Effective theories for thin elastic films

Discrete-to-continuum limits for membranes and plates and minimal energy configurations of strained multi-layers

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Chapter 1

Introduction

The main focus of this thesis is on the derivation and discussion of effective theories for thin elastic structures. These objects are of interest not only in technical applications. One also encounters completely new phenomena (as, e.g., large deformations at low energy). To find appropriate energy functionals in the limit of singular geometries is a classical problem in elasticity theory (see, e.g., the work of Euler, Kirchhoff, von Kármán [17, 28, 27] etc., also compare [32]). However, rigorous results deriving membrane, plate, rod or shell theories from three-dimensional elasticity have been obtained only recently (cf. [29, 30, 31, 20, 21, 22, 23, 24]). By now there has emerged a whole hierarchy of plate theories according to different scalings of the stored energy (cf. [22]). For ultra-thin films, i.e., films consisting of only few atomic layers, however, a pure continuum mechanical approach might not be justified any more.

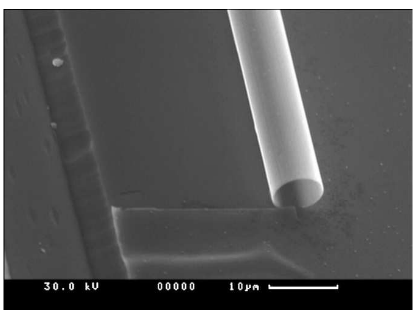
Another area of research in elasticity theory concerns the passage from discrete atomic models to continuum theories. Rigorous Γ-convergence results, especially in one dimension, are proven in [8, 9, 10] for pair potentials under suitable growth assumptions on the atomic interactions. The results in [6, 7] on the other hand deal with both pair potential and quantum mechanical energy models, but assume the Cauchy-Born rule to deduce continuum limits in this general framework.

The main part of this work (see chapters 2, 3, 4) will be devoted to investigating effective theories of thin films starting from atomistic models. Thus, in order to study new effects that may arise for ultra-thin layers, we consider variational convergence schemes that simultaneously take into account the effects of singular geometries and of atomistic particle interactions.

In the membrane energy regime we will prove a rigorous version of a scheme that was proposed by Friesecke and James in [19] (see chapters 2 and 3). The resulting continuum energy expression is obtained by integrating a stored energy density which not only depends on the deformation gradient but also on $\nu - 1$ director fields, where ν is the (fixed) number of atomic film layers. To discuss qualitative aspects of the derived continuum theory, the stored energy density is examined for convexity properties and limiting behavior under large and small strains. A study of the dependence of the theory on relaxation parameters leads to the result that our scale of convergence is in fact the only scale for which a limiting theory that also accounts for atomistic relaxation effects is non-trivial.

For bending dominated deformations the energy scaling is much more subtle. In chapter 4 we will derive Kirchhoff's plate theory for a class of generalized mass-spring models both for thin and ultra-thin layers. While in the 'thick film regime', i.e., when the film consists of many layers of atoms, we recover the well known plate theory derived from 3D-elasticity in [21], for 'thin films' new terms in the limit functional are obtained. These terms are due to the discrete nature of atomic models and surface effects, and cannot be detected from continuum elasticity.

Finally, in chapter 5 we concentrate on thin multi-layers, in particular on roll-up phenomena in thin stressed multi-layers. Recently, in the physics literature there has been much interest in thin multi-layers internally stressed due to mismatching lattice constants. This mismatch can be caused, e.g., by a temperature gradient or differing lattice constants for a film consisting of layers of different materials. If such a film is released from the substrate, it will assume a geometrically non-trivial configuration in order to reduce its elastic energy. This phenomenon is used, e.g., in the waver-curvature measurement, where one tries to deduce material (mismatch) properties from measurements of the curved substrate. Another, more recent application is the fabrication of nanotubes (nanoscrolls, nanobelts, etc.) by growing bi-layers of films with mismatching lattice constants and releasing them from the substrate (see, e.g., [36, 33]).



SEM image of a multi-layer tube (courtesy of H. Paetzelt, V. Gottschalch, J. Bauer, H. Herrnberger, G. Wagner, Universtität Leipzig, cf. [33])

In the physics literature so far (mostly linear) three-dimensional elasticity theory is used to describe the energy of such objects (cf., e.g., [26], [40]); and in order to discuss the geometry of energy minimizers, one uses appropriate ansatz functions (cylinders, belts, etc.) and optimizes with respect to certain parameters (e.g., radius, winding direction).

We take a continuum approach to derive an effective plate theory for internally stressed thin elastic layers. The shape of the energy minimizers of the effective energy functional is investigated without a priori assumptions on the geometry. For configurations in two dimensions (corresponding to Euler-Bernoulli theory) we also take into account a non-interpenetration condition for films of small but non-vanishing thickness.

A more detailed outline of the content of this thesis is as follows.

In chapter 2 we fix $h > 0$, the thickness of the film, and for $k \in \mathbb{N}$ consider the reference configurations

$$\mathcal{L}_k = \mathbb{Z}^3 \cap [0,k] \times [0,k] \times [0,h]$$

(more general lattices are possible, see paragraph 2.2.6) subject to some deformation $y^{(k)} : \mathcal{L}_k \to \mathbb{R}^3$. The elastic energy of such a deformation is denoted by $E(y^{(k)})$. In the membrane energy regime the macroscopic energy scales like the aspect ratio of the film. The natural limiting objects in the limit $k \to \infty$ are argued to be (after rescaling) given by some function $u : [0,1] \times [0,1] \to \mathbb{R}^3$ (the 'single layer deformation') and vector fields $b^i : [0,1] \times [0,1] \to \mathbb{R}^3$, $i = 1, \ldots, \nu - 1$, where the film consists of ν layers of atoms. Having defined a suitable notion of convergence, we are led to the following fundamental

Problem. Find $\varphi : \mathbb{R}^{3\times 2} \times (\mathbb{R}^3)^{\nu-1} \to \mathbb{R}$ such that

$$E(u, b^1, \ldots, b^{\nu-1}) := \lim_{k\to\infty} E(y^{(k)}) = \int_{[0,1]^2} \varphi(\nabla u, b^1, \ldots, b^{\nu-1})$$

whenever $y^{(k)} \to (u, b^1, \ldots, b^{\nu-1})$.

In the spirit of Γ-convergence (cf., e.g., [15]) we do not want to restrict to pointwise limits, but rather calculate a variational limit of the energy that also takes into account microscopic relaxation effects.

In section 2.1 we introduce the model, in particular, we discuss the admissible limiting deformations and energy functions that may be considered. We define precisely in what sense microscopic deformations are understood to converge to their macroscopic representatives.

Section 2.2 is the core of the theory. It shows how to pass from atomic to continuum theory in the framework set up so far. The scheme follows Friesecke and James ([19]):

- Replace u and $\mathbf{b} = (b^1, \ldots, b^{\nu-1})$ by their piecewise affine and piecewise constant approximations u_ε and $\mathbf{b}_\varepsilon$, respectively.
- Partition the body into mesoscopic regions where $u_\varepsilon, \mathbf{b}_\varepsilon$ are affine and constant, respectively, and show that the energy decouples.
- Find minimizers separately on each of these regions.
- Patch them together.
- Obtain an integral expression in terms of ∇u and $\mathbf{b}$.

We give a rigorous version of these steps which in part were derived formally in [19]. Note, however, that there are some major differences. In particular, the (central) notion of weak neighborhood given here is at variance with that of [19], resulting in some technical differences. These neighborhoods are not only of mathematical interest but also describe physically which deformation fluctuations are subject to relaxation and which will be seen in continuum theory. We will therefore study these neighborhoods in some detail. Furthermore, we show that the hypotheses on the decay of the energy and on the regularity of $(u, \mathbf{b})$ made in [19] can be weakened. We also give a proof for the convergence of the relaxed energy on a mesoscale level under homogeneous conditions, thus showing that the continuum theory derived is indeed well-defined. Our study of variants of weak neighborhoods will lead to a representation result for the limiting energy density φ. The results are extended to systems with unbounded interaction potential. This is of physical interest since many interaction potentials contain terms that diverge for two atoms getting too close to each other. Finally, we discuss some extensions, in particular to certain systems of distinguishable particles, and variants of the continuum theory.

In section 2.3 we examine physical energy functions and exhibit conditions under which these fit into the theory. In particular, we treat pair potentials, angular forces (to incorporate materials whose binding energy depends on the bond-angles) and pair functionals (derived by the embedded atom method). We show that, under reasonable hypotheses on the parameters, these energies are admissible for our passage to continuum theory. To give an explicit example we also treat the case of an elementary nearest neighbor model.

Chapter 3 is devoted to studying this continuum theory, i.e., the macroscopic energy density φ, qualitatively. First, cf. section 3.1, we examine the dependence of φ on the relaxation parameter c_0 and study the limiting cases $c_0 \to \infty$ and $c_0 \to 0$. Moreover, we will see that the physically motivated rate of convergence for which continuum theory was derived in chapter 2 is the only scale that leads to a non-trivial limiting theory: more restrictive notions of convergence would not allow for atomistic relaxation, while less restrictive notions lead to constant limiting energy expressions due to fracture.

In the following two sections 3.2 and 3.3 we derive the limiting behavior under large tensile and compressive strains and explore the convexity properties and symmetries of the limiting energy functional. In particular, for strongly compressive deformations we will observe an interesting scaling of the energy.

Finally, in section 3.4, the scaling behavior of certain systems near $O(2,3)$ is examined. We still find non-trivial energy response to compressive strains in this regime; it is, however, weaker than the response calculated without taking into account atomic relaxation effects. In order to prove this result, we are led to study the one-dimensional version, an atomic chain, in detail. The results of this paragraph might be of independent interest.

In order to derive a continuum plate theory in the regime of finite bending energies starting from a microscopic atomistic model in chapter 4, we assume that the energy can be decomposed into certain cell-energies similar as in [13]. The main goal will be to rigorously derive plate theory as the number of particles becomes large and the aspect ratio of the film tends to zero. In particular, we will not make use of the Cauchy-Born rule.

In section 4.1, we first introduce our models of thin and thick films and also some notation that will be used in the sequel. We describe the energy functions that we will consider and define in what sense discrete deformations are understood to converge to continuum deformations as the number of particles tends to infinity and the aspect ratio of the film tends to zero. While the atomic lattice is as in the previous chapters, there are major differences in the definition of convergence of deformations. This is mainly due to the more restrictive assumptions on the energy function which prevents fracture by suitable growth assumptions.

In section 4.2 we prove rigidity estimates for deformations in terms of their elastic energy in the spirit of [21]. The main point will be to estimate the discrete atomic energy in terms of suitable continuum deformations and make use of the continuum estimates obtained in [21]. This builds on work in [39] and [13] and generalizes two-dimensional results in [39] to higher dimensions.

Section 4.3 serves to prove compactness for sequences having finite bending energy, thus complementing the Γ-convergence results in the later sections. We also recall some basic estimates from the continuum theory for later use.

In section 4.4, we specialize to thin films, i.e., films consisting of a fixed number $\nu+1$ of atomic layers. (Unlike in the membrane energy regime, only films of at least 2 atomic layers are of interest here.) The main result is a convergence theorem for the energy as the length k of the lateral directions of the film tends to infinity, i.e., as the aspect ratio tends to zero, in the spirit of Γ-convergence. To leading order in ν, the continuum theory coincides with a formula derived in [21] from three-dimensional continuum elasticity theory. However, for ultra-thin films new terms in the limiting functional appear. These contributions are due to surface terms which can not be neglected in this very thin film regime and to the discrete nature of our underlying atomic model. The derivation is inspired by the work in [21], and we refer to this paper rather than re-deriving the results that are needed here. The main difficulty arises when estimating the cell-to-cell fluctuations of the converging film deformations. Here, continuum theory gives only partial results since usual deformation gradients are 3×3-matrices whereas we have to consider discrete gradients which are elements of $\mathbb{R}^{3\times 8}$. Additional matrix elements have to be identified which lead to new terms in the limiting functional.

Keeping only the leading term in powers of ν, the thickness of the film, we are formally led to a continuum theory for thick films. By thick films we mean the regime $k, \nu \to \infty$, i.e., films of many atomic layers, such that still $\nu/k \to 0$. That this is indeed the correct Γ-limit in the realm of thick films, is the content of section 4.5. This way we obtain the functional of plate theory derived in [21] on the basis of three-dimensional elasticity rigorously as a thick film limit starting from atomistic models.

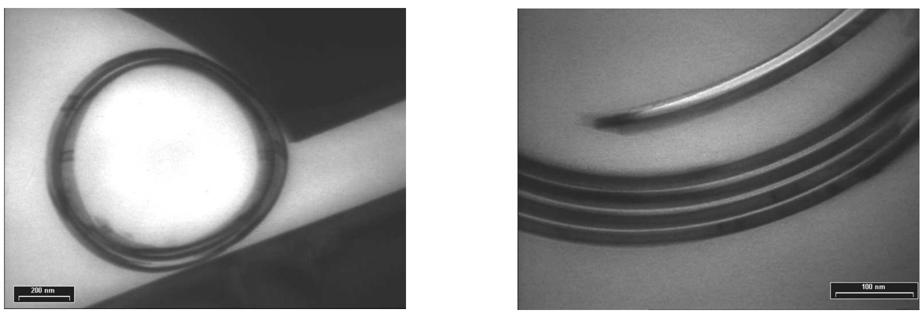
Section 4.6 discusses a mass-spring model as an elementary but physically realistic example of atomic interactions to which the results in the previous sections apply.

In the final chapter 5 we investigate thin elastic films whose (flat) reference configuration $S \times (-h/2, h/2)$, $h \ll 1$, is stressed due to some small mismatch of equilibria in the x_3-direction.

Our aim is first to derive an effective plate theory from three-dimensional nonlinear elasticity theory rigorously as a suitable Γ-limit in the bending energy regime for $h \to 0$, see section 5.1. This is the appropriate energy scale for objects as nanoscrolls etc. mentioned above. We have chosen a model of a heterogeneous film for which this derivation is a rather straightforward extension of the results in [21], yet it models thermally stressed films of a single material or stress induced due to mismatching lattice constants of materials with similar elastic constants (as, e.g., in [33]) reasonably well. We do not re-derive all the steps needed from [21]; rather we focus on those parts of the derivation that are new. (For more general models, the adaption of the methods in [21] is not so straightforward, however still possible as exploratory calculations indicate.) The outcome is an integral expression for the energy in terms of the second fundamental form of the film surface similar as in [21]. However, the reference state is not a state of minimal energy any more; the thin film can reduce energy by rolling up.

The following section 5.2 is devoted to an ansatz free study of minimal energy configurations (for free boundary conditions). An elementary observation shows that indeed one cannot do better than cylinders. Using results of Pakzad (cf. [34]) on the developability of $W^{2,2}$ isometric immersions, it is proven that in fact every minimizer must be a cylinder. We also describe the set of optimal winding directions and radii in detail.

