial cell energy function.

To model surface energy, let $\mathfrak{T}$ be the power set of $\{1,\dots,8\}$. We classify the cells centred at $\hat{\Lambda}_k'^{,\mathrm{ext}} = k\Lambda_k'^{,\mathrm{ext}}$ by the set of corners they share with $\hat{\Lambda}_k$, i.e. $\mathrm{t}_k(\hat{x}) = \left\{i \in \{1,\dots,8\};\ \hat{x} + z^i \in \hat{\Lambda}_k\right\}$ for $\hat{x} \in \hat{\Lambda}_k'^{,\mathrm{ext}}$. (Obviously, $\mathrm{t}_k(\hat{x}) = \{1,\dots,8\}$ iff $\hat{x} \in \hat{\Lambda}_k'$ and $\mathrm{t}_k(\hat{x}) \neq \emptyset$ iff $\hat{x} \in \hat{\Lambda}_k'^{,\mathrm{ext}}$ for the specific choice $m = 1$.) Also note that on the lateral boundary, i.e. for $\hat{x}_1 \notin \{-\frac{1}{2}, kL_k + \frac{1}{2}\}$, we have $i \in \mathrm{t}_k(\hat{x})$ iff $i + 4 \in \mathrm{t}_k(\hat{x})$ for $i = 1,2,3,4$ and so $\mathrm{t}_k(\hat{x}) = \mathrm{t}_k(\hat{x}') := \left\{i \in \{1,\dots,8\} : \hat{x}' + (z^i)' \in \mathcal{L}_k\right\}$. Let $\hat{\Lambda}_k'^{,\mathrm{surf}} = \{\frac{1}{2},\dots,kL_k - \frac{1}{2}\} \times (\mathcal{L}_k'^{,\mathrm{ext}} \setminus \mathcal{L}_k')$ and $\hat{\Lambda}_k'^{,\mathrm{end}} = \{-\frac{1}{2}, kL_k + \frac{1}{2}\} \times \mathcal{L}_k'^{,\mathrm{ext}}$. Our total elastic interaction energy reads

$$\begin{aligned} E^{(k)}(y^{(k)}) = \sum_{\hat{x}\in\hat{\Lambda}_k'} W_{\mathrm{cell}}\Big(\vec{y}^{(k)}(\hat{x})\Big) + \sum_{\hat{x}\in\hat{\Lambda}_k'^{,\mathrm{surf}}} W_{\mathrm{surf}}\Big(\mathrm{t}_k(\hat{x}'), \vec{y}^{(k)}(\hat{x})\Big) \\ + \sum_{\hat{x}\in\hat{\Lambda}_k'^{,\mathrm{end}}} W_{\mathrm{end}}\Big(\mathrm{t}_k(\hat{x}), \vec{y}^{(k)}(\hat{x})\Big), \end{aligned} \tag{3.4}$$

where W_{cell} is a full cell energy and $W_{\mathrm{surf}}(\mathrm{t},\cdot)$, $W_{\mathrm{end}}(\mathrm{t},\cdot)$ with $\mathrm{t} \in \mathfrak{T}$ are partial cell energy functions according to Definition 3.2.1. In order to avoid artificial contributions we assume that the values of $W_{\mathrm{surf}}(\mathrm{t},\vec{y})$ and $W_{\mathrm{end}}(\mathrm{t},\vec{y})$, $\vec{y} = (\hat{y}_1|\cdots|\hat{y}_8)$, may depend on $\hat{y}_i$ only if $i \in \mathrm{t}$.

We remark that the terms involving W_{end} for cells near the rod's endpoints vanish as $k \to \infty$ for both ultrathin and thin rods. While for thin rods also the lateral boundary contributions vanish, this is no longer the case for ultra-thin rods. Our set-up allows us to model extra-cross-sectional interactions of atoms which lie in different atomic cells but which are, in fact, their mutual neighbours due to the cross section's potentially jagged shape.

Hereafter we write Q_{cell} and $Q_{\mathrm{surf}}(\mathrm{t},\cdot)$ for the quadratic forms generated by $\nabla^2 W_{\mathrm{cell}}(\bar{\mathrm{Id}})$ and $\nabla^2 W_{\mathrm{surf}}(\mathrm{t},\bar{\mathrm{Id}})$, $\mathrm{t} \in \mathcal{T}$, respectively.

Example 3.1. To explain the motivation behind W_{surf} and W_{end}, let us consider a simple mass-spring model with harmonic springs for a rod with its cross section determined by $\mathcal{L}'_k \equiv \mathcal{L}' = \{-\frac{1}{2}, \frac{1}{2}, \frac{3}{2}\}^2 \cup \{(\frac{1}{2}, -\frac{3}{2}), (\frac{1}{2}, \frac{5}{2})\}$ ($m := 1$). The aim is to rewrite

$$E^{(k)}(y) = \frac{1}{2} \sum_{\substack{\hat{x}_*, \hat{x}_{**} \in \hat{\Lambda}_k \\ |\hat{x}_* - \hat{x}_{**}| = 1}} \frac{K_1}{2} (|\hat{y}(\hat{x}_*) - \hat{y}(\hat{x}_{**})| - 1)^2 + \frac{1}{2} \sum_{\substack{\hat{x}_*, \hat{x}_{**} \in \hat{\Lambda}_k \\ |\hat{x}_* - \hat{x}_{**}| = \sqrt{2}}} \frac{K_2}{2} (|\hat{y}(\hat{x}_*) - \hat{y}(\hat{x}_{**})| - \sqrt{2})^2$$

using W_{cell}, W_{surf}, and W_{end} ($K_1 > 0$ and $K_2 > 0$ are constant stiffnesses). While in the bulk, we set

$$W_{\mathrm{cell}}(\vec{y}) = \frac{1}{8} \sum_{|\bar{z}^i - \bar{z}^j| = 1} \frac{K_1}{2} (|\hat{y}_i - \hat{y}_j| - 1)^2 + \frac{1}{4} \sum_{|\bar{z}^i - \bar{z}^j| = \sqrt{2}} \frac{K_2}{2} (|\hat{y}_i - \hat{y}_j| - \sqrt{2})^2,$$

the functions $W_{\mathrm{surf}}(\mathrm{t}_k(\frac{5}{2}, \frac{3}{2}), \cdot)$, $W_{\mathrm{surf}}(\mathrm{t}_k(-\frac{3}{2}, \frac{3}{2}), \cdot)$ etc., and W_{end} in turn include surface terms, e.g.

$$W_{\mathrm{surf}}\Big(\mathrm{t}_k\Big(\tfrac{5}{2}, \tfrac{1}{2}\Big), \vec{y}\Big) = W_{\mathrm{surf}}\Big(\{3,4,7,8\}, \vec{y}\Big) = \sum_{i \in \{3,7\}} \frac{K_1}{8} (|\hat{y}_{i+1} - \hat{y}_i| - 1)^2$$

$$+ \sum_{i=3}^{4} \frac{K_1}{8} (|\hat{y}_{i+4} - \hat{y}_i| - 1)^2 + \frac{K_2}{4} (|\hat{y}_7 - \hat{y}_4| - \sqrt{2})^2 + \frac{K_2}{4} (|\hat{y}_8 - \hat{y}_3| - \sqrt{2})^2,$$

$$W_{\mathrm{end}}\Big(\mathrm{t}_k\Big(-\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}\Big), \vec{y}\Big) = W_{\mathrm{end}}\Big(\{5,6,7,8\}, \vec{y}\Big) = \sum_{i=1}^{3} \frac{K_1}{8} (|\hat{y}_{i+1} - \hat{y}_i| - 1)^2$$

$$+ \frac{K_1}{8} (|\hat{y}_4 - \hat{y}_1| - 1)^2 + \sum_{i=1}^{2} \frac{K_2}{4} (|\hat{y}_{i+2} - \hat{y}_i| - \sqrt{2})^2.$$

The auxiliary square $Q'(x'_{\mathrm{e}}) = x'_{\mathrm{e}} + (-\frac{1}{2}, \frac{1}{2})^2$ centred at $x'_{\mathrm{e}} := (\frac{3}{2}, \frac{5}{2})$ is adjacent to two physically relevant cross-sectional squares, so in particular, the atoms with x'-coordinates $(2,2)$ and $(1,3)$, belonging to different 'real' atomic squares $Q'(\frac{1}{2}, \frac{5}{2})$ and $Q'(\frac{3}{2}, \frac{3}{2})$, can still interact – this interaction should be comprised in $W_{\mathrm{surf}}(\mathrm{t}_k(x'_{\mathrm{e}}), \cdot)$. Like this, $E^{(k)}$ is expressible by (3.4). After adding a suitable penalty term positive in a neighbourhood of $\mathrm{O}(3)\bar{\mathrm{Id}} \setminus \bar{\mathrm{SO}}(3)$, such W_{cell}, W_{surf}, and W_{end} fulfil all the assumptions for our results to apply.

Remark 3.2. In a more general case we now find an expression for the quadratic form Q_{cell}. If $E^{(k)}$ is given by

$$E^{(k)}(y) = \frac{1}{2} \sum_{\substack{\hat{x}_*, \hat{x}_{**} \in \hat{\Lambda}_k \\ |\hat{x}_* - \hat{x}_{**}| = 1}} W_{\mathrm{NN}}(|\hat{y}(\hat{x}_*) - \hat{y}(\hat{x}_{**})|) + \frac{1}{2} \sum_{\substack{\hat{x}_*, \hat{x}_{**} \in \hat{\Lambda}_k \\ |\hat{x}_* - \hat{x}_{**}| = \sqrt{2}}} W_{\mathrm{NNN}}\Big(\frac{|\hat{y}(\hat{x}_*) - \hat{y}(\hat{x}_{**})|}{\sqrt{2}}\Big),$$

where $W_{\mathrm{NN(N)}}\colon [0,\infty) \to [0,\infty)$ is continuous on $[0,\infty)$ and $\mathcal{C}^2$ in a neighbourhood of 1 with $W''_{\mathrm{NN(N)}}(1) > 0$ and $W_{\mathrm{NN(N)}}(r) = 0$ if and only if $r = 1$, then the corresponding W_{cell} is

$$W_{\mathrm{cell}}(\vec{y}) = \frac{1}{8} \sum_{|\bar{z}^i - \bar{z}^j| = 1} W_{\mathrm{NN}}(|\hat{y}_i - \hat{y}_j|) + \frac{1}{4} \sum_{|\bar{z}^i - \bar{z}^j| = \sqrt{2}} W_{\mathrm{NNN}}\Big(\frac{|\hat{y}_i - \hat{y}_j|}{\sqrt{2}}\Big)$$

and

$$\begin{aligned} Q_{\mathrm{cell}}(\bar{H}) = \tfrac{1}{4} W''_{\mathrm{NN}}(1)\Big[&(H_{32}-H_{31})^2 + (H_{23}-H_{22})^2 + (H_{34}-H_{33})^2 + (H_{21}-H_{24})^2 \\ &+(H_{15}-H_{11})^2 + (H_{16}-H_{12})^2 + (H_{17}-H_{13})^2 + (H_{18}-H_{14})^2 + \\ &+(H_{36}-H_{35})^2 + (H_{27}-H_{26})^2 + (H_{38}-H_{37})^2 + (H_{25}-H_{28})^2\Big] \\ +\tfrac{1}{4} W''_{\mathrm{NNN}}(1)\Big[&(H_{23}-H_{21}+H_{33}-H_{31})^2 + (H_{22}-H_{24}+H_{34}-H_{32})^2 \\ &+(H_{16}-H_{11}+H_{36}-H_{31})^2 + (H_{15}-H_{12}+H_{32}-H_{35})^2 \\ &+(H_{18}-H_{11}+H_{28}-H_{21})^2 + (H_{14}-H_{15}+H_{25}-H_{24})^2 \\ &+(H_{17}-H_{12}+H_{27}-H_{22})^2 + (H_{13}-H_{16}+H_{26}-H_{23})^2 \\ &+(H_{17}-H_{14}+H_{37}-H_{34})^2 + (H_{13}-H_{18}+H_{38}-H_{33})^2 \\ &+(H_{27}-H_{25}+H_{37}-H_{35})^2 + (H_{26}-H_{28}+H_{38}-H_{36})^2\Big] \end{aligned}$$

for any $\bar{H} \in \mathbb{R}^{3\times 8}$ with components H_{ij}.

Lemma 3.3. *Under the assumptions of Lemma 3.1, let W be a full cell energy function. Then*

$$k^3 h_k^2 \int_{\tilde{Q}(\bar{x})} \mathrm{dist}^2(\nabla_k \tilde{y}^{(k)}(\xi), \mathrm{SO}(3))\mathrm{d}\xi \le C W\big(\bar{\nabla}\hat{y}^{(k)}(\hat{x})\big). \tag{3.5}$$

Proof. See [Sch06, Lemma 3.2]; the claim is only restated in our notation. □

3.2.4 Compactness of low-energy sequences

We provide a compactness theorem that complements our Γ-convergence results in the following sections and is also the first step towards their proofs. It is based on Theorem 1.1 (a now well-known result about geometric rigidity from [FJM02]) and is essentially contained in [MM03].

We fix a null sequence (h_k) with $\frac{1}{k} \le h_k$ and abbreviate $h_k' = \frac{1}{k}\lfloor k h_k \rfloor$. Set $\Omega_k = (0, L_k) \times \frac{1}{k h_k} S_k$.

Theorem 3.4. *Let $(\tilde{y}^{(k)})_{k=1}^{\infty}$ be a sequence with $y^{(k)}\colon \Lambda_k^{\mathrm{ext}} \to \mathbb{R}^3$ such that their interpolations $\tilde{y}^{(k)}$ constructed in Section 3.2.2 satisfy the estimate*

$$\limsup_{k\to\infty} \frac{1}{h_k^2} \int_{\Omega_k} \mathrm{dist}^2(\nabla_k \tilde{y}^{(k)}, \mathrm{SO}(3))\mathrm{d}x < \infty. \tag{3.6}$$

Then, there exist a (not relabelled) subsequence $(\tilde{y}^{(k)})$ and a sequence of piecewise constant mappings $R^{(k)}\colon \mathbb{R} \to \mathrm{SO}(3)$ whose discontinuity set is contained in $\{h'_k, 2h'_k, \ldots, (\lfloor L_k/h'_k \rfloor - 1)h'_k\}$ such that

$$R^{(k)} \to R \text{ in } L^2([0,L];\mathbb{R}^{3\times3}), \tag{3.7}$$

where $R \in \mathrm{SO}(3)$ a.e. and $R(x_1) = \left(\frac{\partial \tilde{y}}{\partial x_1}(x) \middle| d_2(x) \middle| d_3(x)\right)$ for $\tilde{y} \in H^2(\Omega;\mathbb{R}^3)$, $d_s \in H^1(\Omega;\mathbb{R}^3)$, $s = 2,3$, that are independent of x_2 and x_3. Moreover, we have

$$\int_{\Omega_k^{\text{ext}}} |\nabla_k \tilde{y}^{(k)} - R^{(k)}|^2 \mathrm{d}x \le Ch_k^2. \tag{3.8}$$

and

$$|R^{(k)}(ih'_k + \tfrac{3}{2}h'_k) - R^{(k)}(ih'_k + \tfrac{1}{2}h'_k)|^2 \le \frac{C}{h_k} \|\mathrm{dist}(\nabla_k \tilde{y}^{(k)}, \mathrm{SO}(3))\|^2_{L^2((u_i^{(k)}, v_i^{(k)}) \times S_k^{\text{ext}})}, \tag{3.9}$$

where $u_i^{(k)} = ih'_k$, $v_i^{(k)} = u_i^{(k)} + 2h_k$ for $i = 1, \ldots, \lfloor L_k/h'_k \rfloor - 3$, $u_0^{(k)} = -\frac{1}{k}$, $v_0^{(k)} = -\frac{1}{k} + 3h_k$ and $u_i^{(k)} = \min\{(\lfloor L_k/h'_k \rfloor - 2)h'_k, L_k + \frac{1}{k} - 3h_k\}$, $v_i^{(k)} = L_k + \frac{1}{k}$ for $i = \lfloor L_k/h'_k \rfloor - 2$.

Note that in the ultrathin case one has $h_k = 1/k$ and hence $h'_k = \frac{1}{k}$ so that $(\lfloor L_k/h'_k \rfloor - 1)h'_k = L_k - \frac{1}{k}$.

Proof. By Lemma 3.2, property (3.6) is equivalent to

$$\limsup_{k\to\infty} \frac{1}{h_k^2} \int_{\Omega_k^{\text{ext}}} \mathrm{dist}^2(\nabla_k \tilde{y}^{(k)}, \mathrm{SO}(3)) \mathrm{d}x < \infty,$$

hence also to the same inequality with Ω_k^{ext} replaced by $(-\frac{1}{k}, L_k + \frac{1}{k}) \times S$ or $(0,L) \times S$. Except for the specific choice of the discontinuity set, these statements are thus proven in [MM03] by applying Theorem 1.1 to sets of the form $(a, a + bh_k) \times h_k S$.[1] If we do this here for $b = 1$ and the special choices $a = ih'_k$, $i = 1, \ldots, \lfloor L_k/h'_k \rfloor - 2$ as well as $b = 3$ and $a \in \{-\frac{1}{k}, L_k + \frac{1}{k} - 3h_k\}$, we see that $R^{(k)}$ can be arranged to jump only in $\{h'_k, 2h'_k, \ldots, (\lfloor L_k/h'_k \rfloor - 1)h'_k\}$. □

We remark that, for a suitable choice of translation vectors c_k (which does not change the energy), $\tilde{y}^{(k)} - c_k \to \tilde{y}$ in $H^1(\Omega;\mathbb{R}^3)$.

Remark 3.3. The proof mathematically utilizes one idea that already appeared in the investigations of Kirchhoff [Kir59] – he also viewed the rod as a union of short segments with their length comparable to the rod thickness.

[1] Because of lattice squares that only share one corner, in the ultrathin case S_k might not be Lipschitz, but in that case Theorem 1.1 can be first invoked for domains $U_{a,b,h_k}^{(\varepsilon)}$ instead of $U_{a,b,h_k} = (a, a + bh_k) \times h_k S$, where $V^{(\varepsilon)} = \{x \in V;\ \mathrm{dist}(x, \partial V) > \varepsilon\}$ for $V \subset \mathbb{R}^n$. Since $\nabla_k \tilde{y}^{(k)}$ is piecewise constant, the inequality

$$\int_{\tilde{Q}} |\nabla_k \tilde{y}^{(k)} - R^{(k)}|^2 \mathrm{d}\xi \le C \int_{\tilde{Q}^{(\varepsilon)}} |\nabla_k \tilde{y}^{(k)} - R^{(k)}|^2 \mathrm{d}\xi$$

for $\tilde{Q} = \bar{x} + (-\frac{1}{2k}, \frac{1}{2k}) \times (-\frac{1}{2}, \frac{1}{2})^2$ then allows us to extend the rigidity estimate to U_{a,b,h_k}. Thus we can assume $S = S_k$ for ultrathin rods to simplify the presentation.

3.3 Resulting theory for ultrathin rods

We now specialize to ultrathin rods for which the cross sectional lattice $\mathcal{L}_k = \mathcal{L}$ is assumed to be fixed. We set $h_k = 1/k$ and fix $m = 1$. Since also $\mathcal{L}_k^{\text{ext}}$, $\mathcal{L}_k^{\prime,\text{ext}}$, S_k (which equals S without loss of generality) and S_k^{ext} are independent of k, we drop the subscript.

3.3.1 Difference operators

In addition to $\bar{\nabla}$, we define several other difference operators, applicable to any function $f\colon [-\frac{1}{k}, L_k + \frac{1}{k}] \times \mathcal{L}^{\text{ext}} \to \mathbb{R}^\ell$, $\ell \in \mathbb{N}$. If $x \in \overline{\Omega_k^{\text{ext}}}$, we denote by $\bar{x}$ an element of $\tilde{\Lambda}_k^{\prime,\text{ext}}$ that is closest to x. For $x \in \overline{\Omega_k^{\text{ext}}}$ we set

$$\begin{aligned}
\bar{\nabla}_k^{2\text{d}} f(x) &= k\left[f(x_1, (\bar{x} + \tilde{\tilde{z}}^i)') - \frac{1}{4}\sum_{j=1}^{4} f(x_1, (\bar{x} + \tilde{\tilde{z}}^j)')\right]_{i=1}^{4}, \\
\bar{\nabla}^{2\text{d}} f(x) &= \left[f(x_1, (\bar{x} + z^i)') - \frac{1}{4}\sum_{j=1}^{4} f(x_1, (\bar{x} + z^j)')\right]_{i=1}^{4}, \\
\bar{\nabla}_k f(x) &= k\left[f(\bar{x} + \tilde{\tilde{z}}^i) - \frac{1}{8}\sum_{j=1}^{8} f(\bar{x} + \tilde{\tilde{z}}^j)\right]_{i=1}^{8} \\
&= \left(\bar{\nabla}_k^{\text{left}} f(x) | \bar{\nabla}_k^{\text{right}} f(x)\right), \qquad \bar{\nabla}_k^{\text{left}} f(x),\ \bar{\nabla}_k^{\text{right}} f(x) \in \mathbb{R}^{\ell \times 4}, \\
\Delta_1 f(x) &= k\left[\frac{1}{4}\sum_{j=5}^{8} f(\bar{x} + \tilde{\tilde{z}}^j) - \frac{1}{4}\sum_{j=1}^{4} f(\bar{x} + \tilde{\tilde{z}}^j)\right],
\end{aligned}$$

whose interpretations are '2D-differences in the x_2x_3-plane' (divided by $1/k$ or not), '3D-differences' and 'averaged difference in the x_1-direction', respectively. Note that the functions $\bar{\nabla}_k^{2\text{d}} f(x_1, \cdot)$ and $\bar{\nabla}^{2\text{d}} f(x_1, \cdot)$ are piecewise constant on lattice squares of the form $x' + (-\frac{1}{2}, \frac{1}{2})^2$, where $x' \in \mathcal{L}'$, and $\bar{\nabla}^{2\text{d}} f(x)$ is independent of k. The functions $\bar{\nabla}_k f$ and $\Delta_1 f$ are piecewise constant on lattice blocks that are centred in points of $\tilde{\Lambda}_k^{\prime,\text{ext}}$.

Set $\tilde{y}_i^{(k)} = \tilde{y}^{(k)}(\bar{x} + \tilde{\tilde{z}}^i)$, $i = 1, 2, \ldots, 8$, then property (3.2) yields

$$\begin{aligned}
\Delta_1 \tilde{y}^{(k)}(x) &= k\left(\frac{\tilde{y}_5^{(k)} + \tilde{y}_6^{(k)} + \tilde{y}_7^{(k)} + \tilde{y}_8^{(k)}}{4} - \frac{\tilde{y}_1^{(k)} + \tilde{y}_2^{(k)} + \tilde{y}_3^{(k)} + \tilde{y}_4^{(k)}}{4}\right) \\
&= k \fint_{\bar{x}' + (-\frac{1}{2}, \frac{1}{2})^2} \tilde{y}^{(k)}(\bar{x}_1 + \tfrac{1}{2k}, \xi') - \tilde{y}^{(k)}(\bar{x}_1 - \tfrac{1}{2k}, \xi') \mathrm{d}\xi' \qquad (3.10) \\
&= k \fint_{\bar{x}' + (-\frac{1}{2}, \frac{1}{2})^2} \int_{\bar{x}_1 - \frac{1}{2k}}^{\bar{x}_1 + \frac{1}{2k}} \frac{\partial \tilde{y}^{(k)}}{\partial x_1}(\xi_1, \xi') \mathrm{d}\xi_1 \mathrm{d}\xi' = \fint_{\tilde{Q}(x)} \frac{\partial \tilde{y}^{(k)}}{\partial x_1} \mathrm{d}\xi.
\end{aligned}$$

Direct computation shows:

$$\begin{aligned}
\bar{\nabla}_k^{\text{left}} f(x) &= \bar{\nabla}_k^{2\text{d}} f(\bar{x}_1 - \tfrac{1}{2k}, x') - \frac{1}{2}\Delta_1 f(x)(1,1,1,1), \\
\bar{\nabla}_k^{\text{right}} f(x) &= \bar{\nabla}_k^{2\text{d}} f(\bar{x}_1 + \tfrac{1}{2k}, x') + \frac{1}{2}\Delta_1 f(x)(1,1,1,1)
\end{aligned}$$

and so, with all columns grouped together,

$$\bar{\nabla}_k f(x) = \left(\bar{\nabla}_k^{2d} f(\bar{x}_1 - \tfrac{1}{2k}, x') | \bar{\nabla}_k^{2d} f(\bar{x}_1 + \tfrac{1}{2k}, x')\right) + \frac{1}{2}\Delta_1 f(x)(-1,-1,-1,-1,1,1,1,1). \tag{3.11}$$

3.3.2 Gamma-convergence

Recall that $\Omega = (0,L) \times S$. In order to specify an appropriate limit space we first note that in view of Theorem 3.4 and (3.5) it suffices to consider limiting configurations $\tilde{y} \in H^1(\Omega;\mathbb{R}^3)$ and $d_2, d_3 \in L^2(\Omega;\mathbb{R}^3)$ that do not depend on (x_2, x_3). We will then simply write $\tilde{y} \in H^1((0,L);\mathbb{R}^3)$ and $d_2, d_3 \in L^2((0,L);\mathbb{R}^3)$. The following observation shows that the convergence in $L^2(\Omega,\mathbb{R}^3)$ to such $\tilde{y}$ and d_2, d_3 is naturally described in terms of asymptotic atomic positions and independent of our interpolation scheme, cf. also Remark 3.6.

For $\tilde{y} \in H^1((0,L);\mathbb{R}^3)$ and a sequence $(y^{(k)})_{k=1}^{\infty}$ of (extended) lattice deformations the convergence $\tilde{y}^{(k)} \to \tilde{y}$ in $L^2(\Omega;\mathbb{R}^3)$ is equivalent to

$$\tilde{y}^{(k)}(\cdot, x') \to \tilde{y} \text{ in } L^2((0,L);\mathbb{R}^3) \text{ for every } x' \in \mathcal{L}.$$

We note here that for $x' \in \mathcal{L}$ the map $\tilde{y}^{(k)}(\cdot, x')$ is nothing but the piecewise affine interpolation of $\tilde{y}^{(k)}(\cdot, x')$ on $\{-\frac{1}{k}, 0, \ldots, L_k + \frac{1}{k}\}$. If moreover $d_2, d_3 \in L^2((0,L);\mathbb{R}^3)$, then $\nabla_k \tilde{y}^{(k)} \xrightarrow{L^2} R = (\frac{\partial \tilde{y}}{\partial x_1} | d_2 | d_3)$ is equivalent to

$$\bar{\nabla}_k \tilde{y}^{(k)} \to R\,\bar{\mathrm{Id}} \text{ in } L^2(\Omega;\mathbb{R}^{3\times 8})$$

by Lemma 3.1 (recall that $\bar{\nabla}_k \tilde{y}^{(k)}$ is a function in $L^2(\Omega;\mathbb{R}^{3\times 8})$ constant on each cell $\bar{x} + (-\frac{1}{2k}, \frac{1}{2k}) \times (-\frac{1}{2}, \frac{1}{2})^2$, $\bar{x} \in \tilde{\Lambda}_k^{\prime,\mathrm{ext}}$).

Theorem 3.5. *If $k \to \infty$, the functionals $kE^{(k)}$ Γ-converge to the functional E_{ult} defined below, in the following sense:*

(i) (liminf inequality) *Let $(y^{(k)})_{k=1}^{\infty}$ be a sequence of (extended) lattice deformations such that their piecewise affine interpolations $(\tilde{y}^{(k)})_{k=1}^{\infty}$, defined in Section 3.2, converge to $\tilde{y} \in H^1((0,L);\mathbb{R}^3)$ in $L^2(\Omega;\mathbb{R}^3)$. Let us also assume that $k\partial_{x_s}\tilde{y}^{(k)} \to d_s \in L^2((0,L);\mathbb{R}^3)$ in $L^2(\Omega;\mathbb{R}^3)$, $s = 2,3$. Then*

$$E_{\mathrm{ult}}(\tilde{y}, d_2, d_3) \le \liminf_{k\to\infty} kE^{(k)}(y^{(k)}).$$

(ii) (existence of a recovery sequence) *For any $\tilde{y} \in H^1((0,L);\mathbb{R}^3)$ and $d_2, d_3 \in L^2((0,L);\mathbb{R}^3)$ there is a sequence of (extended) lattice deformations $(y^{(k)})_{k=1}^{\infty}$ such that their interpolations $(\tilde{y}^{(k)})$, defined in Section 3.2, satisfy $\tilde{y}^{(k)} \to \tilde{y}$ in $L^2(\Omega;\mathbb{R}^3)$, $k\frac{\partial \tilde{y}^{(k)}}{\partial x_s} \to d_s$ in $L^2(\Omega;\mathbb{R}^3)$ for $s = 2,3$, and*

$$\lim_{k\to\infty} kE^{(k)}(y^{(k)}) = E_{\mathrm{ult}}(\tilde{y}, d_2, d_3).$$

The limit energy functional is given by

$$E_{\mathrm{ult}}(\tilde{y},d_2,d_3) = \begin{cases} \frac{1}{2}\int_0^L Q_{\mathrm{cell}}^{\mathrm{rel}}(R^\top \partial_{x_1} R)\mathrm{d}x_1 & \textit{if } (\tilde{y},d_2,d_3)\in\mathcal{A}, \\ +\infty & \textit{otherwise,} \end{cases}$$

where $R := (\partial_{x_1}\tilde{y}|d_2|d_3)$ *and the class of admissible deformations is*

$$\mathcal{A} := \Big\{(\tilde{y},d_2,d_3)\in H^2(\Omega;\mathbb{R}^3)\times H^1(\Omega;\mathbb{R}^3)\times H^1(\Omega;\mathbb{R}^3); \\ \tilde{y},d_2,d_3 \textit{ do not depend on } x_2,x_3, \quad \Big(\tfrac{\partial\tilde{y}}{\partial x_1}\,|\,d_2\,|\,d_3\Big)\in \mathrm{SO}(3) \textit{ a.e. in } (0,L)\Big\}.$$

The relaxed quadratic form $Q_{\mathrm{cell}}^{\mathrm{rel}}\colon \mathbb{R}^{3\times 3}_{\mathrm{skew}} \to [0,+\infty)$ *is defined as*

$$Q_{\mathrm{cell}}^{\mathrm{rel}}(A) := \min_{\substack{\alpha\colon \mathcal{L}^{\mathrm{ext}}\to\mathbb{R}^3\\ g\in\mathbb{R}^3}} \sum_{x'\in\mathcal{L}'^{,\mathrm{ext}}} Q_{\mathrm{tot}}\Bigg(x', \frac{1}{2}\Bigg(A\begin{pmatrix}0\\x_2\\x_3\end{pmatrix}+g\Bigg)(-1,-1,-1,-1,1,1,1,1) \\ +\frac{1}{4}A\begin{pmatrix}0&0&0&0&0&0&0&0\\1&1&-1&-1&-1&-1&1&1\\1&-1&-1&1&-1&1&1&-1\end{pmatrix}+\Big(\bar{\nabla}^{2\mathrm{d}}\alpha|\bar{\nabla}^{2\mathrm{d}}\alpha\Big)\Bigg) \quad (3.12)$$

with $Q_{\mathrm{tot}}(x',\cdot) = Q_{\mathrm{cell}}$ *if* $x'\in\mathcal{L}'$ *and* $Q_{\mathrm{tot}}(x',\cdot) = Q_{\mathrm{surf}}(\mathrm{t}(x'),\cdot)$ *if* $x'\in\mathcal{L}'^{,\mathrm{ext}}\setminus\mathcal{L}'$.

Remark 3.4. In comparison with the rod theory in [MM03], the functional E_{ult} takes into account the fewer degrees of freedom of the cross section leading to the discrete minimization in (3.12) and it also features an *ultrathin correction* term $\mathfrak{C}$, explicitly given in (3.14) below, which captures effects in our very thin atomic structures that could not be described by a Cauchy–Born continuum approximation.

Remark 3.5. Let us comment on the existence of a minimizer in (3.12). Fix $A\in\mathbb{R}^{3\times3}_{\mathrm{skew}}$ and let

$$C_A(x') = \frac{1}{2}A(0,x')^\top(-1,-1,-1,-1,1,1,1,1) \\ +\frac{1}{4}A\begin{pmatrix}0&0&0&0&0&0&0&0\\1&1&-1&-1&-1&-1&1&1\\1&-1&-1&1&-1&1&1&-1\end{pmatrix}.$$

The mapping $J\colon (\mathbb{R}^3)^{\mathcal{L}^{\mathrm{ext}}}\times\mathbb{R}^3\to\mathbb{R}$ given by

$$J(\alpha,g) = \sum_{x'\in\mathcal{L}'^{,\mathrm{ext}}} Q_{\mathrm{tot}}\Big(x', C_A(x') + \Big(\bar{\nabla}^{2\mathrm{d}}\alpha(x')|\bar{\nabla}^{2\mathrm{d}}\alpha(x')\Big)+\tfrac{1}{2}(-g|\cdots|-g|g|\cdots|g)\Big)$$

is, in fact, a real-valued function of $3\cdot\sharp\mathcal{L}^{\mathrm{ext}}+3$ variables. Since $Q_{\mathrm{tot}}(x',\cdot)$ is positive semidefinite on $\mathbb{R}^{3\times8}$ for any $x'\in\mathcal{L}'^{,\mathrm{ext}}$, the function J is a positive semidefinite quadratic form. It thus attains a minimum and a minimizer (α,g) of J can be chosen in linear dependence on A, so $Q_{\mathrm{cell}}^{\mathrm{rel}}$ is a quadratic form as well. Besides, since the components of $A := R^\top\partial_{x_1}R$ are L^2 in x_1, we obtain

$$(\alpha,g)\in L^2([0,L];(\mathbb{R}^3)^{\mathcal{L}^{\mathrm{ext}}}\times\mathbb{R}^3).$$

Label the points in the 2D lattice $\mathcal{L}^{\text{ext}}$ as $\mathcal{L}^{\text{ext}} = \{p_1, p_2, \ldots, p_{\sharp\mathcal{L}^{\text{ext}}}\}$ and express

$$J(\alpha, g) = J(\alpha^{p_1}, \alpha^{p_2}, \ldots, \alpha^{p_{\sharp\mathcal{L}^{\text{ext}}}}, g),$$

where $\alpha^{p_j} = (\alpha_1^{p_j}, \alpha_2^{p_j}, \alpha_3^{p_j}) \in \mathbb{R}^3$ is the variable corresponding to the value $\alpha(p_j)$ of $\alpha\colon \mathcal{L}^{\text{ext}} \to \mathbb{R}^3$ for every $j = 1, 2, \ldots, \sharp\mathcal{L}^{\text{ext}}$.

If (α, g) is a minimizer of J, it satisfies the condition $\nabla J(\alpha, g) = 0$, which, written componentwise, reads

$$\frac{\partial}{\partial \alpha_i^{p_j}} J(\alpha, g) = \sum_{r=1}^{4} \sum_{\ell=1}^{8} \sum_{m=1}^{3} \sum_{n=1}^{8} 2\Big(\nabla^2 W_{\text{tot}}\big(\mathrm{t}(p_j - (\bar{z}^r)'), \bar{\mathrm{Id}}\big)\Big)_{i\ell mn} \Big(-\frac{1}{4} + \delta_{\ell r} + \delta_{\ell(r+4)}\Big)$$
$$\cdot\Big[(C_A(p_j - (\bar{z}^r)'))_{mn} + \Big(-\frac{1}{2}\Big)^{\lfloor \frac{n-1}{4} \rfloor} g_m$$
$$+\alpha_m^{p_j - (\bar{z}^r)' + (\bar{z}^n)'} - \frac{1}{4} \sum_{q=1}^{4} \alpha_m^{p_j - (\bar{z}^r)' + (\bar{z}^q)'}\Big] = 0,\ i = 1, 2, 3,\ j = 1, 2, \ldots, \sharp\mathcal{L}^{\text{ext}},$$

$$\frac{\partial}{\partial g_i} J(\alpha, g) = \sum_{x' \in \mathcal{L}'^{,\text{ext}}} \sum_{\ell=1}^{8} \sum_{m=1}^{3} \sum_{n=1}^{8} 2\Big(-\frac{1}{2}\Big)^{\lfloor \frac{l-1}{4} \rfloor} (\nabla^2 W_{\text{tot}}(\mathrm{t}(x'), \bar{\mathrm{Id}}))_{i\ell mn}$$
$$\cdot\Big[(C_A(x'))_{mn} + \Big(-\frac{1}{2}\Big)^{\lfloor \frac{n-1}{4} \rfloor} g_m + \alpha_m^{x' + (\bar{z}^n)'} - \frac{1}{4} \sum_{q=1}^{4} \alpha_m^{x' + (\bar{z}^q)'}\Big] = 0,\ i = 1, 2, 3$$

(the terms C_A, $W_{\text{tot}}(\mathrm{t}(\cdot), \vec{y})$ for $\vec{y} \in \mathbb{R}^{3\times 8}$, and α are understood to equal zero outside $\overline{S^{\text{ext}}}$). Thus we have a linear algebraic system for the components of the minimizer (α, g), which can be expressed as

$$M(\alpha_1^{p_1}, \alpha_2^{p_1}, \alpha_3^{p_1}, \alpha_1^{p_2}, \alpha_2^{p_2}, \alpha_3^{p_2}, \ldots, \alpha_1^{p_{\sharp\mathcal{L}^{\text{ext}}}}, \alpha_2^{p_{\sharp\mathcal{L}^{\text{ext}}}}, \alpha_3^{p_{\sharp\mathcal{L}^{\text{ext}}}}, g_1, g_2, g_3)^\top = b_A$$

for a matrix $M \in \mathbb{R}^{(3\sharp\mathcal{L}^{\text{ext}}+3)\times(3\sharp\mathcal{L}^{\text{ext}}+3)}$ and a vector $b_A \in \mathbb{R}^{3\sharp\mathcal{L}^{\text{ext}}+3}$. (The right-hand side b_A, unlike the matrix M, depends on A.)

Basic code for approximating (α, g) can be found in [Zem23].

Remark 3.6. One could also consider limiting configurations with an explicit dependence on x'. Due to the discrete nature of $\mathcal{L}$, however, only a subspace of $H^1(\Omega; \mathbb{R}^3)$ can be realized as limits of interpolated deformations $\tilde{y}^{(k)}$. That is, $\tilde{y}^{(k)}$ can converge to $\tilde{y}$ in $L^2(\Omega; \mathbb{R}^3)$ if and only if $\tilde{y}$ is piecewise affine in x', more precisely, if for a. e. $x_1 \in (0, L)$ and $x' \in \mathcal{L}'$ one has $\tilde{y}(x_1, x') = \frac{1}{4}\sum_{i=1}^{4} \tilde{y}(x_1, x' + (\bar{z}^i)')$ and $\tilde{y}(x_1, \cdot)$ is affine on $\operatorname{conv}\{x', x' + (\bar{z}^i)', x' + (\bar{z}^j)'\}$ if $i, j \in \{1, 2, 3, 4\}$, $|i - j| = 1$. Similarly, limiting directors (d_2, d_3) are restricted to be gradients with respect to x' of such functions. By Theorem 3.4, (3.4) and (3.5) one still has Γ-convergence with such a class of limiting configurations if E_{ult} is extended by the value $+\infty$ outside of $H^1((0, L); \mathbb{R}^3) \times L^2((0, L); \mathbb{R}^3) \times L^2((0, L); \mathbb{R}^3)$.

Remark 3.7. Standard arguments show that forcing terms of the form

$$-k^{-3} h_k^{-2} \sum_{x \in \Lambda_k} f(x_1) \cdot y^{(k)}(x),$$

$f \in L^2((0, L); \mathbb{R}^3)$, could be added to $k^{-3} h_k^{-4} E^{(k)}$ and Γ-convergence as well as compactness claims would still hold (see e.g. [Sch07, Corollary 3.4] or [BS22] for more details).

Correspondence between almost-minimizers of the discrete energies and minimizers of the effective functional E_{ult} is expressed in the corollary below. Analogous statements would also be available in the thin-rod regime or Chapter 4.