While in the previous section all $W^{2,2}$ isometric immersions were admissible, in section 5.3 we will also take into account a non-interpenetration condition for films of small but non-vanishing thickness. Motivated by the results of section 5.2, we study Euler-Bernoulli type deformations that can be described by a planar curve of length L. We investigate the minimal energy configurations in the most interesting regime $L \sim h^{-1}$ in detail and find non-trivial minimal energy configurations. According to the boundary conditions chosen, they will turn out to be spirals or double spirals.



TEM cross sectional images of a BGaAs 7nm / InGaAs 9 nm two layer system rolled up in $(1, 0, 0)$ direction (courtesy of H. Paetzelt, V. Gottschalch, J. Bauer, H. Herrnberger, G. Wagner, Universtität Leipzig, cf. [33])

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Chapter 2

A hybrid atomistic/continuum membrane theory for thin films

2.1 Microscopic model and macroscopic variables

After introducing the atomic model of a thin film subject to some deformation, we identify the variables of continuum theory as limiting points of these deformations. Finally, we collect the basic assumptions on the admissible energy functions.

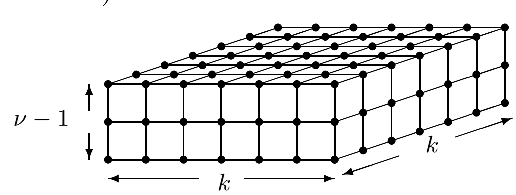
2.1.1 Kinematics

Atomistic model

We consider a film of ν atomic layers. Our reference configuration will be

$$\mathcal{L}_k = \mathcal{L} \cap (\mathcal{S}_k \times [0, h]),$$

where $\mathcal{L} = \mathbb{Z}^3$, $\mathcal{S}_k := [0, k] \times [0, k]$ for $k \in \mathbb{N}$ and $h := \nu - 1$ is the height of the film. (Only minor changes are necessary to treat more general Bravais-lattices $\mathcal{L}$, cf. paragraph 2.2.6.)



It will sometimes be convenient to enumerate these points as $x_1, \ldots, x_{\nu(k+1)^2}$.

The deformations of this configuration will be denoted by

$$y = y^{(k)} : \mathcal{L}_k \to \mathbb{R}^3.$$

(Also write y as $(y_1, \ldots, y_{\nu(k+1)^2})$ for $y_i = y(x_i)$.) In order for y to be defined not only at the atomic positions, we will assume some interpolation between the atomic positions. However, we then have to be careful that our results do not depend on the particular interpolation chosen, see below.

Our aim being to study the limit $k \to \infty$, it is natural to introduce the rescaled functions $\tilde{y}$ defined on the common domain $\mathcal{S}_1 \times [0, h]$:

$$\tilde{y}^{(k)}(x) := \frac{1}{k} y^{(k)}(kx_1, kx_2, x_3).$$

Assume for the moment some interpolation is chosen. As pointed out in [19], imposing regularity assumptions on the deformations y implies existence of limiting deformations in the limit $k \to \infty$. It is argued that these limits have to be considered the natural variables of continuum theory. In detail, the assumptions on the deformations made in [19] are the following. There are constants $c_1, c_2 > 0$ such that,

(a) $|y(x)| \leq c_2 k$ (boundedness),

(b) $|y(x_2) - y(x_1)| \leq c_2 |x_2 - x_1|$ (Lipschitz),

(c) $|y(x_2) - y(x_1)| \geq c_1 |x_2 - x_1|$ (minimal strain hypothesis),

for all $x, x_1, x_2 \in \mathcal{S}_k \times [0, h]$.

While conditions (a) and (b) guarantee the existence of well-defined limiting points by weak*-compactness of the set of admissible deformations as $k \to \infty$, a minimal strain hypothesis is needed in order localize the energy of a deformation. Without that assumption the film could by repeatedly folding back on itself be deformed into a block of bulk material. This would certainly not give rise to film-like behavior.

Macroscopic variables

As indicated above, for fixed c_2 the set of admissible functions $\tilde{y}$ is weak*-compact in $W^{1,\infty}(\mathcal{S}_1 \times [0, h]; \mathbb{R}^3)$. Also, $(k\tilde{y}^{(k)}_{,3})$ is bounded in $L^\infty(\mathcal{S}_1 \times [0, h]; \mathbb{R}^3)$. So there are limit points of these deformations as $k \to \infty$: There is u such that (for a subsequence)

$$\tilde{y}^{(k)} \overset{*}{\rightharpoonup} u, \quad \nabla \tilde{y}^{(k)} \overset{*}{\rightharpoonup} \nabla u \qquad \text{in } L^\infty. \tag{2.1}$$

It is easy to see that u is independent of x_3.

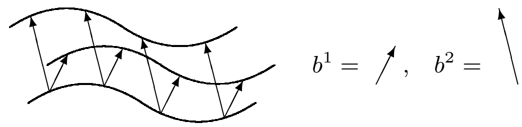
There is also a subsequence such that $(k\tilde{y}^{(k)}_{,3})$ weak*-converges in L^∞. However, this can not become a free variable of our continuum theory since the limit function must be determined by the atomic positions only. We instead follow [19] and consider

$$\Delta^i \tilde{y}^{(k)}(x_p) = \tilde{y}^{(k)}(x_p, i) - \tilde{y}^{(k)}(x_p, 0), \quad i = 1, \ldots \nu - 1,$$

$x_p = (x_1, x_2)$. These quantities measure the relative shift of the layers of the film. By assumption, $(k\Delta^i \tilde{y}^{(k)})$ is a bounded sequence, and so some subsequence weak*-converges to, say, $b^i(x_1, x_2)$:

$$k\left(\tilde{y}^{(k)}(\cdot, i) - \tilde{y}^{(k)}(\cdot, 0)\right) \overset{*}{\rightharpoonup} b^i \qquad \text{in } L^\infty. \tag{2.2}$$

These objects u and $\mathbf{b} = (b^1, \dots, b^{\nu-1})$ constitute the natural variables of a continuum theory.



While the first condition (2.1) does not depend too much on the particular interpolation chosen, we can expect condition (2.2) to hold only for suitable interpolations (cf. below).

In our derivation – deviating from [19] – we will take the point of view that we are given u and $\mathbf{b} = (b^1, \dots, b^{\nu-1})$ and would like to assign an energy to these variables allowing for atomistic relaxation. Thus reflecting the fact that we are interested in energies of macroscopic film-like configurations, we do not restrict the lattice deformations themselves but rather impose the following conditions on u and $\mathbf{b}$.

Definition 2.1.1 *Let $u \in W^{1,\infty}(\mathcal{S}_1; \mathbb{R}^3)$ and $\mathbf{b} \in L^\infty(\mathcal{S}_1; (\mathbb{R}^3)^{\nu-1})$. We say that $(u, \mathbf{b})$ is admissible (for given $c_0 > 0$), i.e., $(u, \mathbf{b}) \in \mathcal{A}$, if there exists $c_1 > 0$ such that*

$$|u(x) - u(z)| \geq c_1 |x - z| \quad \forall x, z \in \mathcal{S}_1 \tag{2.3}$$

(minimal strain hypothesis), and there exists $b^0 \in L^\infty$ such that

$$\|b^0\|_{L^\infty}, \|b^i - b^0\|_{L^\infty} \leq c_0, \quad i = 1, \dots, \nu - 1. \tag{2.4}$$

The first hypothesis ensures the macroscopic deformation to be 'film like'. The meaning of the second condition will become clear when we have specified our convergence scheme. To be able to work also in un-rescaled variables, we define $U : \mathcal{S}_k \to \mathbb{R}^3$ by $\tilde{U}(x) = \frac{1}{k} U(kx) = u(x)$.

The following lemma is elementary but important. In particular, the lower bound in (ii) gives a 'far field minimal strain hypothesis' for deformations close to u.

Lemma 2.1.2 *Suppose u is admissible and $y : \mathcal{L}_k \to \mathbb{R}^3$ some deformation with $\sup_{x \in \mathcal{L}_k} |y(x) - U(x_p)| \leq c$. Then y is Lipschitz. For any (rescaled) Lipschitz interpolation $y : \mathcal{S}_k \times [0, h] \to \mathbb{R}^3$ ($\tilde{y} : \mathcal{S}_1 \times [0, h] \to \mathbb{R}^3$) there are constants $C_1, C_2, C_3 > 0$ such that,*

(i) $\sup_{x \in \mathcal{S}_1 \times [0,h]} |\tilde{y}(x)| \leq C_2$ *and*

(ii) $C_1 |x - z| - C_3 \leq |y(x) - y(z)| \leq C_2 |x - z| \;\forall x, z \in \mathcal{S}_k \times [0, h]$.

Proof. Since u is admissible, there are $0 < c_1 \leq c_2$ such that

$$c_1 |x - z| \leq |u(x) - u(z)| \leq c_2 |x - z| \tag{2.5}$$

for all $x, z \in \mathcal{S}_1$. Then (i) is clear for $x \in \frac{1}{k}\mathcal{L}_k \cap \mathcal{S}_1$: choose $C_2 \geq |u(0)| + \sqrt{2} c_2 + c/k$. For $x, z \in \mathcal{L}_k$, $|y(x) - y(z)|$ on the one hand is greater than or equal to

$$|U(x_p) - U(z_p)| - 2c \geq c_1 |x_p - z_p| - 2c \geq c_1 |x - z| - c_1 h - 2c,$$

which proves the first inequality of (ii) for $x, z \in \mathcal{L}_k$. On the other hand, for $x \neq z \in \mathcal{L}_k$ this is less than or equal to

$$|U(x_p) - U(z_p)| + 2c \leq c_2|x_p - z_p| + 2c \leq c_2|x - z| + 2c \leq C|x - z|$$

since $|x-z| \geq 1$. In particular, y is Lipschitz. Choosing a Lipschitz-interpolation with Lipschitz constant C_2, we get for all $x \in \mathcal{S}_k \times [0, h]$

$$|y(x) - U(x_p)| \leq C_2 + c + |U(\bar{x}_p) - U(x_p)| \leq C' + c + c_2 =: c'$$

where $\bar{x} \in \mathcal{L}_k$ is such that $|\bar{x} - x| \leq 1$. Now repeat the above steps to conclude (i) and the first part of (ii) for y on $\mathcal{S}_k \times [0, h]$ ($\tilde{y}$ on $\mathcal{S}_1 \times [0, h]$). ☐

Remarks:

(i) The constants C_1, C_2, C_3 only depend on u through c, c_1 and c_2 and on the Lipschitz constant of the chosen interpolation. Below, this constant will be chosen independently of k.

(ii) If y is defined only on a subset of $\mathcal{L}_k$ and satisfies $|y - U| \leq c$ on this set, then clearly the implications of the lemma remain valid on this set.

Interpolation & convergence

Weak*-convergence for bounded sequences in L^∞ is equivalent to convergence of averages (e.g., over all sub-squares $a + [0, \alpha]^2$ of the domain, cf. [14]). We will therefore choose our interpolation carefully such that

$$\fint_Q \tilde{y}(z, i)dz \approx \frac{1}{\#(\frac{1}{k}\mathcal{L} \cap Q)} \sum_{z \in \frac{1}{k}\mathcal{L} \cap Q} \tilde{y}(z, i)$$

for Q a square in $\mathcal{S}_1$. For a deformation $y : \mathcal{L}_k \to \mathbb{R}^3$ let $\bar{x} = x + (1/2, 1/2)$ for $x \in \{0, \ldots, k-1\}^2$, and set

$$y(\bar{x}, i) = \frac{1}{4} \sum_{\substack{z \in \mathbb{Z}^2, \\ |z - \bar{x}| = 1/\sqrt{2}}} y(z, i), \quad i = 0, \ldots, \nu - 1.$$

Now on each of the four triangles with corners $(\bar{x}, i), (z, i), (z', i)$, where $z, z' \in \mathbb{Z}^2$ with $|z - \bar{x}| = 1/\sqrt{2}$, $|z - z'| = 1$, interpolate linearly to obtain $y(x, i)$ for $x \in \mathcal{S}_k$. Interpolating in between the layers is not so subtle, for definiteness we choose y to be linear on the segments $[(x, i-1), (x, i)]$.

Note that this choice guarantees that

$$\fint_{\bar{x} + [-\frac{1}{2k}, \frac{1}{2k}]^2} \tilde{y}(z, i)dz = \frac{1}{4} \sum_{z \in \bar{x} + \{-\frac{1}{2k}, \frac{1}{2k}\}^2} \tilde{y}(z, i).$$

Now let $D \subset \mathcal{S}_1$ be some square of fixed side-length l and consider the measure ρ on $\mathbb{R}^2$ defined by $\rho = \sum_{x \in \mathbb{Z}^2} \delta_{x/k}$, where δ_z is the Dirac-measure at z. Supposing $|k\Delta^i \tilde{y}^{(k)}|$ is bounded uniformly in k, we get that

$$\left| \fint_D k\Delta^i \tilde{y}(z_1, z_2) d\rho - \fint_D k\Delta^i \tilde{y}(z_1, z_2) dz_1 dz_2 \right| \leq C\frac{1}{kl}.$$

This shows that the limits b^i are in fact only depending on atomic positions.

In the sequel, we will assume that y (resp. $\tilde{y}$) are interpolated precisely in this manner. As a consequence of the next definition and the previous lemma, all deformations that will be taken into account for atomistic relaxation are Lipschitz with a common Lipschitz constant independent of k.

Definition 2.1.3 *Let $u \in W^{1,\infty}(\mathcal{S}_1;\mathbb{R}^3)$, $\mathbf{b} \in L^\infty(\mathcal{S}_1;\mathbb{R}^3)$. Choose $c_0 > 0$, a constant. We say that $y^{(k)} \to (u, \mathbf{b})$ (w.r.t. c_0) if*

$$\|\tilde{y}^{(k)} - u\| \le c_0/k \quad \text{and} \quad k\Delta^i \tilde{y}^{(k)} \overset{*}{\rightharpoonup} b^i \quad \text{in } L^\infty.$$

Here and in the sequel, we denote by $\|f\|$, respectively $\|\tilde{f}\|$ in rescaled variables,

$$\|f\| := \sup_{x\in\mathcal{L}_k} |f(x)|, \qquad \text{resp.} \qquad \|\tilde{f}\| := \sup_{x\in\mathcal{L}_k} |\tilde{f}(x_p/k, x_3)|.$$

Indeed, $\|\tilde{y}^{(k)} - u\| \to 0$ and $\|\nabla\tilde{y}^{(k)}\|_{L^\infty} \le$ const. imply $\tilde{y}^{(k)} \overset{*}{\rightharpoonup} u$ in $W^{1,\infty}$. Also note, if $\|\tilde{y}^{(k)} - u\| \le c_0/k$, then in fact $k\Delta^i\tilde{y}^{(k)}$ is bounded, so we can describe weak*-convergence in L^∞ by convergence of averages. In order to shed light on the compatibility assumption made for admissible $\mathbf{b}$, we first prove the following lemma.

Lemma 2.1.4 *Suppose $|\tilde{y}^{(k)}(z,i) - u(z)| \le c_0/k$ for all $z \in \frac{1}{k}\mathbb{Z}^2 \cap \mathcal{S}_1$. Then there exist $w^{(k)} \in L^\infty(\mathcal{S}_1;\mathbb{R})$ with $\|w^{(k)}\|_{L^\infty} \le C$ and $w^{(k)} \to 0$ pointwise a.e. as $k \to \infty$ such that*

$$|\tilde{y}^{(k)}(x) - u(x_p)| \le \frac{c_0 + w^{(k)}(x_p)}{k}.$$

Proof. Since there is a common Lipschitz constant for all deformations and $|\tilde{y}(x,i) - u(x)| \le c_0/k$ whenever $x \in \frac{1}{k}\mathbb{Z}^2$, we immediately get a constant $C > c_0$ such that

$$|\tilde{y}(x,i) - u(x)| \le C/k \quad \forall x \in \mathcal{S}_1. \tag{2.6}$$

Let $x \in \mathcal{S}_1$ such that $\nabla u(x)$ exists and define $u'(x,z) = u(x) + \nabla u(x)(z-x)$. Choose $z_0 \in (\frac{1}{k}\mathbb{Z}^2 + (1/2,1/2)) \cap \mathcal{S}_1$ such that $|x - z_0|$ is minimal and let $\{z \in \frac{1}{k}\mathbb{Z}^2 : |z_0 - z| = 1/\sqrt{2}\} = \{z_1, z_2, z_3, z_4\}$. W.l.o.g. suppose x lies in the triangle with corners z_0, z_1, z_2. By our interpolation and since $u'(x,\cdot)$ is affine,

$$\begin{aligned}
|\tilde{y}(z_0,i) - u'(x,z_0)| &= \left| \frac{1}{4}\sum_{j=1}^4 \tilde{y}(z_j,i) - \frac{1}{4}\sum_{j=1}^4 u'(x,z_j) \right| \\
&\le \frac{1}{4}\sum_{j=1}^4 |\tilde{y}(z_j,i) - u(z_j)| + |u(z_j) - u'(x,z_j)| \\
&\le \frac{c_0}{k} + \frac{1}{4}\sum_{j=1}^4 |u(z_j) - u'(x,z_j)|
\end{aligned}$$

Also, for $j = 1,2,3,4$,

$$|\tilde{y}(z_j,i) - u'(x,z_j)| \le \frac{c_0}{k} + |u(z_j) - u'(x,z_j)|.$$

Now since $\tilde{y}(\cdot,i)$ and $u'(x,\cdot)$ are affine on the triangle with corners z_0, z_1, z_2, we deduce from these inequalities that

$$\begin{aligned} |\tilde{y}(x,i)-u(x)| &= |\tilde{y}(x,i)-u'(x,x)| \leq \max_{j\in\{0,1,2\}} |\tilde{y}(z_j,i)-u'(x,z_j)| \\ &\leq \frac{c_0}{k} + \max_{j\in\{1,2,3,4\}} |u(z_j)-u'(x,z_j)|. \end{aligned} \tag{2.7}$$

Choosing

$$w(x) = \min\{C-c_0, k \max_{i\in\{1,2,3,4\}} |u(z_j)-u'(x,z_j)|\},$$

we see by (2.6) and (2.7) and our choice of interpolating linearly between the film layers

$$|\tilde{y}(x_p,x_3)-u(x_p)| \leq \max_{0\leq i\leq \nu-1} |\tilde{y}(x_p,i)-u(x_p)| \leq \frac{c_0}{k} + \frac{w(x_p)}{k}$$

for a.e. (x_1,x_2). To finish the proof just observe that $z_j \to x$ as $k\to\infty$ and $|u(z_j)-u'(x,z_j)| = o(|x-z_j|) = o(1/k)$ since $|x-z_j| \leq \sqrt{2}/k$. □

As a consequence we obtain the following lemma.

Lemma 2.1.5 *Suppose* $u \in W^{1,\infty}(\mathcal{S}_1,\mathbb{R}^3)$. *There exists a sequence of deformations* $y^{(k)} \to (u,\mathbf{b})$ *for* $\mathbf{b} \in L^\infty(\mathcal{S}_1;(\mathbb{R}^3)^{\nu-1})$ *if and only if (2.4) holds.*

Proof. Assume $y^{(k)} \to (u,\mathbf{b})$ and consider $f^{(k)}(z) = ku(z) - k\tilde{y}^{(k)}(z,0)$. By the previous lemma, $f^{(k)}$ is bounded in L^∞, so there is a weak*-convergent subsequence $f^{(k_j)} \overset{*}{\rightharpoonup} b^0$, say. Now if $\chi \in L^1(\mathcal{S}_1)$ with $\|\chi\|_{L^1} = 1$, then by lemma 2.1.4,

$$\int \chi\cdot b^0 = \lim_{j\to\infty}\int \chi\cdot f^{(k_j)} \leq \lim_{j\to\infty}\int |\chi|\cdot|c_0+w^{(k_j)}| = c_0$$

by dominated convergence since the $w^{(k)}$ are uniformly bounded and converge to zero pointwise. It follows that $\|b^0\|_{L^\infty} \leq c_0$. Now considering $k_j\Delta^i\tilde{y}^{(k_j)} - f^{(k_j)} \overset{*}{\rightharpoonup} b^i - b^0$, $|k_j\Delta^i\tilde{y}(z) - f^{(k_j)}(z)| = |k\tilde{y}(z,i) - ku(z)| \leq c_0 + w^{(k)}(z)$, the same reasoning shows that $\|b^i - b^0\|_{L^\infty} \leq c_0$.

Conversely, suppose b^0 satisfying (2.4) exists. Extend b^i boundedly (constantly if b^i is constant) outside $\mathcal{S}_1$. For $0 \leq i \leq \nu-1$ set

$$\bar{b}^i(x) = \fint_{x+[-\frac{1}{2k},\frac{1}{2k}]^2} b^i(z)dz. \tag{2.8}$$

Now consider the function v (V in un-rescaled variables) defined by (interpolation of)

$$v(x_1,x_2,i) = \begin{cases} u(x_1,x_2) - \frac{1}{k}\bar{b}^0(x_1,x_2) & \text{for } i=0, \\ u(x_1,x_2) + \frac{1}{k}(\bar{b}^i(x_1,x_2) - \bar{b}^0(x_1,x_2)) & \text{for } 1\leq i\leq \nu-1, \end{cases} \tag{2.9}$$

for $(x_1,x_2) \in \frac{1}{k}\mathbb{Z}^2 \cap \mathcal{S}_1$. Clearly, $\|v-u\| \leq c_0/k$ since for $x \in \frac{1}{k}\mathbb{Z}^2\cap\mathcal{S}_1$,

$$\left|\bar{b}^0(x)\right| \leq \left\|b^0\right\|_{L^\infty}, \quad \left|\bar{b}^i(x) - \bar{b}^0(x)\right| \leq \left\|b^i - b^0\right\|_{L^\infty}.$$

Also, for each square D of side-length $0 < l \leq 1$, $\fint_D k\Delta^i\tilde{y} = b^i + \mathcal{O}(l/k)$ which implies that $k\Delta^i\tilde{y} \overset{*}{\rightharpoonup} b^i$. □

2.1.2 Energy

The energy of a system of N atoms at positions $y_1, \dots, y_N \in \mathbb{R}^3$ shall be a function $E : (\mathbb{R}^3)^N \to \mathbb{R}$ only depending on atomic positions. To study E we will endow the configuration space $(\mathbb{R}^3)^N$ with the norm

$$\|(y_1, \dots, y_N)\| = \sup_{1 \le i \le N} |y_i|_2.$$

The energy of a deformation y is denoted

$$E(y) = E(y(x) : x \in \mathcal{L}_k).$$

More generally, the energy of the subset $y(\mathcal{K})$, $\mathcal{K} \subset \mathcal{L}_k$, (counted with multiplicities) of all the atoms is

$$E(y(\mathcal{K})) = E(y(x) : x \in \mathcal{K}).$$

We normalize E so that $E(\emptyset) = 0$.

Consider deformations $y : \mathcal{K} \to \mathbb{R}^3$, where $\mathcal{K} = \mathcal{L} \cap (\Omega \times [0, h])$, $\Omega \subset \mathcal{S}_k$. For U with $\tilde{U} = u$ as before we write $\|y - U\| = \max_{x \in \mathcal{K}} |y(x) - U(x_p)|_2$. The main assumption on E is the following – physically reasonable – decay hypothesis.

Assumption 2.1.6 *Suppose u is admissible. There exists a function $\psi : [0, \infty) \to \mathbb{R}$ such that*

$$0 \le \psi \le M \quad \text{and} \quad \psi(r) \le M r^{-q}, \tag{2.10}$$

where M, q are constants, $M > 0$, $q > 3$, such that for disjoint sets $\mathcal{M}$ and $\mathcal{N}$ of atoms we have

$$|E(\mathcal{M} \cup \mathcal{N}) - E(\mathcal{M}) - E(\mathcal{N})| \le \sum_{v \in \mathcal{M}, w \in \mathcal{N}} \psi(|v - w|)$$

whenever $\|y - U\| \le C$. (The function ψ may depend on C and on u through c_1 and c_2 where $c_1|x_1 - x_2| \le |u(x_1) - u(x_2)| \le c_2|x_1 - x_2|$.)

The energy functionals E act on different spaces because of the different number of atoms involved. The following assumption guarantees that, locally near admissible u's, we have control of $\frac{\partial}{\partial y_i} E(y_1, \dots, y_N)$ uniformly in k.

Assumption 2.1.7 *Let u be admissible. We assume that E is locally Lipschitz, and in any C-neighborhood of U we have a.e.*

$$\left| \frac{\partial}{\partial y_i} E(y) \right| \le L$$

where L might depend on C and on U through c_1, c_2 but is independent of the number of atoms involved.

Furthermore, we assume E to be frame indifferent and only depending on the atomic positions, i.e., E remains unchanged after renumbering of atoms and rigid motion of the configuration $y(\mathcal{K})$.

So in particular $E(\{y\})$, the (finite) self-energy of a single atom at $y \in \mathbb{R}^3$, is the same for all $y \in \mathbb{R}^3$.

Remarks:

(i) By assumption 2.1.7 we could restrict to injective y. This would result in energy errors as small as we wish.

(ii) The last requirement can be weakened to situations where E is merely translational invariant and more than one species of atoms is involved. In the latter case one has to assume some periodicity condition. Also systems of distinguishable particles as arise, e.g., in nearest neighbor models can be treated. We will come back to this in paragraph 2.2.6.

(iii) Energy functions E satisfying 2.1.6 and 2.1.7 will be called *admissible* in the sequel. Note that the set of admissible E forms a vector space.

(iv) The assumption on the Lipschitz continuity can be rephrased by requiring that $\|\nabla E\|_{l^\infty(N)}$ be bounded, i.e., there be a universal Lipschitz constant when the state space $\mathbb{R}^N$ is equipped with the $l^1(N)$-norm rather than with the $l^\infty(N)$-norm. Then the Lipschitz constant (for the usual norm) in a C-neighborhood of U can be chosen as $L \cdot \#\mathcal{K}$, where L might depend on C, c_1, c_2, but is independent of $\mathcal{K}$.

(v) In paragraph 2.2.5 we will see that the boundedness assumptions on ψ and $\partial E / \partial y_i$ can be weakened. Then also energies that become infinitely large as the distance between two atoms tends to zero can be considered.

In lemma 2.1.2 we saw how the condition $\|y - U\| \leq C$ led to a "far field minimal strain hypothesis" $|y(x) - y(z)| \geq C_1|x - z| - C_3$ (with C_1, C_3 depending on C). In fact, many interesting systems satisfy the above assumptions in a more restrictive sense:

Assumption 2.1.8 *Assume that ψ and L of assumption 2.1.6 resp. 2.1.7 depend only on C_1 and C_3 where y satisfies $|y(x) - y(z)| \geq C_1|x - z| - C_3$.*

This assumption has far reaching consequences as will be detailed in chapter 3. For the derivation of continuum theory in this chapter, we will not make use of this.

2.2 Passage to continuum theory

Having defined the variables of continuum theory u and $b^1, \dots, b^{\nu-1}$, our aim is to calculate a limit energy $E(u, \mathbf{b})$ as a variational limit of $E(y^{(k)})$ as $y^{(k)}$ tends to $(u, \mathbf{b})$. We will prove that this limit exists and give an integral expression in terms of some macroscopic energy density φ. Furthermore, we will prove a representation formula for φ. The results will be extended to other atomic systems, in particular to systems with unbounded (pair-) interaction potential.

2.2.1 Main results

Suppose E satisfies assumptions 2.1.6 and 2.1.7, and a relaxation parameter $c_0 > 0$ is chosen. Our main result is the following variational convergence result in the spirit of Γ-convergence:

Theorem 2.2.1 *There exists a macroscopic stored energy function φ such that,*

(i) if $y^{(k)} \to (u, \mathbf{b})$, $(u, \mathbf{b})$ admissible, then

$$\liminf_{k\to\infty} E(y^{(k)}) \geq E(u, \mathbf{b}).$$

(ii) For all admissible $(u, \mathbf{b})$ there exists a sequence $y^{(k)} \to (u, \mathbf{b})$ such that

$$\lim_{k\to\infty} E(y^{(k)}) = E(u, \mathbf{b}).$$

Here, $E(u, \mathbf{b})$ is the macroscopic energy

$$E(u, \mathbf{b}) = \int_{\mathcal{S}_1} \varphi(\nabla u, b^1, \ldots, b^{\nu-1}). \tag{2.11}$$

In proving this theorem our strategy will be to first reduce to homogeneous conditions and study the limit for affine u and constant b^i. Assuming this in (2.11) leads to defining φ by solving a cell problem

$$\varphi(A, \mathbf{b}) = \liminf \frac{1}{\nu k^2} E(y^{(k)}) \quad \text{ as } y^{(k)} \to (A, \mathbf{b}) \tag{2.12}$$

for matrices $A \in \mathbb{R}^{3\times 2}$ of rank 2 and admissible vectors $b^i \in \mathbb{R}^3$. However, it turns out that there is a more explicit formula for φ. Let

$$\hat{\mathcal{N}}_k^{0,1}(A, \mathbf{b}) = \left\{ y : \mathcal{L}_k \to \mathbb{R}^3 : \|y - A\| \leq c_0 \text{ and } \frac{1}{(k+1)^2} \sum_{x \in \mathbb{Z}^2 \cap \mathcal{S}_k} \Delta^i y(x) = b^i \right\}. \tag{2.13}$$

Then we have the following representation result:

Theorem 2.2.2 *The macroscopic energy density φ of theorem 2.2.3 (and formula (2.12)) is given by*

$$\varphi(A, \mathbf{b}) = \lim_{k\to\infty} \frac{1}{\nu k^2} \inf_{y \in \hat{\mathcal{N}}_k^{0,1}(A, \mathbf{b})} E(y). \tag{2.14}$$

This limit is uniform on compact subsets of $\mathcal{A}_{\mathrm{hom}}$ and depends continuously on $A, \mathbf{b}$.