Corollary 3.6. *Suppose that $kE^{(k)} \xrightarrow{\Gamma} E_{\mathrm{ult}}$ as $k \to \infty$ and that the following property holds:*

$$\begin{aligned}(\exists\, C > 0\, \exists\, (y^{(k)});\, y^{(k)}\colon \Lambda_k \to \mathbb{R}^3\, \forall\, k \in \mathbb{N}\colon\, kE^{(k)}(y^{(k)}) \le C)\\ \Rightarrow \exists\, (k_j) \subset \mathbb{N}\, \exists\, R \in L^2([0,L];\mathrm{SO}(3))\colon\ \nabla_{k_j}\tilde{y}^{(k_j)} \to R \text{ in } L^2([0,L];\mathbb{R}^3).\end{aligned} \tag{3.13}$$

Then any sequence $(y^{(k)})$, $y^{(k)}\colon \Lambda_k \to \mathbb{R}^3$, with

$$\lim_{k\to\infty}\Big(kE^{(k)}(y^{(k)}) - \inf_{z\colon \Lambda_k \to \mathbb{R}^3} kE^{(k)}(z)\Big) = 0$$

has a subsequence $(y^{(k_j)})$ such that $\nabla_{k_j}\tilde{y}^{(k_j)} \to R \in L^2([0,L];\mathrm{SO}(3))$ in $L^2([0,L];\mathbb{R}^3)$ and for every such cluster point $R = (\tilde{y}'|d_2|d_3)$ and $\tilde{y}$ being a primitive function of $\tilde{y}'$ it follows that $(\tilde{y}, d_2, d_3)$ is a minimizer of E_{ult}.

Condition (3.13) is satisfied due to compactness Theorem 3.4 and Lemma 3.3. The proof of Corollary 3.6 is based on classical arguments.

3.3.3 Proof of the lower bound

In this section, we prove Theorem 3.5(i). We may assume that $kE^{(k)}(y^{(k)}) \le C$ and so (3.6) holds true by (3.4) and (3.5). We set $\Omega^{\mathrm{ext}} = (0,L) \times S^{\mathrm{ext}}$. Let $R^{(k)}$ be as in Theorem 3.4. By (3.8) and in analogy with [MM03], for

$$G^{(k)}(x) := \frac{(R^{(k)})^\top(x_1)\nabla_k\tilde{y}^{(k)}(x) - \mathrm{Id}}{1/k}, \quad x \in \Omega_k^{\mathrm{ext}},$$

we have $G^{(k)} \rightharpoonup G \in L^2(\Omega^{\mathrm{ext}};\mathbb{R}^{3\times 3})$ in $L^2(\Omega^{\mathrm{ext}};\mathbb{R}^{3\times 3})$, up to a subsequence.

Remark 3.8. The quantity $G^{(k)}$ can be interpreted as a measure of strain. More specifically, note the resemblance of $G^{(k)}$ to a rescaled approximation of the Biot strain tensor $E_{1/2} = U - \mathrm{Id}$ from the Seth–Hill family of strain measures [Ogd97, p. 119], where $F = RU$ is the polar decomposition of the deformation gradient F.

In our discrete setting we instead need to study

$$\bar{G}^{(k)}(x) := \frac{(R^{(k)})^\top(x_1)\bar{\nabla}_k\tilde{y}^{(k)} - \bar{\mathrm{Id}}}{1/k}, \quad x \in \Omega_k^{\mathrm{ext}}.$$

By virtue of (3.3), the L^2-boundedness of $(G^{(k)})$ implies the boundedness of $(\bar{G}^{(k)})$ in $L^2(\Omega^{\mathrm{ext}};\mathbb{R}^{3\times 8})$. Hence $\bar{G}^{(k)} \rightharpoonup \bar{G}$ for a subsequence, which we do not relabel. We state a proposition about the structure of $\bar{G}$.

Proposition 3.7. *$\bar{G}^{(k)} \rightharpoonup \bar{G}$ in $L^2(\Omega^{\text{ext}};\mathbb{R}^{3\times 8})$ for*

$$\bar{G}(x) = \frac{1}{2}\Big[G_1(x_1) + R^\top(x_1)\frac{\partial R}{\partial x_1}(x_1)\begin{pmatrix}0\\ \bar{x}_2\\ \bar{x}_3\end{pmatrix}\Big](-1,-1,-1,-1,1,1,1,1)$$
$$+ \mathfrak{C}(x_1) + \Big(\bar{\nabla}^{2\text{d}}\alpha(x)|\bar{\nabla}^{2\text{d}}\alpha(x)\Big),$$

where $G_1 \in L^2((0,L);\mathbb{R}^3)$, $\alpha \in L^2((0,L)\times\mathcal{L}^{\text{ext}};\mathbb{R}^3) \cong L^2((0,L);(\mathbb{R}^3)^{\mathcal{L}^{\text{ext}}})$ and $\mathfrak{C}$ is explicitly given by

$$\mathfrak{C} = \frac{1}{4}\begin{pmatrix} -\kappa_2-\kappa_3 & \kappa_3-\kappa_2 & \kappa_2+\kappa_3 & \kappa_2-\kappa_3 & \kappa_2+\kappa_3 & \kappa_2-\kappa_3 & -\kappa_2-\kappa_3 & \kappa_3-\kappa_2\\ -\tau & \tau & \tau & -\tau & \tau & -\tau & -\tau & \tau\\ \tau & \tau & -\tau & -\tau & -\tau & -\tau & \tau & \tau \end{pmatrix} \tag{3.14}$$

with $\kappa_2(x_1) = \frac{\partial^2\tilde{y}}{\partial x_1^2}\cdot d_2$, $\kappa_3(x_1) = \frac{\partial^2\tilde{y}}{\partial x_1^2}\cdot d_3$, $\tau(x_1) = \frac{\partial d_2}{\partial x_1}\cdot d_3$, and R from Theorem 3.5.

Proof. Formula (3.11) enables us to find the longitudinal and transversal contributions separately.
1. *Longitudinal contributions.* We consider the piecewise constant function

$$\bar{G}^{(k)}_{\text{long}} := \frac{k}{2}\Big[(R^{(k)})^\top\Delta_1\tilde{y}^{(k)}(-1,-1,-1,-1,1,1,1,1) - e_1e_1^\top\bar{\text{Id}}\Big]$$

and observe that for each $x\in\Omega_k^{\text{ext}}$ with $\tilde{Q}(x) := \tilde{Q}(\bar{x}) = \bar{x} + (-\frac{1}{2k},\frac{1}{2k})\times(-\frac{1}{2},\frac{1}{2})^2$ property (3.10) of the piecewise affine interpolation $\tilde{y}^{(k)}$ yields

$$\begin{aligned}\bar{G}^{(k)}_{\text{long}} &= \frac{k}{2}\Big((R^{(k)})^\top\fint_{\tilde{Q}}\frac{\partial\tilde{y}^{(k)}}{\partial x_1}\mathrm{d}\xi - e_1\Big)(-1,-1,-1,-1,1,1,1,1)\\ &= \frac{1}{2}\fint_{\tilde{Q}} G^{(k)}e_1\,\mathrm{d}\xi(-1,-1,-1,-1,1,1,1,1).\end{aligned}$$

This converges weakly to

$$\frac{1}{2}\fint_{\tilde{Q}'(x')} G(x_1,\xi')e_1\,\mathrm{d}\xi'(-1,-1,-1,-1,1,1,1,1),$$

where $\tilde{Q}'(x') = (\bar{x}_2-\frac{1}{2},\bar{x}_2+\frac{1}{2})\times(\bar{x}_3-\frac{1}{2},\bar{x}_3+\frac{1}{2})$, since for any $\varphi\in C_c^\infty(\Omega^{\text{ext}})$

$$\begin{aligned}\int_{\Omega^{\text{ext}}}\fint_{\tilde{Q}(\bar{x})} G^{(k)}(\xi)\mathrm{d}\xi\,\varphi(x)\mathrm{d}x &= \int_{\Omega^{\text{ext}}} G^{(k)}(\xi)\fint_{\tilde{Q}(\bar{\xi})}\varphi(x)\mathrm{d}x\mathrm{d}\xi\\ &\to \int_{\Omega^{\text{ext}}} G(\xi)\int_{\tilde{Q}'(\xi')}\varphi(\xi_1,x')\mathrm{d}x'\mathrm{d}\xi\\ &= \int_{\Omega^{\text{ext}}}\int_{\tilde{Q}'(x')} G(x_1,\xi')\mathrm{d}\xi'\varphi(x)\mathrm{d}x.\end{aligned}$$

(A similar property is also used in [BS22, Proposition 4.6].) In view of [MM03, equation (3.10)], the first column of G reads

$$Ge_1 = G_1(x_1) + R^\top(x_1)\frac{\partial R}{\partial x_1}(x_1)\begin{pmatrix}0\\ x_2\\ x_3\end{pmatrix}$$

for some $G_1 \in L^2((0,L);\mathbb{R}^3)$ and hence

$$\fint_{\tilde{Q}'(x')} G(x_1,\xi')e_1 \mathrm{d}\xi' = G_1(x_1) + R^\top(x_1)\frac{\partial R}{\partial x_1}(x_1)\begin{pmatrix}0\\ \bar{x}_2\\ \bar{x}_3\end{pmatrix}.$$

It follows that in $L^2(\Omega^{\mathrm{ext}};\mathbb{R}^{3\times 8})$,

$$\bar{G}^{(k)}_{\mathrm{long}} \rightharpoonup \frac{1}{2}\Big(G_1(x_1) + R^\top(x_1)\frac{\partial R}{\partial x_1}(x_1)\begin{pmatrix}0\\ \bar{x}_2\\ \bar{x}_3\end{pmatrix}\Big)(-1,-1,-1,-1,1,1,1,1).$$

2. *Transversal contributions.* Here the left 3×4 submatrix of some $\bar{A} \in \mathbb{R}^{3\times 8}$ is referred to as the *left part* of $\bar{A}$, whereas the other 3×4 submatrix as the *right part* of $\bar{A}$.

First let us look at the left part

$$\bar{G}^{(k)}_{\mathrm{left}}(x) := k\Big[(R^{(k)})^\top(x_1)\,\bar{\nabla}^{2\mathrm{d}}_k\,\tilde{y}^{(k)}(\bar{x}_1 - \tfrac{1}{2k},\bar{x}') - \begin{pmatrix}0 & 0 & 0 & 0\\ (\bar{z}^1)' & (\bar{z}^2)' & (\bar{z}^3)' & (\bar{z}^4)'\end{pmatrix}\Big].$$

We define the auxiliary function

$$\alpha^{(k)}_{\mathrm{left}}(x) := k\Big[kR^{(k)}(x_1)^\top\tilde{y}^{(k)}(\bar{x}_1 - \tfrac{1}{2k},x') - x_2e_2 - x_3e_3\Big], \quad x \in \overline{\Omega^{\mathrm{ext}}_k},$$

whose average over the cross-sectional lattice is

$$\alpha^{(k)}_{\mathrm{left},0}(x_1) := \frac{1}{\sharp\mathcal{L}^{\mathrm{ext}}}\sum_{x'\in\mathcal{L}^{\mathrm{ext}}}\alpha^{(k)}_{\mathrm{left}}(x_1,x')$$

and its two-dimensional discrete gradient is equal to $\bar{G}^{(k)}_{\mathrm{left}}$, since

$$\bar{\nabla}^{2\mathrm{d}}\,\alpha^{(k)}_{\mathrm{left}}(x) = k\Big[(R^{(k)}(x_1)^\top\,\bar{\nabla}^{2\mathrm{d}}_k\,\tilde{y}^{(k)}(\bar{x}_1 - \tfrac{1}{2k},\bar{x}') - \frac{1}{2}\begin{pmatrix}0 & 0 & 0 & 0\\ -1 & -1 & 1 & 1\\ -1 & 1 & 1 & -1\end{pmatrix}\Big].$$

Since S^{ext} is a polygonal domain, setting $\nabla' f = (\partial_{x_2}f\,|\,\partial_{x_3}f)$ and bounding the $\max_{S^{\mathrm{ext}}}$ with a successive maximization over $\mathcal{L}'^{,\mathrm{ext}}$ and over the interpolation tetrahedra, we have

$$\begin{aligned}
|\alpha^{(k)}_{\mathrm{left}}(x) - \alpha^{(k)}_{\mathrm{left},0}(x_1)|^2 &\le C\max_{\zeta'\in S^{\mathrm{ext}}}|\nabla'\alpha^{(k)}_{\mathrm{left}}(x_1,\zeta')|^2\\
&= C\max_{\zeta'\in S^{\mathrm{ext}}} k^2\Big|R^{(k)}(x_1)^\top\Big[k\nabla'\tilde{y}^{(k)}(\bar{x}_1 - \tfrac{1}{2k},\zeta')\Big] - \begin{pmatrix}0 & 0\\ 1 & 0\\ 0 & 1\end{pmatrix}\Big|^2\\
&\le 24\max_{\zeta'\in\mathcal{L}'^{,\mathrm{ext}}} C\fint_{\tilde{Q}(\bar{x}_1,\zeta')} k^2\Big|R^{(k)}(\xi_1)^\top\nabla_k\tilde{y}^{(k)}(\xi) - \mathrm{Id}\Big|^2\mathrm{d}\xi\\
&\le C\fint_{\bar{x}_1-\frac{1}{2k}}^{\bar{x}_1+\frac{1}{2k}}\int_{S^{\mathrm{ext}}}\Big|G^{(k)}(\xi)\Big|^2\mathrm{d}\xi.
\end{aligned}$$

Integrating over Ω_k^{ext} shows that $\alpha_{\mathrm{left}}^{(k)} - \alpha_{\mathrm{left},0}^{(k)}$ and $\partial_{x_s}(\alpha_{\mathrm{left}}^{(k)} - \alpha_{\mathrm{left},0}^{(k)}) = \partial_{x_s}\alpha_{\mathrm{left}}^{(k)}$, $s = 2,3$, are bounded in $L^2(\Omega_k^{\mathrm{ext}};\mathbb{R}^3)$. We thus find $\alpha_{\mathrm{left}} \in L^2(\Omega^{\mathrm{ext}};\mathbb{R}^3)$ with $\nabla'\alpha_{\mathrm{left}} \in L^2(\Omega^{\mathrm{ext}};\mathbb{R}^{3\times 2})$ such that, passing to a subsequence,

$$\alpha_{\mathrm{left}}^{(k)} - \alpha_{\mathrm{left},0}^{(k)} \rightharpoonup \alpha_{\mathrm{left}} \quad \text{and} \quad \partial_{x_s}\Big(\alpha_{\mathrm{left}}^{(k)} - \alpha_{\mathrm{left},0}^{(k)}\Big) \rightharpoonup \partial_{x_s}\alpha_{\mathrm{left}},\ s = 2,3,$$

in $L^2(\Omega^{\mathrm{ext}};\mathbb{R}^3)$. In particular, for any $\bar{x}' \in \mathcal{L}'^{,\mathrm{ext}}$ and $i,j \in \{1,2,3,4\}$ with $|\bar{z}^i - \bar{z}^j| = 1$ considering the triangle $T = \operatorname{conv}\{\bar{x}', \bar{x}' + (\bar{z}^i)', \bar{x}' + (\bar{z}^j)'\} \subset S^{\mathrm{ext}}$ we still have

$$\nabla'\Big(\alpha_{\mathrm{left}}^{(k)} - \alpha_{\mathrm{left},0}^{(k)}\Big) \rightharpoonup \nabla'\alpha_{\mathrm{left}} \quad \text{in } L^2((0,L)\times T;\mathbb{R}^{3\times 2}).$$

Our piecewise affine interpolation scheme and the definition of $\alpha_{\mathrm{left}}^{(k)}$ guarantee that $\nabla'\alpha_{\mathrm{left}}^{(k)}(x)$ is independent of x' and piecewise constant in x_1 for $x \in (0,L)\times T$. Therefore $\nabla'\alpha_{\mathrm{left}}(x)$ does not depend on $x' \in T$ either and we may conclude that

$$\Big[\bar{\nabla}^{2\mathrm{d}}\Big(\alpha_{\mathrm{left}}^{(k)} - \alpha_{\mathrm{left},0}^{(k)}\Big)\Big]_{\bullet i} = \nabla'\Big(\alpha_{\mathrm{left}}^{(k)} - \alpha_{\mathrm{left},0}^{(k)}\Big)(\bar{z}^i)' \rightharpoonup \nabla'\alpha_{\mathrm{left}}(\bar{z}^i)' = \Big[\bar{\nabla}^{2\mathrm{d}}\,\alpha_{\mathrm{left}}\Big]_{\bullet i}$$

in $L^2((0,L)\times T;\mathbb{R}^3)$. As both $\bar{\nabla}^{2\mathrm{d}}(\alpha_{\mathrm{left}}^{(k)} - \alpha_{\mathrm{left},0}^{(k)})$ and $\bar{\nabla}^{2\mathrm{d}}\,\alpha_{\mathrm{left}}$ are in fact independent of $x' \in \tilde{Q}' = \bar{x}' + (-\frac{1}{2},\frac{1}{2})^2$, we even have $[\bar{\nabla}^{2\mathrm{d}}(\alpha_{\mathrm{left}}^{(k)} - \alpha_{\mathrm{left},0}^{(k)})]_{\bullet i} \rightharpoonup [\bar{\nabla}^{2\mathrm{d}}\,\alpha_{\mathrm{left}}]_{\bullet i}$ in $L^2((0,L)\times\tilde{Q}';\mathbb{R}^3)$ and so, since $\bar{x}'$ and i were arbitrary,

$$\bar{\nabla}^{2\mathrm{d}}(\alpha_{\mathrm{left}}^{(k)} - \alpha_{\mathrm{left},0}^{(k)}) = \bar{G}_{\mathrm{left}}^{(k)} \rightharpoonup \bar{\nabla}^{2\mathrm{d}}\,\alpha_{\mathrm{left}} \text{ in } L^2(\Omega^{\mathrm{ext}};\mathbb{R}^{3\times 4})$$

and the restriction of α_{left} to $(0,L)\times\mathcal{L}^{\mathrm{ext}}$ is well defined. Similarly we find $\alpha_{\mathrm{right}} \in L^2(\Omega^{\mathrm{ext}};\mathbb{R}^3)$, the weak limit of $\alpha_{\mathrm{right}}^{(k)} - \alpha_{\mathrm{right},0}^{(k)}$, so that

$$\bar{G}_{\mathrm{right}}^{(k)} = k\Bigg[(R^{(k)})^\top\,\bar{\nabla}_k^{2\mathrm{d}}\,\tilde{y}^{(k)}(\bar{\cdot} + \tfrac{1}{2k}e_1) - \begin{pmatrix} 0 & 0 & 0 & 0 \\ (\bar{z}^5)' & (\bar{z}^6)' & (\bar{z}^7)' & (\bar{z}^8)' \end{pmatrix}\Bigg] \rightharpoonup \bar{\nabla}^{2\mathrm{d}}\,\alpha_{\mathrm{right}}.$$

It would be nice to express α_{right} in terms of α_{left} and R. We see that

$$\alpha_{\mathrm{right}}^{(k)}(x - \tfrac{1}{k}e_1) = k\Big[k(R^{(k)}(x_1 - \tfrac{1}{k})^\top\tilde{y}^{(k)}(\bar{x}_1 - \tfrac{1}{2k}, x') - x_2e_2 - x_3e_3\Big]$$

and so

$$\alpha_{\mathrm{right}}^{(k)}(x - \tfrac{1}{k}e_1) - \alpha_{\mathrm{left}}^{(k)}(x) = k^2\Big[(R^{(k)})(x_1 - \tfrac{1}{k}) - (R^{(k)})(x_1)\Big]^\top\tilde{y}^{(k)}(\bar{x}_1 - \tfrac{1}{2k}, x').$$

For the discrete gradient of the above expression, we have

$$\begin{aligned} &\bar{\nabla}^{2\mathrm{d}}\Big(\alpha_{\mathrm{right}}^{(k)}(x - \tfrac{1}{k}e_1) - \alpha_{\mathrm{left}}^{(k)}(x)\Big) \\ &\quad = \frac{(R^{(k)})^\top(x_1 - \frac{1}{k}) - (R^{(k)})^\top(x_1)}{1/k}\,\bar{\nabla}_k^{2\mathrm{d}}\,\tilde{y}^{(k)}(\bar{x}_1 - \tfrac{1}{2k}, x'). \end{aligned} \tag{3.15}$$

From (3.9) and (3.6), we see that $\Big(k(R^{(k)}(\cdot - \frac{1}{k}) - R^{(k)})\Big)_{k\in\mathbb{N}}$ is bounded in L^2 and therefore has a subsequence weakly converging to, say, F. Moreover, convergence (3.7) gives $F = -\frac{\partial R}{\partial x_1}$, thus

$$k\Big(R^{(k)}(\cdot - \tfrac{1}{k}) - R^{(k)}\Big) \rightharpoonup -\frac{\partial R}{\partial x_1} \text{ in } L^2(\Omega^{\mathrm{ext}};\mathbb{R}^{3\times 3}). \tag{3.16}$$

Now we notice that

$$\bar{\nabla}_k^{2\mathrm{d}}\,\tilde{y}^{(k)}(\bar{x}_1-\tfrac{1}{2k},x')\to R(x_1)\begin{pmatrix}0&0&0&0\\(\bar{z}^1)'&(\bar{z}^2)'&(\bar{z}^3)'&(\bar{z}^4)'\end{pmatrix}\text{ in }L^2(\Omega^{\mathrm{ext}};\mathbb{R}^{3\times4}).\quad(3.17)$$

Indeed, for $\bar{x}'\in\mathcal{L}'^{,\mathrm{ext}}$ and $i,j\in\{1,2,3,4\}$ with $|\bar{z}^i-\bar{z}^j|=1$ we let $T_\ell=(\frac{\ell}{k}+\frac{1}{2k},\bar{x}')+\mathrm{conv}\{0,-\frac{1}{2k}e_1,\tilde{z}^i,\tilde{z}^j\}$, $\ell=-1,0,\ldots,kL_k$, so that $\tilde{y}^{(k)}$ is affine on every T_ℓ. Also set $T=\bigcup_\ell T_\ell$ and let χ_k be the characteristic function of T. Since $\bar{\nabla}_k^{2\mathrm{d}}\,\tilde{y}^{(k)}(\bar{x}_1-\frac{1}{2k},\cdot)$ is constant on each $\tilde{Q}'(\bar{x}')=\bar{x}'+(-\frac{1}{2},\frac{1}{2})^2$ and $R^{(k)}$ is independent of x', we have

$$\begin{aligned}\int_{(-\frac{1}{k},L_k+\frac{1}{k})\times\tilde{Q}'(\bar{x}')}&\Big|\Big[\bar{\nabla}_k^{2\mathrm{d}}\,\tilde{y}^{(k)}(\bar{x}_1-\tfrac{1}{2k},\xi')\Big]_{\bullet i}-R^{(k)}(x_1)(0,(\bar{z}^i)')^\top\Big|^2\mathrm{d}x_1\mathrm{d}\xi'\\&=24\int_{\Omega_k^{\mathrm{ext}}}\chi_k\Big|\Big(\nabla_k\tilde{y}^{(k)}(x)-R^{(k)}(x_1)\Big)(0,(\bar{z}^i)')^\top\Big|^2\mathrm{d}x\to0\end{aligned}$$

as $k\to\infty$ by (3.8). Since $\bar{x}'$ and i were arbitrary, (3.17) now follows from (3.7).

Thus in (3.15), we combine (3.16) with (3.17) to obtain the limit

$$\bar{\nabla}^{2\mathrm{d}}\,\alpha_{\mathrm{right}}-\bar{\nabla}^{2\mathrm{d}}\,\alpha_{\mathrm{left}}=R^\top\frac{\partial R}{\partial x_1}\begin{pmatrix}0&0&0&0\\(\bar{z}^1)'&(\bar{z}^2)'&(\bar{z}^3)'&(\bar{z}^4)'\end{pmatrix},\qquad(3.18)$$

as $-(\partial_{x_1}R^\top)R=-(R^\top\partial_{x_1}R)^\top=R^\top\partial_{x_1}R$.

3. Finally we bring all contributions together:

$$\begin{aligned}\bar{G}^{(k)}&=\bar{G}^{(k)}_{\mathrm{long}}+\Big(\bar{G}^{(k)}_{\mathrm{left}}\,|\,\bar{G}^{(k)}_{\mathrm{right}}\Big)\\&\rightharpoonup\frac{1}{2}\left(G_1(x_1)+R^\top(x_1)\frac{\partial R}{\partial x_1}(x_1)\begin{pmatrix}0\\\bar{x}_2\\\bar{x}_3\end{pmatrix}\right)(-1,-1,-1,-1,1,1,1,1)\\&\quad+\Big(\bar{\nabla}^{2\mathrm{d}}\,\alpha_{\mathrm{left}}\,|\,\bar{\nabla}^{2\mathrm{d}}\,\alpha_{\mathrm{right}}\Big).\end{aligned}$$

To finish the proof, we set $\alpha:=(\alpha_{\mathrm{left}}+\alpha_{\mathrm{right}})/2$ (restricted to $(0,L)\times\mathcal{L}^{\mathrm{ext}}$), and use (3.18) as well as

$$R^\top\frac{\partial R}{\partial x_1}=\begin{pmatrix}0&-\kappa_2&-\kappa_3\\\kappa_2&0&-\tau\\\kappa_3&\tau&0\end{pmatrix}.$$

□

With the help of Proposition 3.7, the proof of Theorem 3.5(i) can now be completed following [FJM02] (see also [MM03, Sch06]). For $\vec{y}\in\mathbb{R}^{3\times8}$ we set $W_{\mathrm{tot}}(x',\vec{y})=W_{\mathrm{cell}}(\vec{y})$ if $x'\in S$ and $W_{\mathrm{tot}}(x',\vec{y})=W_{\mathrm{surf}}(\mathrm{t}(x'),\vec{y})$ if $x'\in S^{\mathrm{ext}}\setminus S$ so that $Q_{\mathrm{tot}}(x',\cdot)$ is the quadratic form generated by $\nabla^2W_{\mathrm{tot}}(x',\bar{\mathrm{Id}})$. Using (3.4), the non-negativity of W_{end} and the frame-indifference of W_{tot}, we can write

$$\begin{aligned}E^{(k)}(y^{(k)})&\geq\sum_{\hat{x}\in\hat{\Lambda}_k'\cup\hat{\Lambda}_k'^{,\mathrm{surf}}}W_{\mathrm{tot}}\Big(\hat{x}',\vec{y}^{(k)}(\hat{x})\Big)\\&=\int_{(0,kL_k)\times S^{\mathrm{ext}}}W_{\mathrm{tot}}\Big(\hat{x}',[R^{(k)}(\frac{\hat{x}_1}{k})]^\top\bar{\nabla}\hat{y}^{(k)}(\hat{x})\Big)\mathrm{d}\hat{x}\\&=k\int_{(0,L_k)\times S^{\mathrm{ext}}}W_{\mathrm{tot}}\Big(x',R^{(k)}(x_1)^\top\bar{\nabla}_k\tilde{y}^{(k)}(x)\Big)\mathrm{d}x\\&=k\int_{(0,L_k)\times S^{\mathrm{ext}}}W_{\mathrm{tot}}\Big(x',\bar{\mathrm{Id}}+\tfrac{1}{k}\bar{G}^{(k)}(x)\Big)\mathrm{d}x\end{aligned}\qquad(3.19)$$

We let χ_k be the characteristic function of $\{|\bar{G}^{(k)}| \le \sqrt{k}\} \cap [(0, L_k) \times S^{\text{ext}}]$ and note that $\chi_k \to 1$ boundedly in measure on Ω^{ext}. As both $W_{\text{tot}}(x', \cdot)$ and $\nabla W_{\text{tot}}(x', \cdot)$ vanish at $\bar{\text{Id}}$, a Taylor expansion yields

$$\chi_k W_{\text{tot}}\Big(x', \bar{\text{Id}} + \tfrac{1}{k}\bar{G}^{(k)}\Big) \ge \frac{1}{2k^2}\chi_k Q_{\text{tot}}(x', \bar{G}^{(k)}) - \chi_k \omega\Big(\tfrac{1}{k}|\bar{G}^{(k)}|\Big),$$

where $\omega(t) = o(t^2)$, $t \to 0$. We deduce that

$$kE^{(k)}(y^{(k)}) \ge \frac{1}{2}\int_{\Omega^{\text{ext}}} \chi_k Q_{\text{tot}}(x', \bar{G}^{(k)})\mathrm{d}x - k\int_{\Omega^{\text{ext}}} \chi_k |\bar{G}^{(k)}|^2 \frac{\omega(\frac{1}{k}|\bar{G}^{(k)}|)}{(\frac{1}{k}|\bar{G}^{(k)}|)^2}\mathrm{d}x. \tag{3.20}$$

We can move χ_k inside the second argument of Q_{tot}. Further, as $W_{\text{tot}}(x', \cdot)$ has a local minimum at $\bar{\text{Id}}$, $Q_{\text{tot}}(x', \cdot)$ is positive semidefinite and therefore, convex. The convergence $\chi_k \bar{G}^{(k)} \rightharpoonup \bar{G}$ thus yields

$$\liminf_{k\to\infty} kE^{(k)}(y^{(k)}) \ge \frac{1}{2}\int_{\Omega^{\text{ext}}} Q_{\text{tot}}(x', \bar{G})\mathrm{d}x$$

if the second term in (3.20) goes to zero. But that follows from the boundedness of $\bar{G}^{(k)}$ in $L^2(\Omega^{\text{ext}}; \mathbb{R}^{3\times 8})$ and the cut-off by χ_k forcing L^∞-convergence of the fraction involving ω.

We substitute in Q_{tot} the representation of $\bar{G}$. By Proposition 3.7,

$$\int_{S^{\text{ext}}} Q_{\text{tot}}(x', \bar{G})\mathrm{d}x' = \int_{S^{\text{ext}}} Q_{\text{tot}}\Bigg(x', \frac{1}{2}\Bigg[G_1 + R^\top \frac{\partial R}{\partial x_1}\begin{pmatrix} 0 \\ \bar{x}_2 \\ \bar{x}_3 \end{pmatrix}\Bigg](-1,-1,-1,-1,1,1,1,1)$$
$$\underbrace{+\frac{1}{4}R^\top \frac{\partial R}{\partial x_1}\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 \end{pmatrix}}_{\mathfrak{C}} + (\bar{\nabla}^{2\text{d}}\alpha | \bar{\nabla}^{2\text{d}}\alpha)\Bigg)\mathrm{d}x'.$$

The definition of $Q_{\text{cell}}^{\text{rel}}$ lets us eliminate G_1, which only depends on x_1, and conclude that

$$\liminf_{k\to\infty} kE^{(k)}(y^{(k)}) \ge \frac{1}{2}\int_{\Omega^{\text{ext}}} Q_{\text{tot}}(x', \bar{G})\mathrm{d}x \ge \frac{1}{2}\int_0^L Q_{\text{cell}}^{\text{rel}}\Big(R^\top \frac{\partial R}{\partial x_1}\Big)\mathrm{d}x_1.$$

Remark 3.9. Although in continuum theories with homogeneous materials, it can be proved that (an analogue of) the minimizing x_1-stretch g in (3.12) is 0 [Sca06], here in ultrathin rods it does not seem so clear how to investigate this question.

3.3.4 Proof of the upper bound

Proof of Theorem 3.5(ii). Thanks to the Γ-liminf inequality, it is enough to show

$$\limsup_{k\to\infty} kE^{(k)}(y^{(k)}) \le E_{\text{ult}}(\tilde{y}, d_2, d_3).$$

This trivially holds if $(\tilde{y}, d_2, d_3) \notin \mathcal{A}$. By contrast, if $(\tilde{y}, d_2, d_3) \in \mathcal{A}$, we first additionally suppose that $\tilde{y} \in \mathcal{C}^3([0,L];\mathbb{R}^3)$, $d_2, d_3 \in \mathcal{C}^2([0,L];\mathbb{R}^3)$. Define the sequence of lattice deformations

$$\tilde{y}^{(k)}(x) := \tilde{y}(x_1) + \frac{1}{k} x_2 d_2(x_1) + \frac{1}{k} x_3 d_3(x_1) + \frac{1}{k} q(x_1) + \frac{1}{k^2}\beta(x), \quad x \in \{0, \tfrac{1}{k}, \dots, L_k\} \times \mathcal{L}^{\text{ext}},$$

where $\beta(\cdot, x') \in \mathcal{C}^1([0,L];\mathbb{R}^3)$ for each $x' \in \mathcal{L}^{\text{ext}}$ and $q \in \mathcal{C}^2([0,L];\mathbb{R}^3)$ are arbitrary for the time being. We interpolate and extend the sequence $\tilde{y}^{(k)}$ to a piecewise affine mapping on Ω_k^{ext} as in Section 3.2.2 (by now applying Lemma 3.2 to S_k^{ext} instead of S_k and then restricting $\tilde{y}^{(k)}$ to Ω_k^{ext}, as no new external atomic layers are needed) so that

$$\operatorname{ess\,sup}_{\Omega_k^{\text{ext}}} \operatorname{dist}^2(\nabla_k \tilde{y}^{(k)}, \mathrm{SO}(3)) \le C \operatorname{ess\,sup}_{(0,L_k)\times \frac{1}{kh_k} S_k^{\text{ext}}} \operatorname{dist}^2(\nabla_k \tilde{y}^{(k)}, \mathrm{SO}(3)). \tag{3.21}$$

The rescaled discrete gradient of $\tilde{y}^{(k)}$ is

$$\begin{aligned} [\bar{\nabla}_k \tilde{y}^{(k)}(x)]_{\bullet i} = k\Big[&\tilde{y}(\bar{x}_1 + \tfrac{1}{k} z_1^i) - \frac{1}{2}\Big(\tilde{y}(\bar{x}_1 - \tfrac{1}{2k}) + \tilde{y}(\bar{x}_1 + \tfrac{1}{2k})\Big)\Big] \\ &+ \sum_{s=2}^{3} \Big[(\bar{x}_s + z_s^i) d_s(\bar{x}_1 + \tfrac{1}{k} z_1^i) - \frac{1}{2}\bar{x}_s\Big(d_s(\bar{x}_1 - \tfrac{1}{2k}) + d_s(\bar{x}_1 + \tfrac{1}{2k})\Big)\Big] \\ &+ q(\bar{x}_1 + \tfrac{1}{k} z_1^i) - \frac{1}{2}\Big(q(\bar{x}_1 - \tfrac{1}{2k}) + q(\bar{x}_1 + \tfrac{1}{2k})\Big) + \tfrac{1}{k}\Big(\tilde{\beta}(\bar{x} + \tilde{z}^i) - \tilde{\beta}(\bar{x})\Big), \end{aligned}$$

where $\tilde{\beta}$ denotes the usual piecewise affine interpolation of β. Let furthermore $R = (\frac{\partial \tilde{y}}{\partial x_1} \,|\, d_2 \,|\, d_3)$. As in (3.19), frame-indifference for the energy defined in (3.4) yields

$$\begin{aligned} E^{(k)}(y^{(k)}) = k \int_{(0,L_k)\times S^{\text{ext}}} & W_{\text{tot}}\Big(x', \bar{\mathrm{Id}} + \tfrac{1}{k}\bar{F}^{(k)}(x)\Big)\mathrm{d}x \\ &+ \sum_{x \in \{-\frac{1}{2k}, L_k + \frac{1}{2k}\} \times \mathcal{L}'^{,\text{ext}}} W_{\text{end}}\Big(\mathrm{t}_k(kx_1, x'), \bar{\nabla}_k \tilde{y}^{(k)}(x)\Big), \end{aligned} \tag{3.22}$$

where

$$\bar{F}^{(k)}(x) = \frac{R(\bar{x}_1)^\top \bar{\nabla}_k \tilde{y}^{(k)}(x) - \bar{\mathrm{Id}}}{1/k}.$$

We would like to find the limits of $\bar{F}^{(k)}$ and $\frac{1}{k}\bar{F}^{(k)}$ so that we can let $k \to \infty$ in (3.22). Fix $i \in \{1, 2, \dots, 8\}$. For $x' \in S^{\text{ext}}$ we denote by $\bar{x}'$ an element of $\mathcal{L}'^{,\text{ext}}$ that is closest to x. Taylor expanding the functions $d_2, d_3, q \in \mathcal{C}^2([0,L];\mathbb{R}^3)$ about $\bar{x}_1$ we deduce that

$$\begin{aligned} k\Big[&(\bar{x}_s + z_s^i) d_s(\bar{x}_1 + \tfrac{1}{k} z_1^i) \\ &\quad - \frac{\bar{x}_s}{2}\Big(d_s(\bar{x}_1 - \tfrac{1}{2k}) + d_s(\bar{x}_1 + \tfrac{1}{2k})\Big) - d_s(\bar{x}_1) z_s^i\Big] \to (\bar{x}_s + z_s^i)\frac{\partial d_s}{\partial x_1}(x_1) z_1^i, \\ k\Big[&q(\bar{x}_1 + \tfrac{1}{k} z_1^i) - \frac{1}{2}\Big(q(\bar{x}_1 - \tfrac{1}{2k}) + q(\bar{x}_1 + \tfrac{1}{2k})\Big)\Big] \to z_1^i \frac{\partial q}{\partial x_1}(x_1), \end{aligned}$$

$s = 2,3$, uniformly in $x \in \Omega^{\text{ext}}$. Similarly, we get by the $\mathcal{C}^3$-regularity of $\tilde{y}$

$$k^2\Big[\tilde{y}(\bar{x}_1 + \tfrac{1}{k}\bar{z}_1^i) - \frac{1}{2}(\tilde{y}(\bar{x}_1 - \tfrac{1}{2k}) + \tilde{y}(\bar{x}_1 + \tfrac{1}{2k}))\Big] \\ - k\frac{\partial \tilde{y}}{\partial x_1}(\bar{x}_1)\bar{z}_1^i \to \Big(\frac{1}{2}(\bar{z}_1^i)^2 - \frac{1}{8}\Big)\frac{\partial^2 \tilde{y}}{\partial x_1^2}(x_1) = 0$$

uniformly in $x \in \Omega^{\text{ext}}$. Finally, the function β, being uniformly continuous, satisfies

$$\tilde{\beta}(\bar{x} + \tilde{\bar{z}}^i) - \tilde{\beta}(\bar{x}) \to \Big[\bar{\nabla}^{2\text{d}}\beta(x) \,|\, \bar{\nabla}^{2\text{d}}\beta(x)\Big]_{\bullet i},$$

uniformly in $x \in \Omega^{\text{ext}}$. Summing up gives

$$k\Big[\Big[\bar{\nabla}_k \tilde{y}^{(k)}(x)\Big]_{\bullet i} - \Big(\tfrac{\partial \tilde{y}}{\partial x_1}\Big|d_2\Big|d_3\Big)(\bar{x}_1)\bar{z}^i\Big] \\ \to \sum_{s=2}^{3}(\bar{x}_s + \bar{z}_s^i)\frac{\partial d_s}{\partial x_1}\bar{z}_1^i + \frac{\partial q}{\partial x_1}\bar{z}_1^i + [\bar{\nabla}^{2\text{d}}\beta(x) \,|\, \bar{\nabla}^{2\text{d}}\beta(x)]_{\bullet i} \tag{3.23}$$

for any $i \in \{1, 2, \ldots, 8\}$ and so

$$\bar{F}^{(k)}(x) \to R^\top(x_1)\Big(\frac{\partial R}{\partial x_1}(x_1)(0, \bar{x}_2, \bar{x}_3)^\top + \frac{\partial q}{\partial x_1}(x_1)\Big)e_1^\top \bar{\text{Id}} \\ + R^\top(x_1)\frac{\partial R}{\partial x_1}(x_1)\Big[\bar{z}_1^i(0, \bar{z}_2^i, \bar{z}_3^i)^\top\Big]_{i=1}^8 + R^\top(x_1)\Big(\bar{\nabla}^{2\text{d}}\beta(x)|\bar{\nabla}^{2\text{d}}\beta(x)\Big)$$

and $\frac{1}{k}\bar{F}^{(k)}(x) \to 0$ uniformly in $x \in \Omega^{\text{ext}}$.

We first note that by $W_{\text{end}}(\mathrm{t}, \cdot) \le C\text{dist}^2(\cdot, \bar{\text{SO}}(3))$, (3.23) and (3.21),

$$\sum_{x \in \{-\frac{1}{2k}, L_k + \frac{1}{2k}\} \times \mathcal{L}'^{,\text{ext}}} W_{\text{end}}\Big(\mathrm{t}_k(kx_1, x'), \bar{\nabla}_k \tilde{y}^{(k)}(x)\Big) \le \frac{C}{k^2},$$

so that this term can be neglected in what follows. Now Taylor's approximation in (3.22) gives

$$kE^{(k)}(y^{(k)}) \to \frac{1}{2}\int_{\Omega^{\text{ext}}} Q_{\text{tot}}\Bigg(x', R^\top(x_1)\Bigg(\frac{\partial R}{\partial x_1}(x_1)\begin{pmatrix}0\\ \bar{x}_2\\ \bar{x}_3\end{pmatrix} + \frac{\partial q}{\partial x_1}(x_1)\Bigg)e_1^\top \bar{\text{Id}} \\ + R^\top(x_1)\frac{\partial R}{\partial x_1}(x_1)\Big[\bar{z}_1^i(0, \bar{z}_2^i, \bar{z}_3^i)^\top\Big]_{i=1}^8 + R^\top(x_1)\Big(\bar{\nabla}^{2\text{d}}\beta(x)|\bar{\nabla}^{2\text{d}}\beta(x)\Big)\Bigg)\text{d}x. \tag{3.24}$$

Next we turn to the case that $(\tilde{y}, d_2, d_3) \in \mathcal{A}$, but $R = (\partial_{x_1}\tilde{y}|d_2|d_3)$ only belongs to $H^1((0, L); \mathbb{R}^{3\times 3})$. Approximation will allow us to build upon the already finished part of the proof. The procedure is analogous to [MM03].