Here, $\mathcal{A}_{\mathrm{hom}} \subset \mathbb{R}^{3\times 2} \times (\mathbb{R}^3)^{\nu-1}$, the homogeneous version of $\mathcal{A}$ consisting of *admissible* matrices A and vectors $\mathbf{b}$, is defined by

$$\begin{aligned} \mathcal{A}_{\mathrm{hom}} := \{ & (A, b^1, \ldots, b^{\nu-1}) : \mathrm{rank}(A) = 2, \\ & \exists\, b^0 \in \mathbb{R}^3 \text{ s.t. } |b^0|, \max_{1\leq i\leq \nu-1} |b^i - b^0| \leq c_0 \}. \end{aligned}$$

Measuring convergence of $k\Delta^i \tilde{y}^{(k)}$ in terms of negative Sobolev norms, we get the following sharper version of theorem 2.2.1. In terms of the weak neighborhoods to be introduced in the next paragraph, we will see that this amounts to arbitrarily prescribing the scale of convergence of averages as long as the areas over which to take averages are large compared to atomic dimensions.

Theorem 2.2.3 *Suppose $l = l(k)$ is such that $l(k) \to 0$ and $kl(k) \to \infty$ as $k \to \infty$. Let*

$$\mathcal{W}_k^l(u, \mathbf{b}) := \{y : \|\tilde{y} - u\| \le c_0/k,\ \|k\Delta^i \tilde{y} - b^i\|_{W^{-1,\infty}} \le l\},$$

where $\|f\|_{W^{-1,\infty}} := \sup\left\{\int f \cdot \chi \ : \ \chi \in W_0^{1,1},\ \|\chi\|_{W_0^{1,1}} = \int |\nabla\chi|_2 = 1\right\}$. *Then*

$$\lim_{k\to\infty} \frac{1}{\nu k^2} \inf_{y \in \mathcal{W}_k^l(u,\mathbf{b})} E(y) = \int_{\mathcal{S}_1} \varphi(\nabla u(x), \mathbf{b}) dx.$$

In paragraph 2.2.6 we will sketch how to extend these results to certain finite range interaction models for distinguishable particle systems.

For many physically interesting models the requirement that the splitting function ψ be bounded (cf. (2.10)) is too restrictive. More generally, we should allow for energy contributions tending to infinity when atoms are getting very close.

Theorem 2.2.4 *Suppose the energy is of the form*

$$E(y) = \frac{1}{2} \sum_{i \neq j} W(|y_i - y_j|) + E_0(y), \tag{2.15}$$

where E_0 satisfies the usual assumptions (cf. paragraph 2.1.2, also interactions as in (2.49) are allowed for E_0), but $W(r)$ becomes infinitely large as r tends to zero. For any $r_0 > 0$ we assume that W is Lipschitz on $[r_0, \infty)$ and there exist $M = M(r_0) \in \mathbb{R}$ and $q = q(r_0) > 3$ such that for (a.e.) $r \ge r_0$

$$|W(r)| \le M r^{-q} \quad \text{and} \quad |W'(r)| \le M r^{-q+1}.$$

Then theorem 2.2.1 extends to energy functions of the form (2.15) where, as in theorem 2.2.2, $\varphi : \mathcal{A}_{\mathrm{hom}} \to (-\infty, \infty]$ is given by (2.14) and is continuous as a function with values in $\mathbb{R} \cup \{\infty\}$.

Considering $W^{1,\infty}$-weak*-converging sequences $\tilde{y}^{(k)}$, it is natural to measure deviations from u in L^∞-norm, resp. $\|\cdot\|$. Our choice

$$\|\tilde{y} - u\| \le l_1(k)$$

with $l_1(k) := c_0/k$ corresponds to a relaxation regime where the individual atoms are allowed to move in a region comparable to atomic dimensions. As is shown in theorem 3.1.4, if assumption 2.1.8 holds, $l_1 = c_0/k$ is in fact the only scale which both accounts for atomistic relaxation and yields a non-trivial continuum theory. Moreover, we can not relax sending the parameter c_0 to infinity. This is due to our (physically reasonable) decay assumptions on the energy (cf. assumption 2.1.6). The main point is that finite c_0 prevents fracture from happening. Mathematically this could also be achieved by assuming growth conditions on the inter-atomic forces tending to infinity as the distance between initially close atoms becomes large. But this is physically not realistic. In our approach c_0 enters as a parameter. By its physical interpretation as an upper bound for the deviation of atoms from their macroscopic limit, however, applicability of the theory should be decidable on physical grounds.

Following the proofs in the next paragraphs, it is possible (but tedious) to give explicit error bounds under suitable regularity assumptions on ∇u and $\mathbf{b}$ (e.g., requiring them to be (Hölder-)continuous).

2.2.2 Preparations

We are now going to prove these results. Note that in all that follows, k is understood to be sufficiently large, even if not explicitly stated. The constants that will appear in the energy estimates for deformations near some limiting deformation u will depend on u, but only through the constants c_1, c_2 (cf. below and assumptions 2.1.6 and 2.1.7). If in addition assumption 2.1.8 is satisfied, they will only depend on C_1, C_3 (cf. assumption 2.1.8).

Splitting lemmas

We begin our derivation by proving some preparatory lemmas on deformations being close to some admissible u on a part of $\mathcal{S}_1$. So let $\Omega \subset \mathcal{S}_1$ (usually some mesoscopic sub-square), and consider deformations $y : k\Omega \times [0,h] \to \mathbb{R}^3$. Throughout this paragraph $u : \Omega \to \mathbb{R}^3$ (U in un-rescaled variables) shall satisfy

$$c_1|x - z| \leq |u(x) - u(z)| \leq c_2|x - z|$$

for some $0 < c_1 \leq c_2$ and all $x, z \in \Omega$.

From assumption 2.1.6, the following lemma is easily proven by induction.

Lemma 2.2.5 *If $\mathcal{M}_1, \ldots, \mathcal{M}_n \subset y(\mathcal{L} \cap (\Omega \times [0,h]))$ are pairwise disjoint sets of atoms and $\|\tilde{y} - u\| \leq c/k$, then the following inequality holds:*

$$\left| E(\mathcal{M}_1 \cup \ldots \cup \mathcal{M}_n) - \sum_{j=1}^{n} E(\mathcal{M}_j) \right| \leq \sum_{1 \leq i < j \leq n} \sum_{\substack{v \in \mathcal{M}_i, \\ w \in \mathcal{M}_j}} \psi(|v - w|).$$

The next lemma quantifies the energy for subsets of atoms. It is important as it allows to control the loss of energy when neglecting a (small) set of atoms of the configuration. In particular we will see that $E(\mathcal{M}) = \mathcal{O}(\#\mathcal{M})$. Again we are considering deformations $y : k\Omega \times [0,h] \to \mathbb{R}^3$.

Lemma 2.2.6 *Let y be a deformation satisfying $|\tilde{y} - u| \leq c/k$ and $\mathcal{K} \subset \mathcal{L} \cap (k\Omega \times [0,h])$. Then there is a constant C (not depending on $\mathcal{K}$) such that, if $\mathcal{K} = \mathcal{K}_1 \cup \mathcal{K}_2$ for disjoint $\mathcal{K}_1$ and $\mathcal{K}_2$, then*

$$|E(y(x) : x \in \mathcal{K}) - E(y(x) : x \in \mathcal{K}_1)| \leq C\#\mathcal{K}_2.$$

Proof. From lemma 2.2.5 we deduce that

$$\left| E(y(\mathcal{K})) - E(y(\mathcal{K}_1)) - \sum_{z\in\mathcal{K}_2} E(\{y(z)\}) \right| \le \sum_{\substack{x\in\mathcal{K}\\ z\in\mathcal{K}_2}} \psi(|y(x)-y(z)|).$$

By (remark (ii) after) lemma 2.1.2 there are constants C_1 and C_3 such that

$$C_1|x-z| - C_3 \le |y(x)-y(z)| \ \forall x, z \in \mathcal{S}_k \times [0,h].$$

Now fix $z_0 \in \mathcal{K}_2$, $y_0 = y(z_0)$. We will estimate $\sum_{x\in\mathcal{K}} \psi(|y(x)-y_0|)$ by splitting it into a short-range and a long-range part. Let $\delta = 2C_3/C_1$. Since the number of $x \in \mathcal{K}$ such that $|z_0 - x| \le \delta$ is bounded, we find

$$\sum_{\{x:|x-z_0|\le\delta\}} \psi(|y(x)-y_0|) \le CM,$$

M being the global bound on ψ.

Now if $|x-z_0| > \delta$, then $\frac{C_1}{2}|x-z_0| < |y(x)-y_0|$, and we can estimate

$$\begin{aligned}
\sum_{\{x:|x-z_0|>\delta\}} \psi(|y(x)-y_0|) &\le \sum_{\{x:|x-z_0|>\delta\}} M|y(x)-y_0|^{-q} \\
&\le \sum_{\{x:|x-z_0|>\delta\}} M\left(\frac{C_1}{2}\right)^{-q} |x-z_0|^{-q} \\
&\le C \sum_{\substack{\{x\in\mathcal{L}:\ x\neq 0,\\ 0\le x_3\le h\}}} |x|^{-q}.
\end{aligned}$$

Since $q > 2$, this last expression is bounded by lemma A.1 (with $a = 1$).

It follows that

$$|E(y(\mathcal{K})) - E(y(\mathcal{K}_1))| \ \le \ \left|\sum_{z\in\mathcal{K}_2} E(\{y(z)\})\right| + \sum_{z\in\mathcal{K}_2} C \ \le \ C\#\mathcal{K}_2$$

by frame indifference of the energy. □

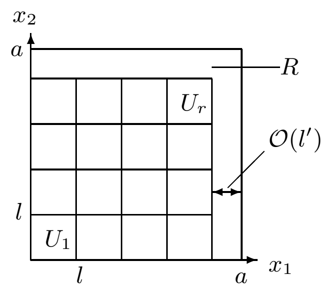
As an immediate consequence we get

Corollary 2.2.7 *Let y, y' be two deformations satisfying the hypotheses of lemma 2.2.6 and $\mathcal{K} \subset \mathcal{L} \cap (k\Omega \times [0,h])$. Then there is a constant C such that*

$$\big|E(y(x) : x \in \mathcal{K}) - E(y'(x) : x \in \mathcal{K})\big| \le C\#\{x \in \mathcal{K} : y(x) \neq y'(x)\}.$$

Proof. Apply lemma 2.2.6 with $\mathcal{K}_2 = \{x \in \mathcal{K} : y(x) \neq y'(x)\}$ to y and y'. □

Suppose $Q = [0,a)^2$, $a \le 1$, is partitioned by squares $U_1, \dots, U_r$ of side-length l where $1/k \le l \le a$ plus some rest R with $|R| = \mathcal{O}(a \cdot l')$, $l' \ll a$, as in the following picture. (Then $r \sim (a/l)^2$.)



We need to estimate the error when replacing the full energy by the sum of the energies over the sets U_i. Let $\mathcal{K}_i = \mathcal{L} \cap (kU_i \times [0,h])$, $\mathcal{K} = \mathcal{L} \cap (kQ \times [0,h])$.

Lemma 2.2.8 *Suppose $y : kQ \times [0,h]$ satisfies $|\tilde{y} - u| \leq c/k$ for some admissible u. Then*

$$E(y(x) : x \in \mathcal{K}) = \sum_{i=1}^{r} E(y(x) : x \in \mathcal{K}_i) + \mathcal{O}(ka^2/l) + \mathcal{O}(k^2 a l').$$

Proof. By lemma 2.2.6 we get

$$\left| E(y(x) : x \in \mathcal{K}) - E(y(x) : x \in \bigcup_{i=1}^{r} \mathcal{K}_i) \right| = \mathcal{O}(k^2 a l'). \tag{2.16}$$

Lemma 2.2.5 implies that

$$\left| E(y(x) : x \in \bigcup_{i=1}^{r} \mathcal{K}_i) - \sum_{i=1}^{r} E(y(x) : x \in \mathcal{K}_i) \right| \leq \frac{1}{2} \sum_{i \neq j} \sum_{\substack{x \in \mathcal{K}_i \\ z \in \mathcal{K}_j}} \psi(|y(x) - y(z)|).$$

Again we will estimate this error term on the right hand side by splitting it into a short range term (1) where $|x - z| \leq \delta$ and a long range term (2) where $|x - z| > \delta$, $\delta := 2C_3/C_1$.

1. Short range term: Since $|\psi| \leq M$, we have

$$\frac{1}{2} \sum_{i \neq j} \sum_{\substack{x \in \mathcal{K}_i \\ z \in \mathcal{K}_j \\ |x-z| \leq \delta}} \psi(|y(x) - y(z)|) \leq \frac{1}{2} \sum_{i \neq j} \sum_{\substack{x \in \mathcal{K}_i \\ z \in \mathcal{K}_j \\ |x-z| \leq \delta}} M.$$

For fixed $x \in \mathcal{K}_i$, the number of $z \in \mathcal{L}$ with $|x - z| \leq \delta$ is bounded. On the other hand, in order to have at least one $z \in \mathcal{K}_j$ with $|x - z| \leq \delta$ and $i \neq j$, we must have $\operatorname{dist}(x_p, \partial(kU_i)) \leq \delta$. For fixed i, the number of these x is bounded by Ckl, C constant. This yields

$$\frac{1}{2} \sum_{i \neq j} \sum_{\substack{x \in \mathcal{K}_i \\ z \in \mathcal{K}_j \\ |x-z| \leq \delta}} M \;\leq\; \frac{1}{2} \sum_{i} \sum_{\substack{x \in \mathcal{K}_i \\ \operatorname{dist}(x_p, \partial kU_i) \leq \delta}} CM \;\leq\; \frac{1}{2} \sum_{i} Ckl \;\leq\; Cka^2/l.$$

2. Long range term: As in the proof of lemma 2.2.6, $|x-z|>\delta$ implies $|y(x)-y(z)|>\frac{C_1}{2}|x-z|$ and thus

$$\frac{1}{2}\sum_{i\neq j}\sum_{\substack{x\in\mathcal{K}_i\\ z\in\mathcal{K}_j\\ |x-z|>\delta}}\psi(|y(x)-y(z)|)\ \le\ C\sum_{i\neq j}\sum_{\substack{x\in\mathcal{K}_i\\ z\in\mathcal{K}_j\\ |x-z|>\delta}}|x-z|^{-q},$$

C some constant. Now for fixed $x\in\mathcal{K}_i$ with $\mathrm{dist}(x_p,\partial(kU_i)) =: d(x)=d$ we have by lemma A.1 (i fixed)

$$C\sum_{j\neq i}\sum_{\substack{z\in\mathcal{K}_j\\ |x-z|>\delta}}|x-z|^{-q}\le C\sum_{\substack{z\in\mathcal{L},0\le z_3\le h\\ |x-z|\ge\max\{\delta,d\}}}|x-z|^{-q}\le C\left(\max\{\delta,d\}\right)^{2-q}.$$

So we obtain for i fixed:

$$\frac{1}{2}\sum_{j\neq i}\sum_{\substack{x\in\mathcal{K}_i\\ z\in\mathcal{K}_j\\ |x-z|>\delta}}\psi(|y(x)-y(z)|)\le C\sum_{x\in\mathcal{K}_i}\left(\max\{\delta,d(x)\}\right)^{2-q}. \tag{2.17}$$

The number of x with $d(x)\le\delta$ is bounded by Ckl. So summing over these x will give a term of order $C\delta^{2-q}kl=Ckl$ in (2.17). Now let x be such that $d(x)>\delta$. There exists a unique $m\in\mathbb{N}_0$ such that $d\in(\delta+m,\delta+m+1]$. The number of points x corresponding to the same m is bounded by $C\nu(kl-2(\delta+m))\le Ckl$. So ($i$ fixed)

$$\begin{aligned}\sum_{\substack{x\in\mathcal{K}_i\\ \text{with } d(x)>\delta}}d^{2-q}\ &\le\ \sum_m\sum_{\substack{x\in\mathcal{K}_i\text{with}\\ d(x)\in(\delta+m,\delta+m+1]}}(\delta+m)^{2-q}\ \le\ \sum_{m=0}^{\infty}Ckl\,(\delta+m)^{2-q}\\ &\le\ Ckl\left[\delta^{2-q}+\sum_{m\ge\delta}m^{2-q}\right]\ \le\ Ckl[\delta^{2-q}+C\delta^{3-q}]\end{aligned}$$

by lemma A.1 with $c=0$. Hence this part of the sum is also bounded by Ckl.