Let $(\alpha(x_1, \cdot), g(x_1))$ be a solution of the minimizing problem in the definition of $Q_{\text{cell}}^{\text{rel}}$. Recall that $\alpha \in L^2((0, L) \times \mathcal{L}^{\text{ext}}; \mathbb{R}^3)$, $g \in L^2((0, L); \mathbb{R}^3)$. It would be desirable to see α instead of $R^\top\beta$ and g instead of $R^\top\partial_{x_1}q$ on the right-hand side of (3.24). Hence, find approximating sequences $(\alpha^{(j)}) \subset \mathcal{C}^1([0,L] \times \mathcal{L}^{\text{ext}};\mathbb{R}^3)$, $(\tilde{R}^{(j)}) \subset \mathcal{C}^2([0,L];\mathbb{R}^{3\times3})$, $(g^{(j)}) \subset \mathcal{C}^2([0,L];\mathbb{R}^3)$ such that $\alpha^{(j)} \to \alpha$ in $L^2((0,L) \times \mathcal{L}^{\text{ext}};\mathbb{R}^3)$, $g^{(j)} \to g$ in $L^2((0,L);\mathbb{R}^3)$ and $\tilde{R}^{(j)} \to R$ in $H^1([0,L];\mathbb{R}^{3\times3})$ so that also $\tilde{R}^{(j)} \to R$ uniformly in $[0,L]$ by the Sobolev embedding.

It cannot be guaranteed straight away, though, that $\tilde{R}^{(j)}(x_1)$, $x_1 \in [0,L]$, are orthogonal matrices. To sidestep this issue, we project $\tilde{R}^{(j)}(x_1)$ for every $x_1 \in [0,L]$ smoothly onto SO(3) (if j is large enough, projecting is possible on the basis of the tubular neighbourhood theorem, see [Lee02, p. 137–140]) and get a sequence $(R^{(j)}) \subset \mathcal{C}^2([0,L];\mathbb{R}^{3\times3})$ of mappings with values in SO(3). Then $R^{(j)} \to R$ in $H^1([0,L];\mathbb{R}^{3\times3})$ by smoothness of the projection map.

Further, write $R^{(j)} = (\partial_{x_1}\tilde{y}^{(j)}|d_2^{(j)}|d_3^{(j)})$ with $d_2^{(j)}, d_3^{(j)} \in \mathcal{C}^2([0,L];\mathbb{R}^3)$ and $\tilde{y}^{(j)}$ belonging to $\mathcal{C}^3([0,L];\mathbb{R}^3)$ such that $\tilde{y}^{(j)}(0) = \tilde{y}(0)$; this gives $(\tilde{y}^{(j)}|d_2^{(j)}|d_3^{(j)}) \in \mathcal{A}$.

For every $j \in \mathbb{N}$, $\beta := R^{(j)}\alpha^{(j)}$ and $\partial_{x_1}q := R^{(j)}g^{(j)}$ we can construct, by the first part of the proof, $(\tilde{y}^{(k,j)})_{k=1}^{\infty}$ such that

$$\tilde{y}^{(k,j)} \to \tilde{y}^{(j)} \text{ in } L^2(\Omega^{\text{ext}};\mathbb{R}^3),\ k \to \infty,$$
$$k\frac{\partial \tilde{y}^{(k,j)}}{\partial x_s} \to d_s^{(j)} \text{ in } L^2(\Omega^{\text{ext}};\mathbb{R}^3),\ s = 2,3,\ k \to \infty$$

so that (3.24) holds with $y^{(k)}$, d_2, d_3, β and $\partial_{x_1}q$ replaced with $y^{(k,j)}$, $d_2^{(j)}$, $d_3^{(j)}$, $R^{(j)}\alpha^{(j)}$ and $R^{(j)}g^{(j)}$, respectively. Finally, diagonalize (take $\tilde{y}^{(k,j_k)}$ for a suitable sequence (j_k)) and the proof is finished, since the integral in (3.24) behaves continuously in R, β and $\partial_{x_1}q$ with respect to the required topologies. □

3.4 Resulting theory for thin rods

We now consider the situation of 'thin rods' when the cross section of the rod is not given by a fixed 2D lattice $\mathcal{L}$ but rather by a macroscopic set $hS \subset \mathbb{R}^2$ whose diameter $h = h_k$ satisfies $\frac{1}{k} \ll h \ll 1$ so that $(0,L) \times hS$ is eventually filled with atoms. Again, $L > 0$ stands for the rod's length and the cross section is defined in terms of S and S_k as described in Section 3.2.1. For convenience we also suppose that $|S| = 1$ and that the axes are oriented in such a way that

$$\int_S x_2x_3\mathrm{d}x' = \int_S x_2\mathrm{d}x' = \int_S x_3\mathrm{d}x' = 0. \tag{3.25}$$

(For ultrathin rods this was not assumed.) Since S has a Lipschitz boundary, we can fix $m \geq 1$ such that $S_k^{\text{ext}} \supset kh_kS$ for all k.

3.4.1 Gamma-convergence

As in Section 3.3.2 in view of Theorem 3.4 and (3.5) the convergence in Theorem 3.8 is stated in terms of the piecewise affine interpolations $\tilde{y}^{(k)}$ and their rescaled gradients $\nabla_k\tilde{y}^{(k)}$ on $\Omega = (0,L) \times S$ and it suffices to consider limiting configurations $\tilde{y} \in H^1((0,L);\mathbb{R}^3)$ and $d_2, d_3 \in L^2((0,L);\mathbb{R}^3)$. We remark that, by

Theorem 3.4, one could equivalently consider the Γ-limit in the $L^2_{\mathrm{loc}}(\Omega)$ topology. Also, the convergence could be alternatively formulated in terms of L^2 convergence of piecewise constant interpolations of $\tilde{y}^{(k)}|_{\bar{\Lambda}_k}$ and the piecewise constant $\bar{\nabla}_k \tilde{y}^{(k)}$ to $\tilde{y}$ and $R\bar{\mathrm{Id}}$, respectively; see [BS22].

Theorem 3.8. *If $k \to \infty$ and $h_k \to 0+$ with $kh_k \to \infty$, the functionals $\frac{1}{k^3 h_k^4} E^{(k)}$ Γ-converge to the functional E_{th} defined below, in the following sense:*

(i) Let $(y^{(k)})_{k=1}^{\infty}$ be a sequence of lattice deformations such that their piecewise affine interpolated extensions $(\tilde{y}^{(k)})_{k=1}^{\infty}$, defined in Section 3.2, converge to $\tilde{y} \in H^1((0,L);\mathbb{R}^3)$ in $L^2(\Omega;\mathbb{R}^3)$. Let us also assume that $\frac{1}{h_k}\partial_{x_s}\tilde{y}^{(k)} \to d_s \in L^2((0,L);\mathbb{R}^3)$ in $L^2(\Omega;\mathbb{R}^3)$, $s = 2,3$. Then

$$E_{\mathrm{th}}(\tilde{y}, d_2, d_3) \le \liminf_{k\to\infty} \frac{1}{k^3 h_k^4} E^{(k)}(y^{(k)}).$$

(ii) For every $\tilde{y} \in H^1((0,L);\mathbb{R}^3)$, $d_2, d_3 \in L^2((0,L);\mathbb{R}^3)$ there is a sequence of lattice deformations $(y^{(k)})_{k=1}^{\infty}$ such that their piecewise affine interpolated extensions $(\tilde{y}^{(k)})_{k=1}^{\infty}$, defined in Section 3.2, satisfy $\tilde{y}^{(k)} \to \tilde{y}$ in $L^2(\Omega;\mathbb{R}^3)$, $\frac{1}{h_k}\frac{\partial \tilde{y}^{(k)}}{\partial x_s} \to d_s$ in $L^2_{\mathrm{loc}}(\Omega;\mathbb{R}^3)$ for $s = 2,3$, and

$$\lim_{k\to\infty} \frac{1}{k^3 h_k^4} E^{(k)}(y^{(k)}) = E_{\mathrm{th}}(\tilde{y}, d_2, d_3).$$

The limit energy functional is given by

$$E_{\mathrm{th}}(\tilde{y}, d_2, d_3) = \begin{cases} \frac{1}{2}\int_0^L Q_{\mathrm{cell}}^{\mathrm{rel}}(R^\top \partial_{x_1} R)\mathrm{d}x_1 & \text{if } (\tilde{y}, d_2, d_3) \in \mathcal{A}, \\ +\infty & \text{otherwise,} \end{cases}$$

where $R := (\partial_{x_1}\tilde{y}|d_2|d_3)$ and the class $\mathcal{A}$ of admissible deformations is as in Theorem 3.5. The relaxed quadratic form $Q_{\mathrm{cell}}^{\mathrm{rel}} : \mathbb{R}^{3\times 3}_{\mathrm{skew}} \to [0,+\infty)$ is defined as

$$Q_{\mathrm{cell}}^{\mathrm{rel}}(A) := \min_{\alpha \in H^1(S;\mathbb{R}^3)} \int_S Q_{\mathrm{cell}}\left(\left(A\begin{pmatrix} 0 \\ x_2 \\ x_3 \end{pmatrix}\Big|\frac{\partial \alpha}{\partial x_2}\Big|\frac{\partial \alpha}{\partial x_3}\right)\bar{\mathrm{Id}}\right)\mathrm{d}x'. \tag{3.26}$$

Remark 3.10. Theorem 3.8 is in direct correspondence with the Γ-limit derived in [MM03]. In fact, the work [CDKM06] shows that for W_{cell} admissible as *full* in Definition 3.2.1 and boundary conditions close to a rigid motion, defining the 3D continuum stored energy density $\mathcal{W}$ as $\mathcal{W}(F) = W_{\mathrm{cell}}(F\bar{\mathrm{Id}})$, $F \in \mathbb{R}^{3\times 3}$, is justified (the Cauchy–Born rule is valid). If $\mathcal{W}$ is defined this way, then $A : \partial_F^2 \mathcal{W}(\mathrm{Id}) : A = Q_{\mathrm{cell}}(A\bar{\mathrm{Id}}) := Q_3(A)$ and with Q_2 derived from Q_3 by the auxiliary minimization (3.1) in [MM03], we get the bending-torsion functional from [MM03], since $Q_{\mathrm{cell}}^{\mathrm{rel}}(A) = Q_2(A)$.

Remark 3.11. Like in [MM03], it can be proved that a solution to the minimum problem in (3.26) exists. Since all skew-symmetric matrices are in the kernel of $F \mapsto \nabla^2 W_{\mathrm{cell}}(\bar{\mathrm{Id}}) : F\bar{\mathrm{Id}}$, we can replace the components of $\nabla\alpha$ by the components of $\frac{1}{2}(\nabla\alpha+\nabla^\top\alpha)$ on the right-hand side of (3.26) and get H^1-bounds by a version of Korn's inequality [OSY92, Theorem 2.5] if we require that α belong to the class

$$\mathcal{V}=\Big\{\beta\in H^1(S;\mathbb{R}^3);\ \int_S \beta\,\mathrm{d}x'=0,\ \int_S \nabla\beta\,\mathrm{d}x'=0\Big\}.$$

Since Q_{cell} is convex, we obtain the existence of a minimizer α by the direct method of the calculus of variations. Strict convexity of Q_{cell} on $\mathbb{R}^{3\times3}_{\mathrm{sym}}\bar{\mathrm{Id}}$ implies that the minimizer is unique in $\mathcal{V}$. Further, by analyzing the Euler-Lagrange equations we see that α depends linearly on the entries of A so that $Q^{\mathrm{rel}}_{\mathrm{cell}}$ is a quadratic form and if $\alpha(x_1,\cdot)$ is the solution of (3.26) in $\mathcal{V}$ and $A:=[R^\top R'](x_1)$, $x_1\in[0,L]$, we get $\alpha\in L^2(\Omega;\mathbb{R}^3)$ and $\partial_{x_s}\alpha\in L^2(\Omega;\mathbb{R}^3)$, $s=2,3$, thanks to $R^\top R'\in L^2([0,L];\mathbb{R}^{3\times3})$.

In fact, the Euler-Lagrange equations for this minimum problem can be derived by a straightforward computation as in [MM08] (note that the integrand in (3.26) has quadratic growth). For $k=1,2,3$, the minimizer α is a weak solution to the Neumann problem

$$\begin{aligned}
&\sum_{r,s=2}^{3}\sum_{i=1}^{3}\sum_{j,\ell=1}^{8}\frac{\partial}{\partial x_s}\Big(z_r^j[\nabla^2 W_{\mathrm{cell}}(\bar{\mathrm{Id}})]_{ijk\ell}z_s^\ell\frac{\partial\alpha_i}{\partial x_r}\Big)=\\
&\qquad=-\sum_{s=2}^{3}\sum_{i=1}^{3}\sum_{j,\ell=1}^{8}[\nabla^2 W_{\mathrm{cell}}(\bar{\mathrm{Id}})]_{ijk\ell}z_1^jA_{is}z_s^\ell\quad\text{in } S,\\
&\sum_{r,s=2}^{3}\sum_{i=1}^{3}\sum_{j,\ell=1}^{8}\frac{\partial\alpha_i}{\partial x_r}z_r^j[\nabla^2 W_{\mathrm{cell}}(\bar{\mathrm{Id}})]_{ijk\ell}n_sz_s^\ell=\\
&\qquad=-\sum_{p,s=2}^{3}\sum_{i=1}^{3}\sum_{j,\ell=1}^{8}A_{ip}x_pz_1^j[\nabla^2 W_{\mathrm{cell}}(\bar{\mathrm{Id}})]_{ijk\ell}n_sz_s^\ell\quad\text{on } \partial S,
\end{aligned}$$

where $n=(n_2,n_3)^\top\in\mathbb{R}^2$ denotes the unit outward normal to S. Introducing the tensor $\mathbb{K}=(K^{ki}_{sr})_{s,r,k,i}$ and vectors $\phi,\gamma\in\mathbb{R}^3$ (which depend on x' and A) by

$$\begin{aligned}
K^{ki}_{sr}&=\sum_{j,\ell=1}^{8}z_r^j[\nabla^2 W_{\mathrm{cell}}(\bar{\mathrm{Id}})]_{ijk\ell}z_s^\ell,\quad r,s\in\{2,3\},\ i,k\in\{1,2,3\},\\
\phi_k&=-\sum_{s=2}^{3}\sum_{i=1}^{3}\sum_{j,\ell=1}^{8}[\nabla^2 W_{\mathrm{cell}}(\bar{\mathrm{Id}})]_{ijk\ell}z_1^jA_{is}z_s^\ell,\\
\gamma_k&=-\sum_{p,s=2}^{3}\sum_{i=1}^{3}\sum_{j,\ell=1}^{8}A_{ip}x_pz_1^j[\nabla^2 W_{\mathrm{cell}}(\bar{\mathrm{Id}})]_{ijk\ell}n_sz_s^\ell,\quad k\in\{1,2,3\},
\end{aligned}$$

we can write the system in the more compact form

$$\begin{aligned}
\mathrm{div}_{x_2,x_3}\Big(\mathbb{K}\nabla_{x_2,x_3}\alpha\Big)&=\phi\quad\text{in } S,\\
\mathbb{K}\nabla_{x_2,x_3}\alpha\cdot n&=\gamma\quad\text{on } \partial S.
\end{aligned}\tag{3.27}$$

The structure of eigenspaces of $\nabla^2 W_{\mathrm{cell}}(\bar{\mathrm{Id}})$ gives an ellipticity condition

$$(F\bar{\mathrm{Id}}):\nabla^2 W_{\mathrm{cell}}(\bar{\mathrm{Id}}):(F\bar{\mathrm{Id}})\ge C|\mathrm{sym}F|^2$$

for any $F \in \mathbb{R}^{3\times3}$ so by the aforementioned Korn's inequality and standard PDE theory, we discover that the minimizer α is a weak solution of system (3.27) unique in $\mathcal{V}$. For physical background of this system of PDEs, see Chapter 2.

Remark 3.12. As mentioned in Example 3.1, cell energies given by a sum of pairwise interactions may not satisfy assumption (E2) if they do not include an additional penalty term which prevents them from being minimized on improper rotations. Besides, a deficiency of our approach in terms of physical modelling is that interatomic potentials from molecular dynamics are typically bounded near infinity, so the growth assumption (E4) does not apply. However, even energies that are O(3)-invariant and do not grow quadratically away from $\bar{\mathrm{SO}}(3)$ can be treated in case of 'sufficiently thin' rods. Following [BS22, Section 2.4], let us suppose that W_{cell} only fulfils (E1), (E3), but also the following alternative assumptions:

(E1.1) $W_{\mathrm{cell}}(\vec{y}) = W_{\mathrm{cell}}(-\vec{y})$ for all $\vec{y} \in V_0^\perp$,

(E2.1) $\min_{\vec{y}\in\mathbb{R}^{3\times8}} W_{\mathrm{cell}}(\vec{y}) = 0$ and $W_{\mathrm{cell}}(\vec{y}) = \min W_{\mathrm{cell}}$ if and only if $\vec{y} = O\bar{\mathrm{Id}} + \vec{c}$ for some $O \in \mathrm{O}(3)$ and $\vec{c} \in V_0$,

(E4.1) there is a constant $\eta > 0$ such that $W_{\mathrm{cell}}(\vec{y}) \geq \eta$ for every $\vec{y} \in V_0^\perp \setminus \mathcal{U}^\pm$, where $\mathcal{U}$ is the neighbourhood of $\bar{\mathrm{SO}}(3)$ from (E3) and $\mathcal{U}^\pm := \mathcal{U} \cup (-\mathcal{U})$.

Since reflections may lead to unnatural folded configurations with zero energy, we also add a nonlocal term to $E^{(k)}$ to avoid colliding atoms, see [BS22]. Moreover, if we assume that $k^3h_k^4 \to 0+$ (in particular, this also holds in the ultrathin case), then due to our energy scaling, $W_{\mathrm{cell}}(\vec{y}^{(k)})$ must be small on every atomic cell. As a result, W_{cell} is never evaluated at points for which a growth assumption would manifest itself. In this setting, Theorem 3.8 holds with $R^{(k)}, R \in \mathrm{O}(3)$ (analogously in Theorem 3.5 and up to replacing $\tilde{y}^{(k)}$ with $-\tilde{y}^{(k)}$ in Theorem 3.4).

3.4.2 Proof of the lower bound

To prove Theorem 3.8(i), let us assume that $k^{-3}h_k^{-4}E^{(k)}(y^{(k)}) \leq C$, whence (3.6) holds due to (3.4) and (3.5). Without loss of generality passing to a suitable subsequence, we obtain the piecewise constant $R^{(k)}$ converging to $R(x_1) = (\frac{\partial\tilde{y}}{\partial x_1}(x)\,|\,d_2(x)\,|\,d_3(x))$ as in Theorem 3.4. From (3.8), for

$$G^{(k)}(x) := \frac{(R^{(k)})^\top(x_1)\nabla_k\tilde{y}^{(k)}(x) - \mathrm{Id}}{h_k}, \quad x \in \Omega_k^{\mathrm{ext}},$$

we have $G^{(k)} \rightharpoonup G \in L^2(\Omega;\mathbb{R}^{3\times3})$ in $L^2(\Omega;\mathbb{R}^{3\times3})$, up to a subsequence. Its discrete version

$$\bar{G}^{(k)}(x) := \frac{k(R^{(k)})^\top(x_1)(\tilde{y}^{(k)}(\bar{x}+\tilde{z}^i) - \tilde{y}^{(k)}(\bar{x}))_{i=1}^8 - \bar{\mathrm{Id}}}{h_k}, \quad x \in \Omega_k^{\mathrm{ext}}.$$

is again bounded in $L^2(\Omega;\mathbb{R}^{3\times8})$ (cf. (3.3)). Thus $\bar{G}^{(k)} \rightharpoonup \bar{G}$ in $L^2(\Omega;\mathbb{R}^{3\times8})$ for a (not relabelled) subsequence.

The following proposition is contained in [MM03].

Proposition 3.9. *Suppose $G^{(k)} \rightharpoonup G \in L^2(\Omega;\mathbb{R}^{3\times 3})$ in $L^2(\Omega;\mathbb{R}^{3\times 3})$. Then there are $G_1 \in L^2((0,L);\mathbb{R}^3)$ and $\alpha \in L^2(\Omega;\mathbb{R}^3)$ with $\nabla'\alpha \in L^2(\Omega;\mathbb{R}^{3\times 2})$ such that*

$$G(x) = \Big(G_1(x_1) + R^\top \frac{\partial R}{\partial x_1}(0,x_2,x_3)^\top \Big| \nabla'\alpha(x)\Big).$$

Proof. See [MM03, (3.10) and (3.13)]. □

Now we explore how the limits G and $\bar{G}$ are connected. Recall the notation $\bar{G}_{\bullet i}$ for the i-th column of $\bar{G}$.

Proposition 3.10. *The representation $\bar{G}_{\bullet i} = G z^i$ holds for every $i \in \{1,2,\ldots,8\}$.*

Proof. Our method is, loosely speaking, to shift everything to a neighbouring lattice block by a direction vector a and handle the resulting remainder. The approach is inspired by [Sch06]. Recall that for $x \in \overline{\Omega_k^{\text{ext}}}$, we denote by $\bar{x}$ an element of $\tilde{\Lambda}_k^{\prime,\text{ext}}$ that is closest to x. Take $\bar{x}, \bar{x}_+ = \bar{x} + a \in \tilde{\Lambda}_k^{\prime,\text{ext}}$, where $a := \tilde{z}^i - \tilde{z}^j$, and compute

$$\begin{aligned}k(R^{(k)})^\top\Big(\tilde{y}^{(k)}(\bar{x}+\tilde{z}^i) - \tilde{y}^{(k)}(\bar{x})\Big) - z^i = {} & k(R^{(k)})^\top\Big(\tilde{y}^{(k)}(\bar{x}_+ + \tilde{z}^j) - \tilde{y}^{(k)}(\bar{x}_+)\Big) - z^j \\ & + k(R^{(k)})^\top\Big(\tilde{y}^{(k)}(\bar{x}_+) - \tilde{y}^{(k)}(\bar{x})\Big) + (z^j - z^i)\end{aligned} \tag{3.28}$$

(note that $\bar{x} + \tilde{z}^i = \bar{x}_+ + \tilde{z}^j$). Let $\tilde{Q} = \tilde{Q}(\bar{x}) = \bar{x} + (-\frac{1}{2k}, \frac{1}{2k}) \times (-\frac{1}{2kh_k}, \frac{1}{2kh_k})^2$. Property (3.2) of the piecewise affine interpolation gives

$$\begin{aligned}k(\tilde{y}^{(k)}(\bar{x}_+) - \tilde{y}^{(k)}(\bar{x})) &= k\fint_{\tilde{Q}} \tilde{y}^{(k)}(\xi_+) - \tilde{y}^{(k)}(\xi)\mathrm{d}\xi \\ &= \fint_{\tilde{Q}} \int_0^1 k\frac{\mathrm{d}}{\mathrm{d}t}(\tilde{y}^{(k)}(\xi + ta))\mathrm{d}t\mathrm{d}\xi = \fint_{\tilde{Q}} \int_0^1 k\nabla\tilde{y}^{(k)}(\xi + ta)a\mathrm{d}t\mathrm{d}\xi.\end{aligned} \tag{3.29}$$

Dividing (3.28) by the rod thickness h_k and using (3.29), we derive

$$\bar{G}^{(k)}_{\bullet i} = [\bar{G}^{(k)}_+]_{\bullet j} + \frac{1}{h_k}\Big[(R^{(k)})^\top \fint_{\tilde{Q}} \int_0^1 \nabla_k \tilde{y}^{(k)}(\xi + ta)\mathrm{d}t\mathrm{d}\xi(z^i - z^j) - (z^i - z^j)\Big], \tag{3.30}$$

where we have set

$$[\bar{G}^{(k)}_+(x)]_{\bullet j} := \frac{1}{h_k}[k(R^{(k)}(x_1))^\top\Big(\tilde{y}^{(k)}(\bar{x}_+ + \tilde{z}^j) - \tilde{y}^{(k)}(\bar{x}_+)\Big) - z^j].$$

Fix $\Omega' \subset\subset \Omega$. Let us prove that

$$\bar{G}^{(k)}_+ \rightharpoonup \bar{G} \text{ in } L^1(\Omega';\mathbb{R}^{3\times 8}). \tag{3.31}$$

In the first place, shifts by a preserve weak convergence so that in $L^2(\Omega';\mathbb{R}^{3\times 8})$,

$$\frac{1}{h_k}\Big[k\Big(R^{(k)}(\cdot + a_1)\Big)^\top \Big(\tilde{y}^{(k)}(\cdot + a + \tilde{z}^i) - \tilde{y}^{(k)}(\cdot + a)\Big)_{i=1}^8 - \bar{\mathrm{Id}}\Big] \rightharpoonup \bar{G}. \tag{3.32}$$

In the second place, due to our construction of $R^{(k)}$ as constant on intervals of length h'_k, the difference $R^{(k)}(\cdot + a_1) - R^{(k)}$ can only be nonzero on interfaces of those intervals of constancy. The length of each such interface equals $|a_1| \leq \frac{1}{k}$. Estimate (3.9) then implies that

$$\begin{aligned}\int_{\Omega'} |R^{(k)}(x_1 + a_1) - R^{(k)}(x_1)|^2 \mathrm{d}x &\leq \frac{|S|}{k} \sum_{i=0}^{\lfloor L_k/h'_k \rfloor - 2} \left| R^{(k)}(ih'_k + \tfrac{3}{2}h'_k) - R^{(k)}(ih'_k + \tfrac{1}{2}h'_k) \right|^2 \\ &\leq \frac{C}{kh_k} \int_{\Omega_k^{\mathrm{ext}}} \mathrm{dist}^2\big(\nabla_k \tilde{y}^{(k)}, \mathrm{SO}(3)\big) \mathrm{d}x \leq \frac{Ch_k}{k},\end{aligned}$$

where the last step followed from (3.6). Thus $\frac{1}{h_k}(R^{(k)}(\cdot + a_1) - R^{(k)})$ tends to 0 in L^2. As $(k(\tilde{y}^{(k)}(\cdot + a + \tilde{z}^\ell) - \tilde{y}^{(k)}(\cdot + a))_{\ell=1}^8)$ is L^2-bounded for an analogous reason as $(\bar{G}^{(k)})$, the convergence

$$\frac{1}{h_k}\Big(R^{(k)}(\cdot + a_1)^\top - (R^{(k)})^\top\Big) k\Big(\tilde{y}^{(k)}(\cdot + a + \tilde{z}^\ell) - \tilde{y}^{(k)}(\cdot + a)\Big)_{\ell=1}^8 \xrightarrow{L^1} 0$$

combined with (3.32) establishes (3.31).

By definition, $R^{(k)}$ is constant on $\tilde{Q}$, so the remainder term in (3.30) equals

$$\begin{aligned}&\int_0^1 \fint_{\tilde{Q}} \frac{1}{h_k}\Big[(R^{(k)}(\xi_1))^\top \nabla_k \tilde{y}^{(k)}(\xi + ta)(z^i - z^j) - (z^i - z^j)\Big] \mathrm{d}\xi \mathrm{d}t \\ &\quad = \fint_{\tilde{Q}} \int_0^1 G^{(k)}(\xi + ta)(z^i - z^j) \mathrm{d}t \mathrm{d}\xi \qquad (3.33) \\ &\quad + \int_0^1 \fint_{\tilde{Q}} \Big[\frac{1}{h_k}\Big(\Big(R^{(k)}(\xi_1) - R^{(k)}(\xi_1 + ta_1)\Big)^\top \nabla_k \tilde{y}^{(k)}(\xi + ta)(z^i - z^j)\Big)\Big] \mathrm{d}t. \qquad (3.34)\end{aligned}$$

Term (3.33) weakly converges to $G(z^i - z^j)$ since for any $\varphi \in C_c^\infty(\Omega)$

$$\begin{aligned}\int_\Omega \fint_{\tilde{Q}(\bar{x})} \int_0^1 G^{(k)}(\xi + ta) \mathrm{d}t \mathrm{d}\xi \varphi(x) \mathrm{d}x &= \int_\Omega \int_0^1 G^{(k)}(\xi + ta) \mathrm{d}t \fint_{\tilde{Q}(\bar{\xi})} \varphi(x) \mathrm{d}x \mathrm{d}\xi \\ &\to \int_\Omega G(\xi)\varphi(\xi) \mathrm{d}\xi.\end{aligned}$$

In (3.34), $\nabla_k \tilde{y}^{(k)}(\cdot + ta)$ is L^2-bounded uniformly in t by (3.8) and as above we see that $\frac{1}{h_k}(R^{(k)}(\cdot + ta_1) - R^{(k)})$ converges to 0 in $L^2(\Omega'; \mathbb{R}^{3\times3})$ uniformly in t, so the whole term vanishes in the limit.

Thus, passing to the limit in (3.30), we conclude that

$$\bar{G}_{\bullet i} - \bar{G}_{\bullet j} = G(z^i - z^j).$$

The assertion now follows by summing over j and using the fact that the columns satisfy $\sum_{j=1}^8 \bar{G}_{\bullet j} = \sum_{j=1}^8 z^j = 0$. □

We can now finish the proof of Theorem 3.8(i).

By (3.4), the non-negativity of $W_{\rm surf}$ and $W_{\rm end}$, and the frame-indifference of $W_{\rm cell}$, we estimate as in (3.19)

$$E^{(k)}(y^{(k)}) \geq \sum_{\hat{x}\in\hat{\Lambda}_k'} W_{\rm cell}\Big(\vec{y}^{(k)}(\hat{x})\Big) = k^3 h_k^2 \int_\Omega \chi_k(x) W_{\rm cell}\Big(\bar{\rm Id} + h_k \bar{G}^{(k)}(x)\Big) {\rm d}x,$$

where now χ_k is the characteristic function of $\{|\bar{G}^{(k)}| \leq \sqrt{1/h_k}\} \cap [(0, L_k) \times \frac{1}{kh_k} S_k]$. The same arguments as in the ultrathin case, cf. also [FJM02, MM03, Sch06], lead to

$$\liminf_{k\to\infty} \frac{1}{k^3 h_k^4} E^{(k)}(y^{(k)}) \geq \int_\Omega \frac{1}{2} Q_{\rm cell}(\bar{G}) {\rm d}x.$$

By Proposition 3.10, $Q_{\rm cell}(\bar{G}) = Q_{\rm cell}(G\bar{\rm Id})$. The proof is completed as in [MM03]: Setting $c_s(x_1) = \int_S \frac{\partial \alpha}{\partial x_s} {\rm d}x'$, $s = 2, 3$, invoking Proposition 3.9 and (3.25), and using the fact that certain quantities are independent of x_2, x_3, we find

$$\begin{aligned}\int_S Q_{\rm cell}(\bar{G}) {\rm d}x' = &\int_S Q_{\rm cell}\Big((G_1(x_1)\,\big|\,c_2(x_1)\big|c_3(x_1))\bar{\rm Id}\Big) {\rm d}x' \\ &+ \int_S Q_{\rm cell}\Big(\Big(R^\top \frac{\partial R}{\partial x_1}(0, x_2, x_3)^\top \Big| \frac{\partial \bar{\alpha}}{\partial x_2} \Big| \frac{\partial \bar{\alpha}}{\partial x_3}\Big)\bar{\rm Id}\Big) {\rm d}x',\end{aligned}$$

where $\bar{\alpha}(x) := \alpha(x) - x_2 c_2(x_1) - x_3 c_3(x_1)$. Thus the definition of $Q_{\rm cell}^{\rm rel}$ lets us conclude that

$$\liminf_{k\to\infty} \frac{1}{k^3 h_k^4} E^{(k)}(y^{(k)}) \geq \int_\Omega \frac{1}{2} Q_{\rm cell}(\bar{G}) {\rm d}x \geq 0 + \frac{1}{2}\int_0^L Q_{\rm cell}^{\rm rel}\left(R^\top \frac{\partial R}{\partial x_1}\right) {\rm d}x_1.$$

3.4.3 Proof of the upper bound

Proof of Theorem 3.8(ii). In the nontrivial case that $(\tilde{y}, d_2, d_3) \in \mathcal{A}$, we first additionally suppose that $\tilde{y} \in \mathcal{C}^3([0, L]; \mathbb{R}^3)$, $d_2, d_3 \in \mathcal{C}^2([0, L]; \mathbb{R}^3)$. For $\beta \in \mathcal{C}^1(\mathbb{R}^3; \mathbb{R}^3)$ to be fixed later, define the sequence

$$\tilde{y}^{(k)}(x) := \tilde{y}(x_1) + h_k x_2 d_2(x_1) + h_k x_3 d_3(x_1) + h_k^2 \beta(x), \quad x \in \{0, \tfrac{1}{k}, \ldots, L_k\} \times \frac{1}{kh_k}\mathcal{L}_k^{\rm ext}.$$

We extend and interpolate the sequence $\tilde{y}^{(k)}$ on $\Omega_k^{\rm ext}$ in the same way as in Section 3.3.4 so that, in particular, (3.21) holds true again. The rescaled discrete gradient $\bar{\nabla}_k \tilde{y}^{(k)}(x) = k[\tilde{y}^{(k)}(\bar{x} + \tilde{z}^i) - \frac{1}{8}\sum_{j=1}^8 \tilde{y}^{(k)}(\bar{x} + \tilde{z}^j)]_{i=1}^8$ of $\tilde{y}^{(k)}$ reads

$$\begin{aligned}[\bar{\nabla}_k \tilde{y}^{(k)}(x)]_{\bullet i} = &\,k\Big[\tilde{y}(\bar{x}_1 + \tfrac{1}{k}z_1^i) - \frac{1}{2}\Big(\tilde{y}(\bar{x}_1 - \tfrac{1}{2k}) + \tilde{y}(\bar{x}_1 + \tfrac{1}{2k})\Big)\Big] \\ &+ \sum_{s=2}^3 kh_k\Big[(\bar{x}_s + \tilde{z}_s^i) d_s(\bar{x}_1 + \tfrac{1}{k}z_1^i) - \frac{1}{2}\bar{x}_s\Big(d_s(\bar{x}_1 - \tfrac{1}{2k}) + d_s(\bar{x}_1 + \tfrac{1}{2k})\Big)\Big] \\ &+ kh_k^2\Big(\tilde{\beta}(\bar{x} + \tilde{z}^i) - \tilde{\beta}(\bar{x})\Big),\end{aligned}$$

where $\tilde{\beta}$ denotes the piecewise affine discretization of $\beta|_{\tilde{\Lambda}_k^{\rm ext}}$ described in Section 3.2.

As in (3.22) we obtain

$$E^{(k)}(y^{(k)}) = k^3 h_k^2 \int_{(0,L_k)\times S_k} W_{\mathrm{cell}}\Big(x', \bar{\mathrm{Id}} + h_k \bar{F}^{(k)}(x)\Big)\mathrm{d}x + \sum_{\hat{x}\in\hat{\Lambda}_k'^{,\mathrm{surf}}} W_{\mathrm{surf}}\Big(\mathrm{t}_k(\hat{x}'), \bar{\nabla}\hat{y}^{(k)}(\hat{x})\Big)$$
$$+ \sum_{x\in\{-\frac{1}{2k}, L_k+\frac{1}{2k}\}\times\mathcal{L}_k'^{,\mathrm{ext}}} W_{\mathrm{end}}\Big(\mathrm{t}_k(kx_1, x'), \bar{\nabla}_k \tilde{y}^{(k)}(x)\Big), \tag{3.35}$$

where

$$\bar{F}^{(k)}(x) = \frac{R^\top(\bar{x}_1)\bar{\nabla}_k \tilde{y}^{(k)}(x) - \bar{\mathrm{Id}}}{h_k}.$$

Fixing $i \in \{1,2,\ldots,8\}$, we deduce the following convergences, analogous to their counterparts in ultrathin rods, uniformly in $x \in [0,L]\times S'$ for each bounded domain $S' \supset\supset S$:

$$k h_k\Big(\tilde{\beta}(\bar{x}+\tilde{z}^i) - \tilde{\beta}(\bar{x})\Big) \to \frac{\partial\beta}{\partial x_2}(x) z_2^i + \frac{\partial\beta}{\partial x_3}(x) z_3^i$$

and

$$k\Big[(\bar{x}_s + \tilde{z}_s^i) d_s(\bar{x}_1 + \tfrac{1}{k} z_1^i) - \frac{1}{2}\bar{x}_s\Big(d_s(\bar{x}_1 - \tfrac{1}{2k}) + d_s(\bar{x}_1 + \tfrac{1}{2k})\Big)\Big]$$
$$- \frac{1}{h_k} d_s(\bar{x}_1) z_s^i \to x_s \frac{\partial d_s}{\partial x_1}(x_1) z_1^i$$

for $s = 2,3$, as well as

$$\frac{k}{h_k}\Big[\tilde{y}(\bar{x}_1 + \tfrac{1}{k} z_1^i) - \frac{1}{2}\Big(\tilde{y}(\bar{x}_1 - \tfrac{1}{2k}) + \tilde{y}(\bar{x}_1 + \tfrac{1}{2k})\Big)\Big] - \frac{1}{h_k}\frac{\partial\tilde{y}}{\partial x_1}(\bar{x}_1) z_1^i \to 0.$$

Summing them up leads to

$$\frac{1}{h_k}\Big[\Big[\bar{\nabla}_k \tilde{y}^{(k)}(x)\Big]_{\bullet i} - \Big(\tfrac{\partial\tilde{y}}{\partial x_1}\Big| d_2 \Big| d_3\Big)(\bar{x}_1) z^i\Big] \to \sum_{s=2}^{3} x_s \frac{\partial d_s}{\partial x_1} z_1^i + \frac{\partial\beta}{\partial x_s} z_s^i \tag{3.36}$$

for any $i \in \{1,2,\ldots,8\}$.

Now we first notice that $\max_{\mathrm{t}\in\Upsilon}\Big(W_{\mathrm{surf}}(\mathrm{t},\cdot) + W_{\mathrm{end}}(\mathrm{t},\cdot)\Big) \le C\mathrm{dist}^2(\cdot, \bar{\mathrm{SO}}(3))$, (3.36), (3.21), and the estimate $\sharp(\Lambda_k^{\mathrm{ext}} \setminus \Lambda_k) \le C(k^2 h_k + k^2 h_k^2) \le C k^2 h_k$ give

$$\sum_{\hat{x}\in\hat{\Lambda}_k'^{,\mathrm{surf}}} W_{\mathrm{surf}}\Big(\mathrm{t}_k(\hat{x}'), \bar{\nabla} y^{(k)}(\hat{x})\Big) + \sum_{\hat{x}\in\{-\frac{1}{2}, kL_k+\frac{1}{2}\}\times\mathcal{L}_k'^{,\mathrm{ext}}} W_{\mathrm{end}}\Big(\mathrm{t}_k(\hat{x}), \bar{\nabla} y^{(k)}(\hat{x})\Big) \le C k^2 h_k^3.$$

Hence, Taylor's approximation in (3.35) yields

$$\frac{1}{k^3 h_k^4} E^{(k)}(y^{(k)}) \to \frac{1}{2}\int_\Omega Q_{\mathrm{cell}}\Big(R^\top\Big(x_2 \tfrac{\partial d_2}{\partial x_1} + x_3 \tfrac{\partial d_3}{\partial x_1} \Big| \tfrac{\partial\beta}{\partial x_2} \Big| \tfrac{\partial\beta}{\partial x_3}\Big)\bar{\mathrm{Id}}\Big)\mathrm{d}x.$$

For general $(\tilde{y}, d_2, d_3) \in \mathcal{A}$ with $R = (\partial_{x_1}\tilde{y}|d_2|d_3) \in H^1((0,L);\mathbb{R}^{3\times3})$ we may proceed by approximation exactly as in Section 3.3.4, now using that the solution $\alpha(x_1,\cdot)$ of the minimizing problem in the definition of $Q_{\mathrm{cell}}^{\mathrm{rel}}$ is such that $\alpha \in L^2(\Omega;\mathbb{R}^3)$ and $\partial_{x_s}\alpha \in L^2(\Omega;\mathbb{R}^3)$, $s = 2,3$. □

4. A continuum model for brittle nanowires derived from an atomistic description by Γ-convergence

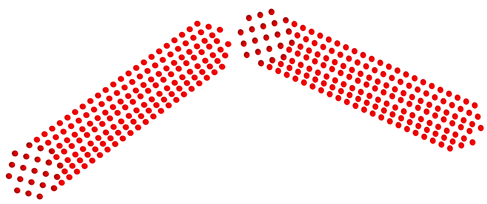
'There's more than one way to crack an egg.'