So finally summing over i we get the following upper bound for the long range term:

$$Crkl\le Cka^2/l.$$

This is the same bound as for the short range term. We have thus shown that the remaining error term is indeed $\mathcal{O}(ka^2/l)$. Together with (2.16) this yields the desired estimate. □

Weak neighborhoods

It is illuminating to describe deformations that we will take into account for atomic energy relaxation more directly by weak neighborhoods about the limit points u and $\mathbf{b}$ in terms of the atomic positions. To do so, we consider mesoscopic local averages. As before, set $\rho=\rho^{(k)}=\sum_{x\in\mathbb{Z}^2}\delta_{x/k}$. Let $Q\subset\mathcal{S}_1$ be a sub-square of side-length l_4, and recall the definition of $\bar{\mathbf{b}}$ from (2.8). For admissible u, $\mathbf{b}$ define:

Definition 2.2.9 *A deformation $y : \mathcal{L} \cap (kQ \times [0,h]) \to \mathbb{R}^3$ (resp. its interpolation) belongs to the weak neighborhood*

(i) $\mathcal{N}_{k,Q}^{l_1,l_2,l_3}(u,\mathbf{b})$ of $(u,\mathbf{b})$, $l_3 < l_4$ if

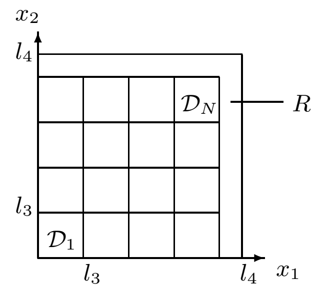
$$\|\tilde{y} - u\| \le l_1 \quad \text{and} \quad \left| \fint_{\mathcal{D}} k\Delta^i \tilde{y} - \bar{b}^i d\rho \right| \le l_2 \tag{2.18}$$

for all translates $\mathcal{D}$ of $[0,l_3)^2$ with $\mathcal{D} \subset \mathcal{S}_1$, or

(ii) $\hat{\mathcal{N}}_{k,Q}^{l_1,l_2,l_3}(u,\mathbf{b})$ of $(u,\mathbf{b})$, $l_3 < l_4$ if

$$\|\tilde{y} - u\| \le l_1 \quad \text{and} \quad \left| \fint_{\mathcal{D}_j} k\Delta^i \tilde{y} - \bar{b}^i d\rho \right| \le l_2 \tag{2.19}$$

for all $j = 1, \dots, N$, where $\{\mathcal{D}_j\}$ is a partition of Q into squares $\mathcal{D}_j$ of side-length l_3 (up to some rest R of measure $|R| = \mathcal{O}(l_3 l_4)$) as in the following picture.



In case $l_3 = l_4$ we require that (2.18) resp. (2.19) holds with $\mathcal{D} = Q$ resp. $\mathcal{D}_1 = Q$.

Remark: Clearly, $\mathcal{N}_{k,Q}^{l_1,l_2,l_3}(u,\mathbf{b}) \subset \hat{\mathcal{N}}_{k,Q}^{l_1,l_2,l_3}(u,\mathbf{b})$, and V as defined in (2.9) lies in $\mathcal{N}_{k,Q}^{l_1,l_2,l_3}(u,\mathbf{b})$ for admissible $(u,\mathbf{b})$ and $l_1 = c_0/k$. Since we will mainly deal with the choice $l_1 = c_0/k$, we will drop l_1 from our notation.

Suppose $\Omega \subset \mathcal{S}_1$, and for the next lemma assume $\mathbf{b} \in L^\infty(\Omega; (\mathbb{R}^3)^{\nu-1})$ satisfies a stronger compatibility condition: there exists $b^0 \in L^\infty(\Omega;\mathbb{R}^3)$ such that

$$\|b^0\|_\infty, \|b^i - b^0\|_\infty \le c_3 \tag{2.20}$$

for all $i \in \{1, \dots, \nu - 1\}$ and some constant $0 < c_3 < c_0$. So $v : \Omega \to \mathbb{R}^3$ as defined in (2.9) satisfies $\|v - u\| \le c_3$.

Lemma 2.2.10 *Suppose $\|y - U\| \le c_0 + \delta$, $0 \le \delta \le c$. Then there exists y' with $\|y' - U\| \le c_0$ such that*

$$\left| \fint_D k\Delta^i \tilde{y}' d\rho - \fint_D \bar{b}^i d\rho \right| \le \frac{c_0 - c_3}{c_0 - c_3 + \delta} \left| \fint_D k\Delta^i \tilde{y} d\rho - \fint_D \bar{b}^i d\rho \right|$$

whenever $D \subset \Omega$, $\rho(D) > 0$, and

$$|E(y(x) : x \in \mathcal{L} \cap (k\Omega \times [0,h])) - E(y'(x) : x \in \mathcal{L} \cap (k\Omega \times [0,h]))| \le C\rho(\Omega)\delta,$$

where $C = L\nu\frac{c_0+c_3}{c_0-c_3}$, L as in assumption 2.1.7.

Proof. Let v be as in (2.9), and define y' such that

$$\tilde{y}' := \lambda \tilde{y} + (1-\lambda)v, \quad \lambda = \frac{c_0 - c_3}{c_0 - c_3 + \delta}. \tag{2.21}$$

Then indeed by (2.20),

$$\|\tilde{y}' - u\| \le \lambda \|\tilde{y} - u\| + (1-\lambda)\|v - u\| \le \lambda \frac{c_0+\delta}{k} + (1-\lambda)\frac{c_3}{k},$$

whence $\|y' - U\| \le c_0$. For the local averages observe that

$$\int_D k\Delta^i \tilde{y}' - \bar{b}^i d\rho = \lambda \int_D k\Delta^i \tilde{y} - \bar{b}^i d\rho.$$

Now since $\tilde{y} = \frac{1}{\lambda}\tilde{y}' - \frac{1-\lambda}{\lambda}v$,

$$\|\tilde{y} - \tilde{y}'\| \le \frac{1-\lambda}{\lambda}(\|\tilde{y}' - u\| + \|u - v\|) \le \frac{\delta}{c_0 - c_3}(c_0/k + c_3/k).$$

By (remark (iv) after) assumption 2.1.7 the claim follows. □

In general, such a uniform bound c_3 on $\mathbf{b}$ does not exist. So we prove:

Lemma 2.2.11 *Let $\mathcal{D}_j$ be as in definition 2.2.9. Suppose $|⨍_{\mathcal{D}_j}(k\Delta^i\tilde{y} - \bar{b}^i)d\rho| \le \delta \le 1$, $j = 1, \ldots, N$, and $\|y - U\| \le c_0 + \varepsilon$, $\varepsilon \le 1$. Then there exists y' with $\|y' - U\| \le c_0$,*

$$\left| ⨍_{\mathcal{D}_j} (k\Delta^i \tilde{y}' - \bar{b}^i) d\rho \right| \le \delta, \quad \textit{and} \quad |E(y) - E(y')| \le C(\varepsilon^{1/5} + \delta^{1/4})(kl_4)^2.$$

Proof. We may assume that $\bar{b}^i$ is constant on the sets $\mathcal{D}_j$ (else for $x \in \mathcal{D}_j$ replace $\bar{b}^i(x)$ by $⨍_{\mathcal{D}_j} \bar{b}^i d\rho$ in the sequel). Let $\varepsilon' = \varepsilon^{4/5}$. First consider those $\mathcal{D}_j$ where there do not exist b^0 and $c_3 \le c_0 - \varepsilon'$ as in the previous lemma. Choose $\bar{b}^0 \in \mathbb{R}^3$ minimizing

$$\max\left\{ \max_{1 \le i \le \nu - 1} |\bar{b}^i - \bar{b}^0|, |\bar{b}^0| \right\} \qquad (\le c_0).$$

Set

$$B^i = \bar{b}^{i-1} - \bar{b}^0 \quad \text{for } i = 2, \ldots, \nu, \qquad B^1 = -\bar{b}^0, \tag{2.22}$$

and define Y^i and $\overline{Y^i}$ by

$$Y^i(x_p) = k(\tilde{y}(x_p, i-1) - u(x_p)), \quad \overline{Y^i} = ⨍_{\mathcal{D}_j} Y^i d\rho \tag{2.23}$$

for $i = 1, \ldots, \nu$. Then

$$\left| (\overline{Y^i} - \overline{Y^j}) - (B^i - B^j) \right| \le 2\delta \quad \text{for } i, j \in \{1, \ldots, \nu\},$$

in particular for $a = \overline{Y^1} - B^1$,

$$\left| \overline{Y^i} - (B^i + a) \right| \le 2\delta.$$

Since $|Y^i| \le c_0 + \varepsilon$, we also have $|\overline{Y^i}| \le c_0 + \varepsilon$, and it follows that $|B^i + a| \le c_0 + \varepsilon + 2\delta$. By our choice of $\bar{b}^0$ there is an i_0 with $|B^{i_0}| \ge c_0 - \varepsilon'$ such that $a \cdot B^{i_0} \ge 0$, so $|B^{i_0} + a|^2 \ge (c_0 - \varepsilon')^2 + a^2$. But then $|a| = \mathcal{O}(\sqrt{\varepsilon + \varepsilon' + 2\delta})$, i.e.,

$$\left|\overline{Y^i} - B^i\right| \le C\sqrt{\varepsilon' + \delta} \qquad \text{for } i = 1, \dots, \nu. \tag{2.24}$$

Now suppose i is such that $|B^i| \ge c_0 - \varepsilon'$. To estimate $|Y^i - B^i|$, assume without loss of generality that $\overline{Y^i} = (\overline{Y^i_1}, 0, 0)$, $\overline{Y^i_1} \ge c_0 - C\sqrt{\varepsilon' + \delta}$. Since $|Y^i(z)| \le c_0 + \varepsilon$ for $z \in \frac{1}{k}\mathbb{Z}^2 \cap \mathcal{D}_j$,

$$\begin{aligned}
\sum_{z \in \frac{1}{k}\mathbb{Z}^2 \cap \mathcal{D}_j} \left|Y^i_1(z) - \overline{Y^i_1}\right| &\le \sum_{\substack{z \in \frac{1}{k}\mathbb{Z}^2 \cap \mathcal{D}_j \\ Y^i_1(z) > \overline{Y^i_1}}} Y^i_1(z) - \overline{Y^i_1} + \sum_{\substack{z \in \frac{1}{k}\mathbb{Z}^2 \cap \mathcal{D}_j \\ Y^i_1(z) \le \overline{Y^i_1}}} \overline{Y^i_1}(z) - Y^i_1 \\
&= 2 \sum_{\substack{z \in \frac{1}{k}\mathbb{Z}^2 \cap \mathcal{D}_j \\ Y^i_1(z) > \overline{Y^i_1}}} Y^i_1(z) - \overline{Y^i_1} + \sum_{z \in \frac{1}{k}\mathbb{Z}^2 \cap \mathcal{D}_j} \overline{Y^i_1}(z) - Y^i_1 \\
&\le 2 \sum_{\substack{z \in \frac{1}{k}\mathbb{Z}^2 \cap \mathcal{D}_j \\ Y^i_1(z) > \overline{Y^i}_1}} C\sqrt{\varepsilon' + \delta} + 0 \\
&\le C(kl_3)^2\sqrt{\varepsilon' + \delta}.
\end{aligned}$$

The second and third component can be estimated by noting that

$$|Y^i_m(z)|^2 \le 2(c_0 + \varepsilon)(c_0 + \varepsilon - Y^i_1(z)) \le C(c_0 + \varepsilon)(|\overline{Y^i_1} - Y^i_1(z)| + \sqrt{\varepsilon' + \delta})$$

for $m = 2, 3$, hence also

$$\begin{aligned}
\sum_{z \in \frac{1}{k}\mathbb{Z}^2 \cap \mathcal{D}_j} \left|Y^i_m(z) - \overline{Y^i_m}\right| &\le C \sum_{z \in \frac{1}{k}\mathbb{Z}^2 \cap \mathcal{D}_j} \sqrt{\left|Y^i_1(z) - \overline{Y^i_1}\right|} + \sqrt[4]{\varepsilon' + \delta} \\
&\le C\left(\# \frac{1}{k}\mathbb{Z}^2 \cap \mathcal{D}_j\right)^{1/2} \left(\sum_{z \in \frac{1}{k}\mathbb{Z}^2 \cap \mathcal{D}_j} \left|Y^i_1(z) - \overline{Y^i_1}\right|\right)^{1/2} \\
&\quad + C(kl_3)^2\sqrt[4]{\varepsilon' + \delta} \\
&\le Ckl_3\left(C(kl_3)^2\sqrt{\varepsilon' + \delta}\right)^{1/2} + C(kl_3)^2\sqrt[4]{\varepsilon' + \delta} \\
&= C(kl_3)^2\sqrt[4]{\varepsilon' + \delta}.
\end{aligned}$$

Together with (2.24) this proves that

$$\sum_{z \in \frac{1}{k}\mathbb{Z}^2 \cap \mathcal{D}_j} \left|Y^i(z) - B^i\right| \le C(kl_3)^2(\sqrt[4]{\varepsilon'} + \sqrt[4]{\delta}). \tag{2.25}$$

Now define a new configuration y'' by replacing Y^i by B^i for those i with $|B^i| \ge c_0 - \varepsilon'$, i.e., Y''^i defined analogously to Y^i equals to B^i for these i and equals Y^i for the other i. By (remark (iv) after) assumption 2.1.7,

$$|E(y'') - E(y)| \le C(\sqrt[4]{\varepsilon'} + \sqrt[4]{\delta})(kl_4)^2.$$

Finally, exactly as in the proof of lemma 2.2.10, we choose $\tilde{y}'$ as a convex combination of $\tilde{y}''$ and v with $c_3 = c_0 - \varepsilon'$. Noting that

$$|E(y') - E(y'')| \leq C\frac{\varepsilon}{\varepsilon'}(kl_4)^2 = C\varepsilon^{1/5}(kl_4)^2$$

finishes the proof. $\square$

We can now investigate the relationship of the various weak neighborhoods.