English proverb

By changing the assumptions on interaction potentials seen in the previous chapter, we obtain a model that can also describe brittle fracture of ultrathin rods (see Figure 4 for an illustration).

After specifying the discrete model in Section 2, we prove a compactness theorem for sequences of bounded energy in Section 3. The lower bound in the Γ-convergence result from Section 4 is shown in Section 5 and then followed in Section 6 by an analysis of the cell formula and the construction of recovery sequences for Theorem 4.3(ii). A simplified model is treated in Section 7. Section 8 provides examples of interatomic potentials to which the presented approach applies. In Section 9, we show that for full cracks and a class of mass-spring models there is an explicit expression for the cell formula. Moreover, it is proved that in such models, the energy needed to produce a full crack is strictly greater than the energy of a mere kink.

Figure 4.1: Fracture of a thin rod composed of atoms.



4.1 Model assumptions and preliminaries

Notation here does not differ much from that used for ultrathin rods in Section 3.3. Nevertheless, we will go through all important definitions now so that this chapter can be read independently.

4.1.1 Atomic lattice and discrete gradients

In our particle interaction model, $\Lambda_k = ([0,L] \times \frac{1}{k}\bar{S}) \cap \frac{1}{k}\mathbb{Z}^3$, $k \in \mathbb{N}$, is a cubic atomic lattice – the reference configuration of a thin rod of length $L > 0$. The interatomic distance $1/k$ is directly proportional to the thickness of the rod.

The rod's cross section is represented with a bounded domain $\emptyset \neq S \subset \mathbb{R}^2$. We assume that there is a set $\mathcal{L}' \subset (\frac{1}{2}+\mathbb{Z})^2$ such that

$$S = \operatorname{Int} \bigcup_{x' \in \mathcal{L}'} \Big(x' + \Big[-\frac{1}{2}, \frac{1}{2}\Big]^2 \Big).$$

Moreover, should it happen that $x' + \{-\frac{1}{2}, \frac{1}{2}\} \subset \mathcal{L} := \bar{S} \cap \mathbb{Z}^2$, it is assumed that $x' \in \mathcal{L}'$ as well. The symbol Λ_k' is used for the lattice of midpoints of open lattice cubes with sidelength $1/k$ and corners in Λ_k.

Our lattice Λ_k undergoes a static deformation $y^{(k)} \colon \Lambda_k \to \mathbb{R}^3$. The main aim in this chapter is to investigate the asymptotic behaviour as k becomes large and to establish an effective continuum model as $k \to +\infty$.

Sometimes it will be advantageous to work with a rescaled lattice that has unit distances between neighbouring atoms. The points of this lattice are written with hats over their coordinates, i.e. if $x = (x_1, x_2, x_3) \in \Lambda_k$ we introduce $\hat{x}_1 := kx_1$, $\hat{x}' = (\hat{x}_2, \hat{x}_3) := kx' = k(x_2, x_3)$ and $\hat{y}^{(k)}(\hat{x}_1, \hat{x}_2, \hat{x}_3) := ky^{(k)}(\frac{1}{k}\hat{x}_1, \frac{1}{k}\hat{x}')$ so that $\hat{y}^{(k)} \colon k\Lambda_k \to \mathbb{R}^3$. Then $\hat{\Lambda}_k$ and $\hat{\Lambda}_k'$ denote the sets of all $\hat{x} = (\hat{x}_1, \hat{x}_2, \hat{x}_3)$ such that the corresponding downscaled points x are elements of the sets Λ_k and Λ_k', respectively. Again we will use the eight direction vectors $z^1, z^2, \ldots, z^8$, the discrete gradient $\bar{\nabla}\hat{y}^{(k)}$, the matrix $\bar{\mathrm{Id}} = (z^1|\cdots|z^8)$, and the sets $\bar{\mathrm{SO}}(3)$, V_0 as in Subsection 3.2.1.

4.1.2 Rescaling, interpolation and extension of deformations

To handle sequences of deformations defined on a common domain $\Omega = (0, L) \times S$, we set $\tilde{y}^{(k)}(x_1, x_2, x_3) := y^{(k)}(x_1, \frac{1}{k}x')$ for $(x_1, \frac{1}{k}x') \in \Lambda_k$ and interpolate $\tilde{y}^{(k)}$ as in Subsection 3.2.2 so that it is defined even outside lattice points.

Like this, $\tilde{y}^{(k)}$ is differentiable almost everywhere, so we can define

$$\nabla_k \tilde{y}^{(k)} := \Big(\frac{\partial \tilde{y}^{(k)}}{\partial x_1} \,|\, k\frac{\partial \tilde{y}^{(k)}}{\partial x_2} \,|\, k\frac{\partial \tilde{y}^{(k)}}{\partial x_3} \Big).$$

For any face $\tilde{F}$ of $\tilde{Q}(\bar{x}) = \bar{x} + (-\frac{1}{2k}, \frac{1}{2k}) \times (-\frac{1}{2}, \frac{1}{2})^2$, $\bar{x} \in \tilde{\Lambda}_k'$, with face centre $x_{\tilde{F}}$, the piecewise affine interpolation satisfies

$$\tilde{y}^{(k)}(x_{\tilde{F}}) = \fint_{\tilde{F}} \tilde{y}^{(k)} \mathrm{d}\mathcal{H}^2 \text{ and } \tilde{y}^{(k)}(\bar{x}) = \fint_{\tilde{Q}(\bar{x})} \tilde{y}^{(k)}(\xi) \mathrm{d}\xi. \tag{4.1}$$

We also set $\bar{\nabla}_k \tilde{y}^{(k)}(\bar{x}) := k(\tilde{y}^{(k)}(\bar{x}_1 + \frac{1}{k}z_1^i, \bar{x}' + (z^i)') - \sum_{j=1}^8 \tilde{y}^{(k)}(\bar{x}_1 + \frac{1}{k}z_1^j, \bar{x}' + (z^j)'))_{i=1}^8$.

For the following reasons we now extend deformations to certain auxiliary surface lattices:

- surface energy needs to be modelled;
- in part we would like to apply Γ-convergence results from Chapter 3;
- a fixed domain on which the convergence of $(\tilde{y}^{(k)})$ is formulated sometimes does not match with its inscribed crystalline lattice (specifically in the x_1-direction).

We present here the necessary tools, without too much emphasis on this technical issue later, referring to Subsection 3.2.2 for more details and a proof, adapted from [Sch09]. Consider a portion $(a,b)\times S \subset (0,L)\times S$ of the rod. Let $a_k = \frac{1}{k}\lceil ka\rceil$, $b_k = \frac{1}{k}\lfloor kb\rfloor$, and

$$
\begin{aligned}
\mathcal{L}^{\mathrm{ext}} &= \mathcal{L} + \{-1,0,1\}^2, & \Lambda_k^{\mathrm{ext}} &= \{a_k - \tfrac{1}{k}, a_k, \dots, b_k + \tfrac{1}{k}\} \times \tfrac{1}{k}\mathcal{L}^{\mathrm{ext}},\\
\mathcal{L}'^{,\mathrm{ext}} &= \mathcal{L}' + \{-1,0,1\}^2, & \Lambda_k'^{,\mathrm{ext}} &= \{a_k - \tfrac{1}{2k}, a_k + \tfrac{1}{2k}, \dots, b_k + \tfrac{1}{2k}\} \times \tfrac{1}{k}\mathcal{L}'^{,\mathrm{ext}},\\
S^{\mathrm{ext}} &= S + (-1,1)^2, & \Omega_k^{\mathrm{ext}} &= (a_k - \tfrac{1}{k}, b_k + \tfrac{1}{k}) \times S^{\mathrm{ext}},\\
\tilde{\Lambda}_k^{\mathrm{ext}} &= \{a_k - \tfrac{1}{k}, a_k, \dots, b_k + \tfrac{1}{k}\} \times \mathcal{L}^{\mathrm{ext}}, & \tilde{\Lambda}_k'^{,\mathrm{ext}} &= \{a_k - \tfrac{1}{2k}, a_k + \tfrac{1}{2k}, \dots, b_k + \tfrac{1}{2k}\} \times \mathcal{L}'^{,\mathrm{ext}}.
\end{aligned}
$$

Lemma 4.1. *There are extensions $y^{(k)}\colon \Lambda_k^{\mathrm{ext}} \to \mathbb{R}^3$ of $y^{(k)}\colon \Lambda_k \to \mathbb{R}^3$ such that their interpolations $\tilde{y}^{(k)}$ satisfy*

$$
\operatorname*{ess\,sup}_{\Omega_k^{\mathrm{ext}}} \operatorname{dist}^2(\nabla_k \tilde{y}^{(k)}, \mathrm{SO}(3)) \le C \operatorname*{ess\,sup}_{(a_k,b_k)\times S} \operatorname{dist}^2(\nabla_k \tilde{y}^{(k)}, \mathrm{SO}(3))
$$

and

$$
\int_{\Omega_k^{\mathrm{ext}}} \operatorname{dist}^2(\nabla_k \tilde{y}^{(k)}, \mathrm{SO}(3))\mathrm{d}x \le C \int_{(a_k,b_k)\times S} \operatorname{dist}^2(\nabla_k \tilde{y}^{(k)}, \mathrm{SO}(3))\mathrm{d}x.
$$

For $x \in \overline{\Omega_k^{\mathrm{ext}}}$, we denote by $\bar{x}$ an element of $\tilde{\Lambda}_k'^{,\mathrm{ext}}$ that is closest to x. In what follows we always understand the symbols Λ_k^{ext}, $\Lambda_k'^{,\mathrm{ext}}$ etc. with $a := 0$ and $b := L$, unless stated otherwise. We also set $\Omega^{\mathrm{ext}} := (0,L)\times S^{\mathrm{ext}}$.

4.1.3 Energy

Let $L_k = \frac{1}{k}\lfloor kL\rfloor$, $\hat{\Lambda}_k'^{,\mathrm{surf}} = \{\frac{1}{2}, \dots, kL_k - \frac{1}{2}\} \times (\mathcal{L}'^{,\mathrm{ext}} \setminus \mathcal{L}')$, and $\hat{\Lambda}_k'^{,\mathrm{end}} = \{-\frac{1}{2}, kL_k + \frac{1}{2}\} \times \mathcal{L}'^{,\mathrm{ext}}$. We give this definition of strain energy $E^{(k)}$:

$$
\begin{aligned}
E^{(k)}(y^{(k)}) = \sum_{\hat{x}\in\hat{\Lambda}_k'} W_{\mathrm{cell}}^{(k)}\Big(\vec{y}^{(k)}(\hat{x})\Big) &+ \sum_{\hat{x}\in\hat{\Lambda}_k'^{,\mathrm{surf}}} W_{\mathrm{surf}}^{(k)}\Big(\hat{x}', \vec{y}^{(k)}(\hat{x})\Big)\\
&+ \sum_{\hat{x}\in\hat{\Lambda}_k'^{,\mathrm{end}}} W_{\mathrm{end}}^{(k)}\Big(\frac{1}{k}\hat{x}_1, \hat{x}', \vec{y}^{(k)}(\hat{x})\Big)
\end{aligned}
\tag{4.2}
$$

with $W_{\mathrm{cell}}^{(k)}\colon \mathbb{R}^{3\times 8} \to [0,\infty]$, $W_{\mathrm{surf}}^{(k)}\colon (\mathcal{L}'^{,\mathrm{ext}}\setminus\mathcal{L}')\times\mathbb{R}^{3\times 8} \to [0,\infty]$ and $W_{\mathrm{end}}^{(k)}\colon \{-\frac{1}{2k}, L_k + \frac{1}{2k}\} \times \mathcal{L}'^{,\mathrm{ext}} \times \mathbb{R}^{3\times 8} \to [0,\infty]$. The terms with $W_{\mathrm{surf}}^{(k)}$ and $W_{\mathrm{end}}^{(k)}$ are useful for incorporating surface energy (see Chapter 3 for further clarification). For convenience we assume that for every $\vec{y} \in \mathbb{R}^{3\times 8}$, $W_{\mathrm{surf}}^{(k)}(\cdot, \vec{y})$ is extended to a piecewise constant function on $S^{\mathrm{ext}} \setminus \bar{S}$ which is equal to $W_{\mathrm{surf}}^{(k)}(\hat{x}', \vec{y})$ on $\hat{x}' + (-\frac{1}{2}, \frac{1}{2})^2$. Sometimes it will be useful to group the terms, so for $\vec{y} \in \mathbb{R}^{3\times 8}$ we set

$$
W_{\mathrm{tot}}^{(k)}(\hat{x}', \vec{y}) = \begin{cases} W_{\mathrm{cell}}^{(k)}(\vec{y}) & \hat{x}' \in \bar{S},\\ W_{\mathrm{surf}}^{(k)}(\hat{x}', \vec{y}) & \hat{x}' \in (S^{\mathrm{ext}} \setminus \bar{S}). \end{cases}
$$

In our Γ-convergence statement, we consider the rescaled energy $\frac{1/k^3}{1/k^4} E^{(k)} = kE^{(k)}$, where k^3 is the order of the number of particles per unit volume in a bulk system and $1/k^4$ is the appropriate power of a rod's thickness for studying the *bending/torsion energy regime* (see e.g. [MM04] for more context).

Assumptions on the cell energy functions $W^{(k)}_{\mathrm{cell}}$, $W^{(k)}_{\mathrm{surf}}$, and $W^{(k)}_{\mathrm{end}}$.

Hereafter $\mathscr{W}^{(k)}$ stands for $W^{(k)}_{\mathrm{cell}}$, $W^{(k)}_{\mathrm{surf}}(\hat{x}',\cdot)$ with $\hat{x}' \in \mathcal{L}'^{,\mathrm{ext}} \setminus \mathcal{L}'$, and for $W^{(k)}_{\mathrm{end}}(\frac{\hat{x}_1}{k},\hat{x}',\cdot)$ with $\hat{x} \in \hat{\Lambda}_k'^{,\mathrm{end}}$.

(W1) Frame-indifference: $\mathscr{W}^{(k)}(R\vec{y} + (c|\cdots|c)) = \mathscr{W}^{(k)}(\vec{y})$ for all $R \in \mathrm{SO}(3)$, $\vec{y} \in \mathbb{R}^{3\times 8}$, $c \in \mathbb{R}^3$, and $k \in \mathbb{N}$.

(W2) Energy well: For every $k \in \mathbb{N}$, $\mathscr{W}^{(k)}$ attains a minimum (equal to 0) at rigid deformations, i.e. deformations $\vec{y} = (\hat{y}_1|\cdots|\hat{y}_8)$ with $\hat{y}_i = Rz^i + c$ for all $i \in \{1,\dots,8\}$ and some $R \in \mathrm{SO}(3)$, $c \in \mathbb{R}^3$.

(W3) Independence of k in the elastic regime: There are parameters $c^{(k)}_{\mathrm{frac}} \searrow 0$ such that $\lim_{k\to\infty} k(c^{(k)}_{\mathrm{frac}})^2 \in (0,\infty)$ and an elastic stored energy function $W_0 \colon \mathcal{L}'^{,\mathrm{ext}} \times \mathbb{R}^{3\times 8} \to [0,\infty]$ such that we have $\forall\, k \in \mathbb{N}\ \forall\, \vec{y} \in \mathbb{R}^{3\times 8}\ \forall x' \in \mathcal{L}'^{,\mathrm{ext}}$:

$$W^{(k)}_{\mathrm{tot}}(x',\vec{y}) = W_0(x',\vec{y}) \quad \text{if } \operatorname{dist}(\bar{\nabla}\hat{y}, \bar{\mathrm{SO}}(3)) \le c^{(k)}_{\mathrm{frac}}.$$

Further, there exists a $C > 0$ independent of $k \in \mathbb{N}$ such that

$$W^{(k)}_{\mathrm{end}}(\tfrac{1}{k}\hat{x}_1,\hat{x}',\vec{y}) \le C\operatorname{dist}^2(\bar{\nabla}\hat{y}, \bar{\mathrm{SO}}(3))$$

for any $\hat{x} \in \hat{\Lambda}_k'^{,\mathrm{end}}$, $\vec{y} = (\hat{y}_1|\cdots|\hat{y}_8) \in \mathbb{R}^{3\times 8}$, and $\bar{\nabla}\hat{y} = \vec{y} - (\sum_{j=1}^8 \hat{y}_j)(1,\dots,1)$ with $\operatorname{dist}(\bar{\nabla}\hat{y}, \bar{\mathrm{SO}}(3)) \le c^{(k)}_{\mathrm{frac}}$.

(W4) Regularity in k: $W^{(k+1)}_{\mathrm{tot}}(x',\vec{y}) \ge \frac{k}{k+1} W^{(k)}_{\mathrm{tot}}(x',\vec{y})$ for all $k \in \mathbb{N}$, $\vec{y} \in \mathbb{R}^{3\times 8}$, and $x' \in \mathcal{L}'^{,\mathrm{ext}}$.

(W5) Non-degeneracy in the elastic and the fracture regime: The function $W_0|_{\mathcal{L}'\times\mathbb{R}^{3\times 8}}$ is independent of x' (hence we omit it from the notation in this region) and satisfies

$$W_0(\vec{y}) \ge c_{\mathrm{W}}\operatorname{dist}^2(\bar{\nabla}\hat{y}, \bar{\mathrm{SO}}(3)) \quad \forall\, \tilde{y} \in \mathbb{R}^{3\times 8}$$

for a constant $c_{\mathrm{W}} > 0$. Writing $W^{(k)}_{\mathrm{cell}}(\vec{y}) = \bar{W}^{(k)}(\vec{y})$ if $\operatorname{dist}(\bar{\nabla}\hat{y}, \bar{\mathrm{SO}}(3)) > c^{(k)}_{\mathrm{frac}}$, we assume that the mappings $\bar{W}^{(k)}$ can be chosen such that

$$\bar{W}^{(k)}(\vec{y}) \ge \bar{c}^{(k)}_1 \quad \forall\, k \in \mathbb{N}\ \forall\, \vec{y} \in \mathbb{R}^{3\times 8}$$

for a sequence $(\bar{c}^{(k)}_1)_{k=1}^\infty$ of positive numbers with $\lim_{k\to\infty} k\bar{c}^{(k)}_1 \in (0,\infty)$.

(W6) $\mathscr{W}^{(k)}$ is everywhere Borel measurable and $W_0(\hat{x}',\cdot)$, $\hat{x}' \in \mathcal{L}'^{,\mathrm{ext}}$, is of class $\mathcal{C}^2$ in a neighbourhood of $\bar{\mathrm{SO}}(3)$.

(W7) If $i \in \{1,2,\dots,8\}$, $\hat{x}' \in \mathcal{L}'^{,\mathrm{ext}} \setminus \mathcal{L}'$, and $\vec{y} = (\hat{y}_1|\cdots|\hat{y}_8)$, then $\vec{y} \mapsto W^{(k)}_{\mathrm{surf}}(\hat{x}',\vec{y})$ may depend on $\hat{y}_i$ only if $\hat{x}' + (z^i)' \in \mathcal{L}$. If $x_1 \in \{-\frac{1}{2k}, L_k + \frac{1}{2k}\}$, then $\vec{y} \mapsto W^{(k)}_{\mathrm{end}}(x_1,\hat{x}',\vec{y})$ may depend on $\hat{y}_i$ only if $(x_1,\hat{x}') + \tilde{z}^i \in \tilde{\Lambda}_k$.

The quadratic form associated with $\nabla^2 W_{\mathrm{surf}}^{(k)}(x', \bar{\mathrm{Id}})$ is denoted by $Q_{\mathrm{surf}}(x', \cdot)$.

Throughout we will assume that Assumptions (W1)–(W7) are satisfied. We also introduce conditions which imply that long-range interactions of atoms are bounded or even are negligible.

(W8) We say that inelastic interactions are *bounded* if

$$\mathcal{W}^{(k)}(\vec{y}) \leq \bar{C}_1^{(k)} \quad \forall\, k \in \mathbb{N}\ \forall\, \vec{y} \in \mathbb{R}^{3\times 8}$$

for a sequence $(\bar{C}_1^{(k)})_{k=1}^{\infty}$ of positive numbers with $\lim_{k\to\infty} k\bar{C}_1^{(k)} \in (0,\infty)$.

(W9) We say that the cell energies have *maximum interaction range* scaling with (M_k), where $M_k \to 0$, $M_k k \to \infty$, if the following holds true: If there is a partition $\{1,\dots,8\} = J_1 \,\dot\cup\, J_2 \,\dot\cup \cdots \dot\cup\, J_{n_{\mathrm{C}}}$ such that for some $\vec{y}, \vec{y}\,' \in \mathbb{R}^{3\times 8}$ one has

$$\min_{1\leq \ell < m \leq n_{\mathrm{C}}} \mathrm{dist}(\{\hat{y}_{i_\ell}\}_{i_\ell \in J_\ell}, \{\hat{y}_{i_m}\}_{i_m \in J_m}) \geq M_k k \quad \text{and}$$
$$\min_{1\leq \ell < m \leq n_{\mathrm{C}}} \mathrm{dist}(\{\hat{y}'_{i_\ell}\}_{i_\ell \in J_\ell}, \{\hat{y}'_{i_m}\}_{i_m \in J_m}) \geq M_k k$$

and there are rigid motions given by $R_m \in SO(3)$ and $c_m \in \mathbb{R}^3$ such that

$$\hat{y}'_{i_m} = R_m \hat{y}_{i_m} + c_m \quad \forall\, i_m \in J_m,\ m = 1,\dots,n_{\mathrm{C}},$$

then

$$|\mathcal{W}^{(k)}(\vec{y}\,') - \mathcal{W}^{(k)}(\vec{y})| \leq \frac{C_{\mathrm{far}}}{M_k k^2}$$

for a uniform constant $C_{\mathrm{far}} > 0$.

Remark 4.1. We remark that the assumption in (W4) is a monotonicity assumption only for $kW_{\mathrm{tot}}^{(k)}(x', \cdot)$ but not for $W_{\mathrm{tot}}^{(k)}(x', \cdot)$ itself. It is in line with our assuming that the elastic energy is independent of k in (W3) and the fracture toughness scales with $\frac{1}{k}$, cf. (W5).

Remark 4.2. By (W2), (W3), and (W6) have

$$\mathcal{W}^{(k)}(\vec{y}) \leq c_{\mathrm{w}} \mathrm{dist}^2(\bar{\nabla}\hat{y}, \bar{SO}(3))$$

for a constant c_{w} and all $\vec{y} \in \mathbb{R}^{3\times 8}$ such that $\mathrm{dist}(\bar{\nabla}\hat{y}, \bar{SO}(3)) \leq c_{\mathrm{frac}}^{(k)}$. Moreover, by (W2), (W5) and (W6) the quadratic form Q_3 associated with $\nabla^2 W_0(\bar{\mathrm{Id}})$ is positive definite on $\mathrm{span}\{V_0 \cup \mathbb{R}^{3\times 3}_{\mathrm{skew}} \bar{\mathrm{Id}}\}^{\perp}$.

4.1.4 Piecewise Sobolev functions

We work with the linear spaces $P\text{-}H^m(0,L;\mathbb{R}^\ell)$, $m = 1,2$, $\ell \in \mathbb{N}$, of functions that are piecewise Sobolev in the following sense:

$$P\text{-}H^m(0,L;\mathbb{R}^\ell) := \Big\{\tilde{y} \in L^1((0,L);\mathbb{R}^\ell);\ \exists \text{ partition } (\sigma^i)_{i=0}^{n+1} \text{ of } [0,L]$$
$$\forall i \in \{1,2,\dots,n+1\}\colon \tilde{y}|_{(\sigma_{i-1},\sigma_i)} \in H^m((\sigma_{i-1},\sigma_i);\mathbb{R}^\ell)\Big\}. \quad (4.3)$$

Here we say that $(\sigma^i)_{i=0}^{n+1}$ is a partition of $[0,L]$ if $0=\sigma^0<\sigma^1<\cdots<\sigma^{n+1}=L$. Suppose $\tilde y\in P\text{-}H^m(0,L;\mathbb{R}^\ell)$ and $\{\sigma^i\}_{i=0}^{n+1}$ is the minimal set with property (4.3). For $m=1$ one has

$$S_{\tilde y}:=\{\sigma\in(0,L);\ \tilde y(\sigma-)\neq\tilde y(\sigma+)\}=\{\sigma^i\}_{i=0}^{n+1}.$$

For $m=2$ we have

$$S_{\tilde y'}:=\{\sigma\in\{\sigma^i\}_{i=1}^{n};\ \tilde y(\sigma-)=\tilde y(\sigma+)\},\qquad S_{\tilde y}:=\{\sigma^i\}_{i=1}^{n}\setminus S_{\tilde y'},$$

where the set $S_{\tilde y}$ is the *jump set* of $\tilde y$ and $S_{\tilde y'}$ the jump set of the derivative $\partial_{x_1}\tilde y$.

4.2 Compactness

Theorem 4.2. *Suppose the sequence $(y^{(k)})_{k=1}^\infty$ of lattice deformations fulfils*

$$\limsup_{k\to\infty}\Big(kE^{(k)}(y^{(k)})+\|y^{(k)}\|_{\ell^\infty(\Lambda_k;\mathbb{R}^3)}\Big)<+\infty. \tag{4.4}$$

Then after applying the extension scheme from Subsection 4.1.2 we can find an increasing sequence $(k_j)_{j=1}^\infty\subset\mathbb{N}$, functions $\tilde y\in P\text{-}H^2(0,L;\mathbb{R}^3)$, $d_2,d_3\in P\text{-}H^1(0,L;\mathbb{R}^3)$ with $R=(\partial_{x_1}\tilde y|d_2|d_3)\in\mathrm{SO}(3)$ a.e., and a partition $(\sigma^i)_{i=0}^{\bar n_{\mathrm f}+1}$ of $[0,L]$ such that for any

$$\eta\in(0,\frac12\min_{0\le i\le\bar n_f}|\sigma^{i+1}-\sigma^i|)$$

and every $0\le i\le\bar n_{\mathrm f}$ we have:

(i) $\tilde y^{(k_j)}\to\tilde y$ *in* $L^2(\Omega^{\mathrm{ext}};\mathbb{R}^3)$;

(ii) $\nabla_{k_j}\tilde y^{(k_j)}\to R=(\partial_{x_1}\tilde y|d_2|d_3)$ *in* $L^2((\sigma^i+\eta,\sigma^{i+1}-\eta)\times S^{\mathrm{ext}};\mathbb{R}^{3\times3})$;

(iii) $\mathrm{dist}(\bar\nabla_{k_j}\tilde y^{(k_j)},\bar{\mathrm{SO}}(3))\le c^{(k)}_{\mathrm{frac}}$ *on* $(\sigma^i+\eta,\sigma^{i+1}-\eta)\times S^{\mathrm{ext}}$*, for j sufficiently large;*

(iv) if we define the measures μ_k on $[0,L]$ by

$$\mu_k(A)=\sum_{\substack{\hat x\in\hat\Lambda_k^{\prime,\mathrm{ext}},\\ \hat x_1\in kA}}kW^{(k)}_{\mathrm{tot}}\Big(\hat x',\vec y^{(k)}(\hat x)\Big),$$

for Borel sets A, then $\mu_{k_j}\rightharpoonup^*\mu$ for a Radon measure μ ($\hat\Lambda_k^{\prime,\mathrm{ext}}:=k\Lambda_k^{\prime,\mathrm{ext}}$).

Proof. By properties of the extension scheme from Subsection 4.1.2 (see Remark 3.1) there is a constant $\hat C_e\ge1$ such that for any $x\in\tilde\Lambda_k^{\prime,\mathrm{ext}}$, setting $\mathcal U(x)=\Big(\{x_1-\frac1k,x_1,x_1+\frac1k\}\times\mathcal L'\Big)\cap\tilde\Lambda_k'$ we have

$$\mathrm{dist}^2(\bar\nabla_k\tilde y^{(k)}(x),\bar{\mathrm{SO}}(3))\le\hat C_e^2\sum_{\xi\in\mathcal U(x)}\mathrm{dist}^2(\bar\nabla_k\tilde y^{(k)}(\xi),\bar{\mathrm{SO}}(3)). \tag{4.5}$$

Let $S_k(x_1)$ denote a slice of the rod at the point x_1:

$$S_k(x_1) = \Big(\frac{1}{k}\lfloor kx_1\rfloor, \frac{1}{k}\lfloor kx_1\rfloor + \frac{1}{k}\Big) \times S^{\mathrm{ext}}, \quad x_1 \in [0, L].$$

A slice $S_k(x_1)$ is regarded as *broken* if there is an $x' \in S$ such that

$$\operatorname{dist}\Big(\bar{\nabla}\hat{y}^{(k)}(kx_1, x'), \bar{\mathrm{SO}}(3)\Big) > \frac{c_{\mathrm{frac}}^{(k)}}{\sqrt{3\sharp\mathcal{L}'}\hat{C}_{\mathrm{e}}}.$$

Like this, for any x such that the slice $S_k(x_1)$ and, if existent, the neighbouring slices $S_k(x_1 \pm \frac{1}{k})$ are not broken, $\bar{\nabla}_k \tilde{y}^{(k)}(x)$ is at most $c_{\mathrm{frac}}^{(k)}$-far from $\bar{\mathrm{SO}}(3)$ even if $x \in \Omega_k^{\mathrm{ext}} \setminus (0, L_k) \times S$. Write $X_1^{(k)}$ for the set of all midpoints of the x_1-projections of broken slices:

$$X_1^{(k)} = \Big\{x_1 \in \Big(\frac{1}{2k} + \frac{1}{k}\mathbb{Z}\Big) \cap [0, L);\ S_k(x_1) \text{ is broken}\Big\}.$$

We have $\sharp X_1^{(k)} \leq C_{\mathrm{f}}$ with $C_{\mathrm{f}} > 0$ independent of k, since by Assumptions (W3) and (W5)

$$\begin{aligned}\min\Big\{W_{\mathrm{cell}}^{(k)}(\vec{y});\ \vec{y} \in \mathbb{R}^{3\times 8},\ \operatorname{dist}(\bar{\nabla}\hat{y}, \bar{\mathrm{SO}}(3)) \geq \frac{c_{\mathrm{frac}}^{(k)}}{\sqrt{3\sharp\mathcal{L}'}\hat{C}_{\mathrm{e}}}\Big\} \\ \geq \min\Big\{\frac{c_{\mathrm{W}}(c_{\mathrm{frac}}^{(k)})^2}{3\sharp\mathcal{L}'\hat{C}_{\mathrm{e}}^2},\ \bar{c}_1^{(k)}\Big\} \geq \frac{c}{k}\end{aligned}$$

for a constant $c > 0$ and so

$$C \geq kE^{(k)}(y^{(k)}) \geq \sum_{\hat{x}\in\hat{\Lambda}_k^{\prime,\mathrm{ext}}} kW_{\mathrm{tot}}^{(k)}\Big(\hat{x}', \vec{y}^{(k)}(\hat{x})\Big) \tag{4.6}$$

$$\geq c\sharp X_1^{(k)} + k \underbrace{\sum_{\hat{x}\in\hat{\Lambda}_k^{\prime,\mathrm{ext}},\ \hat{x}_1 \notin kX_1^{(k)}} W_{\mathrm{tot}}^{(k)}\Big(\hat{x}', \vec{y}^{(k)}(\hat{x})\Big)}_{\text{elastic part } (\geq 0)}. \tag{4.7}$$

If we pass to a subsequence $\{k_j\}_{j=1}^\infty \subset \mathbb{N}$, we find $n_{\mathrm{f}} \in \mathbb{N}$, $0 \leq n_{\mathrm{f}} \leq C/c$, such that for every $j \in \mathbb{N}$, there are always precisely n_{f} broken slices, i.e. $\forall j \in \mathbb{N}$: $\sharp X_1^{(k_j)} = n_{\mathrm{f}}$, and

$$X_1^{(k_j)} = \{s_j^1, s_j^2, \ldots, s_j^{n_{\mathrm{f}}}\}, \quad s_j^1 < s_j^2 < \cdots < s_j^{n_{\mathrm{f}}}.$$

We observe that the location s_j^i of the i-th broken slice, $1 \leq i \leq n_{\mathrm{f}}$, remains in the compact interval $[0, L]$, so we construct a further subsequence, which we still denote by $(k_j)_{j=1}^\infty$, so that

$$\forall i \in \{1, 2, \ldots, n_{\mathrm{f}}\}:\ \lim_{j\to\infty} s_j^i = s^i \in [0, L].$$

Naturally it can be that some of the limiting positions of cracks s^i, $i = 1, 2, \ldots n_{\mathrm{f}}$, coincide or appear at the endpoints of the rod, hence we rewrite

$$X_1 := \{s^i;\ 0 < s^i < L,\ 1 \le i \le n_{\mathrm{f}}\} = \{\sigma^i\}_{i=1}^{\bar{n}_{\mathrm{f}}},$$

where the number $\bar{n}_{\mathrm{f}} \le n_{\mathrm{f}}$. Further, $\sigma^0 := 0$ and $\sigma^{\bar{n}_{\mathrm{f}}+1} := L$.

Suppose $0 < \eta < \frac{1}{2} \min_{0 \le i \le \bar{n}_f} |\sigma^{i+1} - \sigma^i|$. If j is large enough, then for all i, $0 \le i \le \bar{n}_{\mathrm{f}}$,

$$[\sigma^i + \eta, \sigma^{i+1} - \eta] \cap \Big(x_1 - \frac{3}{2k_j}, x_1 + \frac{3}{2k_j}\Big) = \emptyset.$$

Thus the regions $[\sigma^i + \eta, \sigma^{i+1} - \eta] \times S$ are intact, so we can replace $W^{(k)}_{\mathrm{cell}}$ by W_0 and safely apply the results about purely elastic rods here (see Theorem 3.4). Specifically, $\tilde{y}^{(k_j)} \to \tilde{y}$ in $L^2((\sigma^i + \eta, \sigma^{i+1} - \eta) \times S^{\mathrm{ext}}; \mathbb{R}^3)$, $\nabla_{k_j} \tilde{y}^{(k_j)} \to R = (\partial_{x_1} \tilde{y} | d_2 | d_3)$ in $L^2((\sigma^i + \eta, \sigma^{i+1} - \eta) \times S^{\mathrm{ext}}; \mathbb{R}^{3\times 3})$, and the x'-independent limit satisfies $\tilde{y} \in H^2((\sigma^i + \eta, \sigma^{i+1} - \eta); \mathbb{R}^3)$, $d_2, d_3 \in H^1((\sigma^i + \eta, \sigma^{i+1} - \eta); \mathbb{R}^3)$, and $R \in \mathrm{SO}(3)$ a.e. (We extracted another subsequence without changing the subindices.) By passing to a diagonal sequence we find a single sequence that satisfies convergence properties (i)–(ii) for any choice of η. Moreover, the L^∞ bound in (4.4) and the uniform energy bound in (4.7) show that indeed $\tilde{y} \in P\text{-}H^2(0, L; \mathbb{R}^3)$ and $R \in P\text{-}H^1(0, L; \mathbb{R}^{3\times 3})$.

Finally, every μ_k, $k \in \mathbb{N}$, is a Radon measure (i.e. Borel regular with compacts having finite measure). Passing to yet another subsequence (not relabelled), we find $\mu_{k_j} \rightharpoonup^* \mu$ for some Radon measure μ by [EG15, Theorem 1.41] since (4.6) implies $\sup_k \mu_k([0, L]) < \infty$. □

4.3 Main result

Theorem 4.3. *If $k \to \infty$, we have $kE^{(k)} \xrightarrow{\Gamma} E_{\mathrm{lim}}$, more precisely:*

(i) (liminf inequality) *Let $(y^{(k)})_{k=1}^\infty$ be a sequence of lattice deformations such that their piecewise aff. interpolations and extensions $(\tilde{y}^{(k)}) \subset H^1(\Omega_k^{\mathrm{ext}}; \mathbb{R}^3)$, defined in Subsection 4.1.2, converge in $L^2(\Omega^{\mathrm{ext}}; \mathbb{R}^3)$ to $\tilde{y} \in L^2((0, L); \mathbb{R}^3)$ for which there is a partition $(\varsigma^i)_{i=0}^{\tilde{n}_{\mathrm{f}}+1}$ of $[0, L]$ such that $\tilde{y}|_{(\varsigma^i, \varsigma^{i+1})} \in H^1((\varsigma^i, \varsigma^{i+1}) \times S^{\mathrm{ext}}; \mathbb{R}^3)$, $0 \le i \le \tilde{n}_{\mathrm{f}}$.*

Assume further that there are $d_s \in L^2((0, L); \mathbb{R}^3)$ such that for any $\eta > 0$ sufficiently small, we have $k \partial_{x_s} \tilde{y}^{(k)} \to d_s$ in $L^2((\varsigma^i + \eta, \varsigma^{i+1} - \eta) \times S^{\mathrm{ext}}; \mathbb{R}^3)$, $s = 2, 3$, $0 \le i \le \tilde{n}_{\mathrm{f}}$ (L^2_{loc}-convergence). Then

$$E_{\mathrm{lim}}(\tilde{y}, d_2, d_3) \le \liminf_{k \to \infty} kE^{(k)}(y^{(k)}).$$

(ii) (existence of a recovery sequence) *Let $\tilde{y} \in L^2((0, L); \mathbb{R}^3)$ be such that there is a partition $(\varsigma^i)_{i=0}^{\tilde{n}_{\mathrm{f}}+1}$ of $[0, L]$ for which $\tilde{y}|_{(\varsigma^i, \varsigma^{i+1})} \in H^1((\varsigma^i, \varsigma^{i+1}); \mathbb{R}^3)$, and let $d_2, d_3 \in L^2((0, L); \mathbb{R}^3)$. Then there exists a sequence of lattice deformations $(y^{(k)})_{k=1}^\infty$ such that their piecewise affine interpolations and extensions $(\tilde{y}^{(k)}) \subset$*

$H^1(\Omega_k^{\mathrm{ext}};\mathbb{R}^3)$ satisfy $\tilde{y}^{(k)} \to \tilde{y}$ in $L^2(\Omega^{\mathrm{ext}};\mathbb{R}^3)$, $k\frac{\partial \tilde{y}^{(k)}}{\partial x_s} \to d_s$ in $L^2_{\mathrm{loc}}((\varsigma^i,\varsigma^{i+1})\times S^{\mathrm{ext}};\mathbb{R}^3)$ for $s = 2,3$, $0 \le i \le \tilde{n}_{\mathrm{f}}$, and

$$\lim_{k\to\infty} kE^{(k)}(y^{(k)}) = E_{\lim}(\tilde{y}, d_2, d_3).$$

Moreover, if $\|\tilde{y}\|_{L^\infty((0,L);\mathbb{R}^3)} \le M$ and the cell energies satisfy the maximum interaction range property (W9), then for any $(\zeta_k)_{k=1}^\infty \subset (0,1)$ with $\zeta_k \searrow 0$ and $\zeta_k/M_k \to \infty$ one can choose $y^{(k)}$ such that $\|y^{(k)}\|_{\ell^\infty(\Lambda_k;\mathbb{R}^3)} \le M + \zeta_k$.

The limit energy functional is given by

$$E_{\lim}(\tilde{y}, d_2, d_3) = \begin{cases} \displaystyle\frac{1}{2}\int_0^L Q_3^{\mathrm{rel}}(R^\top \partial_{x_1} R)\,\mathrm{d}x_1 \\ \displaystyle\quad + \sum_{\sigma\in S_{\tilde{y}}\cup S_R} \varphi\Big(\tilde{y}(\sigma+) - \tilde{y}(\sigma-), (R(\sigma-))^{-1}R(\sigma+)\Big) & \text{if } (\tilde{y}, d_2, d_3) \in \mathcal{A}, \\ +\infty & \text{otherwise,} \end{cases}$$

where $R := (\partial_{x_1}\tilde{y}|d_2|d_3)$, $S_R := S_{\tilde{y}'} \cup S_{d_2} \cup S_{d_3}$, and the class of admissible deformations

$$\begin{aligned} \mathcal{A} := \Big\{&(\tilde{y}, d_2, d_3) \in (L^1(\Omega;\mathbb{R}^3))^3;\ \tilde{y}, d_2, d_3 \text{ do not depend on } x_2, x_3, \\ &(\tilde{y}, d_2, d_3) \in P\text{-}H^2(0,L;\mathbb{R}^3) \times (P\text{-}H^1(0,L;\mathbb{R}^3))^2 \text{ as functions of } x_1 \text{ only}, \\ &\qquad\qquad \Big(\frac{\partial \tilde{y}}{\partial x_1}\Big| d_2 \Big| d_3\Big) \in \mathrm{SO}(3) \text{ a.e. in } (0,L)\Big\}. \end{aligned}$$

The relaxed quadratic form $Q_3^{\mathrm{rel}} \colon \mathbb{R}^{3\times 3}_{\mathrm{skew}} \to [0,+\infty)$ is defined as

$$\begin{aligned} Q_3^{\mathrm{rel}}(A) := \min_{\substack{\alpha\colon \mathcal{L}^{\mathrm{ext}}\to\mathbb{R}^3 \\ g\in\mathbb{R}^3}} \sum_{x'\in\mathcal{L}'^{,\mathrm{ext}}} Q_{\mathrm{tot}}\Bigg(x', \frac{1}{2}\Bigg(A\begin{pmatrix}0\\x_2\\x_3\end{pmatrix} + g\Bigg)(-1,-1,-1,-1,1,1,1,1) \\ + \frac{1}{4}A\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 \end{pmatrix} + (\bar{\nabla}^{2\mathrm{d}}\alpha|\bar{\nabla}^{2\mathrm{d}}\alpha)\Bigg) \end{aligned} \tag{4.8}$$

with $Q_{\mathrm{tot}}(x',\cdot) = Q_3 + Q_{\mathrm{surf}}(x',\cdot)$, and $\varphi\colon \mathbb{R}^3 \times \mathrm{SO}(3) \to [0,\infty]$ is introduced in (4.11).

Remark 4.3. It follows from the positive semidefiniteness of Q_{tot} that the minimum in (4.8) is attained (see Remark 3.5).

Remark 4.4. The elastic part of our limiting functional includes a matrix expressing what we call an *ultrathin correction* – it is the first term on the second line of (4.8). The term is responsible for atomic effects that a continuum theory merely based on the Cauchy–Born rule would not capture.

Remark 4.5. Assumptions (W3), (W5) and compactness Theorem 3.4 in the elastic case imply that $\varphi \ge \bar{c}_1$ for some constant $\bar{c}_1 > 0$ on $\mathbb{R}^3 \times \mathrm{SO}(3) \setminus \{(0,\mathrm{Id})\}$ (and $\varphi(0,\mathrm{Id}) = 0$). If (W8) holds true, then we also have $\varphi \le \bar{C}_1$ for a constant $\bar{C}_1 < \infty$.

Remark 4.6. The universality of the sequence ζ_k obtained in (ii) would allow to impose an L^∞ constraint energetically by simply setting $E^{(k)}(y^{(k)}) = +\infty$ if $\|y^{(k)}\|_\infty > M + \zeta_k$. One then has a directly matching compactness result in Theorem 4.2.

Remark 4.7. The convergence of deformations used in Theorem 4.3 is equivalent to

$$\tilde{y}^{(k)}(\cdot, x') \to \tilde{y} \text{ in } L^2((0,L);\mathbb{R}^3) \text{ for every } x' \in \mathcal{L} \text{ and}$$
$$\bar{\nabla}_k \tilde{y}^{(k)} \to R\bar{\mathrm{Id}} \text{ in } L^2_{\mathrm{loc}}((\varsigma^i, \varsigma^{i+1}) \times S; \mathbb{R}^{3\times 8}) \text{ for } 0 \le i \le \tilde{n}_{\mathrm{f}},$$

which shows the limit's independence of our interpolation scheme.

4.4 Proof of the lower bound

The proof of Theorem 4.3(i) is divided into four parts.

4.4.1 First step – elastic part

Since the conclusion is immediate if the liminf is infinite, let us assume the contrary; $\tilde{y}^{(k)} \to \tilde{y}$ in $L^2(\Omega^{\mathrm{ext}};\mathbb{R}^3)$ and after extracting a subsequence,

$$\lim_{k\to\infty} kE^{(k)}(y^{(k)}) = \liminf_{k\to\infty} kE^{(k)}(y^{(k)}) < \infty. \tag{4.9}$$

Let $(\sigma^i)_{i=0}^{\tilde{n}_{\mathrm{f}}+1}$, $\nabla_{k_j}\tilde{y}^{(k_j)}$, μ_k, μ be as in Theorem 4.2 and fix $\eta > 0$ small (note that the assumption that $\|y^{(k)}\|_\infty \le C$ is not necessary here, because we know that $\tilde{y} \in L^2((0,L);\mathbb{R}^3)$). Then by the results about purely elastic rods (Theorem 3.5), the bound

$$\liminf_{k\to\infty} \sum_{\substack{\hat{x}\in\hat{\Lambda}_k'^{,\mathrm{ext}} \\ \hat{x}_1 \in k[\sigma^i+\eta, \sigma^{i+1}-\eta]}} kW_{\mathrm{tot}}^{(k)}\left(\hat{x}', \vec{y}^{(k)}(\hat{x})\right)$$
$$\ge \frac{1}{2}\int_{\sigma^i+\eta}^{\sigma^{i+1}-\eta} Q_3^{\mathrm{rel}}(R^\top \partial_{x_1} R)\mathrm{d}x_1, \quad i = 0, 1, \ldots, \tilde{n}_{\mathrm{f}},$$

holds true. Since this is fulfilled for any η, we can let $\eta \to 0+$ and use the monotone convergence theorem, as we will see later.

4.4.2 Second step – w^*-limit in measures

For the crack contribution to the strain energy, we use the *blow-up method* of Fonseca and Müller [FM92]. We will not make a notational distinction between $(\tilde{y}^{(k)})$ and its hitherto constructed subsequence $(\tilde{y}^{(k_j)})$ any more, as this is not relevant for our Γ-convergence proof.

Now note that $S_{\tilde{y}} \cup S_R \subset X_1$, where the set $X_1 = \{\sigma^i\}_{i=1}^{\tilde{n}_{\mathrm{f}}}$ is from the proof of Theorem 4.2. Write $\tilde{\mathcal{H}} := \mathcal{H}^0 \llcorner S_{\tilde{y}} \cup S_R$. Decomposing μ into an absolutely continuous part and a singular part, we have

$$\mu = \frac{\mathrm{d}\mu}{\mathrm{d}\tilde{\mathcal{H}}}\tilde{\mathcal{H}} + \mu_{\mathrm{s}}$$

with $\mu_{\mathrm{s}} \geq 0$. The w^*-convergence then gives (cf. [EG15, Theorem 1.40])

$$\liminf_{k\to\infty} \sum_{i=1}^{\tilde{n}_{\mathrm{f}}} \sum_{\substack{\hat{x}\in\hat{\Lambda}_k^{\prime,\mathrm{ext}} \\ \hat{x}_1\in k(\sigma^i-\eta,\sigma^i+\eta)}} kW_{\mathrm{tot}}^{(k)}\Big(\hat{x}', \vec{y}^{(k)}(\hat{x})\Big) \geq \mu\Big(\bigcup_{i=1}^{\tilde{n}_{\mathrm{f}}}(\sigma^i-\eta, \sigma^i+\eta)\Big) \geq \sum_{\sigma\in S_{\tilde{y}}\cup S_R} \frac{\mathrm{d}\mu}{\mathrm{d}\tilde{\mathcal{H}}}(\sigma).$$

The goal now is to find the *asymptotic minimal energy* $\varphi = \varphi(\tilde{y}^+ - \tilde{y}^-, (R^-)^{-1}R^+)$ *necessary to produce a crack or kink* and for every $1 \leq i \leq n_{\mathrm{f}}$, show that

$$\frac{\mathrm{d}\mu}{\mathrm{d}\tilde{\mathcal{H}}}(\sigma^i) \geq \varphi\Big(\tilde{y}(\sigma^i+) - \tilde{y}(\sigma^i-), (R(\sigma^i-))^{-1}R(\sigma^i+)\Big).$$

Let us expand the definition of the derivative of μ:

$$\frac{\mathrm{d}\mu}{\mathrm{d}\tilde{\mathcal{H}}}(\sigma^i) \overset{\mathrm{def}}{=} \lim_{r\to 0+} \frac{\mu([\sigma^i - r, \sigma^i + r])}{\tilde{\mathcal{H}}([\sigma^i - r, \sigma^i + r])} = \lim_{r\to 0+} \frac{\mu([\sigma^i - r, \sigma^i + r])}{1}.$$

By [FL07, Prop. 1.15] and [EG15, Th. 1.40], we can find $r_n \searrow 0$ such that

$$\begin{aligned}\frac{\mathrm{d}\mu}{\mathrm{d}\tilde{\mathcal{H}}}(\sigma^i) &= \lim_{n\to\infty}\lim_{k\to\infty} \mu_k((\sigma^i - r_n, \sigma^i + r_n)) \\ &= \lim_{n\to\infty}\lim_{k\to\infty} \sum_{\substack{\hat{x}\in\hat{\Lambda}_k^{\prime,\mathrm{ext}} \\ \hat{x}_1\in k(\sigma^i-r_n,\sigma^i+r_n)}} kW_{\mathrm{tot}}^{(k)}\Big(\hat{x}', \vec{y}^{(k)}(\hat{x})\Big).\end{aligned}$$

4.4.3 Third step – prelim. cell formula obtained by blowup

First we shall find a preliminary lower bound ψ by rescaling $(\sigma^i - r_n, \sigma^i + r_n)$ to a fixed interval (cf. [AFP00, proof of Theorem 5.14, Step 3]). There is a sequence $(k_n)_{n=1}^{\infty}$ such that $k_n \geq n$, $r_n k_n \to \infty$,

$$\frac{\mathrm{d}\mu}{\mathrm{d}\tilde{\mathcal{H}}}(\sigma^i) = \lim_{n\to\infty} \sum_{\substack{\hat{x}\in\hat{\Lambda}_{k_n}^{\prime,\mathrm{ext}} \\ \hat{x}_1\in k_n(\sigma^i-r_n,\sigma^i+r_n)}} k_n W_{\mathrm{tot}}^{(k_n)}\Big(\hat{x}', \vec{y}^{(k_n)}(\hat{x})\Big),$$

as well as

$$\begin{aligned}&\int_{(\sigma^i-2r_n,\sigma^i+2r_n)\times S^{\mathrm{ext}}} |\tilde{y}^{(k_n)} - \tilde{y}|^2 \mathrm{d}x_1 \mathrm{d}x' \\ &\qquad + \int_{\{\sigma^i+[(-2r_n,-\frac{1}{4}r_n)\cup(\frac{1}{4}r_n,2r_n)]\}\times S^{\mathrm{ext}}} |\nabla_{k_n}\tilde{y}^{(k_n)} - R|^2 \mathrm{d}x \leq r_n^2 \qquad (4.10)\end{aligned}$$

and $\sigma^i - \frac{r_n}{2} + \frac{2}{k_n} < s_{k_n}^j < \sigma^i + \frac{r_n}{2} - \frac{2}{k_n}$ for every $n \in \mathbb{N}$ and each of the (finitely many) sequences $(s_{k_n}^j)_{n=1}^{\infty}$ of midpoints of broken slices satisfying $s_{k_n}^j \to \sigma^i$ as $n \to \infty$. Since the restrictions of $\tilde{y}$ and R to left and right neighbourhoods of σ^i are H^1, we get for the rescaled functions

$$\begin{aligned}y^{\ddagger,n}(w_1) &:= \tilde{y}(\sigma^i + r_n w_1), \\ R^{\ddagger,n}(w_1) &:= R(\sigma^i + r_n w_1),\ w_1 \in [-1,1],\end{aligned}$$

the convergences $y^{\ddagger,n} \to y_{\mathrm{PC}}$ in $L^2([-1,1];\mathbb{R}^3)$ and $R^{\ddagger,n} \to R_{\mathrm{PC}}$ in $L^2([-1,1];\mathbb{R}^{3\times 3})$ for $n \to \infty$, where the piecewise constant functions y_{PC}, R_{PC} are defined by

$$y_{\mathrm{PC}}(w_1) := \begin{cases} \tilde{y}(\sigma^i-) = \tilde{y}^- & w_1 < 0, \\ \tilde{y}(\sigma^i+) = \tilde{y}^+ & w_1 \geq 0, \end{cases} \quad \text{and} \quad R_{\mathrm{PC}}(w_1) := \begin{cases} R(\sigma^i-) = R^- & w_1 < 0, \\ R(\sigma^i+) = R^+ & w_1 \geq 0. \end{cases}$$

We also set, for $w_1 \in [-1,1]$,

$$\begin{aligned} \mathcal{y}^{(k_n)}(w_1, x') &:= \tilde{y}^{(k_n)}(\sigma^i_{k_n} + r_n w_1, x'), \\ \nabla_{r_n,k_n} \mathcal{y}^{(k_n)}(w_1, x') &:= \Big(\frac{1}{r_n}\partial_{w_1}\mathcal{y}^{(k_n)} | k_n \partial_{x_2}\mathcal{y}^{(k_n)} | k_n \partial_{x_3}\mathcal{y}^{(k_n)}\Big) = \nabla_{k_n}\tilde{y}^{(k_n)}(\sigma^i_{k_n} + r_n w_1, x'), \end{aligned}$$

where $\sigma^i_{k_n} = \frac{1}{k_n}\lfloor k_n \sigma^i \rfloor$. Then using (4.10), we get $\mathcal{y}^{(k_n)} \to y_{\mathrm{PC}}$ in $L^2([-1,1] \times S^{\mathrm{ext}};\mathbb{R}^3)$ and $\nabla_{r_n,k_n}\mathcal{y}^{(k_n)} \to R_{\mathrm{PC}}$ in $L^2([I^-_\psi \cup I^+_\psi] \times S^{\mathrm{ext}}];\mathbb{R}^{3\times 3})$, where $I^-_\psi = [-1, -\frac{1}{2}]$ and $I^+_\psi = [\frac{1}{2}, 1]$. This gives the preliminary estimate with 'converging boundary conditions':

$$\begin{aligned} \frac{\mathrm{d}\mu}{\mathrm{d}\tilde{\mathcal{H}}}(\sigma^i) \geq \min\Big\{ &\limsup_{n\to\infty} \sum_{(w_1,x') \in \Lambda'_{r_n,k_n}} k_n W^{(k_n)}_{\mathrm{tot}}\big(x', \vec{\mathcal{y}}^{(k_n)}(w_1,x')\big); \\ &\mathcal{y}^{(k_n)} \in \mathrm{PAff}(\Lambda_{r_n,k_n}),\ r_n \searrow 0,\ r_n k_n \to \infty, \\ &\|\mathcal{y}^{(k_n)} - y_{\mathrm{PC}}\|_{L^2(I^\pm_\psi \times S^{\mathrm{ext}})} \to 0,\ \|\nabla_{r_n,k_n}\mathcal{y}^{(k_n)} - R_{\mathrm{PC}}\|_{L^2(I^\pm_\psi \times S^{\mathrm{ext}})} \to 0 \Big\} \\ =: \tilde{\psi}(\tilde{y}^-, \tilde{y}^+, R^-, R^+), \end{aligned}$$

where

$$\begin{aligned} \vec{\mathcal{y}}^{(k_n)}(w_1, x') &:= k_n\Big(\mathcal{y}^{(k_n)}\Big(w_1 + \frac{1}{r_n k_n} z^i_1, x' + (z^i)'\Big)\Big)_{i=1}^8, \\ \Lambda_{r_n,k_n} &:= \Big(\frac{1}{r_n k_n}\mathbb{Z} \cap \Big(-1 - \frac{1}{r_n k_n}, 1 + \frac{1}{r_n k_n}\Big)\Big) \times \mathcal{L}^{\mathrm{ext}}, \\ \Lambda'_{r_n,k_n} &:= \Big(\Big(\frac{1}{2 r_n k_n} + \frac{1}{r_n k_n}\mathbb{Z}\Big) \cap \Big(-1 - \frac{1}{2 r_n k_n}, 1 + \frac{1}{2 r_n k_n}\Big)\Big) \times \mathcal{L}'^{,\mathrm{ext}}, \end{aligned}$$

and $\mathrm{PAff}(\Lambda_{r_n,k_n})$ denotes the class of piecewise affine mappings $\mathcal{v}\colon [-1 - \frac{1}{r_n k_n}, 1 + \frac{1}{r_n k_n}] \times \overline{S^{\mathrm{ext}}} \to \mathbb{R}^3$ which are generated by interpolating their values from Λ_{r_n,k_n} by the scheme from Subsection 4.1.2. The minimum in $\tilde{\psi}$ runs over all sequences $(r_n) \subset (0,\infty)$, $(k_n) \subset \mathbb{N}$ and $(\mathcal{y}^{(k_n)})$ with the above properties.

It can be shown by a diagonalization argument that the minimum is attained; this is also the case in (4.11). From the translation and rotation invariance of $W^{(k)}_{\mathrm{tot}}$ we see that $\tilde{\psi}(\tilde{y}^-, \tilde{y}^+, R^-, R^+) = \psi(\tilde{y}^+ - \tilde{y}^-, (R^-)^{-1}R^+)$ for a function $\psi\colon \mathbb{R}^3 \times \mathrm{SO}(3) \to [0,\infty]$.

4.4.4 Fourth step – rigid boundary conditions in the cell formula

At last, we relate the preliminary cell formula ψ to the final cell formula which uses rigid boundary conditions instead of L^2-converging ones:

$$\varphi\big(\tilde{y}^+ - \tilde{y}^-, (R^-)^{-1}R^+\big) = \min\Big\{\limsup_{n\to\infty} \sum_{(w_1,x')\in\Lambda'_{r_n,k_n}} k_n W_{\mathrm{tot}}^{(k_n)}\big(x', \vec{y}^{(k_n)}(w_1,x')\big); \\ \big((r_n)_{n=1}^\infty, (k_n)_{n=1}^\infty, (y^{(k_n)})_{n=1}^\infty\big) \in \mathcal{V}_{\tilde{y}^+-\tilde{y}^-,(R^-)^{-1}R^+}\Big\} \tag{4.11}$$

with

$$\mathcal{V}_{\tilde{y}^+-\tilde{y}^-,(R^-)^{-1}R^+} = \Big\{\big((r_n)_{n=1}^\infty, (k_n)_{n=1}^\infty, (y^{(k_n)})_{n=1}^\infty\big) \in (0,\infty)^{\mathbb{N}} \times \mathbb{N}^{\mathbb{N}} \times \mathrm{PAff}(\Lambda_{r_n,k_n})^{\mathbb{N}}; \\ y^{(k_n)}(w_1,x') = R_\pm^{(k_n)}\Big(r_n w_1, \frac{1}{k_n}x'\Big)^\top + y_\pm^{(k_n)} \text{ on } I^\pm \times \overline{S^{\mathrm{ext}}},\ r_n \searrow 0, \\ r_n k_n \to \infty,\ y_\pm^{(k_n)} \in \mathbb{R}^3,\ R_\pm^{(k_n)} \in \mathrm{SO}(3),\ y_\pm^{(k_n)} \to \tilde{y}^\pm,\ R_\pm^{(k_n)} \to R^\pm\Big\},$$

$I^- = [-1, -\frac{3}{4}]$ and $I^+ = [\frac{3}{4}, 1]$.

Remark 4.8. The particular choice

$$y^{(k_n)}(w_1,x') = \begin{cases} R_-^{(k_n)}(r_n w_1, \frac{1}{k_n}x')^\top + y_-^{(k_n)} & \text{if } w_1 \le 0, \\ R_+^{(k_n)}(r_n w_1, \frac{1}{k_n}x')^\top + y_+^{(k_n)} & \text{if } w_1 > 0 \end{cases}$$

for given $\tilde{y}^+, \tilde{y}^- \in \mathbb{R}^3$ and $R^-, R^+ \in \mathrm{SO}(3)$ shows that, in case inelastic interactions are bounded (see (W8)), one has $\varphi \le \bar{C}_1$ for some $\bar{C}_1 < \infty$.

We now show that we have $\psi \ge \varphi$. Suppose $\varepsilon > 0$ and that $(r_n) \subset (0,\infty)$, $(k_n) \subset \mathbb{N}$, and $(y^{(k_n)})_{n=1}^\infty$ in $\mathrm{PAff}(\Lambda_{r_n,k_n})$ are sequences such that $r_n \searrow 0$ with $r_n k_n \to \infty$,

$$\|y^{(k_n)} - y_{\mathrm{PC}}\|_{L^2(I_\psi^\pm \times S^{\mathrm{ext}})} \to 0, \quad \|\nabla_{r_n,k_n} y^{(k_n)} - R_{\mathrm{PC}}\|_{L^2(I_\psi^\pm \times S^{\mathrm{ext}})} \to 0 \tag{4.12}$$

and

$$\limsup_{n\to\infty} \mathcal{E}_{k_n}(y^{(k_n)}, [-1,1]) \le \psi(\tilde{y}^+ - \tilde{y}^-, (R^-)^{-1}R^+) + \varepsilon,$$

where for any $I \subset [-1,1]$ we set

$$\mathcal{E}_{k_n}(y^{(k_n)}, I) := \sum_{\substack{w_1 \in \mathcal{L}'_n(I) \\ x' \in \mathcal{L}'^{,\mathrm{ext}}}} k_n W_{\mathrm{tot}}^{(k_n)}\big(x', \vec{y}^{(k_n)}(w_1,x')\big)$$

and $\mathcal{L}'_n(I) = (\frac{1}{2r_nk_n} + \frac{1}{r_nk_n}\mathbb{Z}) \cap I$. The definition of a rod slice in this section reads

$$S_{k_n}(w_1) = \Big[\bar{w}_1 - \frac{1}{2r_nk_n}, \bar{w}_1 + \frac{1}{2r_nk_n}\Big) \times \overline{S^{\mathrm{ext}}}, \quad \text{where} \quad \bar{w}_1 = \frac{1}{r_nk_n}\lfloor r_nk_nw_1\rfloor + \frac{1}{2r_nk_n}.$$

Our goal now is to find a sequence $v^{(k_n)}$ which is admissible as a competitor in the definition of φ and has asymptotically lower energy than $y^{(k_n)}$. We provide the construction only for $v^{(k_n)}|_{[-1,0]\times\overline{S^{\mathrm{ext}}}}$, as for $v^{(k_n)}|_{(0,1]\times\overline{S^{\mathrm{ext}}}}$ we could proceed analogously. Writing $I_{0,n}^- := \frac{1}{r_nk_n}(\lfloor -\frac{3}{4}r_nk_n\rfloor + 1, \lfloor -\frac{1}{2}r_nk_n\rfloor)$ for a discrete approximation of $I_\psi^- \setminus I^-$ from inside and $N_n^- = \lfloor -\frac{1}{2}r_nk_n\rfloor - \lfloor -\frac{3}{4}r_nk_n\rfloor - 3 = \sharp\mathscr{L}'(I_{0,n}^-) - 2$ for the number of (interior) slices intersecting $I_{0,n}^- \times \overline{S^{\mathrm{ext}}}$, we introduce the sets

$$W_1^{(n)} = \Big\{ w_1 \in \mathscr{L}'(I_{0,n}^-);\ w_1 \pm \tfrac{i}{r_nk_n} \in \mathscr{L}'(I_{0,n}^-),$$
$$\sum_{i\in\{-1,0,1\}} \sum_{x'\in\mathcal{L}'^{,\mathrm{ext}}} k_n W_{\mathrm{tot}}^{(k_n)}\Big(x', \bar\nabla_{r_n,k_n} y^{(k_n)}(w_1 + \tfrac{i}{r_nk_n}, x')\Big) \le \frac{12}{N_n^-}\mathcal{E}_{k_n}(y^{(k_n)}, I_{0,n}^-)\Big\}, \tag{4.13a}$$

$$W_2^{(n)} = \Big\{ w_1 \in \mathscr{L}'(I_{0,n}^-);\ w_1 \pm \tfrac{i}{r_nk_n} \in \mathscr{L}'(I_{0,n}^-),$$
$$\int_{S_{k_n}(w_1)} |\nabla_{r_n,k_n} y^{(k_n)} - R^-|^2 \mathrm{d}w_1 \mathrm{d}x' \le \frac{4}{N_n^-}\|\nabla_{r_n,k_n} y^{(k_n)} - R^-\|^2_{L^2(I_{0,n}^-\times S^{\mathrm{ext}};\mathbb{R}^{3\times3})}\Big\}, \tag{4.13b}$$

$$W_3^{(n)} = \Big\{ w_1 \in \mathscr{L}'(I_{0,n}^-);\ w_1 \pm \tfrac{i}{r_nk_n} \in \mathscr{L}'(I_{0,n}^-),$$
$$\int_{S_{k_n}(w_1)} |y^{(k_n)} - \tilde y^-|^2 \mathrm{d}w_1 \mathrm{d}x' \le \frac{4}{N_n^-}\|y^{(k_n)} - \tilde y^-\|^2_{L^2(I_{0,n}^-\times S^{\mathrm{ext}};\mathbb{R}^{3})}\Big\}, \tag{4.13c}$$

where $\bar\nabla_{r_n,k_n} y^{(k_n)}(w_1,x') = k_n\big(y^{(k_n)}(\bar w_1 + \frac{1}{r_nk_n}z_1^i, \bar x' + (z^i)') - \sum_{j=1}^8 y^{(k_n)}(\bar w_1 + \frac{1}{r_nk_n}z_1^j, \bar x' + (z^j)')\big)_{i=1}^8$. The sets $W_i^{(n)}$, $i = 1,2,3$, are comprised of the centres of the w_1-projections of slices on which, loosely speaking, a certain quantity is below four times its average. By Lemma 4.5 with $p = 4$ we see that for every $i \in \{1,2,3\}$ and $n \in \mathbb{N}$, the set $W_i^{(n)}$ contains at least $\lfloor (3/4)N_n^-\rfloor$ elements. The pigeonhole principle then implies that for every n large enough there is $w_-^{(n)} \in W_1^{(n)} \cap W_2^{(n)} \cap W_3^{(n)}$. Since $N_n^- \ge \frac{1}{4}r_nk_n - 4$, the inequality in (4.13a) and the finiteness in (4.9) imply an estimate in integral form:

$$\sum_{i\in\{-1,0,1\}} r_nk_n \int_{S_{k_n}(w_-^{(n)} + \frac{i}{r_nk_n})} k_n W_{\mathrm{tot}}^{(k_n)}\Big(x', \bar\nabla_{r_n,k_n} y^{(k_n)}\Big)\mathrm{d}w_1\mathrm{d}x' \le \frac{48}{r_nk_n - 16}\mathcal{E}_{k_n}(y^{(k_n)}, I_{0,n}^-) \le \frac{C_{\mathrm{e}}}{r_nk_n} \tag{4.14}$$

for a constant $C_{\mathrm{e}} > 0$. Hence we can employ growth assumption (W5) on the elastic cell energy W_0, properties of the extension scheme (cf. (4.5)), and Theorem 1.1 (in unrescaled variables) to get $R_-^{(k_n)} \in \mathrm{SO}(3)$ such that

$$\frac{1}{C}\|\nabla_{r_n,k_n} y^{(k_n)} - R_-^{(k_n)}\|^2_{L^2(S_{k_n}(w_-^{(n)});\mathbb{R}^{3\times3})} \le \sum_{i\in\{-1,0,1\}} \int_{S_{k_n}(w_-^{(n)} + \frac{i}{r_nk_n})} W_{\mathrm{tot}}^{(k_n)}\Big(x', \bar\nabla_{r_n,k_n} y^{(k_n)}\Big)\mathrm{d}w_1\mathrm{d}x'$$

for a constant $C > 0$. Combining the previous inequality with (4.14) we deduce that

$$\|\nabla_{r_n,k_n} y^{(k_n)} - R_-^{(k_n)}\|_{L^2(S_{k_n}(w_-^{(n)});\mathbb{R}^{3\times3})} = O\Big(\frac{1}{r_nk_n^{3/2}}\Big). \tag{4.15}$$

Setting

$$y_-^{(k_n)} = \fint_{S_{k_n}(w_-^{(n)})} y^{(k_n)}(w_1, x') - R_-^{(k_n)}\Big(r_n w_1, \frac{1}{k_n}x'\Big)^\top \mathrm{d}w_1 \mathrm{d}x',$$

we achieve that a Poincaré inequality is satisfied, with a $C > 0$:

$$\begin{aligned}\sqrt{\int_{S_{k_n}(w_-^{(n)})} |y^{(k_n)}(w_1, x') - R_-^{(k_n)}\Big(r_n w_1, \frac{1}{k_n}x'\Big)^\top - y_-^{(k_n)}|^2 \mathrm{d}w_1 \mathrm{d}x'} \\ \leq C\frac{1}{k_n}\|\nabla_{r_n,k_n} y^{(k_n)} - R_-^{(k_n)}\|_{L^2(S_{k_n}(w_-^{(n)});\mathbb{R}^{3\times 3})}.\end{aligned} \tag{4.16}$$

Define $v^{(k_n)} \colon [-1, 0] \times \overline{S^{\mathrm{ext}}} \to \mathbb{R}^3$ as follows:

$$v^{(k_n)}(w_1, x') = \begin{cases} R_-^{(k_n)}(r_n w_1, \frac{1}{k_n}x')^\top + y_-^{(k_n)} & -1 \leq w_1 \leq w_-^{(n)} - \frac{1}{2r_n k_n} \\ \text{pcw. affine (24 simplices/cell)} & w_-^{(n)} - \frac{1}{2r_n k_n} < w_1 < w_-^{(n)} + \frac{1}{2r_n k_n} \\ y^{(k_n)}(w_1, x') & 0 \geq w_1 \geq w_-^{(n)} + \frac{1}{2r_n k_n}. \end{cases}$$

We claim that

$$\limsup_{n\to\infty} \mathcal{E}_{k_n}\Big(v^{(k_n)}, [-1, 0)\Big) \leq \limsup_{n\to\infty} \mathcal{E}_{k_n}\Big(y^{(k_n)}, [-1, 0)\Big), \tag{4.17}$$

$$\lim_{n\to\infty} y_-^{(k_n)} = \tilde{y}^-, \quad \lim_{n\to\infty} R_-^{(k_n)} = R^-. \tag{4.18}$$

Concerning (4.17), we notice that for all $n \in \mathbb{N}$,

$$\mathcal{E}_{k_n}\Big(y^{(k_n)}, \Big(w_-^{(n)} + \frac{1}{2r_n k_n}, 0\Big)\Big) = \mathcal{E}_{k_n}\Big(v^{(k_n)}, \Big(w_-^{(n)} + \frac{1}{2r_n k_n}, 0\Big)\Big)$$

and that $\mathcal{E}_{k_n}(v^{(k_n)}, (-1, w_-^{(n)} - \frac{1}{2r_n k_n})) = 0$ since $\bar{\nabla}_{r_n,k_n} v^{(k_n)} = R_-^{(k_n)}\bar{\mathrm{Id}} \in \bar{\mathrm{SO}}(3)$ on $(-1, w_-^{(n)} - \frac{1}{2r_n k_n}) \times S^{\mathrm{ext}}$. Hence it remains to show that the energy on the transition slice $S_{k_n}(w_-^{(n)})$ vanishes in the limit.

Lemma 4.4. *The following is true:*

$$\lim_{n\to\infty} \mathcal{E}_{k_n}\Big(y^{(k_n)}, w_-^{(n)} + \frac{1}{2r_n k_n}\Big(-1, 1\Big)\Big) + \mathcal{E}_{k_n}\Big(v^{(k_n)}, w_-^{(n)} + \frac{1}{2r_n k_n}\Big(-1, 1\Big)\Big) = 0.$$

Proof. The proof is divided into several steps. Let $Q = [w_-^{(n)} - \frac{1}{2r_n k_n}, w_-^{(n)} + \frac{1}{2r_n k_n}] \times Q'$, where $Q' = x' + [-\frac{1}{2}, \frac{1}{2}]^2$ for some $x' \in \mathcal{L}'^{,\mathrm{ext}}$, be any atomic cell contained in the slice $\overline{S_{k_n}}(w_-^{(n)})$.

Step 1. Using Lemma 3.1 and (4.15), we can obtain the relation

$$c|\bar{\nabla}_{r_n,k_n} y^{(k_n)}(w_-^{(n)}, x') - R_-^{(k_n)}\bar{\mathrm{Id}}|^2 \leq r_n k_n \int_Q |\nabla_{r_n,k_n} y^{(k_n)} - R_-^{(k_n)}|^2 \mathrm{d}w_1 \mathrm{d}w' = O\Big(\frac{1}{r_n k_n^2}\Big) \tag{4.19}$$

with a constant $c > 0$.

Step 2. The symbol $\langle y^{(k_n)}\rangle$ denotes the 'barycentre of the deformation' on Q,

$$\langle y^{(k_n)}\rangle := \frac{1}{8}\sum_{j=1}^{8} y^{(k_n)}\Big(w_-^{(n)} + \frac{1}{r_n k_n} z_1^j, x' + (z^j)'\Big).$$

We now compare $\vec{y}^{(k_n)}(w_-^{(n)}, x')$ and $\vec{v}^{(k_n)}(w_1, x')$. By construction, $[\vec{y}^{(k_n)}]_{\cdot i} = [\vec{v}^{(k_n)}]_{\cdot i}$ for $i = 5, 6, 7, 8$ and from Step 1 we get, for $i = 1, 2, 3, 4$,

$$
\begin{aligned}
&[\vec{y}^{(k_n)}(w_-^{(n)}, x')]_{\cdot i} - [\vec{v}^{(k_n)}(w_-^{(n)}, x')]_{\cdot i} \\
&= \Big|k_n\Big(y^{(k_n)}\Big(w_-^{(n)} + \frac{1}{r_n k_n} z_1^i, x' + (z^i)'\Big) - R_-^{(k_n)}\Big(r_n w_-^{(n)} + \frac{1}{k_n} z_1^i, \frac{1}{k_n}(x + z^i)'\Big)^\top - y_-^{(k_n)}\Big)\Big| \\
&\le \underbrace{\Big|[\bar{\nabla}_{r_n,k_n} y^{(k_n)}(w_-^{(n)}, x')]_{\cdot i} - R_-^{(k_n)} z^i\Big|}_{=O(r_n^{-1/2} k_n^{-1})} + k_n\Big|\langle y^{(k_n)}\rangle - R_-^{(k_n)}\Big(r_n w_-^{(n)}, \frac{1}{k_n} x'\Big)^\top - y_-^{(k_n)}\Big|.
\end{aligned}
$$

Property (4.1) of our piecewise affine interpolation, Hölder's inequality, (4.16) and (4.15) give

$$
\begin{aligned}
&k_n\Big|\langle y^{(k_n)}\rangle - R_-^{(k_n)}\Big(r_n w_-^{(n)}, \frac{1}{k_n} x'\Big)^\top - y_-^{(k_n)}\Big| \\
&\quad = r_n k_n^2 \Big|\int_Q y^{(k_n)}(w_1, w') - R_-^{(k_n)}\Big(r_n w_1, \frac{1}{k_n} w'\Big)^\top - y_-^{(k_n)} \mathrm{d}w_1 \mathrm{d}w'\Big| \\
&\quad \le C\sqrt{|Q|} r_n k_n^2 \frac{1}{k_n} \|\nabla_{r_n,k_n} y^{(k_n)} - R_-^{(k_n)}\|_{L^2(S_{k_n}(w_-^{(n)});\mathbb{R}^{3\times 3})} = O\Big(\frac{1}{\sqrt{r_n} k_n}\Big)
\end{aligned}
$$

so that $|\vec{y}^{(k_n)}(w_-^{(n)}, x') - \vec{v}^{(k_n)}(w_-^{(n)}, x')| = O(r_n^{-1/2} k_n^{-1})$ and, in particular,

$$
|\bar{\nabla}_{r_n,k_n} y^{(k_n)}(w_-^{(n)}, x') - \bar{\nabla}_{r_n,k_n} v^{(k_n)}(w_-^{(n)}, x')| = O\Big(\frac{1}{\sqrt{r_n} k_n}\Big)
$$

as $\bar{\nabla}_{r_n,k_n} y^{(k_n)}(w_-^{(n)}, x') = \vec{y}^{(k_n)}(w_-^{(n)}, x') - \frac{1}{8}\sum_{i=1}^8 [\vec{y}^{(k_n)}(w_-^{(n)}, x')]_{\cdot i}(1, \ldots, 1)$ and likewise for $v^{(k_n)}$. Together with (4.19) this shows that also $v^{(k_n)}$ satisfies

$$
|\bar{\nabla}_{r_n,k_n} v^{(k_n)}(w_-^{(n)}, x') - R_-^{(k_n)} \bar{\mathrm{Id}}| = O\Big(\frac{1}{\sqrt{r_n} k_n}\Big). \tag{4.20}
$$

Step 3. Now we use that $W_{\mathrm{tot}}^{(k_n)}$ is independent of k_n on a tubular neighbourhood of SO(3) of size $O(k_n^{-1})$ and, by Taylor expansion, satisfies an estimate of the form $W_{\mathrm{tot}}^{(k_n)} \le C \mathrm{dist}^2(\cdot, \mathrm{SO}(3))$ there. Thus, (4.19) and (4.20) give

$$
k_n W_{\mathrm{tot}}^{(k_n)}\Big(x', \bar{\nabla}_{r_n,k_n} y^{(k_n)}\Big) + k_n W_{\mathrm{tot}}^{(k_n)}\Big(x', \bar{\nabla}_{r_n,k_n} v^{(k_n)}\Big) = O\Big(\frac{1}{r_n k_n}\Big).
$$

This implies the assertion. □

The second convergence in (4.18) is a consequence of (4.13b), (4.12), and (4.15):

$$
\begin{aligned}
|R_-^{(k_n)} - R^-|^2 &= \frac{r_n k_n}{|S^{\mathrm{ext}}|} \int_{S_{k_n}(w_-^{(n)})} |R_-^{(k_n)} - R^-|^2 \mathrm{d}w_1 \mathrm{d}x' \\
&\le \frac{2 r_n k_n}{|S^{\mathrm{ext}}|}\Big(\int_{S_{k_n}(w_-^{(n)})} |R^- - \nabla_{r_n,k_n} y^{(k_n)}|^2 \mathrm{d}w_1 \mathrm{d}x' \\
&\qquad + \int_{S_{k_n}(w_-^{(n)})} |R_-^{(k_n)} - \nabla_{r_n,k_n} y^{(k_n)}|^2 \mathrm{d}w_1 \mathrm{d}x'\Big) \\
&\le \frac{2 r_n k_n}{|S^{\mathrm{ext}}|} \cdot \frac{4}{\frac{1}{4} r_n k_n - 4} \|\nabla_{r_n,k_n} y^{(k_n)} - R^-\|_{L^2(I_{0,n}^- \times S;\mathbb{R}^{3\times 3})}^2 + O\Big(\frac{1}{r_n k_n^2}\Big) \longrightarrow 0.
\end{aligned}
$$

The first convergence in (4.18) follows similarly from (4.13c) and (4.12) if we use (4.16) and (4.15) to show that

$$\frac{2r_nk_n}{|S^{\text{ext}}|}\int_{S_{k_n}(w_-^{(n)})}|y_-^{(k_n)}-\underset{\sim}{y}^{(k_n)}|^2\mathrm{d}w_1\mathrm{d}x'\leq C\Big[r_n\|\nabla_{r_n,k_n}\underset{\sim}{y}^{(k_n)}-R_-^{(k_n)}\|^2_{L^2(S_{k_n}(w_-^{(n)});\mathbb{R}^{3\times3})}$$
$$+|R_-^{(k_n)}|^2r_nk_n\frac{1}{|S^{\text{ext}}|r_nk_n}\Big|\Big(r_n,\frac{1}{k_n},\frac{1}{k_n}\Big)\Big|^2\Big]\longrightarrow 0,$$

with a constant $C>0$.

In the same way, we could construct $(R_+^{(k_n)})_{n=1}^\infty$, $(y_+^{(k_n)})_{n=1}^\infty$, and $\underset{\sim}{v}^{(k_n)}|_{(0,1]\times S^{\text{ext}}}$ and prove a version of (4.17)–(4.18) on $(0,1]$. Thus, as

$$\varphi\Big(\tilde{y}^+-\tilde{y}^-,(R^-)^{-1}R^+\Big)\leq\limsup_{n\to\infty}\mathcal{E}_{k_n}\Big(\underset{\sim}{v}^{(k_n)},[-1,1]\Big)$$
$$\leq\limsup_{n\to\infty}\mathcal{E}_{k_n}\Big(\underset{\sim}{y}^{(k_n)},[-1,1]\Big)\leq\psi\Big(\tilde{y}^+-\tilde{y}^-,(R^-)^{-1}R^+\Big)+\varepsilon$$

and $\varepsilon>0$ was arbitrary, the claim that $\varphi\leq\psi$ is proved.