Lemma 2.2.12 *Suppose u and $\mathbf{b}$ are admissible, and scales $0 \leq l_2, l_2' \leq 1$ and $1/k \leq l_3, l_3' \leq l_4$ are given with $l_2' \gg l_3/l_3'$.*

(i) For all $y \in \hat{\mathcal{N}}^{l_2,l_3}_{k,Q}(u,\mathbf{b})$ there exists $y' \in \hat{\mathcal{N}}^{0,l_3}_{k,Q}(u,\mathbf{b})$ such that

$$|E(y') - E(y)| \leq Cl_2^{1/5}(kl_4)^2.$$

If there is $c_3 < c_0$ such that (2.20) holds, then the error term $\mathcal{O}(k^2 l_4^2 l_2^{1/5})$ may be replaced by $\mathcal{O}(k^2 l_4^2 l_2)$.

(ii) $\hat{\mathcal{N}}^{0,l_3}_{k,Q}(u,\mathbf{b}) \subset \mathcal{N}^{l_2',l_3'}_{k,Q}(u,\mathbf{b})$.

Proof. Let $y \in \hat{\mathcal{N}}^{l_2,l_3}_{k,Q}(u,\mathbf{b})$ be arbitrary. Write Q as a disjoint union of N translates of $[0,l_3)^2$, $\mathcal{D}_1,\ldots,\mathcal{D}_N$, and a rest R whose area is of order $\mathcal{O}(l_3\cdot l_4)$ as in definition 2.2.9 (ii). Set $m_j^i = \fint_{\mathcal{D}_j} k\Delta^i\tilde{y} - \bar{b}^i d\rho$, and define $y_0 : kQ\times[0,h] \to \mathbb{R}^3$ by (interpolation of)

$$\tilde{y}_0(x_p,i) = \begin{cases} \tilde{y}(x_p,0) & \text{for } i=0,\ x_p \in \frac{1}{k}\mathcal{L}\cap\mathcal{D}_j, \\ \tilde{y}(x_p,i) - \frac{1}{k}m_j^i & \text{for } 1\leq i\leq \nu-1,\ x_p \in \frac{1}{k}\mathcal{L}\cap\mathcal{D}_j, \\ \tilde{y}_0(x_p,i) & \text{for } 0\leq i\leq \nu-1,\ x_p \in \frac{1}{k}\mathcal{L}\cap R. \end{cases} \tag{2.26}$$

Then we have

$$\|y_0 - y\| \leq \max_{\substack{1\leq i\leq\nu-1 \\ 1\leq j\leq N}} |m_j^i| \leq l_2 \tag{2.27}$$

since $y \in \hat{\mathcal{N}}^{l_2,l_3}_{k,Q}(u,\mathbf{b})$. In particular, $\|y_0 - U\| \leq c_0 + l_2$. So because $\fint_{\mathcal{D}_j} k\Delta^i\tilde{y}_0 - \bar{b}^i d\rho = 0$ by construction of y_0, invoking lemma 2.2.11 (resp. 2.2.10), we find $y' \in \hat{\mathcal{N}}^{0,l_3}_{k,Q}(u,\mathbf{b})$ satisfying

$$|E(y') - E(y_0)| \leq Cl_2^{1/5}(kl_4)^2 \qquad (\text{resp. } \leq Cl_2(kl_4)^2).$$

Now by (2.27) and the Lipschitz assumption 2.1.7 on E we also have

$$|E(y) - E(y_0)| \leq C(kl_4)^2 l_2.$$

This proves (i).

In order to prove (ii), suppose $y \in \hat{\mathcal{N}}^{0,l_3}_{k,Q}(u,\mathbf{b})$ and $\mathcal{D} \subset \mathcal{S}_1$ is some translate of $[0,l_3')^2$. Let $\mathcal{J}$ be the set of those indices of sets $\mathcal{D}_j$ that intersect $\mathcal{D}$, and set

$$\mathcal{D}' = \bigcup_{j\in\mathcal{J}} \mathcal{D}_j.$$

Then $\rho((\mathcal{D}' \setminus \mathcal{D}) \cup (\mathcal{D} \setminus \mathcal{D}')) \leq Ck^2 l_3 l_3'$, hence since $|k\Delta^i y - b^i|$ is bounded,

$$\begin{aligned}
&\left|\frac{1}{\rho(\mathcal{D})}\int_{\mathcal{D}} k\Delta^i y - \bar{b}^i d\rho - \frac{1}{\rho(\mathcal{D}')}\int_{\mathcal{D}'} k\Delta^i y - \bar{b}^i d\rho\right| \\
&\leq\ C\frac{\rho(\mathcal{D}\setminus\mathcal{D}')}{\rho(\mathcal{D})} + C\frac{\rho(\mathcal{D}'\setminus\mathcal{D})}{\rho(\mathcal{D}')} + \left|\left(\frac{1}{\rho(\mathcal{D})} - \frac{1}{\rho(\mathcal{D}')}\right)\int_{\mathcal{D}\cap\mathcal{D}'} k\Delta^i y - \bar{b}^i d\rho\right| \\
&\leq\ C\frac{k^2 l_3 l_3'}{(kl_3')^2} + C\frac{k^2 l_3 l_3'}{(kl_3')^2} + C\frac{k^2 l_3 l_3'}{(kl_3')^4}(kl_3')^2 \\
&=\ \mathcal{O}(l_3/l_3').
\end{aligned}$$

But $\int_{\mathcal{D}'} k\Delta^i y - \bar{b}^i d\rho = 0$, so

$$\left|⨍_{\mathcal{D}} k\Delta^i y - \bar{b}^i d\rho\right| \leq C\frac{l_3}{l_3'} \leq l_2',$$

i.e., $y \in \mathcal{N}_{k,Q}^{l_2',l_3'}(u, \mathbf{b})$. □

The connection between $\mathcal{W}_k^l(u, \mathbf{b})$ (see theorem 2.2.3) and the neighborhoods defined in definition 2.2.9 is described by the following lemma.

Lemma 2.2.13 *Let $u, \mathbf{b}$ be admissible. Assume $1/k \leq l_3 \ll l$, and $1/k \leq l' \ll l_2' l_3'$. Then*

$$\hat{\mathcal{N}}_k^{0,l_3}(u, \mathbf{b}) \subset \mathcal{W}_k^l(u, \mathbf{b}) \quad \textit{and} \quad \mathcal{W}_k^{l'}(u, \mathbf{b}) \subset \mathcal{N}_k^{l_2',l_3'}(u, \mathbf{b}).$$

Proof. Suppose $y \in \hat{\mathcal{N}}_k^{0,l_3}$ and $f \in W_0^{1,1}(\mathcal{S}_1; \mathbb{R}^3)$ with $\|f\|_{W_0^{1,1}} = 1$, w.l.o.g. f smooth. Choose $x_j \in \mathcal{D}_j$ such that $|\nabla f(x_j)| \cdot |\mathcal{D}_j| \leq \int_{\mathcal{D}_j} |\nabla f(x_j)|$. Then

$$\begin{aligned}
&\int_{\mathcal{S}_1} f \cdot (k\Delta^i \tilde{y} - b^i) \\
&=\ \frac{1}{k^2}\int_{\mathcal{S}_1} f \cdot (k\Delta^i \tilde{y} - \bar{b}^i) d\rho + \mathcal{O}(1/k) \\
&=\ \frac{1}{k^2}\sum_j \int_{\mathcal{D}_j} f \cdot (k\Delta^i \tilde{y} - \bar{b}^i) d\rho + \mathcal{O}(1/k + l_3) \\
&=\ \frac{1}{k^2}\sum_j \int_{\mathcal{D}_j} \Big(f(x_j) + \nabla f(x_j)(x - x_j) + o(l_3)\Big) \cdot (k\Delta^i \tilde{y} - \bar{b}^i) d\rho + \mathcal{O}(l_3) \\
&\leq\ \frac{1}{k^2}\sum_j \int_{\mathcal{D}_j} |\nabla f(x_j)||x - x_j| \cdot |(k\Delta^i \tilde{y} - \bar{b}^i)| d\rho + \mathcal{O}(l_3) \\
&\leq\ \frac{1}{k^2}\sum_j \int_{\mathcal{D}_j} C|\nabla f(x_j)|\sqrt{2} l_3 + \mathcal{O}(l_3) \\
&\leq\ C(1 + \|\nabla f\|_{L^1}) l_3 \ \leq\ C l_3 \ \ll\ l,
\end{aligned}$$

i.e., $y \in \mathcal{W}_k^l(u, \mathbf{b})$. This proves $\hat{\mathcal{N}}_k^{0,l_3}(u, \mathbf{b}) \subset \mathcal{W}_k^l(u, \mathbf{b})$.

Now suppose $y \in \mathcal{W}_k^{l'}(u, \mathbf{b})$, and let $\mathcal{D}$ be some translate of $[0, l_3')^2 \subset \mathcal{S}_1$. Consider the function f_a with support in $\mathcal{D}$ and

$$f_a(x) = \frac{1}{4l_3'} \min\{1, \frac{1}{a}\text{dist}(x, \partial\mathcal{D})\} e$$

for $x \in \mathcal{D}$, $e \in \mathbb{R}^3$ a unit vector. Then for $a \le l_3'/2$,

$$\|f\|_{W_0^{1,1}} = \|\nabla f\|_{L^1} = \frac{1}{4l_3' a} \cdot 4(l_3' - a)a \le 1.$$

In particular, sending $a \to 0$,

$$\left| \frac{1}{4l_3'} \int_{\mathcal{D}} e \cdot (k\Delta^i \tilde{y} - b^i) \right| = \lim_{a \to 0} \left| \int f_a \cdot (k\Delta^i \tilde{y} - b^i) \right| \le l'.$$

This implies

$$\left| \fint_{\mathcal{D}} (k\Delta^i \tilde{y} - \bar{b}^i) d\rho \right| \le \left| \fint_{\mathcal{D}} (k\Delta^i \tilde{y} - b^i) \right| + \frac{C}{kl_3'} \le \frac{Cl'}{l_3'} + \frac{C}{kl_3'} \ll l_2',$$

i.e., $y \in \mathcal{N}_k^{l_2',l_3'}(u, \mathbf{b})$. Therefore, $\mathcal{W}_k^{l'}(u, \mathbf{b}) \subset \mathcal{N}_k^{l_2',l_3'}(u, \mathbf{b})$. □

2.2.3 Proof of theorem 2.2.2

In this paragraph we will prove theorem 2.2.2, the representation formula for φ. Setting

$$\varphi_k(A, \mathbf{b}) = \frac{1}{\nu k^2} \inf_{y \in \hat{\mathcal{N}}_k(A, \mathbf{b})} E(y), \tag{2.28}$$

we need to show that φ_k converges uniformly on compact subsets of $\mathcal{A}_{\text{hom}}$ to some continuous function φ. First, we will show that φ exists as a pointwise limit (cf. proposition 2.2.15), then in the second part of this paragraph we will investigate the continuity properties of the functions φ_k (cf. corollary 2.2.19) leading to the final result.

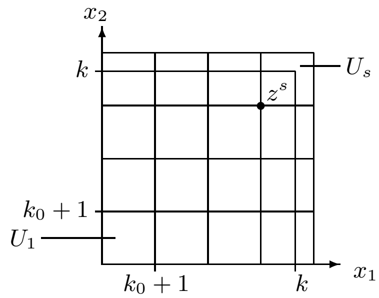
Existence

We start with a preparatory lemma. Throughout this paragraph, $A \in \mathbb{R}^{3\times 2}$ is some admissible matrix and $\mathbf{b} \in (\mathbb{R}^3)^{\nu-1}$ some admissible vector. Set for short $\hat{\mathcal{N}}_k(A, \mathbf{b}) := \hat{\mathcal{N}}_{k,\mathcal{S}_1}^{0,1}(A, \mathbf{b})$.

Lemma 2.2.14 *Suppose $k_0 \in \mathbb{N}$. Then there is a constant C (independent of k_0) such that, if $k > k_0$ is sufficiently large, for every $y \in \hat{\mathcal{N}}_{k_0}(A, \mathbf{b})$ there is a $\hat{y} \in \hat{\mathcal{N}}_k(A, \mathbf{b})$ with*

$$\left| \frac{1}{\nu k^2} E(\hat{y}(x) : x \in \mathcal{L}_k) - \frac{1}{\nu k^2} E(y(x) : x \in \mathcal{L}_{k_0}) \right| \le C \left(\frac{1}{k_0} + \frac{k_0}{k} \right)^{1/5}.$$

Proof. Let $y \in \hat{\mathcal{N}}_{k_0}(A, \mathbf{b})$, and cover $\mathcal{S}_k$ by translates of $[0, k_0 + 1)^2$, denoted $U_1, \ldots, U_s$ as in the following picture:



Let $z^j \in \mathbb{Z}^2$ be the lower left corner of U_j and set $f^j = Az^j$. Then define $y' : S \times [0,h] \to \mathbb{R}^3$ by (interpolation of)

$$y'(x) := y(x - (z_1^j, z_2^j, 0)) + f^j$$

for $x \in \mathcal{L} \cap ((U_j \cap S) \times [0,h]),\ 1 \le j \le s$. It is easy to see that

$$\|y' - A\| \le c_0 \quad \text{and} \quad \left| \fint_{\mathcal{S}_1} k\Delta^i \tilde{y}' d\rho^{(k)} - b^i \right| = \mathcal{O}\left(\frac{k_0}{k}\right).$$

So by lemma 2.2.12 there exists $\hat{y} \in \hat{\mathcal{N}}_k(A, \mathbf{b})$ with

$$\left| \frac{1}{k^2} E(\hat{y}) - \frac{1}{k^2} E(y') \right| \le C \left(\frac{k_0}{k}\right)^{1/5}. \tag{2.29}$$

We estimate the energy of y'. Using lemma 2.2.8 for translates of $[0, \frac{k_0+1}{k})^2$ and denoting the set of indices i for which $U_i \subset \mathcal{S}_k$ by $\mathcal{I}$, we see that

$$\begin{aligned} E(y'(x) : x \in \mathcal{L}_k) &= \sum_{i \in \mathcal{I}} E(y'(x) : x \in \mathcal{L} \cap (U_i \times [0,h])) + \mathcal{O}(k^2/k_0 + kk_0) \\ &= \#\mathcal{I} \cdot E(y(x) : x \in \mathcal{L}_{k_0}) + \mathcal{O}(k^2/k_0 + k_0 k). \end{aligned} \tag{2.30}$$

by the periodic construction of y' and frame indifference. Since $\#\mathcal{I} = \lfloor k/k_0 \rfloor^2 = (k/k_0)^2(1 + \mathcal{O}(k_0/k))$, we obtain from (2.30), noting that $E(y(x) : x \in \mathcal{L}_{k_0}) = \mathcal{O}(k_0^2)$ by lemma 2.2.6,

$$\frac{1}{\nu k^2} E(y'(x) : x \in \mathcal{L}_k) = \frac{1}{\nu k_0^2} E(y(x) : x \in \mathcal{L}_{k_0}) + \mathcal{O}\left(\frac{1}{k_0}\right) + \mathcal{O}\left(\frac{k_0}{k}\right).$$

This finishes the proof by (2.29). □

Recall the definition of φ_k from (2.28).