Lemma 4.5. *Let $c_1, c_2, \dots, c_N$ be nonnegative reals and $p\geq 1$. Then*

$$\sharp\Big\{i\in\{1,\dots,N\};\ c_i\leq\frac{p}{N}\sum_{j=1}^N c_j\Big\}>\Big\lfloor\Big(1-\frac{1}{p}\Big)N\Big\rfloor.$$

Proof. We denote by $\bar{c}$ the average $N^{-1}\sum_j c_j$. If the statement were not true, the number of c_j's such that $c_j>p\bar{c}$ would be greater than or equal to N/p. Hence

$$\bar{c}\geq\frac{1}{N}\sum_{j;\,c_j>p\bar{c}}c_j>\frac{1}{N}p\bar{c}\frac{N}{p}=\bar{c},$$

but that is a contradiction. □

Summing up the elastic and crack energy contributions, we get

$$\lim_{k\to\infty}kE^{(k)}(y^{(k)})\geq\liminf_{k\to\infty}k\Bigg[\sum_{i=0}^{\bar{n}_{\text{f}}}\sum_{\substack{\hat{x}\in\hat{\Lambda}_k^{\prime,\text{ext}}\\ \hat{x}_1\in k[\sigma^i+\eta,\sigma^{i+1}-\eta]}}W_{\text{tot}}^{(k)}\Big(\hat{x}',\vec{y}^{(k)}(\hat{x})\Big)$$
$$+\sum_{i=1}^{\bar{n}_{\text{f}}}\sum_{\substack{\hat{x}\in\hat{\Lambda}_k^{\prime,\text{ext}}\\ \hat{x}_1\in k(\sigma^i-\eta,\sigma^i+\eta)}}W_{\text{tot}}^{(k)}\Big(\hat{x}',\vec{y}^{(k)}(\hat{x})\Big)\Bigg]$$
$$\geq\sum_{i=0}^{\bar{n}_{\text{f}}}\frac{1}{2}\int_{\sigma^i+\eta}^{\sigma^{i+1}-\eta}Q_3^{\text{rel}}(R^\top\partial_{x_1}R)\mathrm{d}x_1+\sum_{\sigma\in S_{\tilde{y}}\cup S_R}\varphi\Big(\tilde{y}(\sigma+)-\tilde{y}(\sigma-),(R(\sigma-))^{-1}R(\sigma+)\Big).$$

To obtain the Γ-liminf inequality, we apply the monotone convergence theorem with $\eta\to0+$.

4.5 Proof of the upper bound

For a construction of recovery sequences it is crucial to first analyze the cell formula more precisely. In particular, we will need to prove that the crack set is essentially localized on the atomic scale.

4.5.1 Analysis of the cell formula

Lemma 4.6 (localization of crack). *Let $\tilde{y}^-, \tilde{y}^+ \in \mathbb{R}^3$ and $R^-, R^+ \in \mathrm{SO}(3)$. Then for any $\varepsilon_* > 0$, there is an $N_* \in \mathbb{N}$, sequences $(k_n)_{n=1}^\infty \subset \mathbb{N}$, $(r_n) \subset (0,\infty)$ and mappings $\overset{+}{\underline{y}}{}^{(k_n)} \in \mathrm{PAff}(\Lambda_{r_n,k_n})$, $n \in \mathbb{N}$, with the following properties:*

$$\limsup_{n\to\infty} \mathcal{E}_{k_n}(\overset{+}{\underline{y}}{}^{(k_n)}, [-1,1]) \le \varphi\Big(\tilde{y}^+ - \tilde{y}^-, (R^-)^{-1}R^+\Big) + \varepsilon_*, \tag{4.21}$$

$r_n \searrow 0$, $r_n k_n \to \infty$, and, for suitable $\overset{+}{y}{}_\pm^{(k_n)} \in \mathbb{R}^3$, $\overset{+}{R}{}_\pm^{(k_n)} \in \mathrm{SO}(3)$ with $\overset{+}{y}{}_\pm^{(k_n)} \to \tilde{y}^\pm$, $\overset{+}{R}{}_\pm^{(k_n)} \to R^\pm$,

$$\overset{+}{\underline{y}}{}^{(k_n)}(w_1, x') = \begin{cases} \overset{+}{R}{}_-^{(k_n)}\Big(r_n w_1, \frac{x'}{k_n}\Big)^\top + \overset{+}{y}{}_-^{(k_n)} & \text{on } \Big([-1,0] \setminus I_{\mathrm{c}}^{(n)}\Big) \times \overline{S^{\mathrm{ext}}}, \\ \overset{+}{R}{}_+^{(k_n)}\Big(r_n w_1, \frac{x'}{k_n}\Big)^\top + \overset{+}{y}{}_+^{(k_n)} & \text{on } \Big((0,1] \setminus I_{\mathrm{c}}^{(n)}\Big) \times \overline{S^{\mathrm{ext}}}, \end{cases}$$

where $I_{\mathrm{c}}^{(n)} = \frac{1}{r_n k_n}[-N_*, N_*]$.

Proof. Find $(k_n)_{n=1}^\infty \subset \mathbb{N}$, $(r_n)_{n=1}^\infty \subset (0,\infty)$ with $r_n \searrow 0$ and $\lim_{n\to\infty} r_n k_n = \infty$, and $(\underline{y}^{(k_n)})$ in $\mathrm{PAff}(\Lambda_{r_n,k_n})$ such that

$$\lim_{n\to\infty} \mathcal{E}_{k_n}(\underline{y}^{(k_n)}, [-1,1]) = \varphi\Big(\tilde{y}^+ - \tilde{y}^-, (R^-)^{-1}R^+\Big)$$

and, for some $y_\pm^{(k_n)} \in \mathbb{R}^3$, $R_\pm^{(k_n)} \in \mathrm{SO}(3)$ with $y_\pm^{(k_n)} \to \tilde{y}^\pm$, $R_\pm^{(k_n)} \to R^\pm$,

$$\underline{y}^{(k_n)}(w_1, x') = R_\pm^{(k_n)}\Big(r_n w_1, \frac{1}{k_n}x'\Big)^\top + y_\pm^{(k_n)} \text{ on } I^\pm \times \overline{S^{\mathrm{ext}}}.$$

Recalling assumption (W5) on $W_{\mathrm{cell}}^{(k_n)}$ and passing to a subsequence (without relabelling it), we can assert that there is an $N_{\mathrm{f}} \in \mathbb{N}_0$, $N_{\mathrm{f}} \le C\varphi(\tilde{y}^+ - \tilde{y}^-, (R^-)^{-1}R^+)$, such that for every n, only the slices

$$S_{k_n}(s_n^j) := \Big[s_n^j - \frac{1}{2r_n k_n}, s_n^j + \frac{1}{2r_n k_n}\Big) \times \overline{S^{\mathrm{ext}}}, \quad j \in \{1, \dots, N_{\mathrm{f}}\},$$

are *broken* in the sense from the proof of Theorem 4.2, where $s_n^1 < \dots < s_n^{N_{\mathrm{f}}}$ are the midpoints of the w_1-projections of the broken slices and $\lim_{n\to\infty} s_n^j = s^j \in [-3/4, 3/4]$. This means that $\bar{\nabla}_{r_n,k_n}\underline{y}^{(k_n)}$ on the remaining 'intact' slices is at most $c_{\mathrm{frac}}^{(k_n)}$-far from $\bar{\mathrm{SO}}(3)$. Then

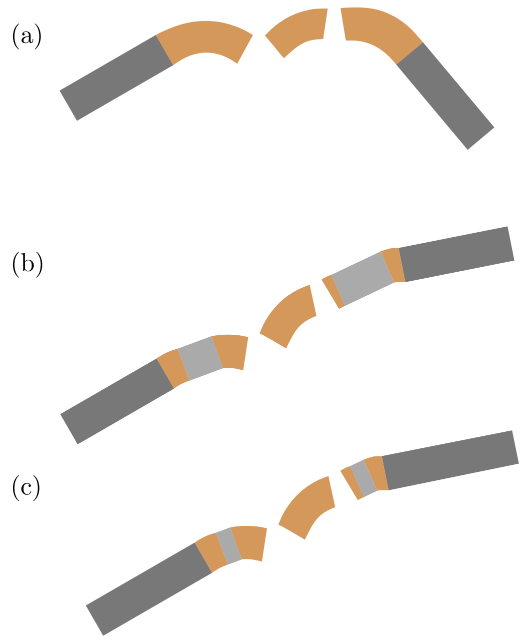
$$\tilde{I}_1^{(n)} = \Big[-\frac{\lfloor \frac{3}{4} r_n k_n \rfloor}{r_n k_n} + \frac{1}{r_n k_n}, s_n^1 - \frac{1}{2r_n k_n}\Big],$$

$$\tilde{I}_2^{(n)} = \Big[s_n^1 + \frac{1}{2r_n k_n}, s_n^2 - \frac{1}{2r_n k_n}\Big], \; \dots, \; \tilde{I}_{N_{\mathrm{f}}+1}^{(n)} = \Big[s_n^{N_{\mathrm{f}}} + \frac{1}{2r_n k_n}, \frac{\lfloor \frac{3}{4} r_n k_n \rfloor}{r_n k_n}\Big]$$

are the w_1-projections of elastically deformed parts of the region surrounding the crack. We fix a number $N_*' := \lfloor 2N_\mathrm{f}C_\mathrm{E}/\varepsilon_* \rfloor + 1$, where C_E is a positive constant (independent of n and ε_*) that will be introduced in (4.25). Let $\{\tilde{I}_{j_i}^{(n)}\}_{i=1}^{N_\mathrm{U}} \subset \{\tilde{I}_j^{(n)}\}_{j=1}^{N_\mathrm{f}+1}$ denote those intervals $\tilde{I}_{j_i}^{(n)}$ for which $r_n k_n |\tilde{I}_{j_i}^{(n)}| \geq 2N_*' + 4$ (the 'too long' intervals). On extracting a further subsequence, $N_\mathrm{U} = N_\mathrm{U}(N_*')$ is independent of n. We assume $N_\mathrm{U} > 0$, since otherwise the next 'rigidification' procedure is redundant and it is enough to construct $\overset{+}{y}^{(k_n)}$ directly from $y^{(k_n)}$ later. To shorten notation, we set $\tilde{I}_{j_i}^{(n)} =: I_i^{(n)} = [a_i^{(n)} - \frac{1}{r_n k_n}, b_i^{(n)} + \frac{1}{r_n k_n}]$.

As an intermediate step, we now construct mappings $\overset{\leftharpoonup}{y}^{(k_n)}$ (illustrated in Figure 4.2(b)) which have the property that middle parts of the segments $I_i^{(n)} \times \overline{S^\mathrm{ext}}$ are only subject to a rigid motion, instead of an elastic deformation. The complements of these middle parts contain no more than $2N_*' + 2$ slices. Below, the rigidifying procedure is presented for an arbitrary but fixed $i \in \{1, \ldots, N_\mathrm{U}\}$.

Figure 4.2: Main steps in the proof of Lemma 4.6. Rigid parts of the rod are drawn in grey. (a) The original mapping $y^{(k_n)}$. (b) Rigidification of rod segments to construct $\overset{\leftharpoonup}{y}^{(k_n)}$. (c) Subsequent shortening of the rigid parts to obtain $\overset{+}{y}^{(k_n)}$.



Procedure (R). As in Theorem 3.4, we get piecewise constant mappings $R^{(k_n)}$ defined on $I_i^{(n)}$ with discontinuity set contained in $\frac{1}{r_n k_n}\mathbb{Z}$ and values in SO(3), fulfilling

$$
\begin{aligned}
r_n \int_{S_{k_n}(\bar w_1)} & |\nabla_{r_n,k_n} y^{(k_n)} - R^{(k_n)}|^2 \mathrm{d}w_1 \mathrm{d}x' \\
&\le \sum_{m=-1}^{1} C r_n \int_S \int_{\bar w_1 + \frac{m}{r_n k_n}}^{\bar w_1 + \frac{m+1}{r_n k_n}} \operatorname{dist}^2(\nabla_{r_n,k_n} y^{(k_n)}, \mathrm{SO}(3)) \mathrm{d}w_1 \mathrm{d}x' \qquad (4.22)\\
&\qquad \le 3 C r_n |S_{k_n}(\bar w_1)| (c_{\mathrm{frac}}^{(k_n)})^2 \le \frac{C}{k_n^2}
\end{aligned}
$$

for all $w_1 \in [a_i^{(n)}, b_i^{(n)})$ by Theorem 1.1, growth assumptions on W_0, and bounds related to our extension scheme (cf. (4.5)). Moreover, Theorem 3.4 implies

$$
\begin{aligned}
\frac{1}{r_n k_n} & \Big| R^{(k_n)}(w_1) - R^{(k_n)}\Big(w_1 \pm \frac{1}{r_n k_n}\Big)\Big|^2 \\
&\le C \int_{\bigcup_{m=-1}^{1} S_{k_n}(\bar w_1 + \frac{m}{r_n k_n})} \operatorname{dist}^2(\nabla_{r_n,k_n} y^{(k_n)}, \mathrm{SO}(3)) \mathrm{d}w_1 \mathrm{d}x' \qquad (4.23)
\end{aligned}
$$

for all $w_1 \in [a_i^{(n)}, b_i^{(n)})$.

We now define points that delimit the middle part of $I_i^{(n)} \times \overline{S^{\mathrm{ext}}}$ (where $y^{(k_n)}$ has to be 'rigidified') and the sets $W_-^{(n)}$, $W_+^{(n)}$ containing the w_1-coordinates of cell midpoints left of or right of this middle part:

$$
\begin{aligned}
a_{0,i}^{(n)} = a_i^{(n)} + \frac{N_*'}{r_n k_n}, \quad & b_{0,i}^{(n)} = b_i^{(n)} - \frac{N_*'}{r_n k_n} \\
W_-^{(n)} &= \Big(\frac{1}{2 r_n k_n} + \frac{1}{r_n k_n}\mathbb{Z}\Big) \cap (a_i^{(n)}, a_{0,i}^{(n)}) \\
W_+^{(n)} &= \Big(\frac{1}{2 r_n k_n} + \frac{1}{r_n k_n}\mathbb{Z}\Big) \cap (b_{0,i}^{(n)}, b_i^{(n)}).
\end{aligned}
$$

The next few steps, till (4.25), are similar to the proof of the inequality $\varphi \le \psi$ (cf. Subsection 4.4.4), so not all computations will be described in full here. We find $w_-^{(n)} \in W_-^{(n)}$ and $w_+^{(n)} \in W_+^{(n)}$ such that

$$
\begin{aligned}
\sum_{\ell=-1}^{1} \sum_{x' \in \mathcal{L}'^{,\mathrm{ext}}} k_n W_{\mathrm{tot}}^{(k_n)}\Big(x', \bar\nabla_{r_n,k_n} y^{(k_n)}(w_-^{(n)} + \tfrac{\ell}{r_n k_n}, x')\Big) \le \frac{3}{N_*'} \mathcal{E}_{k_n}\Big(y^{(k_n)}, (a_i^{(n)}, a_{0,i}^{(n)})\Big), \\
\sum_{\ell=-1}^{1} \sum_{x' \in \mathcal{L}'^{,\mathrm{ext}}} k_n W_{\mathrm{tot}}^{(k_n)}\Big(x', \bar\nabla_{r_n,k_n} y^{(k_n)}(w_+^{(n)} + \tfrac{\ell}{r_n k_n}, x')\Big) \le \frac{3}{N_*'} \mathcal{E}_{k_n}\Big(y^{(k_n)}, (b_{0,i}^{(n)}, b_i^{(n)})\Big).
\end{aligned}
$$

Writing $R_\pm^{(i,k_n)}$ in place of $R^{(k_n)}(w_\pm^{(n)})$ for short and using that all the slices centred in $W_\pm^{(n)}$ are intact, from the first inequality in (4.22) we get

$$
\|\nabla_{r_n,k_n} y^{(k_n)} - R_\pm^{(i,k_n)}\|_{L^2(S_{k_n}(w_\pm^{(n)}); \mathbb{R}^{3\times 3})} = O\Big(\frac{1}{\sqrt{N_*' r_n} k_n}\Big).
$$

Choosing vectors $c_-^{(n)}$, $c_+^{(n)}$ as

$$
c_\pm^{(n)} = \fint_{S_{k_n}(w_\pm^{(n)})} y^{(k_n)}(w_1, x') - R_\pm^{(i,k_n)}\Big(r_n(w_1 - w_\pm^{(n)}), \frac{1}{k_n} x'\Big)^\top \mathrm{d}w_1 \mathrm{d}x',
$$

we get Poincaré inequalities

$$\sqrt{\int_{S_{k_n}(w_\pm^{(n)})} |y^{(k_n)}(w_1,x') - R_\pm^{(i,k_n)}\Big(r_n(w_1 - w_\pm^{(n)}), \frac{1}{k_n}x'\Big)^\top - c_\pm^{(n)}|^2 \mathrm{d}w_1 \mathrm{d}x'}$$
$$\leq C\frac{1}{k_n}\|\nabla_{r_n,k_n} y^{(k_n)} - R_\pm^{(i,k_n)}\|_{L^2(S_{k_n}(w_\pm^{(n)});\mathbb{R}^{3\times 3})}$$

with a constant $C > 0$.

With the rotated and shifted version of $y^{(k_n)}$, given by

$$y_\mathrm{r}^{(k_n)}(w_1,x') := R_-^{(i,k_n)}\left[\Big(R_+^{(i,k_n)}\Big)^\top(y^{(k_n)}(w_1,x') - c_+^{(n)}) + \begin{pmatrix} r_n(w_+^{(n)} - w_-^{(n)}) \\ 0 \end{pmatrix}\right] + c_-^{(n)}, \quad (4.24)$$

set

$$\overleftarrow{y}^{(k_n)}(w_1,x') = \begin{cases} y^{(k_n)}(w_1,x') & a_i^{(n)} - \frac{1}{r_nk_n} \leq w_1 \leq w_-^{(n)} - \frac{1}{2r_nk_n} \\ \text{pcw. affine (24 simplices/cell)} & w_-^{(n)} - \frac{1}{2r_nk_n} < w_1 < w_-^{(n)} + \frac{1}{2r_nk_n} \\ R_-^{(i,k_n)}(r_n(w_1 - w_-^{(n)}), \frac{1}{k_n}x')^\top + c_-^{(n)} & w_-^{(n)} + \frac{1}{2r_nk_n} \leq w_1 \leq w_+^{(n)} - \frac{1}{2r_nk_n} \\ \text{pcw. affine (24 simplices/cell)} & w_+^{(n)} - \frac{1}{2r_nk_n} < w_1 < w_+^{(n)} + \frac{1}{2r_nk_n} \\ y_\mathrm{r}^{(k_n)}(w_1,x') & w_+^{(n)} + \frac{1}{2r_nk_n} < w_1 \leq b_i^{(n)} + \frac{1}{r_nk_n} \end{cases}$$

so that $\overleftarrow{y}^{(k_n)}$ is defined on $I_i^{(n)} \times \overline{S^\mathrm{ext}}$. Besides, to prepare future rigidification on possible next intervals, we redefine $y^{(k_n)}$ by $y^{(k_n)} := y_\mathrm{r}^{(k_n)}$ on $[b_i^{(n)} + \frac{1}{r_nk_n}, 1] \times \overline{S^\mathrm{ext}}$.

After calculations as in the proof of Lemma 4.4 we deduce that on any atomic cell Q such that $\operatorname{Int} Q \subset S_{k_n}(w_-^{(k_n)})$,

$$\Big|\bar{\nabla}_{r_n,k_n} y^{(k_n)}|_Q - R_-^{(i,k_n)}\bar{\mathrm{Id}}\Big| = O\Big(\frac{1}{\sqrt{N_*'k_n}}\Big) \quad \text{and consequently,}$$
$$\Big|\bar{\nabla}_{r_n,k_n} \overleftarrow{y}^{(k_n)}|_Q - R_-^{(i,k_n)}\bar{\mathrm{Id}}\Big| = O\Big(\frac{1}{\sqrt{N_*'k_n}}\Big),$$

which implies that for all n sufficiently large, the energetic error occurring on the transition slice $S_{k_n}(w_-^{(k_n)})$ is controlled by our choice of N_*':

$$\Big|\mathcal{E}_{k_n}\Big(y^{(k_n)}, w_-^{(n)} + \frac{1}{2r_nk_n}(-1,1)\Big) - \mathcal{E}_{k_n}\Big(\overleftarrow{y}^{(k_n)}, w_-^{(n)} + \frac{1}{2r_nk_n}(-1,1)\Big)\Big| \leq \frac{C_\mathrm{E}}{N_*'}. \quad (4.25)$$

It should be stressed that the constant C_E above does not depend on n or ε_*. Due to the definition of $y_\mathrm{r}^{(k_n)}$, an analogous computation reveals that (4.25) also holds if $w_-^{(n)}$ is replaced with $w_+^{(n)}$.

Later we will have to check that $(\overleftarrow{y}^{(k_n)})_{n=1}^\infty$ is an admissible competitor of $(y^{(k_n)})_{n=1}^\infty$ in the cell formula. Therefore we now show that the error incurred by the boundary condition due to the previous steps of Procedure (R) tends to zero.

By our interpolation scheme, on any atomic cell Q contained in $I_i^{(n)} \times \overline{S^{\text{ext}}}$ we have (cf. Lemma 3.1)

$$\left\|\nabla_{r_n,k_n} y^{(k_n)}|_Q\right\|_\infty \leq 24 \fint_Q |\nabla_{r_n,k_n} y^{(k_n)}| \mathrm{d}w_1 \mathrm{d}x' \leq C \left|\bar{\nabla}_{r_n,k_n} y^{(k_n)}|_Q\right| \leq C$$

since $\mathrm{dist}^2(\bar{\nabla}_{r_n,k_n} y^{(k_n)}, \bar{\mathrm{SO}}(3)) \leq (\mathrm{c}_{\mathrm{frac}}^{(\mathrm{k_n})})^2$. This proves that the mappings $y^{(k_n)}$ are Lipschitz on $I_i^{(n)} \times \overline{S^{\text{ext}}}$ with the uniform constant Cr_n. In particular,

$$\lim_{n\to\infty} |c_+^{(n)} - c_-^{(n)}| = 0.$$

Since by iterating (4.23) we derive a 'pointwise curvature estimate' (as in [MM03, FJM02])

$$|R_+^{(i,k_n)} - R_-^{(i,k_n)}|^2 \leq Cr_n^2 k_n^2 \int_{I_i^{(n)} \times S} \mathrm{dist}^2(\nabla_{r_n,k_n} y^{(k_n)}, \mathrm{SO}(3)) \mathrm{d}w_1 \mathrm{d}x' = O(r_n)$$

we obtain for $y_{\mathrm{r}}^{(k_n)}$ from (4.24) that $|y_{\mathrm{r}}^{(k_n)} - y^{(k_n)}| \to 0$ uniformly.

This finishes Procedure (R) for the chosen i.

We construct $\overleftarrow{y}^{(k_n)}$ by letting $\overleftarrow{y}^{(k_n)}(w_1, x') := y^{(k_n)}(w_1, x')$ for every $-1 \leq w_1 \leq a_1^{(n)} - \frac{1}{r_n k_n}$ and $x' \in \overline{S^{\text{ext}}}$ and then by successively applying Procedure (R) for $i = 1, 2, \ldots, N_{\mathrm{U}}$ (it should be kept in mind that after each invocation of Procedure (R), $y^{(k_n)}$ is redefined on $[b_i^{(n)} + \frac{1}{r_n k_n}, 1] \times \overline{S^{\text{ext}}}$ so that in step $i+1$ we get the modified mapping $y^{(k_n)}$ from step i as input).

On $(\frac{1}{r_n k_n} \lfloor \frac{3}{4} r_n k_n \rfloor, 1] \times \overline{S^{\text{ext}}}$, we define $\overleftarrow{y}^{(k_n)}$ as $\overleftarrow{y}^{(k_n)} := y^{(k_n)}$, where $y^{(k_n)}$ is understood as the transformed mapping after the N_{U}-th step of rigidification.

As we have seen above, the affine transformations given by (4.24) at each step vanish in the limit. Hence, $((r_n)_{n=1}^\infty, (k_n)_{n=1}^\infty, (\overleftarrow{y}^{(k_n)})_{n=1}^\infty) \in \mathcal{V}_{\tilde{y}^+ - \tilde{y}^-, (R^-)^{-1} R^+}$.

To summarize, the sequence $(\overleftarrow{y}^{(k_n)})_{n=1}^\infty$ satisfies

$$\begin{aligned}\varphi\Big(\tilde{y}^+ - \tilde{y}^-, (R^-)^{-1} R^+\Big) &\leq \limsup_{n\to\infty} \mathcal{E}_{k_n}\Big(\overleftarrow{y}^{(k_n)}, [-1,1]\Big) \\ &\leq \varphi\Big(\tilde{y}^+ - \tilde{y}^-, (R^-)^{-1} R^+\Big) + 2N_{\mathrm{U}} \frac{C_{\mathrm{E}}}{N_*'} \leq \varphi\Big(\tilde{y}^+ - \tilde{y}^-, (R^-)^{-1} R^+\Big) + \varepsilon_*.\end{aligned}$$

Now we proceed to construct the modifications $\overset{+}{y}^{(k_n)}$ of $\overleftarrow{y}^{(k_n)}$ which will have more localized non-rigid parts (as depicted in Figure 4.2(c)).

Since no confusion arises, we again use $R_\pm^{(k_n)}$ and $y_\pm^{(k_n)}$ to denote the rigid deformations near the interval boundaries, i.e.

$$\overleftarrow{y}^{((k_n))}(w_1, x') = R_\pm^{(k_n)}\Big(r_n w_1, \frac{1}{k_n} x'\Big)^\top + y_\pm^{(k_n)} \text{ on } I^\pm \times \overline{S^{\text{ext}}}.$$

Now we first extend $\overleftarrow{y}^{(k_n)}$ rigidly to a function on $\mathbb{R} \times \overline{S^{\text{ext}}}$ by requiring this formula to hold true on $(-\infty, -\frac{3}{4}) \times \overline{S^{\text{ext}}}$ and $(\frac{3}{4}, \infty) \times \overline{S^{\text{ext}}}$, with the obvious interpretation of the $\pm$ sign.

If $j = j_i$ for some $i \in \{1, 2, \ldots, N_{\mathrm{U}}\}$, then we write $w_-^{(i,n)}$, $w_+^{(i,n)}$ in place of $w_-^{(n)}$, $w_+^{(n)}$ from Procedure (R), respectively, to stress the dependence on i. We set

$d^{(i,n)} = w_+^{(i,n)} - w_-^{(i,n)} - \frac{1}{r_n k_n}$ and also recall the definition of $R_-^{(i,k_n)}$ on this interval. Now consecutively do the following steps for $i \in \{1, 2, \dots, N_{\mathrm{U}}\}$, in reverse order starting with $i = N_{\mathrm{U}}$:

$$\overset{+}{y}^{(k_n)}(w_1, x') := \begin{cases} \overset{\leftarrow}{y}^{(k_n)}(w_1, x') & w_1 \le w_-^{(i,n)} + \frac{1}{2r_n k_n}, \\ \overset{\leftarrow}{y}^{(k_n)}(w_1 + d^{(i,n)}, x') - r_n d^{(i,n)} R_-^{(i,k_n)} e_1 & w_1 > w_-^{(i,n)} + \frac{1}{2r_n k_n}, \end{cases}$$
$$\overset{\leftarrow}{y}^{(k_n)}(w_1, x') := \overset{+}{y}^{(k_n)}(w_1, x'), \qquad w_1 \ge w_-^{(i,n)} + \frac{1}{2r_n k_n},\ x' \in \overline{S^{\mathrm{ext}}}.$$

This finally results in a configuration with

$$\overset{+}{y}^{(k_n)}(w_1, x') = \overset{\leftarrow}{y}^{(k_n)}(w_1, x') = R_-^{(k_n)}\Big(r_n w_1, \frac{1}{k_n} x'\Big)^\top + y_-^{(k_n)}$$

if $w_1 \le -\frac{3}{4}$, $x' \in \overline{S^{\mathrm{ext}}}$, and

$$\begin{aligned} \overset{+}{y}^{(k_n)}(w_1, x') &= \overset{\leftarrow}{y}^{(k_n)}(w_1 + d^{(n)}, x') - r_n c^{(n)} \\ &= R_+^{(k_n)}\Big(r_n w_1, \frac{1}{k_n} x'\Big)^\top + r_n d^{(n)} R_+^{(k_n)} e_1 + y_+^{(k_n)} - r_n c^{(n)} \end{aligned}$$

where $d^{(n)} = \sum_{i=1}^{N_{\mathrm{U}}} d^{(i,n)}$ and $c^{(n)} = \sum_{i=1}^{N_{\mathrm{U}}} d^{(i,n)} R_-^{(i,k_n)} e_1$, if $w_1 \ge \frac{3}{4} - d^{(n)}$ and $x' \in \overline{S^{\mathrm{ext}}}$.

Observe that $\mathcal{E}_{k_n}(\overset{+}{y}^{(k_n)}, [-1,1]) = \mathcal{E}_{k_n}(\overset{\leftarrow}{y}^{(k_n)}, [-1,1])$ for every $n \in \mathbb{N}$ as we have only shortened the intermediate rigid parts. Also, the length of the non-rigid part now satisfies

$$\frac{1}{r_n k_n}\Big\lfloor \frac{3}{4} r_n k_n \Big\rfloor - d^{(n)} - \frac{1}{r_n k_n}\Big(-\Big\lfloor \frac{3}{4} r_n k_n \Big\rfloor + 1\Big) \le \frac{1}{r_n k_n}\Big((2N_*' + 4)(N_{\mathrm{f}} + 1) + N_{\mathrm{f}}\Big).$$

Setting $N_* = (2N_* + 4)(N_{\mathrm{f}} + 1) + N_{\mathrm{f}}$ and shifting we finally obtain $\overset{+}{y}^{(k_n)}$ as claimed. □

Remark 4.9. Lemma 4.6 shows that the choice of $I^\pm$ in the definition of φ was arbitrary and that a different positive length of $I^\pm$ which still leaves a nonempty middle interval for fracture would give the same value of φ.

Our next task is to prove that the passages to subsequences (k_n) can be avoided when approximating the value of the cell formula.

Proposition 4.7. *Suppose that $\tilde{y}^-, \tilde{y}^+ \in \mathbb{R}^3$ and $R^-, R^+ \in \mathrm{SO}(3)$. Then for any $\varepsilon_* > 0$ and any nonincreasing sequence $(\rho_k)_{k=1}^\infty \subset (0,\infty)$ with $\lim_{k\to\infty} \rho_k = 0$ and $\lim_{k\to\infty} \rho_k k = \infty$ there exist deformations $\bar{y}^{(k)} \colon ([-1,1] \times \overline{S^{\mathrm{ext}}}) \to \mathbb{R}^3$ such that $((\rho_k)_{k=1}^\infty, (k)_{k=1}^\infty, (\bar{y}^{(k)})_{k=1}^\infty) \in \mathcal{V}_{\tilde{y}^+ - \tilde{y}^-, (R^-)^{-1} R^+}$ and*

$$\limsup_{k\to\infty} \mathcal{E}_k(\bar{y}^{(k)}, [-1,1]) \le \varphi\Big(\tilde{y}^+ - \tilde{y}^-, (R^-)^{-1} R^+\Big) + \varepsilon_*.$$

Proof. For a given $\varepsilon_* > 0$ we choose $N_* \in \mathbb{N}$, a (without loss of generality nondecreasing) sequence $(k_n)_{n=1}^\infty$, and mappings $\overset{+}{y}^{(k_n)} \in \mathrm{PAff}(\Lambda_{r_n,k_n})$ as in Lemma 4.6 so that

$$\limsup_{n\to\infty} \mathcal{E}_{k_n}(\overset{+}{y}^{(k_n)}, [-1,1]) \le \varphi\Big(\tilde{y}^+ - \tilde{y}^-, (R^-)^{-1} R^+\Big) + \varepsilon_*,$$

and, for suitable $\overset{+}{y}^{(k_n)}_{\pm} \in \mathbb{R}^3$, $\overset{+}{R}^{(k_n)}_{\pm} \in \mathrm{SO}(3)$ with $\overset{+}{y}^{(k_n)}_{\pm} \to \tilde{y}^{\pm}$, $\overset{+}{R}^{(k_n)}_{\pm} \to R^{\pm}$, after a rigid extension to the left and to the right,

$$\overset{+}{y}^{(k_n)}(w_1, x') = \overset{+}{R}^{(k_n)}_{\pm}\Big(r_n w_1, \frac{x'}{k_n}\Big)^{\top} + \overset{+}{y}^{(k_n)}_{\pm} \text{ on } \Big(\mathbb{R} \setminus I_{\mathrm{c}}^{(n)}\Big) \times \overline{S^{\mathrm{ext}}}$$

where $I_{\mathrm{c}}^{(n)} = \frac{1}{r_n k_n}[-N_*, N_*]$.

For each $k \in \mathbb{N}$ find $n_k \in \mathbb{N}$ such that $k_{n_k}^{-1} \leq k^{-1} \leq k_{n_k - 1}^{-1}$. Set

$$\bar{y}^{(k)}(w_1, x') := \frac{k_{n_k}}{k} \overset{+}{y}^{(k_{n_k})}\Big(\frac{\rho_k k}{r_{n_k} k_{n_k}} w_1, x'\Big), \quad (w_1, x') \in [-1, 1] \times \overline{S^{\mathrm{ext}}}.$$

Like this, $\bar{y}^{(k)}$ is well-defined (as far as the boundary condition on $I^{\pm} \times \overline{S^{\mathrm{ext}}}$ is concerned), at worst for all k larger than a certain $\bar{k} \in \mathbb{N}$. If it is the case that $\bar{k} > 1$, we define $y^{(1)}, \ldots, y^{(\bar{k}-1)}$ as we like, e.g. by extending the boundary rigid motions to all of $[-1, 1] \times \overline{S^{\mathrm{ext}}}$. Then for $k \geq \bar{k}$,

$$\bar{\nabla}_{\rho_k, k} y^{(k)}(w_1, x') = \bar{\nabla}_{r_{n_k}, k_{n_k}} \overset{+}{y}^{(k_{n_k})}\Big(\frac{\rho_k k}{r_{n_k} k_{n_k}} w_1, x'\Big)$$

and

$$k W_{\mathrm{tot}}^{(k)}\Big(x', \bar{\nabla}_{\rho_k, k} y^{(k)}(w_1, x')\Big) \leq k_{n_k} W_{\mathrm{tot}}^{(k_{n_k})}\Big(x', \bar{\nabla}_{r_{n_k}, k_{n_k}} \overset{+}{y}^{(k_{n_k})}\Big(\frac{\rho_k k}{r_{n_k} k_{n_k}} w_1, x'\Big)\Big)$$

by assumption (W4) on the cell energy. This yields

$$\begin{aligned}\varphi\Big(\tilde{y}^+ - \tilde{y}^-, (R^-)^{-1} R^+\Big) &\leq \limsup_{k \to \infty} \mathcal{E}_k(\bar{y}^{(k)}, [-1, 1]) \\ &\leq \limsup_{k \to \infty} \mathcal{E}_{k_{n_k}}(\overset{+}{y}^{(k_{n_k})}, [-1, 1]) \leq \varphi\Big(\tilde{y}^+ - \tilde{y}^-, (R^-)^{-1} R^+\Big) + \varepsilon_*. \square\end{aligned}$$

The approximating sequence $(y^{(k)})$ in the vicinity of crack points can be chosen to be bounded in L^∞ in a universal way – this is the content of

Proposition 4.8. *Suppose that* $\tilde{y}^-, \tilde{y}^+ \in \mathbb{R}^3$, $R^-, R^+ \in \mathrm{SO}(3)$ *and* $(r_k)_{k=1}^\infty \subset (0, \infty)$ *is a nonincreasing sequence with* $\lim_{k \to \infty} r_k = 0$ *and* $\lim_{k \to \infty} r_k k = \infty$. *Assume that* $y^{(k)}\colon ([-1, 1] \times \overline{S^{\mathrm{ext}}}) \to \mathbb{R}^3$ *is such that* $((r_k)_{k=1}^\infty, (k)_{k=1}^\infty, (y^{(k)})_{k=1}^\infty) \in \mathcal{V}_{\tilde{y}^+ - \tilde{y}^-, (R^-)^{-1} R^+}$ *with*

$$y^{(k)}(w_1, x') = R_{\pm}^{(k)}\Big(r_n w_1, \frac{1}{k} x'\Big)^{\top} + y_{\pm}^{(k)} \text{ on } I^{\pm} \times \overline{S^{\mathrm{ext}}}$$

for $R_{\pm}^{(k)} \to R^{\pm}$, $y_{\pm}^{(k)} \to \tilde{y}^{\pm}$. *If the maximum interaction range property (W9) with rate* $(M_k)_{k=1}^\infty$ *holds true, then there exists a modification* $\bar{y}^{(k)}$ *of* $y^{(k)}$ *with the corresponding triple* $((r_k)_{k=1}^\infty, (k)_{k=1}^\infty, (\bar{y}^{(k)})_{k=1}^\infty) \in \mathcal{V}_{\tilde{y}^+ - \tilde{y}^-, (R^-)^{-1} R^+}$ *such that*

$$|\mathcal{E}_k(\bar{y}^{(k)}, [-1, 1]) - \mathcal{E}_k(y^{(k)}, [-1, 1])| \leq \frac{C}{k M_k} \mathcal{E}_k(y^{(k)}, [-1, 1]),$$

$\bar{y}^{(k)} = y^{(k)}$ *on* $(I^- \cup I^+) \times \overline{S^{\mathrm{ext}}}$ *and*

$$\|\mathrm{dist}(\bar{y}^{(k)}, \{y_-^{(k)}, y_+^{(k)}\})\|_\infty \leq C r_k M_k k \mathcal{E}_k(y^{(k)}, [-1, 1]).$$

Proof. We write $D(\bar{x}) = \bar{x} + \{(\frac{1}{r_k k}z_1^i, (z^i)'); \ i = 1, \dots, 8\}$ for the corners of the cell with midpoint $\bar{x} \in \Lambda'_{r_k,k}$. Our strategy is to move back all pieces of the rod that are too far from $\{y_-^{(k)}, y_+^{(k)}\}$. Fix $k \in \mathbb{N}$ and consider the undirected graph $\mathfrak{G} = (\mathfrak{V}, \mathfrak{E})$, where $\mathfrak{V} = \Lambda_{r_k,k}$ and

$$\{x, x^\dagger\} \in \mathfrak{E} \Leftrightarrow (\exists\, \bar{x} \in \Lambda'_{r_k,k} \colon x, x^\dagger \in D(\bar{x}) \wedge |y^{(k)}(x) - y^{(k)}(x^\dagger)| < M_k).$$

Let $\mathfrak{G}_1, \mathfrak{G}_2, \dots, \mathfrak{G}_{n_\mathrm{G}}$ be the connected components of $\mathfrak{G}$, numbered in such a way that $(I^- \times \overline{S^{\mathrm{ext}}}) \cap \Lambda_{r_k,k} \in \mathfrak{G}_1$ and $(I^+ \times \overline{S^{\mathrm{ext}}}) \cap \Lambda_{r_k,k} \in \mathfrak{G}_{n_\mathrm{G}}$. Accordingly we partition $\{z^1, \dots, z^8\} = Z_1(\bar{x}) \dot\cup Z_2(\bar{x}) \dot\cup \cdots \dot\cup Z_{n_{\bar{x}}}(\bar{x})$ for every $\bar{x} \in \Lambda'_{r_k,k}$, where $Z_i(\bar{x}) \neq \emptyset$, so that $z^j, z^m \in Z_\ell(\bar{x})$ for some $\ell \in \{1, 2, \dots, n_{\bar{x}}\}$ if and only if there is $i_\mathrm{V} \in \{1, 2, \dots, n_\mathrm{G}\}$ such that $\bar{x} + \frac{1}{k}z^j, \bar{x} + \frac{1}{k}z^m \in \mathfrak{V}_{i_\mathrm{V}}$, the set of vertices of $\mathfrak{G}_{i_\mathrm{V}}$. Then the induced components of atomic cells are far apart: for any $\bar{x} \in \Lambda'_{r_k,k}$ and $1 \leq i < j \leq n_{\bar{x}}$, we have $\mathrm{dist}(y^{(k)}(\bar{x} + Z_i(\bar{x})), y^{(k)}(\bar{x} + Z_j(\bar{x}))) \geq M_k$.

Similarly as before we observe that the number of atomic cells 'broken' by $y^{(k)}$ is controlled by the energy so that the number n_G of connected components of $\mathfrak{G}$ satisfies a bound of the form

$$n_\mathrm{G} \leq C_1 \mathcal{E}_k(y^{(k)}, [-1, 1])$$

with a constant $C_1 > 0$. The construction further implies that the diameter of each component after deformation is bounded by

$$\mathrm{diam}\, y^{(k)}(\mathfrak{V}_i) \leq C_2 M_k r_k k, \quad i = 1, \dots, n_\mathrm{G},$$

with another constant $C_2 > 0$.

For the first and last component we have

$$\mathrm{dist}(y^{(k)}(\mathfrak{V}_1), \{y_-^{(k)}\}) \leq C_3 M_k r_k k \quad \text{and} \quad \mathrm{dist}(y^{(k)}(\mathfrak{V}_{n_\mathrm{G}}), \{y_+^{(k)}\}) \leq C_3 M_k r_k k.$$

If $n_\mathrm{G} \geq 3$, we can shift graph components $\mathfrak{G}_i$, $i = 2, \dots, n_\mathrm{G} - 1$, without considerably changing the total energy, provided we do not put the components at a distance less than M_k. Specifically, for $\gamma = 2M_k + (C_2 + C_3)M_k r_k k \leq (2 + C_2 + C_3)M_k r_k k$ and $|e| = 1$ with $e \perp y_+^{(k)} - y_-^{(k)}$ the points $y_-^{(k)} + (i-1)\gamma e$, $i = 2, \dots, n_\mathrm{G} - 1$, have a distance $\geq \gamma$ from each other and from $\{y_+^{(k)}, y_-^{(k)}\}$. We then define $\bar{y}^{(k)}$ by shifting $\mathfrak{G}_i$ rigidly in such a way that $y_-^{(k)} + (i-1)\gamma e \in \bar{y}^{(k)}(\mathfrak{V}_i)$, $i = 2, \dots, n_\mathrm{G} - 1$.

Then indeed the shifted components have the required minimal distances and moreover

$$\mathrm{dist}(y^{(k)}(\mathfrak{V}_i), \{y_-^{(k)}\}) \leq n_\mathrm{G}\gamma \leq C_1 \mathcal{E}_k(y^{(k)}, [-1, 1])(2 + C_2 + C_3)M_k r_k k,$$

$i = 2, \dots, n_\mathrm{G} - 1$. The assertion follows now by noting that $\bar{y}^{(k)} = y^{(k)}$ on $\mathfrak{V}_1 \cup \mathfrak{V}_{n_\mathrm{G}}$ and

$$\tfrac{1}{k}|\mathcal{E}_k(\bar{y}^{(k)}, [-1, 1]) - \mathcal{E}_k(y^{(k)}, [-1, 1])| \leq C\mathcal{E}_k(y^{(k)}, [-1, 1]) \frac{C_\mathrm{far}}{k^2 M_k},$$

as only broken cells have been altered. □

4.5.2 Construction of recovery sequences

Proof of Theorem 4.3(ii). It is known from the theory of Γ-convergence that for any $\varepsilon > 0$ it suffices to find a recovery sequence with $\limsup_{k\to\infty} kE^{(k)}(y^{(k)}) \leq E_{\lim}(\tilde{y}, d_2, d_3) + \varepsilon$, which is trivial if $(\tilde{y}, d_2, d_3) \notin \mathcal{A}$. In the case that $(\tilde{y}, d_2, d_3) \in \mathcal{A}$, let $(\sigma^i)_{i=0}^{\bar{n}_f+1}$ be the partition of $[0,L]$ such that $\{\sigma^i\}_{i=1}^{\bar{n}_f} = S_{\tilde{y}} \cup S_R$, where $S_R := S_{\tilde{y}'} \cup S_{d_2} \cup S_{d_3}$. Depending on the assumptions on $\tilde{y}$, d_2, d_3, we treat two different cases separately.

Piecewise smooth case

Denoting by $\mathcal{UC}^n(U;\mathbb{R}^m)$ the space of functions $f\colon U \to \mathbb{R}^m$, $U \subset \mathbb{R}^\ell$, such that their derivatives of order $0,1,\dots,n$ are uniformly continuous on U, we first additionally suppose that $\tilde{y}|_{(\sigma^{i-1},\sigma^i)} \in \mathcal{UC}^3((\sigma^{i-1},\sigma^i);\mathbb{R}^3)$, $d_s|_{(\sigma^{i-1},\sigma^i)} \in \mathcal{UC}^2((\sigma^{i-1}, \sigma^i);\mathbb{R}^3)$, $s = 2,3$, for all $i \in \{1,2,\dots,\bar{n}_f+1\}$ and that $R = (\partial_1\tilde{y}|d_2|d_3)$ is constant on the sets $(\sigma^0, \sigma^0+\eta)$, $(\sigma^i - \eta, \sigma^i)$, $(\sigma^i, \sigma^i+\eta)$, $i \in \{1,2,\dots,\bar{n}_f\}$, and $(\sigma^{\bar{n}_f+1} - \eta, \sigma^{\bar{n}_f+1})$ for some $\eta > 0$. If $k \in \mathbb{N}$, write $I_0^k := [0, \frac{1}{k}\lfloor k\sigma^1 \rfloor]$, $I_i^k := [\frac{1}{k}\lfloor k\sigma^i \rfloor + \frac{1}{k}, \frac{1}{k}\lfloor k\sigma^{i+1} \rfloor]$ for $i = 1,2,\dots,\bar{n}_f - 1$ and $I_{\bar{n}_f}^k := [\frac{1}{k}\lfloor k\sigma^{\bar{n}_f} \rfloor + \frac{1}{k}, L_k]$.

Let $\beta(\cdot, x') \in \mathcal{C}^1([0,L];\mathbb{R}^3)$ for each $x' \in \mathcal{L}^{\text{ext}}$ and $q \in \mathcal{C}^2([0,L];\mathbb{R}^3)$. It turns out that the sequence

$$\tilde{y}^{(k)}(x) := \tilde{y}(x_1) + \frac{1}{k}x_2 d_2(x_1) + \frac{1}{k}x_3 d_3(x_1) + \frac{1}{k}q(x_1) + \frac{1}{k^2}\beta(x), \quad x \in \{0, \tfrac{1}{k}, \dots, L_k\} \times \mathcal{L}^{\text{ext}}, \tag{4.26}$$

appropriately extended and interpolated on $[-\frac{1}{k}, L_k + \frac{1}{k}] \times \overline{S^{\text{ext}}}$, behaves elastically in every region $I_i^k \times S^{\text{ext}}$, $i = 0,1,\dots,\bar{n}_f$.

To show this, choose $i \in \{0,1,\dots,\bar{n}_f\}$. Excluding the contributions with $W_{\text{end}}^{(k)}$, the strain energy contained in the portion $I_i^k \times S^{\text{ext}}$ is

$$\begin{aligned} k\int_{I_i^k \times S^{\text{ext}}} W_{\text{tot}}^{(k)}(x', \bar{\nabla}_k \tilde{y}^{(k)})\mathrm{d}x &= k\int_{I_i^k \times S^{\text{ext}}} W_{\text{tot}}^{(k)}\Big(x', R^\top(\bar{x}_1)\bar{\nabla}_k\tilde{y}^{(k)}(x)\Big)\mathrm{d}x = \\ &= k\int_{I_i^k \times S^{\text{ext}}} W_{\text{tot}}^{(k)}\Big(x', \bar{\mathrm{Id}} + R^\top(\bar{x}_1)\Big(\bar{\nabla}_k\tilde{y}^{(k)}(x) - R(\bar{x}_1)\bar{\mathrm{Id}}\Big)\Big)\mathrm{d}x. \end{aligned}$$

Using Taylor expansions as in the purely elastic case, we find

$$\|\bar{\nabla}_k\tilde{y}^{(k)} - R(\bar{\cdot})\bar{\mathrm{Id}}\|_{L^\infty(I_i^k \times S^{\text{ext}};\mathbb{R}^{3\times 8})} = O\Big(\frac{1}{k}\Big)$$

due to the sufficient smoothness of the restrictions of $\tilde{y}$, d_2, d_3, q, or β, to (σ^i, σ^{i+1}), or to $(\sigma^i, \sigma^{i+1}) \times S^{\text{ext}}$. But this implies that

$$\mathrm{dist}(\bar{\nabla}_k\tilde{y}^{(k)}\big|_{I_i^k \times S^{\text{ext}}}, \bar{\mathrm{SO}}(3)) \leq c_{\text{frac}}^{(k)}$$

for all k large enough, since $c_{\text{frac}}^{(k)} = O(\frac{1}{\sqrt{k}})$, and $W_{\text{tot}}^{(k)}$ does not enter the fracture regime on any atomic cell in $I_i^k \times S^{\text{ext}}$.

Hence, the analysis of elastic rods in Chapter 3 shows that one has $\tilde{y}^{(k)} \to \tilde{y}$ in L^2 on $(0,L) \times S^{\text{ext}}$ as well as

$$\sum_{x \in \{-\frac{1}{2k}, L_k + \frac{1}{2k}\} \times \mathcal{L}'^{,\text{ext}}} kW_{\text{end}}^{(k)}\Big(x_1, x', \bar{\nabla}_k\tilde{y}^{(k)}(x)\Big) \to 0$$

and, for a suitable choice of β and q,

$$k\int_{I_i^k\times\overline{S^{\mathrm{ext}}}} W_{\mathrm{tot}}^{(k)}(x',\bar\nabla_k\tilde y^{(k)})\mathrm{d}x$$

$$\to \frac{1}{2}\int_{\sigma^i}^{\sigma^{i+1}}\int_{S^{\mathrm{ext}}} Q_{\mathrm{tot}}\Big(x', R^\top(x_1)\Big(\frac{\partial R}{\partial x_1}(x_1)(0,\bar x_2,\bar x_3)^\top + \frac{\partial q}{\partial x_1}(x_1)\Big)e_1^\top \bar{\mathrm{Id}}$$
$$+ R^\top(x_1)\frac{\partial R}{\partial x_1}(x_1)\Big[\bar z_1^i(0,\bar z_2^i,\bar z_3^i)^\top\Big]_{i=1}^8 + R^\top(x_1)\Big(\bar\nabla^{2\mathrm{d}}\beta(x)|\bar\nabla^{2\mathrm{d}}\beta(x)\Big)\Big)\mathrm{d}x \tag{4.27}$$

$$\le \frac{1}{2}\int_{\sigma^i}^{\sigma^{i+1}}\int_{S^{\mathrm{ext}}} Q_3^{\mathrm{rel}}\Big(R^\top(x_1)\frac{\partial R}{\partial x_1}(x_1)\Big)\mathrm{d}x_1+\varepsilon. \tag{4.28}$$

Indeed one can choose $\beta\equiv 0$ and $q\equiv 0$ on $(\sigma^i,\sigma^i+\frac{\eta}{2})\cup(\sigma^{i+1}-\frac{\eta}{2},\sigma^{i+1})$ as R by assumption is constant on a neighbourhood of these sets. So we have

$$\tilde y^{(k)}(x) = \begin{cases}\tilde y(\sigma^i+) + R(\sigma^i+)(x_1-\sigma^i,x')^\top & \text{for } x_1\in(\sigma^i,\sigma^i+\frac{\eta}{2}),\\ \tilde y(\sigma^{i+1}-) + R(\sigma^{i+1}-)(x_1-\sigma^{i+1},x')^\top & \text{for } x_1\in(\sigma^{i+1}-\frac{\eta}{2},\sigma^{i+1}).\end{cases}$$

We now update $\tilde y^{(k)}$ by replacing portions near the jumps σ^i (and matching all parts by applying suitable rigid motions). Fix a sequence $(r_k)_{k=1}^\infty$ such that $r_k\to 0$ and $r_k k\to\infty$. By Proposition 4.7 for each $i=1,\dots,\bar n_{\mathrm{f}}$ we can choose $\mathcal{y}_i^{(k)}\colon([-1,1]\times\overline{S^{\mathrm{ext}}})\to\mathbb{R}^3$ such that $((r_k)_{k=1}^\infty,(k)_{k=1}^\infty,(\mathcal{y}_i^{(k)})_{k=1}^\infty)$ belongs to $\mathcal{V}_{\tilde y(\sigma^i+)-\tilde y(\sigma^i-),(R(\sigma^i-))^{-1}R(\sigma^i+)}$ with

$$\mathcal{y}_i^{(k)}(w_1,x') = R_\pm^{(k,i)}\Big(r_n w_1,\frac{1}{k}x'\Big)^\top + y_\pm^{(k,i)} \text{ on } I^\pm\times\overline{S^{\mathrm{ext}}}$$

for $R_\pm^{(k,i)}\to R(\sigma^i\pm)$, $y_\pm^{(k,i)}\to\tilde y^\pm$ which satisfies the energy estimate

$$\limsup_{k\to\infty}\mathcal{E}_k\Big(\mathcal{y}_i^{(k)},[-1,1]\Big)\le\varphi(\tilde y(\sigma^i+)-\tilde y(\sigma^i-),R(\sigma^i-)^{-1}R(\sigma^i+))+\varepsilon. \tag{4.29}$$

Let $H_{\sigma,r}(x) := (\frac{1}{r}(x_1-\sigma),x')$ for any $r>0$ and recall $\sigma_k^i=\frac{1}{k}\lfloor k\sigma^i\rfloor$. Noticing that $\tilde y^{(k)}$ is rigid near a jump as are the $\mathcal{y}_i^{(k)}$ near ±1, we can now define a modification $\tilde y_{\mathrm{tot}}^{(k)}$ of $\tilde y^{(k)}$ by setting

$$\tilde y_{\mathrm{tot}}^{(k)}(x) = \begin{cases}\tilde y^{(k)}(x) & -\frac{1}{k}\le x_1\le\sigma_k^1-r_k,\\ O_-^{(k,i)}\mathcal{y}_i^{(k)}\circ H_{\sigma_k^i,r_k}(x)+c_-^{(k,i)} & \sigma_k^i-r_k<x_1\le\sigma_k^i+r_k,\ i=1,\dots,\bar n_{\mathrm{f}},\\ O_+^{(k,i)}\tilde y^{(k)}(x)+c_+^{(k,i)} & \sigma_k^i+r_k<x_1\le\sigma_k^{i+1}-r_k,\ i=1,\dots,\bar n_{\mathrm{f}}-1,\\ O_+^{(k,\bar n_{\mathrm{f}})}\tilde y^{(k)}(x)+c_+^{(k,\bar n_{\mathrm{f}})} & \sigma_k^{\bar n_{\mathrm{f}}}+r_k<x_1\le L_k+\frac{1}{k},\end{cases}$$

where $O_\pm^{(k,i)}\in\mathrm{SO}(3)$ and $c_\pm^{(k,i)}\in\mathbb{R}^3$ are such that

$$O_-^{(k,i)}\mathcal{y}_i^{(k)}\circ H_{\sigma_k^i,r_k}+c_-^{(k,i)} = \begin{cases}O_+^{(k,i-1)}\tilde y^{(k)}+c_+^{(k,i-1)} & \text{on } (\sigma_k^i-r_k,\sigma_k^i-\frac{3}{4}r_k)\times S^{\mathrm{ext}},\\ O_+^{(k,i)}\tilde y^{(k)}+c_+^{(k,i)} & \text{on } (\sigma_k^i+\frac{3}{4}r_k,\sigma_k^i+r_k)\times S^{\mathrm{ext}}\end{cases}$$

for $i = 1, \dots, \bar{n}_{\mathrm{f}}$ (and we have set $O_+^{(k,0)} := \mathrm{Id}$, $c_+^{(k,0)} := 0$). Since $R_\pm^{(k,i)} \to R(\sigma^i\pm)$, $y_\pm^{(k,i)} \to \tilde{y}^\pm$ we get $O_\pm^{(k,i)} \to \mathrm{Id}$ and $c_\pm^{(k,i)} \to 0$ as $k \to \infty$. Thus we still have $\tilde{y}_{\mathrm{tot}}^{(k)} \to \tilde{y}$ in $L^2((0,L)\times S^{\mathrm{ext}};\mathbb{R}^3)$. By (4.28) and (4.29) the sequence $\tilde{y}_{\mathrm{tot}}^{(k)}$ satisfies the envisioned energy estimate

$$\limsup_{k\to\infty} kE^{(k)}(\tilde{y}_{\mathrm{tot}}^{(k)}) \le E_{\mathrm{lim}}(\tilde{y}, d_2, d_3) + C\varepsilon.$$

It remains to observe that in case (W9) holds true with a sequence $(M_k)_{k=1}^\infty$ and $\|\tilde{y}\|_\infty \le M$, then for any $(\zeta_k)_{k=1}^\infty \subset (0,1)$ with $\zeta_k \searrow 0$ and $\zeta_k/M_k \to \infty$ one can choose $\tilde{y}_{\mathrm{tot}}^{(k)}$ such that $\|\tilde{y}_{\mathrm{tot}}^{(k)}\|_\infty \le M + \zeta_k$. This is clear by construction for $\tilde{y}^{(k)}$ in (4.26) instead of $\tilde{y}_{\mathrm{tot}}^{(k)}$ since $\zeta_k \gg \frac{1}{k}$. The bound is indeed preserved by the passage to $\tilde{y}_{\mathrm{tot}}^{(k)}$ due to Proposition 4.8 once we have $r_k M_k k \ll \zeta_k$. As Proposition 4.7 allows us to choose $r_k \searrow 0$ as fast as we wish as long as $r_k k \to \infty$, the claim follows.

Nonsmooth case

Now let us assume that $\tilde{y}$, d_2, d_3 are general as in Theorem 4.3(ii). Interestingly, a related approximation problem was treated recently by P. Hornung. [Hor21] However, a more elementary construction is sufficient in our case. By a density argument, it is enough to show that there are sequences $(\tilde{y}_{\mathrm{tot}}^{(j)})_{j=1}^\infty$, $(d_s^{(j)})_{j=1}^\infty$, $s = 2,3$, such that:

(i) for every j and all $i \in \{1,2,\dots,\bar{n}_{\mathrm{f}}+1\}$, the functions satisfy $\tilde{y}_{\mathrm{tot}}^{(j)}|_{(\sigma^{i-1},\sigma^i)} \in \mathcal{UC}^3((\sigma^{i-1},\sigma^i);\mathbb{R}^3)$, $d_2^{(j)}|_{(\sigma^{i-1},\sigma^i)}, d_3^{(j)}|_{(\sigma^{i-1},\sigma^i)} \in \mathcal{UC}^2((\sigma^{i-1},\sigma^i);\mathbb{R}^3)$ with $R_{\mathrm{tot}}^{(j)} = (\partial_{x_1}\tilde{y}_{\mathrm{tot}}^{(j)}|d_2^{(j)}|d_3^{(j)})$ constant on $(\sigma^i - \eta_j, \sigma^i)$ and on $(\sigma^i, \sigma^i + \eta_j)$, $\eta_j > 0$, and $(\tilde{y}_{\mathrm{tot}}^{(j)}, d_2^{(j)}, d_3^{(j)}) \in \mathcal{A}$;

(ii) $\tilde{y}_{\mathrm{tot}}^{(j)} \to \tilde{y}$ in $L^2((0,L);\mathbb{R}^3)$, $R_{\mathrm{tot}}^{(j)} \to R = (\partial_{x_1}\tilde{y}|d_2|d_3)$ in $H^1((\sigma^{i-1},\sigma^i);\mathbb{R}^{3\times3})$ for any $i \in \{1,\dots,\bar{n}_{\mathrm{f}}+1\}$;

(iii) $E_{\mathrm{lim}}(\tilde{y}_{\mathrm{tot}}^{(j)}, d_2^{(j)}, d_3^{(j)}) \to E_{\mathrm{lim}}(\tilde{y}, d_2, d_3)$, $j \to \infty$.

Let (η_j) be a positive null sequence. For each $i \in \{1,2,\dots,\bar{n}_{\mathrm{f}}+1\}$ we find an approximating sequence $(\tilde{R}^{(j)}|_{(\sigma^{i-1},\sigma^i)}) \subset \mathcal{UC}^2([\sigma^{i-1},\sigma^i];\mathbb{R}^{3\times3})$, such that $\tilde{R}^{(j)}$ is constant on $(\sigma^{i-1},\sigma^{i-1}+\eta_j)$ and $(\sigma^i - \eta_j, \sigma^i)$ and $\tilde{R}^{(j)} \to R$ in $H^1((\sigma^{i-1},\sigma^i);\mathbb{R}^{3\times3})$ so that $\tilde{R}^{(j)} \to R$ uniformly in (σ^{i-1},σ^i) by the Sobolev embedding theorem. Then we project $\tilde{R}^{(j)}(x_1)$ for every $x_1 \in (\sigma^{i-1},\sigma^i)$ smoothly onto SO(3) and get a sequence $\{R^{(j)}\} \subset \mathcal{C}^1([\sigma^{i-1},\sigma^i];\mathbb{R}^{3\times3})$ of mappings with values in SO(3). This implies that $R^{(j)} \to R$ in $H^1((\sigma^{i-1},\sigma^i);\mathbb{R}^{3\times3})$ for $i = 1,2,\dots,\bar{n}_{\mathrm{f}}+1$.

We write $R^{(j)} = (\partial_{x_1}\tilde{y}^{(j)}|\bar{d}_2^{(j)}|\bar{d}_3^{(j)})$ for $\bar{d}_2^{(j)}, \bar{d}_3^{(j)} \in \mathcal{C}^2([\sigma^{i-1},\sigma^i];\mathbb{R}^3)$ and $\tilde{y}^{(j)} \in \mathcal{C}^3([\sigma^{i-1},\sigma^i];\mathbb{R}^3)$ such that $\tilde{y}^{(j)}(\sigma^{i-1}+) = \tilde{y}(\sigma^{i-1}+)$; thus we have $(\tilde{y}^{(j)}|\bar{d}_2^{(j)}|\bar{d}_3^{(j)}) \in \mathcal{A}$. To avoid issues with crack terms, we rigidly move the pieces of the rod so as to obtain a j-independent contribution from the cracks that is exactly equal to the limiting crack energy. We set

$$\tilde{y}^{(j)}_{\rm tot}(x) = O^{(j,i)}\tilde{y}^{(j)}(x) + c^{(j,i)} \quad \text{and} \quad d^{(j)}_s = O^{(j,i)}\bar{d}^{(j)}_s,\ s = 2,3,$$

if $\sigma^{i-1} < x_1 < \sigma^i$, $i = 1,2,\dots,\bar{n}_{\rm f}+1$, where $O^{(j,i)} \in \mathrm{SO}(3)$ and $c^{(j,i)} \in \mathbb{R}^3$ are defined consecutively by $O^{(j,0)} = \mathrm{Id}$, $c^{(j,0)} = 0$, and requiring that

$$\tilde{y}^{(j)}_{\rm tot}(\sigma^i+) - \tilde{y}^{(j)}_{\rm tot}(\sigma^i-) = \tilde{y}(\sigma^i+) - \tilde{y}(\sigma^i-) \quad \text{and}$$
$$[R^{(j)}_{\rm tot}(\sigma^i-)]^{-1}R^{(j)}_{\rm tot}(\sigma^i+) = [R(\sigma^i-)]^{-1}R(\sigma^i+)$$

for $i = 1,\dots,\bar{n}_{\rm f}$, $R^{(j)}_{\rm tot} = (\partial_{x_1}\tilde{y}^{(j)}_{\rm tot}|d^{(j)}_2|d^{(j)}_3)$, $j \in \mathbb{N}$. By frame indifference, the elastic energy is not changed by such an operation. Noting that $O^{(j,i)} \to \mathrm{Id}$ and $c^{(j,i)} \to 0$ for $j \to \infty$, we see that these mappings are such that (i)–(iii) hold (for (iii) observe that the integral in (4.27) behaves continuously in R with respect to the topologies used here). □

4.6* A more simple proof for a highly brittle model

If we use stronger assumptions on our interaction potentials, Γ-convergence can be proved more easily. The effective 'highly brittle' continuum model is specified in Theorem 4.9. Due to the explicit expression for crack energy, technical constructions like in Subsections 4.4.4 or 4.5.1 can be avoided.

Our total strain energy $E^{(k)}$ in this section is a sum of x'-dependent cell energies:

$$E^{(k)}(y^{(k)}) = \sum_{\hat{x}\in\hat{\Lambda}'_k} W^{(k)}_{\rm cell}\big(\hat{x}', \vec{y}^{(k)}(\hat{x})\big),$$

where $W^{(k)}_{\rm cell}\colon \mathcal{L}' \times \mathbb{R}^{3\times 8} \to [0,\infty)$, and no stand-alone surface terms are present this time. (Firstly, the dependence on x' allows some basic surface energy modelling by defining $W^{(k)}_{\rm cell}$ differently near the rod's surface; secondly, more sophisticated surface terms would make it difficult to characterize the limiting functional explicitly in the presence of rod kinks.)

These considerations also indicate that it is sufficient to extend lattice deformations only in the longitudinal direction x_1, in order to have $y^{(k)}\colon \Lambda_k \cup (\{L_k + \frac{1}{k}\} \times \mathcal{L}) \to \mathbb{R}^3$.

As for $W^{(k)}_{\rm cell}$, we rely on a new, simplified set of assumptions:

(V1) $W^{(k)}_{\rm cell}(x', R\vec{y} + (c|\cdots|c)) = W^{(k)}_{\rm cell}(x', \vec{y})$ for all $x' \in \mathcal{L}'$, $R \in \mathrm{SO}(3)$, $\vec{y} \in \mathbb{R}^{3\times 8}$, $c \in \mathbb{R}^3$, and $k \in \mathbb{N}$.

(V2) For every $k \in \mathbb{N}$ and $x' \in \mathcal{L}'$, $W^{(k)}_{\rm cell}(x', \cdot)$ attains a minimum (equal to 0) at and only at deformations of the form $\vec{y} = (\hat{y}_1|\cdots|\hat{y}_8)$ with $\hat{y}_i = Rz^i + c$ for all $i \in \{1,\dots,8\}$ and some $R \in \mathrm{SO}(3)$, $c \in \mathbb{R}^3$.

(V3) There are $c_{\mathrm{w}} \geq c_{\mathrm{W}} > 0$, $W_0\colon \mathcal{L}' \times \mathbb{R}^{3\times 8} \to [0,\infty)$, and cut-off values $c_{\mathrm{cut}}^{(k)}(x') > 0$, $k \in \mathbb{N}$, $x' \in \mathcal{L}'$, where

$$\lim_{k\to\infty} k\Big(c_{\mathrm{cut}}^{(k)}(x')\Big)^2 = c_{\mathrm{cut}}(x') \in (0,\infty),$$

such that for any $x' \in \mathcal{L}'$ and $\vec{y} = (\hat{y}_1|\hat{y}_2|\cdots|\hat{y}_8) \in \mathbb{R}^{3\times 8}$, (recall the formula $\vec{y} = \bar{\nabla}\hat{y} + \frac{1}{8}\sum_{i=1}^{8}\hat{y}_i(1,\dots,1)$) we have

$$W_{\mathrm{cell}}^{(k)}(x',\vec{y}) = \min\Big\{W_0(x',\vec{y}), c_{\mathrm{W}}\Big(c_{\mathrm{cut}}^{(k)}(x')\Big)^2\Big\},$$

$$c_{\mathrm{w}}\mathrm{dist}^2(\bar{\nabla}\hat{y}, \bar{\mathrm{SO}}(3)) \geq W_0(x',\vec{y}) \geq c_{\mathrm{W}}\mathrm{dist}^2(\bar{\nabla}\hat{y}, \bar{\mathrm{SO}}(3)).$$

(V4) $W_{\mathrm{cell}}^{(k)}(x',\cdot)$ is everywhere Borel measurable and $W_0(x',\cdot)$, $x' \in \mathcal{L}'$, is of class $\mathcal{C}^2$ in a neighbourhood of $\bar{\mathrm{SO}}(3)$.

Remark 4.10. The sequence $(c_{\mathrm{cut}}^{(k)})_{k=1}^{\infty}$ need not be monotone.

Theorem 4.9. *Under assumptions (V1)–(V4) we have $kE^{(k)} \xrightarrow{\Gamma} E_{\mathrm{hb}}$ as $k \to \infty$, more precisely:*

(i) Let $(y^{(k)})_{k=1}^{\infty}$ be a sequence of lattice deformations such that their piecewise affine interpolations and extensions $(\tilde{y}^{(k)})_{k=1}^{\infty} \subset H^1(\Omega;\mathbb{R}^3)$, defined in Subsection 4.1.2, converge in $L^2(\Omega;\mathbb{R}^3)$ to $\tilde{y} \in L^2((0,L);\mathbb{R}^3)$ for which there is a partition $(\varsigma^i)_{i=0}^{\tilde{n}_{\mathrm{f}}+1}$ of $[0,L]$ such that $\tilde{y}\big|_{(\varsigma^i,\varsigma^{i+1})} \in H^1((\varsigma^i,\varsigma^{i+1});\mathbb{R}^3)$, $0 \leq i \leq \tilde{n}_{\mathrm{f}}$.

Assume further that there are $d_s \in L^2((0,L);\mathbb{R}^3)$ such that for any $\eta > 0$ sufficiently small, we have $k\partial_{x_s}\tilde{y}^{(k)} \to d_s$ in $L^2((\varsigma^i+\eta,\varsigma^{i+1}-\eta)\times S;\mathbb{R}^3)$, $s = 2,3$, $1 \leq i \leq \tilde{n}_{\mathrm{f}}$. Then

$$E_{\mathrm{hb}}(\tilde{y},d_2,d_3) \leq \liminf_{k\to\infty} kE^{(k)}(y^{(k)}).$$

(ii) Let $\tilde{y} \in L^2((0,L);\mathbb{R}^3)$ be such there is a partition $(\varsigma^i)_{i=0}^{\tilde{n}_{\mathrm{f}}+1}$ of $[0,L]$ for which $\tilde{y}\big|_{(\varsigma^i,\varsigma^{i+1})} \in H^1((\varsigma^i,\varsigma^{i+1});\mathbb{R}^3)$, and let $d_2, d_3 \in L^2((0,L);\mathbb{R}^3)$. Then there exists a sequence of lattice deformations $(y^{(k)})_{k=1}^{\infty}$ such that their piecewise affine interpolations and extensions $(\tilde{y}^{(k)})_{k=1}^{\infty} \subset H^1(\Omega;\mathbb{R}^3)$, defined in Subsection 4.1.2, satisfy $\tilde{y}^{(k)} \to \tilde{y}$ in $L^2(\Omega;\mathbb{R}^3)$, $k\frac{\partial \tilde{y}^{(k)}}{\partial x_s} \to d_s$ in $L^2_{\mathrm{loc}}((\varsigma^i,\varsigma^{i+1})\times S;\mathbb{R}^3)$ for $s = 2,3$, $0 \leq i \leq \tilde{n}_{\mathrm{f}}$, and

$$\lim_{k\to\infty} kE^{(k)}(y^{(k)}) = E_{\mathrm{hb}}(\tilde{y},d_2,d_3).$$

The limit energy functional is given by

$$E_{\mathrm{hb}}(\tilde{y},d_2,d_3) = \begin{cases} \dfrac{1}{2}\displaystyle\int_0^L Q_3^{\mathrm{rel}}(R^\top\partial_{x_1}R)\mathrm{d}x_1 \\ \qquad + \sharp(S_{\tilde{y}} \cup S_R)\displaystyle\sum_{x'\in\mathcal{L}'} c_{\mathrm{W}}c_{\mathrm{cut}}(x') & \text{if } (\tilde{y},d_2,d_3) \in \mathcal{A}, \\ +\infty & \text{otherwise,} \end{cases}$$

where $R = (\partial_{x_1}\tilde{y}|d_2|d_3)$, $S_R = S_{\tilde{y}'} \cup S_{d_2} \cup S_{d_3}$, *and the class of admissible deformations* $\mathcal{A}$ *is defined as in Theorem 4.3. Here the relaxed quadratic form* $Q_3^{\mathrm{rel}}\colon \mathbb{R}^{3\times 3}_{\mathrm{skew}} \to [0,+\infty)$ *is*

$$Q_3^{\mathrm{rel}}(A) := \min_{\substack{\alpha\colon \mathcal{L}\to\mathbb{R}^3 \\ g\in\mathbb{R}^3}} \sum_{x'\in\mathcal{L}'} Q_{\mathrm{cell}}\Bigg(x', \frac{1}{2}\Bigg(A\begin{pmatrix}0\\x_2\\x_3\end{pmatrix} + g\Bigg)(-1,-1,-1,-1,1,1,1,1) + \frac{1}{4}A\begin{pmatrix}0&0&0&0&0&0&0&0\\1&1&-1&-1&-1&-1&1&1\\1&-1&-1&1&-1&1&1&-1\end{pmatrix} + (\bar{\nabla}^{2\mathrm{d}}\alpha|\bar{\nabla}^{2\mathrm{d}}\alpha)\Bigg) \quad (4.30)$$

with $Q_{\mathrm{cell}}(x',\cdot)$ *being the quadratic form associated with* $\nabla^2 W_0(x',\bar{\mathrm{Id}})$.

Remark 4.11. In the homogeneous case where c_{cut} is independent of the location $x' \in \mathcal{L}'$, the limiting crack energy $\sum_{x'\in\mathcal{L}'} c_{\mathrm{W}} c_{\mathrm{cut}}(x')$ reduces to $(\sharp\mathcal{L}')c_{\mathrm{W}}c_{\mathrm{cut}}$. This can be viewed as an explicit expression for the associated cell formula $\varphi(u,R)$ from the previous part of this chapter for $(u,R) \in \mathbb{R}^3 \times \mathrm{SO}(3) \setminus \{(0,\mathrm{Id})\}$.

The Γ-convergence is accompanied by a corresponding compactness theorem.

Theorem 4.10. *Suppose the sequence* $(y^{(k)})_{k=1}^{\infty}$ *of lattice deformations fulfils*

$$\limsup_{k\to\infty}\Big(kE^{(k)}(y^{(k)}) + \|y^{(k)}\|_{\ell^\infty(\Lambda_k;\mathbb{R}^3)}\Big) < +\infty \quad (4.31)$$

Then after applying the extension scheme from Subsection 4.1.2 we can find an increasing sequence $(k_j)_{j=1}^{\infty} \subset \mathbb{N}$, *functions* $\tilde{y} \in P\text{-}H^2(0,L;\mathbb{R}^3)$, $d_2, d_3 \in P\text{-}H^1(0,L;\mathbb{R}^3)$ *with* $R = (\partial_{x_1}\tilde{y}|d_2|d_3) \in \mathrm{SO}(3)$ *a.e., and a partition* $(\sigma^i)_{i=0}^{\bar{n}_{\mathrm{f}}+1}$ *of* $[0,L]$ *such that for any*

$$\eta \in \Big(0, \tfrac{1}{2}\min_{0\le i\le \bar{n}_f} |\sigma^{i+1} - \sigma^i|\Big)$$

and every $0 \le i \le \bar{n}_{\mathrm{f}}$ *we have:*

(i) $\tilde{y}^{(k_j)} \to \tilde{y}$ *in* $L^2(\Omega;\mathbb{R}^3)$ *and a.e. in* Ω;

(ii) $\nabla_{k_j}\tilde{y}^{(k_j)} \to R = (\partial_{x_1}\tilde{y}|d_2|d_3)$ *in* $L^2((\sigma^i+\eta, \sigma^{i+1}-\eta)\times S;\mathbb{R}^{3\times 3})$;

(iii) $W_0(x', \bar{\nabla}\hat{y}^{(k_j)}(kx_1,x')) \le c_{\mathrm{W}}(c_{\mathrm{cut}}^{(k_j)}(x'))^2$ *on* $(\sigma^i+\eta,\sigma^{i+1}-\eta)\times S$, *for j sufficiently large.*

Proof. Here a slice $S_k(x_1)$ is called *broken* if there is an $x' \in S$ such that

$$W_0\Big(x', \bar{\nabla}\hat{y}^{(k)}(kx_1,x')\Big) > c_{\mathrm{W}}\Big(c_{\mathrm{cut}}^{(k)}(x')\Big)^2.$$

This ensures that on any slice that is not broken, $W_{\mathrm{cell}}^{(k)}(x', \bar{\nabla}\hat{y}^{(k)}(kx_1,x'))$ remains in the elastic regime ($W_{\mathrm{cell}}^{(k)} = W_0$).

The rest of the proof is omitted due to its similarity with the procedure used for Theorem 4.2. □

4.6.3 Lower bound

In this subsection we show Theorem 4.9(i). We can assume that $\tilde{y}^{(k)} \to \tilde{y}$ in $L^2(\Omega;\mathbb{R}^3)$ and

$$\lim_{k\to\infty} kE^{(k)}(y^{(k)}) = \liminf_{k\to\infty} kE^{(k)}(y^{(k)}) < \infty.$$

Recall $(\sigma^i)_{i=0}^{\bar{n}_f+1}$ and $\nabla_{k_j}\tilde{y}^{(k_j)}$ from Theorem 4.9.

Let $\eta > 0$ be arbitrary, but strictly less than $\min_{0\le i\le \bar{n}_f} |\sigma^{i+1}-\sigma^i|$ (we will fix the precise value by Lemmas 4.11–4.12). If $j \ge j_0$ for j_0 large enough, then the regions $[\sigma^i+\eta, \sigma^{i+1}-\eta]\times S$, $0 \le i \le \bar{n}_f$, are not intersected by any broken slices. By results in the case without fracture (Theorem 3.5(i)), the bound

$$\lim_{k\to\infty} k \sum_{\substack{\hat{x}\in\hat{\Lambda}_k' \\ \hat{x}_1\in k[\sigma^i+\eta,\sigma^{i+1}-\eta]}} W_{\mathrm{cell}}^{(k)}\big(\hat{x}', \vec{y}^{(k)}(\hat{x})\big) \ge \frac{1}{2}\int_{\sigma^i+\eta}^{\sigma^{i+1}-\eta} Q_3^{\mathrm{rel}}(R^\top \partial_{x_1} R)\mathrm{d}x_1$$

holds true.

Now we turn to the crack contribution to the strain energy. For ease of notation, we write k in place of the double subscripts k_j. We have $S_{\tilde{y}} \cup S_R \subset \{\sigma^i\}_{i=1}^{\bar{n}_f}$, where $S_R := S_{\tilde{y}'} \cup S_{d_2} \cup S_{d_3}$. A lower bound on the energy at an arbitrary crack point $\sigma \in S_{\tilde{y}} \cup S_R$ will now be derived.

Case 1: $\sigma \in S_{\tilde{y}}$

As H^1 functions on bounded intervals are uniformly continuous, the limits $\tilde{y}(\sigma+) =: \tilde{y}^+$, $\tilde{y}(\sigma-) =: \tilde{y}^-$ exist and are finite. The goal is to prove that in each prism $(\sigma-\rho, \sigma+\rho)\times\tilde{Q}'$ with $\rho > 0$ and $\tilde{Q}' = x' + (-\frac{1}{2}, \frac{1}{2})^2$ for some $x' \in \mathcal{L}'$, there is a broken atomic cell for all large k's.

Take $x' \in \mathcal{L}'$ and $\tilde{Q}' = x' + (-\frac{1}{2}, \frac{1}{2})^2$.