Proposition 2.2.15 *The limit*

$$\varphi(A, \mathbf{b}) := \lim_{k \to \infty} \varphi_k(A, \mathbf{b})$$

exists in $\mathbb{R}$ *for all admissible* $A, \mathbf{b}$.

Proof. By lemma 2.2.6 we have for $y \in \hat{\mathcal{N}}_k(A, \mathbf{b})$

$$\frac{1}{\nu k^2} E(y(x) : x \in \mathcal{L}_k) = \mathcal{O}(1),$$

so $(\varphi_k(A, \mathbf{b}))_{k \in \mathbb{N}}$ is a bounded sequence. We may therefore define φ by

$$\varphi(A, \mathbf{b}) := \liminf_{k \to \infty} \varphi_k(A, \mathbf{b}).$$

For $\delta > 0$ we may choose arbitrarily large k_0 such that $\varphi_{k_0}(A, \mathbf{b}) < \varphi(A, \mathbf{b}) + \delta/3$. By definition of φ_{k_0}, there also exists $y \in \hat{\mathcal{N}}_{k_0}(A, \mathbf{b})$ satisfying $\frac{1}{\nu k_0^2} E(y) \leq \varphi_{k_0}(A, \mathbf{b}) + \delta/3$. Now let $k > k_0$ be so large that

$$C \left(\frac{1}{k_0} + \frac{k_0}{k} \right)^{1/5} < \delta/3$$

where C is the constant from lemma 2.2.14. Then there is $\hat{y} \in \hat{\mathcal{N}}_k(A, \mathbf{b})$ such that

$$\begin{aligned} \frac{1}{\nu k^2} E(\hat{y}(x) : x \in \mathcal{L}_k) &\leq \frac{1}{\nu k_0^2} E(y(x) : x \in \mathcal{L}_{k_0}) + C \left(\frac{1}{k_0} + \frac{k_0}{k} \right)^{1/5} \\ &< \varphi(A, \mathbf{b}) + \delta/3 + \delta/3 + \delta/3. \end{aligned}$$

It follows $\varphi_k(A, \mathbf{b}) \leq \frac{1}{\nu k^2} E(\hat{y}(x) : x \in \mathcal{L}_k) \leq \varphi(A, \mathbf{b}) + \delta$.

Since, by definition of φ, also $\varphi_k(A, \mathbf{b}) \geq \varphi(A, \mathbf{b}) - \delta$ for k sufficiently large, the proposition is proven. □

Continuity

Here we investigate the remaining parts of theorem 2.2.2, namely if $\varphi_k \to \varphi$ uniformly on compact subsets of $\mathcal{A}_{\text{hom}}$ and if $(A, \mathbf{b}) \mapsto \varphi(A, \mathbf{b})$ is continuous. We start by investigating the continuity properties of φ_k, first with respect to the variables b^i.

Lemma 2.2.16 *Let* $(A, \mathbf{b}), (A, \mathbf{b}') \in \mathcal{A}_{\text{hom}}$. *Then*

$$|\varphi_k(A, \mathbf{b}) - \varphi_k(A, \mathbf{b}')| \leq C \left(\max_{1 \leq i \leq \nu - 1} |b^i - b'^i| \right)^{1/5},$$

C a constant (independent of k, and on A only depending through c_1, c_2 if the singular values $s_1(A) \leq s_2(A)$ of A lie in $[c_1, c_2]$).

Proof. For every $y \in \hat{\mathcal{N}}_k(A, \mathbf{b})$, $|⨍_{\mathcal{S}_1} k \Delta^i \tilde{y} d\rho - b'^i| \leq |b^i - b'^i|$, i.e., $y \in \hat{\mathcal{N}}_{k, \mathcal{S}_1}^{l_2, 1}(A, \mathbf{b}')$ for $l_2 = \max_i |b^i - b'^i|$ fixed. By lemma 2.2.12,

$$\varphi_k(A, \mathbf{b}') = \frac{1}{\nu k^2} \inf_{y' \in \hat{\mathcal{N}}_k(A, \mathbf{b}')} E(y') \leq \frac{1}{\nu k^2} E(y) + C l_2^{1/5}.$$

Taking the infimum over $y \in \hat{\mathcal{N}}_k(A, \mathbf{b})$, we get

$$\varphi_k(A, \mathbf{b}') \leq \varphi_k(A, \mathbf{b}) + C \left(\max_{1 \leq i \leq \nu - 1} |b^i - b'^i| \right)^{1/5}.$$

Now interchanging the roles of $\mathbf{b}$ and $\mathbf{b}'$ finishes the proof. □

In the next lemma we investigate continuity with respect to A.

Lemma 2.2.17 *Let* $(A, \mathbf{b}), (A', \mathbf{b}) \in \mathcal{A}_{\text{hom}}$. *Then there exist constants* $c, C > 0$ *such that*

$$|\varphi_k(A, \mathbf{b}) - \varphi_k(A', \mathbf{b})| \leq k|A - A'|$$

for $|A - A'| < c/k$.

Proof. Let $y \in \hat{\mathcal{N}}_k(A, \mathbf{b})$ and define y' by

$$y'(x) = y(x) - Ax_p + A'x_p.$$

Then $\|y' - y\| \leq |A - A'|\sqrt{2k^2 + h^2} \leq C|A - A'|k$, so by assumption 2.1.7,

$$|E(y') - E(y)| \leq Ck^2|A - A'|k. \tag{2.31}$$

On the other hand, we clearly have $y' \in \hat{\mathcal{N}}_k(A', \mathbf{b})$. Together with (2.31) it follows that $\varphi_k(A', \mathbf{b}) \leq \frac{1}{\nu k^2} E(y) + C|A - A'|k$. Since y was arbitrary, we get

$$\varphi_k(A', \mathbf{b}) \leq \varphi_k(A, \mathbf{b}) + C|A - A'|k.$$

Interchanging the roles of A and A' finishes the proof. □

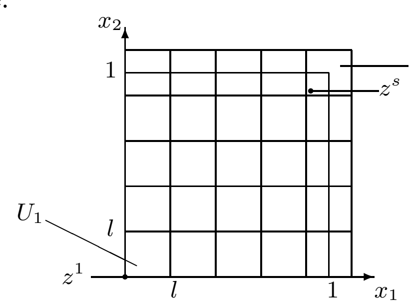
This lemma proves continuity of the φ_k with respect to A. The condition that $|A - A'| \leq c/k$ can easily be dropped considering intermediate points between A and A'. However, the Lipschitz constant Ck obtained this way blows up as $k \to \infty$. In order to prove the main continuity result, we therefore need another preparatory lemma:

Lemma 2.2.18 *Let* $(A, \mathbf{b}), (A', \mathbf{b}) \in \mathcal{A}_{\text{hom}}$ *and* $c > 0$ *a constant. Suppose* $1/k \leq l = l(k) \leq 1$. *Then there is a constant* $C > 0$ *such that*

$$|\varphi_k(A, \mathbf{b}) - \varphi_k(A', \mathbf{b})| \leq C(1/kl + l + kl|A - A'|)$$

whenever $|A - A'| \leq c/kl$.

Proof. Cover $\mathcal{S}_1$ by translates $U_1, \ldots, U_s$ of $[0, l)^2$ with $|\bigcup U_i \setminus \mathcal{S}_1| = \mathcal{O}(l)$ as in the following picture:



Let $z^i \in \mathbb{Z}^2$ be the lower left lattice point of kU_i, and set $f^i = (A - A')z^i$. For $y \in \hat{\mathcal{N}}_k(A, \mathbf{b})$ we define y' by (interpolation and)

$$y'(x) = y(x) - Ax_p + A'x_p + f^i$$

if $x \in \mathcal{L} \cap (kU_i \times [0, h])$. Then

$$\|y' - y\| \leq |A - A'|\sqrt{2(kl)^2 + h^2} \leq C|A - A'|kl \leq Cc,$$

so assumption 2.1.7 shows that

$$|E(y') - E(y)| \leq Ck^2kl|A - A'|. \tag{2.32}$$

Now let $\mathcal{I}$ denote the set of those indices i for which $U_i \subset \mathcal{S}_1$. Applying lemma 2.2.8 to y' first, then using frame indifference, and finally applying lemma 2.2.8 to $y''(x) = y(x) - Ax_p + A'x_p$ gives

$$\begin{aligned} E(y'(x) : x \in \mathcal{L}_k) &= \sum_{i=1}^{r} E(y'(x) : x \in \mathcal{L} \cap (kU_i \times [0,h])) + \mathcal{O}(k/l + k^2 l) \\ &= \sum_{i=1}^{r} E(y''(x) : x \in \mathcal{L} \cap (kU_i \times [0,h])) + \mathcal{O}(k/l + k^2 l) \\ &= E(y''(x) : x \in \mathcal{L}_k) + \mathcal{O}(k/l + k^2 l). \end{aligned}$$

Since clearly $y'' \in \hat{\mathcal{N}}_k(A', \mathbf{b})$, this shows that

$$\varphi_k(A', \mathbf{b}) \leq \frac{1}{\nu k^2} E(y'') \leq \frac{1}{\nu k^2} E(y) + C(1/kl + l + kl|A - A'|)$$

by (2.32). Since y was arbitrary we get

$$\varphi_k(A', \mathbf{b}) \leq \varphi_k(A, \mathbf{b}) + C(1/kl + l + kl|A - A'|).$$

Again interchanging the roles of A and A' concludes the proof. □

As a consequence of lemmas 2.2.16, 2.2.17 and 2.2.18 we get:

Proposition 2.2.19 *The set $\{\varphi_k\}$ is equicontinuous.*

Proof. Let $\delta > 0$ be given. Choose constants c, C as in the previous lemma, and let $l = 3C/k\delta$. Then for k so large that

$$Cl = 3C^2/\delta k \leq \delta/3,$$

we get from the above lemma for $|A - A'| \leq c/kl$, i.e., $|A - A'| \leq c\delta/3C$,

$$\begin{aligned} |\varphi_k(A, \mathbf{b}) - \varphi_k(A', \mathbf{b})| &\leq C(1/kl + l + kl|A - A'|) \\ &\leq \delta/3 + \delta/3 + 3C^2|A - A'|/\delta. \end{aligned}$$

So, for $|A - A'| \leq \min\{\delta^2/9C^2, c\delta/3C\}$, we have for sufficiently large k, say $k > k_0$,

$$|\varphi_k(A, \mathbf{b}) - \varphi_k(A', \mathbf{b})| \leq \delta.$$

This shows equicontinuity of $\{\varphi_k(\cdot, \mathbf{b}) : k \in \mathbb{N}\}$ since the remaining finitely many $\varphi_1(\cdot, \mathbf{b}), \ldots, \varphi_{k_0}(\cdot, \mathbf{b})$ are continuous by lemma 2.2.17. By lemma 2.2.16 the family $\{\varphi_k(A, \cdot) : A \text{ admissible with } s_1(A), s_2(A) \in [c_1, c_2], k \in \mathbb{N}\}$ is also equicontinuous for all $c_2 \geq c_1 > 0$. The claim follows. □

From propositions 2.2.15 and 2.2.19 we can now easily finish the proof of theorem 2.2.2.

Proof of theorem 2.2.2. By proposition 2.2.15, $\varphi_k(A, \mathbf{b}) \to \varphi(A, \mathbf{b})$ pointwise and, by proposition 2.2.19, $\{\varphi_k\}$ is equicontinuous. This implies that $\varphi_k(A, \mathbf{b}) \to \varphi(A, \mathbf{b})$ uniformly on compact subsets of $\mathcal{A}_{\text{hom}}$, in particular that φ is continuous since by Arzela-Ascoli every subsequence has a further subsequence that converges. By the pointwise convergence, its limit must be φ. □

2.2.4 Proofs of theorems 2.2.1 and 2.2.3

First note that theorem 2.2.1 is an immediate consequence of theorem 2.2.3. So we only have to prove the latter result.

Fix admissible $u \in W^{1,\infty}(\mathcal{S}_1), \mathbf{b} \in L^\infty(\mathcal{S}_1)$ and constants $c_1, c_2 > 0$ as in (2.5). We will show that for $l_3 \to 0$ and $kl_3 \to \infty$,

$$\lim_{k\to\infty} \frac{1}{\nu k^2} \inf_{\hat{\mathcal{N}}_k^{0,l_3}(u,\mathbf{b})} E(y) = E(u, \mathbf{b}). \tag{2.33}$$

This will be sufficient since from lemmas 2.2.12 and 2.2.13 (and the obvious inclusions of neighborhoods) we obtain the following corollary which precisely describes our relaxation procedure in terms of weak neighborhoods.

Corollary 2.2.20 *Suppose (2.33) holds. Then in fact*

$$\lim_{k\to\infty} \frac{1}{\nu k^2} \inf_{y\in\mathcal{U}_k(u,\mathbf{b})} E(y) = E(u, \mathbf{b})$$

where the minimum is taken over $\mathcal{U}_k(u,\mathbf{b}) = \hat{\mathcal{N}}_k^{l_2,l_3}(u,\mathbf{b})$ *with* $l_2, l_3 \to 0$ *and* $kl_3 \to \infty$*, or* $\mathcal{U}_k(u,\mathbf{b}) = \mathcal{W}_k^l(u,\mathbf{b})$ *with* $l \to 0$ *and* $kl \to \infty$*, or over* $\mathcal{U}_k(u,\mathbf{b}) = \mathcal{N}_k^{l_2,l_3}(u,\mathbf{b})$ *with* $l_2, l_3 \to 0$ *and* $kl_2l_3 \to \infty$.

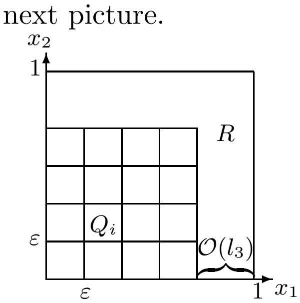
If $Q \subset \mathcal{S}_1$ is some square in $\mathcal{S}_1$ of side-length $l = l(k)$ we write $\hat{\mathcal{N}}_Q(u,\mathbf{b}) := \hat{\mathcal{N}}_{k,Q}^{0,l}(u,\mathbf{b})$.