Lemma 4.11. *For any $\gamma > 0$ there is $\rho > 0$ and $k_0 \in \mathbb{N}$ such that for all $k \ge k_0$ there exists $\tilde{Q} = (\frac{i}{k}, \frac{i+1}{k})\times\tilde{Q}'$ for some $i\in\mathbb{N}$, $\tilde{Q}\cap[(\sigma-\rho,\sigma+\rho)\times\tilde{Q}'] \neq \emptyset$, such that $|\bar{\nabla}_k \tilde{y}^{(k)}\big|_{\tilde{Q}}| > \gamma$.*

Proof. By Lemma 3.1, there exists $C_e > 0$ such that for any $\tilde{Q} = (i/k, (i+1)/k)\times\tilde{Q}'$, $i \in \{0,1,\ldots,\lfloor kL\rfloor\}$,

$$\frac{1}{|\tilde{Q}|}\int_{\tilde{Q}} |\nabla_k \tilde{y}^{(k)}(\xi)|^2 \mathrm{d}\xi \le C_e \left|\bar{\nabla}_k \tilde{y}^{(k)}\big|_{\tilde{Q}}\right|^2. \tag{4.32}$$

Given $\gamma > 0$, choose $0 < \varepsilon < |\tilde{y}^+ - \tilde{y}^-|/4$. Find $\rho > 0$ such that

$$2\sqrt{6C_e}\gamma < (|\tilde{y}^+ - \tilde{y}^-| - 4\varepsilon)/(2\rho), \text{ and}$$
$$\|\tilde{y}-\tilde{y}^+\|_{L^\infty(\sigma,\sigma+\rho;\mathbb{R}^3)} < \varepsilon,\ \|\tilde{y}-\tilde{y}^-\|_{L^\infty(\sigma-\rho,\sigma;\mathbb{R}^3)} < \varepsilon$$

by the uniform continuity of $\tilde{y}$ on one-sided neighbourhoods of σ. As stated in Theorem 4.10(i), we can suppose that $\tilde{y}^{(k)} \to \tilde{y}$ a.e. in Ω. This means that for some $a \in (\sigma-\rho,\sigma)\times S$, $b \in (\sigma,\sigma+\rho)\times S$, such that their orthogonal projections a',

b' onto $\{0\}\times S$ are equal, we have $\lim_{k\to\infty}\tilde{y}^{(k)}(b) = \tilde{y}(b)$ and $\lim_{k\to\infty}\tilde{y}^{(k)}(a) = \tilde{y}(a)$. Let $k_0 \in \mathbb{N}$ be such that for all $k \geq k_0$: $|\tilde{y}^{(k)}(b) - \tilde{y}(b)| < \varepsilon$ and $|\tilde{y}^{(k)}(a) - \tilde{y}(a)| < \varepsilon$. Then, by triangle inequality,

$$
\begin{aligned}
|\tilde{y}^+ - \tilde{y}^-| - 4\varepsilon &\leq |\tilde{y}(b) - \tilde{y}(a)| - |\tilde{y}^{(k)}(b) - \tilde{y}(b)| - |\tilde{y}^{(k)}(a) - \tilde{y}(a)| \\
&\leq |\tilde{y}^{(k)}(b) - \tilde{y}^{(k)}(a)| \leq \|\partial_{x_1}\tilde{y}^{(k)}\|_{L^\infty((\sigma-\rho,\sigma+\rho)\times\tilde{Q}';\mathbb{R}^3)}|b-a| \\
&\leq 2\|\nabla_k\tilde{y}^{(k)}\|_{L^\infty((\sigma-\rho,\sigma+\rho)\times\tilde{Q}';\mathbb{R}^{3\times3})}\rho
\end{aligned}
$$

so that

$$
\|\nabla_k\tilde{y}^{(k)}\|_{L^\infty((\sigma-\rho,\sigma+\rho)\times\tilde{Q}';\mathbb{R}^{3\times3})} \geq \frac{|\tilde{y}^+ - \tilde{y}^-| - 4\varepsilon}{2\rho} > 2\sqrt{6C_\mathrm{e}}\gamma. \tag{4.33}
$$

Inequality (4.33) implies that there is a cell $\tilde{Q} = (i/k, (i+1)/k) \times \tilde{Q}'$, with $i \in \mathbb{N}$, such that $\tilde{Q} \cap (\sigma - \rho, \sigma + \rho) \times \tilde{Q}' \neq \emptyset$, and a simplex $\breve{T} \subset \tilde{Q}$ on which $\nabla_k\tilde{y}^{(k)}$ is constant and

$$
\|\nabla_k\tilde{y}^{(k)}\|_{L^\infty((\sigma-\rho,\sigma+\rho)\times\tilde{Q}';\mathbb{R}^{3\times3})} = |\nabla_k\tilde{y}^{(k)}\big|_{\breve{T}}| > 2\sqrt{6C_\mathrm{e}}\gamma.
$$

Combining this with (4.32), we finally get

$$
\frac{(2\sqrt{6C_\mathrm{e}})^2}{24}\gamma^2 < \frac{1}{24k}k|\nabla_k\tilde{y}^{(k)}\big|_{\breve{T}}|^2 \leq k\int_{\tilde{Q}} |\nabla_k\tilde{y}^{(k)}(\xi)|^2 \mathrm{d}\xi \leq C_\mathrm{e}\left|\bar{\nabla}_k\tilde{y}^{(k)}\big|_{\tilde{Q}}\right|^2. \qquad \square
$$

If we let $\gamma := r_{\bar{\mathrm{SO}}(3)} + \gamma_0$, where the radius $r_{\bar{\mathrm{SO}}(3)} := |\bar{\mathrm{Id}}| = \sqrt{6}$ and $\gamma_0 \geq \max_{x'} c^{(k)}_{\mathrm{cut}}(x')$ for all sufficiently large values of k, then the cell $\hat{Q} = (i, i+1) \times \tilde{Q}'$ is deformed inelastically, as $\mathrm{dist}(\bar{\nabla}\hat{y}^{(k)}\big|_{\hat{Q}}, \bar{\mathrm{SO}}(3)) \geq c^{(k)}_{\mathrm{cut}}(x')$.

Case 2: $\sigma \in S_R$

The function $\tilde{y}$ is continuous at σ and the restriction of $(\partial_{x_1}\tilde{y}|d_2|d_3)$ to a left (or right) neighbourhood of σ is H^1, so there are finite limits $(\partial_{x_1}\tilde{y}|d_2|d_3)(\sigma+) =: R^+ \in \mathrm{SO}(3)$ and $(\partial_{x_1}\tilde{y}|d_2|d_3)(\sigma-) =: R^- \in \mathrm{SO}(3)$. We claim that again, there is a broken cell in any prism $(\sigma - \rho, \sigma + \rho) \times \tilde{Q}'$ if $k \geq k_0$. Consider $x' \in \mathcal{L}'$ and $\tilde{Q}' = x' + (-\frac{1}{2}, \frac{1}{2})^2$.

Lemma 4.12. *There is $\rho > 0$ and $k_0 \in \mathbb{N}$ such that for all $k \geq k_0$ there exists $\tilde{Q} = (\frac{i}{k}, \frac{i+1}{k}) \times \tilde{Q}'$ for some $i \in \mathbb{N}$, $\tilde{Q} \cap [(\sigma - \rho, \sigma + \rho) \times \tilde{Q}'] \neq \emptyset$, such that*

$$
\mathrm{dist}(\bar{\nabla}\hat{y}^{(k)}\big|_{\hat{Q}}, \bar{\mathrm{SO}}(3)) \geq c^{(k)}_{\mathrm{cut}}(x'),
$$

where $\hat{Q} = (i, i+1) \times \tilde{Q}'$.

Proof. We proceed by contradiction. Fix $\rho > 0$ small enough and construct a subsequence, denoted again by $\tilde{y}^{(k)}$, such that for all $\tilde{Q}$ as in the statement, the discrete gradients are close to $\bar{\mathrm{SO}}(3)$: $\mathrm{dist}(\bar{\nabla}\hat{y}^{(k)}\big|_{\hat{Q}}, \bar{\mathrm{SO}}(3)) < \mathrm{c}^{(\mathrm{k})}_{\mathrm{cut}}(\mathrm{x}')$. This means that

$$
\begin{aligned}
W^{(k)}_{\mathrm{cell}}(x', \bar{\nabla}_k\tilde{y}^{(k)}(x)) &= \min\left\{W_0(x', \bar{\nabla}_k\tilde{y}^{(k)}(x)), c_\mathrm{W}[c^{(k)}_{\mathrm{cut}}(x')]^2\right\} \\
&\geq c_\mathrm{W}\mathrm{dist}^2(\bar{\nabla}_k\tilde{y}^{(k)}(x), \bar{\mathrm{SO}}(3))
\end{aligned}
$$

on any such cell $\tilde{Q}$. For the total energy in this region we get

$$C \geq k \sum_{\substack{(x_1,x')\in\tilde{\Lambda}_k' \\ \tilde{Q}(x_1,x')\cap[(\sigma-\rho,\sigma+\rho)\times\tilde{Q}']\neq\emptyset}} W_{\mathrm{cell}}^{(k)}(x',\bar{\nabla}_k\tilde{y}^{(k)}(x))$$

$$\geq k^2 c_{\mathrm{W}} \int_{(\sigma-\rho,\sigma+\rho)\times\tilde{Q}'} \mathrm{dist}^2(\nabla_k\tilde{y}^{(k)}(\xi),\mathrm{SO}(3))\mathrm{d}\xi,$$

setting $\tilde{Q}(x_1,x') = (x_1 - \frac{1}{2k}, x_1 + \frac{1}{2k}) \times \tilde{Q}'$ and using an estimate for the distance to $\bar{\mathrm{SO}}(3)$ [Sch09, Lemma 3.6]. Hence, we deduce that

$$\int_{(\sigma-\rho,\sigma+\rho)\times\tilde{Q}'} \mathrm{dist}^2(\nabla_k\tilde{y}^{(k)},\mathrm{SO}(3))\mathrm{d}x \leq \frac{C}{k^2}.$$

Now as in Theorem 3.4, a further subsequence $(\nabla_k\tilde{y}^{(k)})$ is obtained which L^2-converges to $\tilde{R} \in H^1((\sigma-\rho,\sigma+\rho);\mathbb{R}^{3\times3})$. But this contradicts the fact that the point σ lies in S_R. □

After we have chosen a suitable $\gamma > 0$ in Lemma 4.11 and picked the smaller ρ from Lemmas 4.11–4.12, we let $\eta := \rho$ and sum up the elastic and crack energy contributions:

$$kE^{(k)}(y^{(k)}) = k\sum_{i=0}^{\bar{n}_{\mathrm{f}}}\Bigg[\sum_{\substack{\hat{x}\in\hat{\Lambda}_k' \\ \hat{x}_1-\frac{1}{2k}\geq\sigma^i+\rho,\,\hat{x}_1+\frac{1}{2k}\leq\sigma^{i+1}-\rho}} W_{\mathrm{cell}}^{(k)}\Big(\hat{x}',\vec{y}^{(k)}(\hat{x})\Big) + \sum_{\substack{\hat{x}\in\hat{\Lambda}_k' \\ \hat{Q}(\hat{x})\cap k(\sigma^i-\rho,\sigma^i+\rho)\times S\neq\emptyset}} W_{\mathrm{cell}}^{(k)}\Big(\hat{x}',\vec{y}^{(k)}(\hat{x})\Big)\Bigg]$$

$$\geq \sum_{i=0}^{\bar{n}_{\mathrm{f}}}\Bigg[\sum_{\substack{\hat{x}\in\hat{\Lambda}_k',\,\hat{x}_1-\frac{1}{2k}\geq\sigma^i+\rho, \\ \hat{x}_1+\frac{1}{2k}\leq\sigma^{i+1}-\rho}} kW_{\mathrm{cell}}^{(k)}\Big(\hat{x}',\vec{y}^{(k)}(\hat{x})\Big) + k\sharp(S_{\tilde{y}}\cup S_R)\sum_{x'\in\mathcal{L}'} c_{\mathrm{W}}\Big(c_{\mathrm{cut}}^{(k)}(x')\Big)^2\Bigg].$$

If $k\to\infty$, we get

$$\lim_{k\to\infty} kE^{(k)}(y^{(k)}) \geq \Bigg[\sum_{i=0}^{\bar{n}_{\mathrm{f}}}\frac{1}{2}\int_{\sigma^i+\rho}^{\sigma^{i+1}-\rho} Q_3^{\mathrm{rel}}(R^\top\partial_{x_1}R)\mathrm{d}x_1 + \sharp(S_{\tilde{y}}\cup S_R)\sum_{x'\in\mathcal{L}'} c_{\mathrm{W}}c_{\mathrm{cut}}(x')\Bigg].$$

The Γ-liminf inequality is established by letting $\rho\to 0+$.

4.6.4 Upper bound

Proof of Theorem 4.9(ii). We show $\limsup_{k\to\infty} kE^{(k)}(y^{(k)}) \leq E_{\mathrm{hb}}(y,d_2,d_3)$ for a suitably defined sequence $(y^{(k)})$. Suppose $(\tilde{y},d_2,d_3)\in\mathcal{A}$ and that $(\sigma^i)_{i=0}^{\bar{n}_{\mathrm{f}}+1}$ is the partition of $[0,L]$ such that $\{\sigma^i\}_{i=1}^{\bar{n}_{\mathrm{f}}} = S_{\tilde{y}}\cup S_R$, where $S_R := S_{\tilde{y}'}\cup S_{d_2}\cup S_{d_3}$.

As in Subsection 4.5.2, we first suppose that $\tilde{y}\big|_{(\sigma^{i-1},\sigma^i)} \in \mathcal{UC}^3((\sigma^{i-1},\sigma^i);\mathbb{R}^3)$, $d_2\big|_{(\sigma^{i-1},\sigma^i)}, d_3\big|_{(\sigma^{i-1},\sigma^i)} \in \mathcal{UC}^2((\sigma^{i-1},\sigma^i);\mathbb{R}^3)$ for all $i \in \{1,\dots,\bar{n}_\mathrm{f}+1\}$. For $k \in \mathbb{N}$ we also set $I_0^k := [0, \frac{1}{k}\lfloor k\sigma^1 \rfloor]$, $I_i^k := [\frac{1}{k}\lfloor k\sigma^i \rfloor + \frac{1}{k}, \frac{1}{k}\lfloor k\sigma^{i+1}\rfloor]$ for $i = 1,2,\dots,\bar{n}_\mathrm{f}-1$ and $I_{\bar{n}_\mathrm{f}}^k := [\frac{1}{k}\lfloor k\sigma^{\bar{n}_\mathrm{f}}\rfloor + \frac{1}{k}, L_k]$. Then define the sequence of lattice deformations

$$\tilde{y}^{(k)}(x) := \tilde{y}(x_1) + \frac{1}{k}x_2 d_2(x_1) + \frac{1}{k}x_3 d_3(x_1) + \frac{1}{k}q(x_1) + \frac{1}{k^2}\beta(x), \quad x \in \tilde{\Lambda}_k \cap \Big([0,L]\cap S\Big),$$

where $\beta\colon [0,L]\times\mathcal{L} \to \mathbb{R}^3$ with $\beta(\cdot,x')$ of class $\mathcal{C}^1$ on $[0,L]$ and $q \in \mathcal{C}^2([0,L];\mathbb{R}^3)$ will be used to approximate the minimizers of problem (4.9) as before. On the set $\overline{\Omega}\setminus\tilde{\Lambda}_k$, we extend and interpolate the sequence $\tilde{y}^{(k)}$ in the same way as in Sections 4.1 and 3.3.4 so that $\tilde{y}^{(k)}$ is piecewise affine on $\overline{\Omega}$.

The sequence $\tilde{y}^{(k)}$ satisfies, for every $i = 0,1,\dots,\bar{n}_\mathrm{f}$,

$$\|\bar{\nabla}_k\tilde{y}^{(k)} - R(\cdot)\bar{\mathrm{Id}}\|_{L^\infty(I_i^k\times S;\mathbb{R}^{3\times 8})} = O\left(\frac{1}{k}\right)$$

by Taylor expanding the functions $\tilde{y}$, d_2, d_3, q, and β as in Chapter 3.

Thus

$$\mathrm{dist}(\bar{\nabla}_k\tilde{y}^{(k)}\big|_{I_i^k\times S}, \bar{\mathrm{SO}}(3)) \le \sqrt{\frac{c_\mathrm{W}}{c_\mathrm{w}}}c_\mathrm{cut}^{(k)}$$

for all k large enough, as $c_\mathrm{cut}^{(k)} = O(\frac{1}{\sqrt{k}})$, so we can treat each segment $I_i^k\times S$, $i = 0,1,\dots,\bar{n}_\mathrm{f}$, as purely elastic. By the already proved results, we get

$$k\sum_{i=0}^{\bar{n}_\mathrm{f}}\sum_{\substack{\hat{x}\in\hat{\Lambda}_k' \\ \hat{x}_1\in kI_i^k}} W_\mathrm{cell}^{(k)}\Big(x', \vec{y}^{(k)}(\hat{x})\Big) \to \frac{1}{2}\sum_{i=0}^{\bar{n}_\mathrm{f}}\int_{\sigma^i}^{\sigma^{i+1}}\int_S Q_\mathrm{cell}\Bigg(x', R^\top\frac{\partial R}{\partial x_1}\begin{pmatrix}0\\ \bar{x}_2\\ \bar{x}_3\end{pmatrix}(e^1)^\top\vec{\bar{z}}+$$

$$+\frac{1}{4}\begin{pmatrix}-\kappa_2-\kappa_3 & \kappa_3-\kappa_2 & \kappa_2+\kappa_3 & \kappa_2-\kappa_3 & \kappa_2+\kappa_3 & \kappa_2-\kappa_3 & -\kappa_2-\kappa_3 & \kappa_3-\kappa_2\\ -\tau & \tau & \tau & -\tau & \tau & -\tau & -\tau & \tau\\ \tau & \tau & -\tau & -\tau & -\tau & -\tau & \tau & \tau\end{pmatrix}+$$

$$+R^\top\frac{\partial q}{\partial x_1}(x_1)(e^1)^\top\bar{\mathrm{Id}} + R^\top(\bar{\nabla}^{2\mathrm{d}}\beta(x)|\bar{\nabla}^{2\mathrm{d}}\beta(x))\Bigg)\mathrm{d}x'\mathrm{d}x_1.$$

Near the crack points, regardless of the specific values of $W_\mathrm{cell}^{(k)}$, we have

$$\limsup_{k\to\infty} k\sum_{i=1}^{\bar{n}_\mathrm{f}}\sum_{\substack{\hat{x}\in\hat{\Lambda}_k' \\ \hat{x}_1=\lfloor k\sigma^i\rfloor+\frac{1}{2}}} W_\mathrm{cell}^{(k)}\Big(\hat{x}', \vec{y}^{(k)}(\hat{x})\Big) \le \sharp(S_{\tilde{y}}\cup S_R)\sum_{x'\in\mathcal{L}'} c_\mathrm{W}c_\mathrm{cut}.$$

Repeating the diagonalization as at the end of the proof in the purely elastic case, we reach the conclusion that

$$\limsup_{k\to\infty} kE^{(k)}(y^{(k)}) \le E_\mathrm{hb}(\tilde{y}, d_2, d_3). \qquad \square$$

4.7 Examples

Finally, we list a few examples of mass-spring models treatable by our methods: a model with rather general pair interactions, the so-called truncated and shifted Lennard-Jones potential (LJTS), and a simplified model with 'truncated harmonic springs'.

Example 4.1. We can consider, as general nearest-neighbour (NN) and next-to-nearest-neighbour (NNN) interactions on a cubic lattice,

$$E^{(k)}(y) = \frac{1}{2}\sum_{\substack{\hat{x}_*,\hat{x}_{**}\in\hat{\Lambda}_k\\ |\hat{x}_*-\hat{x}_{**}|=1}} W_{\mathrm{NN}}^{(k)}(|\hat{y}(\hat{x}_*)-\hat{y}(\hat{x}_{**})|)+\frac{1}{2}\sum_{\substack{\hat{x}_*,\hat{x}_{**}\in\hat{\Lambda}_k\\ |\hat{x}_*-\hat{x}_{**}|=\sqrt{2}}} W_{\mathrm{NNN}}^{(k)}\Big(\frac{|\hat{y}(\hat{x}_*)-\hat{y}(\hat{x}_{**})|}{\sqrt{2}}\Big)+\mathcal{X}_k(y), \tag{4.34}$$

where $y\colon \Lambda_k \to \mathbb{R}^3$, $\hat{y}(\hat{x}) = ky(\frac{1}{k}\hat{x})$, $\hat{x}\in\hat{\Lambda}_k$, and $W_{\mathrm{NN}}^{(k)}$, $W_{\mathrm{NNN}}^{(k)}$ satisfy the following list of assumptions:¨

(P1) $W_{\mathrm{NN(N)}}^{(k)}\colon [0,\infty)\to[0,\infty]$ is continuous and finite on $(0,\infty)$ and $W_{\mathrm{NN(N)}}^{(k)}(r)= 0$ if and only if $r=1$;

(P2) there is a sequence $(c_{\mathrm{f}}^{(k)})_{k=1}^{\infty}$ with $c_{\mathrm{f}}^{(k)}\searrow 0$ and $\lim_{k\to\infty} k[c_{\mathrm{f}}^{(k)}]^2\in(0,\infty)$ such that

$$W_{\mathrm{NN(N)}}^{(k)}(r) = W_{0\mathrm{NN(N)}}(r)$$

for all $r\in(1-c_{\mathrm{f}}^{(k)},1+c_{\mathrm{f}}^{(k)})$, where $W_{0\mathrm{NN(N)}}$ is of class $\mathcal{C}^2$ and $W''_{0NN(N)}(1)>0$;

(P3) $W_{\mathrm{NN(N)}}^{(k)}(r) = \bar{W}_{\mathrm{NN(N)}}^{(k)}(r)$ if $r\in[0,1-c_{\mathrm{f}}^{(k)}]\cup[1+c_{\mathrm{f}}^{(k)},\infty)$; the function $\bar{W}_{\mathrm{NN(N)}}^{(k)}$ is bounded from below by $\bar{c}_{\mathrm{NN(N)}}^{(k)}$ such that $k\bar{c}_{\mathrm{NN(N)}}^{(k)}\to\bar{c}_{\mathrm{NN(N)}}>0$ and $(k+1)W_{\mathrm{NN(N)}}^{(k+1)}\geq kW_{\mathrm{NN(N)}}^{(k)}$ for every $k\in\mathbb{N}$;

(P4) $\bar{W}_{\mathrm{NN(N)}}^{(k)}(r) = \omega_{\mathrm{NN(N)}}^{(k)}+\frac{1}{k}\nu_{\mathrm{NN(N)}}(r)$ if $r\geq k\bar{M}_k$ for $\bar{M}_k\to 0$ with $k\bar{M}_k\to\infty$, $\nu_{\mathrm{NN(N)}}(r)=O(r^{-1})$, $r\to\infty$, and $\lim_{k\to\infty}k\omega_{\mathrm{NN(N)}}^{(k)}\in(0,\infty)$.

To guarantee preservation of orientation, in (4.34) we have included a nonnegative term $\mathcal{X}_k(y)$ that gives rise to $\chi^{(k)}$ below. Thus $E^{(k)}$ can be written in the form (4.2) as a sum of cell energies with

$$W_{\mathrm{cell}}^{(k)}(\vec{y}) = \frac{1}{8}\sum_{|z^i-z^j|=1} W_{\mathrm{NN}}^{(k)}(|\hat{y}_i-\hat{y}_j|)+\frac{1}{4}\sum_{|z^i-z^j|=\sqrt{2}} W_{\mathrm{NNN}}^{(k)}\Big(\frac{|\hat{y}_i-\hat{y}_j|}{\sqrt{2}}\Big)+\chi^{(k)}(\vec{y}) \tag{4.35}$$

for $\vec{y}=(\hat{y}_1|\cdots|\hat{y}_8)\in\mathbb{R}^{3\times 8}$ and the functions $W_{\mathrm{surf}}^{(k)}$, $W_{\mathrm{end}}^{(k)}$ constructed in a similar manner to account for surface contributions to atomic bonds lying on the rod's boundary (see Subsection 3.2.3). The frame-indifferent term $\chi^{(k)}$, $C/k\geq\chi^{(k)}\geq 0$, penalizes deformations that are not locally orientation-preserving, i.e. it is greater than or equal to $\bar{c}/k$, $\bar{c}>0$, on a k-independent neighbourhood of $\mathrm{O}(3)\bar{\mathrm{Id}}\setminus\mathrm{S}\bar{\mathrm{O}}(3)$ and vanishes otherwise (see [Sch06, FS15a]). An alternative to penalties such as $\mathcal{X}_k$ and $\chi^{(k)}$ is cell energies with O(3)-invariance, see Remark 3.12 or [BS22, Section 2.4].

It can be shown that potentials $W_{\mathrm{NN}}^{(k)}$, $W_{\mathrm{NNN}}^{(k)}$ as above make the corresponding $W_{\mathrm{cell}}^{(k)}$ admissible, i.e. (W1)–(W6), and (W9) hold ((W9) is a consequence of (P4)). In particular, the *truncated and splined Lennard-Jones potential* from [HE83] and versions thereof fall under this case, with appropriately chosen parameters.

Example 4.2. Let

$$W_{\mathrm{LJ}}(r) = d\left(\frac{1}{r^{12}} - \frac{2}{r^6}\right) + d,$$

where $r \in (0,\infty)$ and $d > 0$ is a parameter (note that $\lim_{r\to\infty} W_{\mathrm{LJ}}(r) = d$ and $\mathrm{argmin}_{r>0}\, W_{\mathrm{LJ}}(r) = 1$). Further we set

$$W_{\mathrm{LJTS}}^{(k)}(r) = \begin{cases} W_{\mathrm{LJ}}(r) & r \in (0,1) \\ \min\{W_{\mathrm{LJ}}(r), \frac{1}{k}\} & r \in [1,\infty) \end{cases}.$$

We again consider pair interactions, so the cell energy function takes the form (4.35) with $W_{\mathrm{LJTS}}^{(k)}$ in place of $W_{\mathrm{NN}}^{(k)}$ and $W_{\mathrm{NNN}}^{(k)}$. The property $(k+1)W_{\mathrm{cell}}^{(k+1)} \geq kW_{\mathrm{cell}}^{(k)}$ can be proved by discussing for each bond if it is deformed elastically or if the truncation is active. Computing the value of r beyond which truncation applies in $W_{\mathrm{LJTS}}^{(k)}$, we observe that assumptions (W3) and (W5) hold with $c_{\mathrm{frac}}^{(k)} = [\sqrt[6]{d+\sqrt{d/k}} - \sqrt[6]{d-(1/k)}]/(2\sqrt[6]{d-(1/k)})$ and W_0 being the sum of Lennard-Jones interactions with no truncation. By the properties of $\nabla^2 W_0(\bar{\mathrm{Id}})$, the estimate $\hat{C}W_0(\vec{y}) \geq \mathrm{dist}^2(\bar\nabla\hat{y}, \mathrm{SO}(3))$ holds with a constant $\hat{C} > 0$ and the usual symbol $\bar\nabla\hat{y}$ denoting the discrete gradient of $\vec{y} \in \mathbb{R}^{3\times 8}$ (cf. [Sch06, Lemma 3.2 and Section 7]).

Moreover, we claim that if $\mathrm{dist}(\bar\nabla\hat{y}, \bar{\mathrm{SO}}(3)) > c_{\mathrm{frac}}^{(k)}$, then $W_{\mathrm{cell}}^{(k)}(\vec{y}) \geq \min\{1/(8k), [c_{\mathrm{frac}}^{(k)}]^2/\hat{C}\} =: \bar{c}_1^{(k)}$. Indeed, as long as $W_{\mathrm{cell}}^{(k)}(\vec{y}) < \bar{c}_1^{(k)}$, the cutoff is not active in any interatomic bond (the arguments of $W_{\mathrm{LJTS}}^{(k)}$ are close enough to 1) and thus $W_{\mathrm{cell}}^{(k)}(\vec{y}) = W_0(\vec{y})$ so that $\mathrm{dist}(\bar\nabla\hat{y}, \bar{\mathrm{SO}}(3)) \leq c_{\mathrm{frac}}^{(k)}$. This shows the second part of assumption (W5).

Example 4.3. For the functions

$$W_{\mathrm{harm}}(r) = K(r-1)^2, \quad W_{\mathrm{TH}}^{(k)}(r) = \begin{cases} \min\{W_{\mathrm{harm}}(r), \frac{c_{\mathrm{TH}}^+}{k}\} & r \geq 1 \\ \min\{W_{\mathrm{harm}}(r), \frac{c_{\mathrm{TH}}^-}{k}\} & r < 1 \end{cases}$$

with positive constants K, c_{TH}^-, c_{TH}^-, one can similarly find $c_{\mathrm{frac}}^{(k)}$ and $\bar{c}_1^{(k)}$ so that $W_{\mathrm{cell}}^{(k)}$ defined by (4.35) with $W_{\mathrm{NN}}^{(k)}$ and $W_{\mathrm{NNN}}^{(k)}$ replaced by $W_{\mathrm{TH}}^{(k)}$ is an admissible cell energy.

4.8 Explicit calculation of crack energy

For mass-spring models, it is possible to simplify further (4.11) in specific situations.

Proposition 4.13. *If $E^{(k)}$ is given by* (4.34) *and assumptions* (P1)–(P4) *hold, together with*

(P5) $\lim_{k\to\infty} k\bar{W}^{(k)}_{\mathrm{NN(N)}}(r_k) = \omega_{\mathrm{NN(N)}}$ *for any sequence* $r_k \to \infty$,

for $W^{(k)}_{\mathrm{NN}}$ *and* $W^{(k)}_{\mathrm{NNN}}$, *then*

$$\varphi(u,R) = (\sharp\mathcal{L})\omega_{\mathrm{NN}} + \sharp\{(x',x'_*) \in \mathcal{L}^2;\ |x'-x'_*| = 1\}\omega_{\mathrm{NNN}}$$

for any $0 \neq u \in \mathbb{R}^3$ *and* $R \in \mathrm{SO}(3)$.

Proof. *Step* 1. The mapping $v^{(k)}$ defined as

$$v^{(k)}(w_1,x') = \begin{cases} R^{(k)}_-(r_k w_1, \frac{1}{k}x')^\top + y^{(k)}_- & \text{on } [-1,0]\times S^{\mathrm{ext}} \\ R^{(k)}_+(r_k w_1, \frac{1}{k}x')^\top + y^{(k)}_+ & \text{on } [r_k^{-1}k^{-1},1]\times S^{\mathrm{ext}}, \end{cases}$$

$$R^{(k)}_\pm \in \mathrm{SO}(3),\ y^{(k)}_\pm \in \mathbb{R}^3,\ (R^{(k)}_-)^{-1}R^{(k)}_+ \to R,\ y^{(k)}_+ - y^{(k)}_- \to u;\ r_k^{-1} \to \infty \text{ as } o(k),$$

and interpolated to be piecewise affine ($v^{(k)} \in \mathrm{PAff}(\Lambda_{r_k,k})$) has the property that

$$\lim_{k\to\infty} \mathcal{E}_k(v^{(k)},[-1,1]) = (\sharp\mathcal{L})\omega_{\mathrm{NN}} + \sharp\{(x',x'_*) \in \mathcal{L}^2;\ |x'-x'_*| = 1\}\omega_{\mathrm{NNN}}.$$

Thus we find that $\varphi(u,R)$ is less than or equal to the right-hand side in the above equation.

Step 2. Given $\varepsilon > 0$, we find sequences $((r_k)_{k=1}^\infty, (k)_{k=1}^\infty, (y^{(k)})_{k=1}^\infty) \in \mathcal{V}_{u,R}$ such that

$$\limsup_{k\to\infty} \mathcal{E}_k(y^{(k)},[-1,1]) \le \varphi(u,R) + \varepsilon, \tag{4.36}$$

using Proposition 4.7. Set

$$\bar{W}^{(k)}_1 := \frac{1}{r_k k}\left\{\lfloor -r_k k\rfloor + \frac{3}{2}, \lfloor -r_k k\rfloor + \frac{5}{2}, \ldots, \lfloor r_k k\rfloor - \frac{1}{2}\right\}.$$

We show that the nature of our pair interactions causes at least one large gap in the spacing of atoms within each fibre which the rod consists of.

Claim 1: For each $x' \in \mathcal{L}$ and every $T > 1$ there is a $k_0 \in \mathbb{N}$ such that whenever $k \ge k_0$, we can find some $\bar{w}_1 \in \bar{W}^{(k)}_1$ satisfying

$$\frac{|y^{(k)}(\bar{w}_1 + \frac{1}{2r_k k}, x') - y^{(k)}(\bar{w}_1 - \frac{1}{2r_k k}, x')|}{1/k} > T.$$

Proof of claim: If the converse were true, there would be a $\tilde{T} > 1$ and an increasing sequence $\{k_n\}_{n=1}^\infty \subset \mathbb{N}$ such that for all $\bar{w}_1 \in \bar{W}^{(k_n)}_1$:

$$k_n|y^{(k_n)}(\bar{w}_1 + \frac{1}{2r_{k_n}k_n}, x') - y^{(k_n)}(\bar{w}_1 - \frac{1}{2r_{k_n}k_n}, x')| \le \tilde{T}.$$

Then we would get

$$\begin{aligned} 0 \neq |u| &= \left|y^{(k_n)}(\max \bar{W}^{(k_n)}_1 + \frac{1}{2r_{k_n}k_n}, x') - y^{(k_n)}(\min \bar{W}^{(k_n)}_1 - \frac{1}{2r_{k_n}k_n}, x')\right| + o_{n\to\infty}(1) \\ &\le \sum_{\bar{w}_1 \in \bar{W}^{(k_n)}_1} \left|y^{(k_n)}(\bar{w}_1 + \frac{1}{2r_{k_n}k_n}, x') - y^{(k_n)}(\bar{w}_1 - \frac{1}{2r_{k_n}k_n}, x')\right| + o_{n\to\infty}(1) \\ &\le 2r_{k_n}\frac{k_n}{k_n}\tilde{T} + o_{n\to\infty}(1) \to 0, \end{aligned}$$

which is a contradiction.

Step 3. A similar argument applies to NNN bonds ('diagonal springs') – if we use zigzag chains of atoms instead of straight atomic fibres. We state the corresponding claim without proof.

Claim $\sqrt{2}$: For each $(x', x'_*) \in \mathcal{L} \times \mathcal{L}$ with $|x'_* - x'| = 1$ and every $T > 1$ there is a $k_0 \in \mathbb{N}$ such that whenever $k \geq k_0$, we can find a $j \in \mathbb{N}$ and $\bar{w}_1 = \frac{1}{r_k k}(\lfloor -r_k k \rfloor + \frac{2j+1}{2}) \in \bar{W}_1^{(k)}$ such that $y^{(k)}$ from (4.36) satisfies:

$$\frac{|y^{(k)}(\bar{w}_1 + (-1)^{j+1}\frac{1}{2r_k k}, x'_*) - y^{(k)}(\bar{w}_1 + (-1)^{j}\frac{1}{2r_k k}, x')|}{\sqrt{2}/k} > T.$$

Step 4. Since Claims 1 and $\sqrt{2}$ hold for every approximating sequence $(y^{(k)})_{k=1}^{\infty}$ fulfilling (4.36), we get

$$(\sharp\mathcal{L})\omega_{\mathrm{NN}} + \sharp\{(x', x'_*) \in \mathcal{L}^2;\ |x' - x'_*| = 1\}\omega_{\mathrm{NNN}} \leq \varphi(u, R) + \varepsilon.$$

As this is valid for any $\varepsilon > 0$, the desired conclusion follows. □

Proposition 4.14. *Under the assumptions of Proposition 4.13 and further supposing*

(P6) $W_{\mathrm{NN}}^{(k)}$, $W_{\mathrm{NNN}}^{(k)}$ *are nondecreasing on* $[1, \infty)$,

we have

$$0 < \varphi(0, R) < \varphi(u, \tilde{R})$$

for any $R, \tilde{R} \in \mathrm{SO}(3)$, $R \neq \mathrm{Id}$ *and* $0 \neq u \in \mathbb{R}^3$.

Proof. The first inequality was shown in Remark 4.5.

As to the second inequality, Proposition 4.13 implies that for a nonzero u, the crack energy $\varphi(u, R)$ is independent of R, hence we limit ourselves to the case $\tilde{R} = R$ without loss of generality. If $R \in \mathrm{SO}(3)$ and $u \in \mathbb{R}^3 \setminus \{0\}$ are fixed, it is enough to find a sequence $(v_0^{(k)})_{k=1}^{\infty}$ of deformations admissible in the definition of $\varphi(0, R)$ such that

$$\limsup_{k\to\infty} \mathcal{E}_k(v_0^{(k)}; [-1, 1]) < (\sharp\mathcal{L})\omega_{\mathrm{NN}} + \sharp\{(x', x'_*) \in \mathcal{L}^2;\ |x' - x'_*| = 1\}\omega_{\mathrm{NNN}}$$

by Proposition 4.13. Fix $k \in \mathbb{N}$ and let $v^{(k)}$, $R_{\pm}^{(k)}$, r_k, and $y_{\pm}^{(k)}$ be as in the proof of Proposition 4.13 with our new definitions of R and u. We define

$$F^{\pm} := \left\{R_{\pm}^{(k)}\Big(\frac{1}{2k} \pm \frac{1}{2k}, \frac{1}{k}x'\Big)^{\top} + y_{\pm}^{(k)};\ x' \in \mathcal{L}\right\}$$

and observe that $\mathrm{dist}(F^+, F^-) = |y_+^{(k)} - y_-^{(k)}| + O(\frac{1}{k}) = |u| + o_{k\to\infty}(1)$. Now we choose $x'_0 \in \mathcal{L}$ and consider configurations with shifted right parts, given by

$$v^{(k)}(w_1, x'; t) = \begin{cases} R_-^{(k)}(r_k w_1, \frac{1}{k}x')^{\top} + y_-^{(k)} & \text{on } [-1, 0] \times S^{\mathrm{ext}} \\ R_+^{(k)}(r_k w_1, \frac{1}{k}x')^{\top} + y_+^{(k)} - c_0^{(k)}(t) & \text{on } [r_k^{-1}k^{-1}, 1] \times S^{\mathrm{ext}}, \end{cases}$$

where $c_0^{(k)}(t) = t[v^{(k)}(\frac{1}{r_k k}, x_0') - v^{(k)}(0, x_0')]$, $t \in [0,1]$. We then define $t_0^{(k)}$ to be the smallest $t \in [0,1]$ such that

$$\Big|v^{(k)}\Big(\frac{1}{r_k k}, x'; t\Big) - v^{(k)}(0, x'; t)\Big| = \frac{1}{k} \qquad \text{or} \qquad \Big|v^{(k)}\Big(\frac{1}{r_k k}, x_*'; t\Big) - v^{(k)}(0, x_{**}'; t)\Big| = \frac{\sqrt{2}}{k}$$

for some $x' \in \mathcal{L}$, or else, $x_*', x_{**}' \in \mathcal{L}$ with $|x_*' - x_{**}'| = 1$, respectively. By construction such $t_0^{(k)} \in (0,1)$ exists if k is large enough and we have $|c_0^{(k)}(t_0^{(k)}) - u| \to 0$ as $k \to \infty$. Setting $v_0^{(k)} = v^{(k)}(\,\cdot\,; t_0^{(k)})$ and recalling (P6) we find

$$\mathcal{E}_k(v_0^{(k)}; [-1,1]) \le (\sharp\mathcal{L})\omega_{\mathrm{NN}} + \sharp\{(x', x_*') \in \mathcal{L}^2;\ |x' - x_*'| = 1\}\omega_{\mathrm{NNN}} - \min\{\omega_{\mathrm{NN}}, \omega_{\mathrm{NNN}}\}. \tag{4.37}$$

We still need to check that the sequence $(v_0^{(k)})_{k=1}^{\infty}$ thus constructed satisfies the correct boundary conditions for $\varphi(0,R)$. But this is clear, since $|y_+^{(k)} - c_0^{(k)}(t_0^{(k)}) - y_-^{(k)}| \to 0$. □

Conclusion and outlook

The main goal this thesis was to derive continuum-mechanical theories for thin rods by performing a dimension reduction and a many-particle limit at the same time. If the frame-invariant discrete energies grow quadratically (Chapter 3), purely elastic models are obtained in the Γ-limit, whereas for interaction potentials with suitably scaled far-field asymptotic values (Chapter 4), the effective strain energy functional also includes a term related to cracks and kinks in the rod. In this way the present work makes a contribution to the modelling of elastic-brittle ultrathin structures, but as such, it could be certainly extended in various directions.

It should be also possible to apply the techniques seen in Chapter 3 to energies scaled by a higher power of the rod thickness, namely $\frac{1}{k^3 h_k^6} E^{(k)}$ instead of $\frac{1}{k h_k^4} E^{(k)}$. The expected Γ-limits would correspond to thin and ultrathin rod theories similar to the von-Kármán theory of plates (see [MM04, BS22]). Although compactness of low-energy sequences $y^{(k)}$ can be proved analogously to [MM04] and otherwise the lower and upper bounds seem deducible, the probably most difficult part of the problem is to identify the discrete limiting strain $\bar{G}$ (cf. [BS22]).

As linearization around a global rigid motion pertains to von-Kármán-like theories, the possibility of combining them with fracture mechanics appears unclear.

Furthermore, the situation from Chapter 4 becomes considerably more difficult for *plates* due to a much richer phenomenology of crack and kink patterns. For bending-dominated configurations also severe geometric obstructions that result from the isometry constraints are encountered. However, a first step has recently been achieved in [SS23], where a 'Blake–Zisserman–Kirchhoff theory' was derived for plates with soft inclusions.

From the point of view of applications, it would be interesting to extend the presented findings to other crystallographic lattices (such as diamond cubic as in [LPS17] or zincblende), heterogeneous nanostructures with several different types of atoms, or to study the influence of lattice defects.

The models could also be studied computationally (e.g. numerical approximations of the cell formula could be implemented). For finite-element discretizations of the purely elastic rod models, the author considered (but did not pursue for time reasons) adapting one of the FEniCS libraries [Bou20, dBD17].

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Following a convention more common in humanities (as yet), authors' names of Far East origin are not abbreviated to enable easier identification.

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