Fix $\sigma > 0$ and $0 < \delta < \min\{1/2, c_1/2\}$. Since $u \in W^{1,\infty}(\mathcal{S}_1)$, we may choose a measurable set $B \subset \mathcal{S}_1$ and $\bar{u} \in C^1(\mathcal{S}_1)$ such that $|B| \le \sigma$ and

$$\mathcal{S}_1 \setminus B = \{x \in \mathcal{S}_1 : u(x) = \bar{u}(x), \nabla u(x) = \nabla \bar{u}(x)\}.$$

Furthermore, there exists $\bar{c}_2$ only depending on c_2 such that $\sup_{x\in\mathcal{S}_1} |\nabla \bar{u}(x)| \le \bar{c}_2$ (cf. [18]).

In order to pass from microscopic to macroscopic dimensions, we will introduce a mesoscale $1/k \ll \varepsilon \le l_3$. As detailed below, we will consider a partition of $\mathcal{S}_1$ by mesoscopic squares Q_i of side-length ε plus some rest R whose area is of the order $\mathcal{O}(l_3)$, see the next picture.



Then $\bar{u} \in C^1(\mathcal{S}_1)$ can be approximated by a piecewise affine function u_ε. More precisely, there is an increasing and continuous function g only depending on the modulus of continuity of $\nabla\bar{u}$ such that $g(\varepsilon) \to 0$ as $\varepsilon \to 0$ and

$$\|\bar{u} - u_\varepsilon\|_\infty < \varepsilon g(\varepsilon), \tag{2.34}$$

where u_ε is affine on each of the squares Q_i. (If $\bar{u} \in C^{1,\alpha}$, one can, e.g., choose $g(\varepsilon) = C\varepsilon^\alpha$.) We fix such a function g satisfying (2.34) from now on.

Let $0 < \gamma < 1$ be a constant. We choose $\varepsilon' = \varepsilon'(k)$ such that

$$k\varepsilon' g(\varepsilon')^\gamma \equiv c_0. \tag{2.35}$$

Note that (2.34) and (2.35) imply that

$$\|\bar{u} - u_\varepsilon\|_\infty \ll c_0/k \quad \text{ if } \varepsilon \leq \varepsilon' \tag{2.36}$$

while $\varepsilon' \to 0$ and $k\varepsilon' \to \infty$.

Lemma 2.2.21 *Let $Q \subset \mathcal{S}_1$ be one of the squares Q_i (on which ∇u_ε is constant). Suppose $c_1 - \delta \leq s_1(\nabla u_\varepsilon) \leq s_2(\nabla u_\varepsilon) \leq c_2 + \delta$ on Q, and let $\mathbf{b}$ be a constant admissible vector in $(\mathbb{R}^3)^{\nu-1}$. Then if $\varepsilon \leq \varepsilon'$,*

$$\left| \inf_{y \in \hat{\mathcal{N}}_Q(u,\mathbf{b})} E(y) - \inf_{y \in \hat{\mathcal{N}}_Q(u_\varepsilon,\mathbf{b})} E(y) \right| \leq C\left(\delta^{1/5}|Q| + \frac{|B \cap Q|}{\delta^3}\right) k^2.$$

Proof. Let $y \in \hat{\mathcal{N}}_Q(u, \mathbf{b})$. We set

$$r_Q := \#\left\{ x \in \frac{1}{k}\mathbb{Z}^2 \cap Q : |u(x) - \bar{u}(x)| > \delta/k \right\}$$

and define y' by

$$\tilde{y}'(x) = \begin{cases} \tilde{y}(x) & \text{if } |u(x_p) - \bar{u}(x_p)| \leq \delta/k, \\ v_\varepsilon(x) & \text{else,} \end{cases}$$

for $x_p \in \frac{1}{k}\mathbb{Z}^2 \cap Q$ and interpolation (v_ε defined analogously to (2.9) with respect to u_ε and $\mathbf{b}$.). Then by (2.36) for $\varepsilon \leq \varepsilon'$,

$$\|\tilde{y}' - u_\varepsilon\| \leq (c_0 + \delta + o(1))/k \leq (c_0 + 2\delta)/k,$$

and since $k\Delta^i \tilde{y}'$ is bounded,

$$\left| \fint_Q \left(k\Delta^i \tilde{y}' - \bar{b}^i\right) d\rho \right| = \left| \fint_Q k\Delta^i \tilde{y}' d\rho - \fint_Q k\Delta^i \tilde{y} d\rho \right| \leq \frac{C r_Q}{|kQ|}.$$

Furthermore, by corollary 2.2.7,

$$|E(y) - E(y')| \leq C r_Q. \tag{2.37}$$

Invoking lemma 2.2.12 (with c_0 replaced by $c_0 + 2\delta$ and c_3 by c_0), we find a deformation y'' on Q with

$$\|\tilde{y}'' - u_\varepsilon\| \leq (c_0 + 2\delta)/k \quad \text{ and } \quad \fint_Q \Delta^i \tilde{y}'' d\rho = \bar{b}^i$$

satisfying

$$E(y'') \leq E(y') + \frac{1}{\delta}\frac{C r_Q}{|kQ|}|kQ|. \tag{2.38}$$

(Note that the constant found in the proof of lemma 2.2.12 by applying lemma 2.2.10 is – in the terminology of this lemma – $Cl_2/(c_0 - c_3)$. Here, this equals $Cr_Q/|kQ|\delta$.) Finally, by lemma 2.2.11 there is yet another deformation y''' with

$$\|\tilde{y}''' - u_\varepsilon\| \leq c_0/k \quad \text{and} \quad \fint_Q \Delta^i \tilde{y}''' = \bar{b}^i$$

and

$$|E(y''') - E(y'')| \leq C\delta^{1/5}|kQ|. \tag{2.39}$$

Since $y''' \in \hat{\mathcal{N}}_Q(u_\varepsilon, \mathbf{b})$ and $y \in \hat{\mathcal{N}}_Q(u, \mathbf{b})$ was arbitrary, we deduce from (2.37), (2.38) and (2.39)

$$\inf_{y \in \hat{\mathcal{N}}_Q(u_\varepsilon, \mathbf{b})} E(y) \leq \inf_{y \in \hat{\mathcal{N}}_Q(u, \mathbf{b})} E(y) + C\left(\delta^{1/5}|kQ| + \frac{r_Q}{\delta}\right).$$

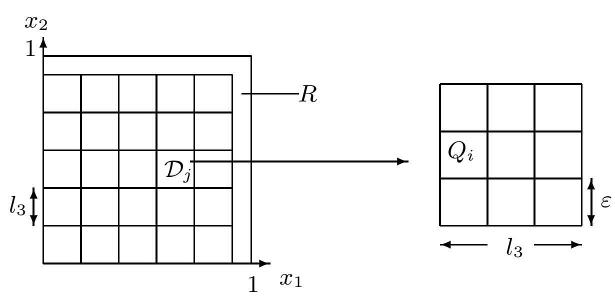
Interchanging the roles of u and u_ε (but defining r_Q as before and only replacing v_ε by v in the definition of y') gives an analogous inequality.

To finish the proof, it remains to estimate r_Q. For δ small enough, the balls $B(x, \delta/(c_2 + \bar{c}_2)k)$ with $x \in \frac{1}{k}\mathbb{Z}^2$ are disjoint. Since $|\nabla u| \leq c_2$ and $|\nabla \bar{u}| \leq \bar{c}_2$, we have $B(x, \delta/(c_2 + \bar{c}_2)k) \cap (\mathcal{S}_1 \setminus B) = \emptyset$ if $|u(x) - \bar{u}(x)| > \delta/k$. So indeed

$$\frac{C\delta^2}{k^2} r_Q \leq |B \cap Q|.$$

□

Now consider a partition of $\mathcal{S}_1$ with squares $\mathcal{D}_j$ of side-length l_3 and R, $|R| \leq 2l_3$ (see the next picture). Since $kl_3 \to \infty$ and $k\varepsilon' \to \infty$ (cf. (2.35)), we may choose $\varepsilon = \varepsilon(k) \leq \varepsilon' \to 0$ with $k\varepsilon \to \infty$ as $k \to \infty$ such that eventually $l_3/\varepsilon \in \mathbb{N}$. This also induces a partition of $\mathcal{S}_1$ into squares Q_i of side-length ε and R as in the picture below.



Proof of Theorem 2.2.3. Define G to be the union of those $\mathcal{D}_j$ where $c_1 - \delta < s_1(\nabla \bar{u}) \leq s_2(\nabla \bar{u}) < c_2 + \delta$. Since $\nabla \bar{u}$ is continuous, for k large enough, $G \supset \{x : c_1 \leq s_1(\nabla \bar{u}(x)) \leq s_2(\nabla \bar{u}(x)) \leq c_2\} \setminus R \supset \mathcal{S}_1 \setminus (B \cup R)$, whence $|G| \geq 1 - |B \cup R| \geq 1 - \sigma - 2l_3$.

Let $\mathcal{M}_j = y(\mathcal{L} \cap (k\mathcal{D}_j \times [0, h]))$. It follows from lemmas 2.2.8 and 2.2.6 that

$$\begin{aligned}\left| \inf_{y \in \hat{\mathcal{N}}_k^{0,l_3}(u,\mathbf{b})} E(y) - \inf_{y \in \hat{\mathcal{N}}_k^{0,l_3}(u,\mathbf{b})} \sum_{\mathcal{D}_j \subset G} E(\mathcal{M}_j) \right| &\leq C\left(\frac{k}{l_3} + k^2 l_3 + \frac{|\mathcal{S}_1 \setminus G|}{l_3^2}(kl_3)^2\right) \\ &\leq Ck^2\left(\frac{1}{kl_3} + l_3 + \sigma\right)\end{aligned}$$

where by definition of $\hat{\mathcal{N}}_k^{0,l_3}$,

$$\inf_{y\in\hat{\mathcal{N}}_k^{0,l_3}(u,\mathbf{b})} \sum_{\mathcal{D}_j\subset G} E(\mathcal{M}_j) = \sum_{\mathcal{D}_j\subset G} \inf_{y\in\hat{\mathcal{N}}_{\mathcal{D}_j}(u,\mathbf{b})} E(y).$$

Now using lemma 2.2.8 again,

$$\left| \inf_{y\in\hat{\mathcal{N}}_{\mathcal{D}_j}(u,\mathbf{b})} E(y) - \min \sum_{Q_i\subset\mathcal{D}_j} \inf_{y\in\hat{\mathcal{N}}_{Q_i}(u,\mathbf{b}_{j,i})} E(y) \right| \le C\frac{kl_3^2}{\varepsilon}, \qquad (2.40)$$

where the minimum is to be taken over admissible vectors $\mathbf{b}_{j,1},\ldots,\mathbf{b}_{j,(l_3/\varepsilon)^2}$ such that $\sum_i \frac{\rho(Q_i)}{\rho(\mathcal{D}_j)}\mathbf{b}_{j,i} = \mathbf{b}_j := ⨍_{\mathcal{D}_j} \bar{\mathbf{b}}\, d\rho$.

Since $\nabla u_\varepsilon \to \nabla\bar{u}$ uniformly, we may choose matrices A_j such that $\sup_j |A_j - \nabla u_\varepsilon| = o(1)$ on $\mathcal{D}_j$. We now want to replace u by A_j in the right hand side of (2.40). First replacing u by u_ε on Q_i leads to an error bounded by $C(\delta^{1/5}|Q_i| + |B\cap Q_i|/\delta^3)k^2$ by lemma 2.2.21. Now replacing ∇u_ε by A_j leads to an additional error of order $o(|kQ_i|)$ because for matrices A,

$$\inf_{y\in\hat{\mathcal{N}}_{Q_i}(A,\mathbf{b}_{j,i})} E(y) = \varphi_m(A,\mathbf{b}_{j,i})\nu|kQ_i| + \mathcal{O}(k\varepsilon),$$

where m is the integer part of $k\varepsilon$ or $k\varepsilon - 1$ (use translational invariance), and $(\varphi_k)_k$ is equicontinuous by proposition 2.2.19, hence also $\{\varphi_k(\cdot,\mathbf{b}) : k \in \mathbb{N}, \mathbf{b} \text{ admissible}\}$ by compactness. It follows that

$$\begin{aligned} &\left| \inf_{y\in\hat{\mathcal{N}}_k^{0,l_3}(u,\mathbf{b})} E(y) - \sum_{\mathcal{D}_j\subset G} \left(\min \sum_{Q_i\subset\mathcal{D}_j} \inf_{y\in\hat{\mathcal{N}}_{Q_i}(A_j,\mathbf{b}_{j,i})} E(y) \right) \right| \\ &\quad\le C \sum_{Q_i\subset G} \left(\left(\delta^{1/5} + o(1)\right)|Q_i|k^2 + \frac{|B\cap Q_i|}{\delta^3}k^2 \right) + Ck^2\left(\frac{1}{k\varepsilon} + l_3 + \sigma\right). \end{aligned}$$

Now reasoning as above, for $n = n(k) = \lfloor kl_3 \rfloor$ or $\lfloor kl_3 \rfloor - 1$,

$$\begin{aligned} \min \sum_{Q_i\subset\mathcal{D}_j} \inf_{y\in\hat{\mathcal{N}}_{Q_i}(A_j,\mathbf{b}_{j,i})} E(y) &= \inf_{y\in\hat{\mathcal{N}}_{\mathcal{D}_j}(A_j,\mathbf{b}_j)} E(y) + \mathcal{O}(kl_3^2/\varepsilon) \\ &= \varphi_n(A_j,\mathbf{b}_j)\nu|k\mathcal{D}_j| + \mathcal{O}(kl_3^2/\varepsilon + kl_3). \end{aligned}$$

Summarizing (using theorem 2.2.2 to choose $n = \lfloor kl_3 \rfloor$ uniquely), we obtain

$$\begin{aligned} \left| \frac{1}{\nu k^2} \inf_{y\in\hat{\mathcal{N}}_k^{0,l_3}(u,\mathbf{b})} E(y) - \sum_{\mathcal{D}_j\subset G} \varphi_n(A_j,\mathbf{b}_j)|\mathcal{D}_j| \right| &\le C(\delta^{1/5} + |B|/\delta^3 + \sigma + o(1)) \\ &\le C(\delta^{1/5} + \sigma/\delta^3). \end{aligned}$$

Let $\Omega = \{x : c_1 - \delta < s_1(\nabla\bar{u}) \le s_2(\nabla\bar{u}) < c_2 + \delta)\}$. Then $\liminf_k G \supset \Omega$. The piecewise linear resp. constant approximations A_j resp. $\mathbf{b}_j$ converge to $\nabla\bar{u}$ uniformly resp. to $\mathbf{b}$ boundedly in measure. (This is not hard to see:

approximate $\mathbf{b}$ by continuous functions in measure.) So we deduce from lemma A.2 and theorem 2.2.2

$$\sum_{\mathcal{D}_j \subset G} \varphi_n(A_j, \mathbf{b}_j) |\mathcal{D}_j \cap \Omega| \to \int_\Omega \varphi(\nabla \bar{u}, \mathbf{b}).$$

Since $\mathcal{S}_1 \setminus \Omega \subset B$, $|B| \leq \sigma$, and φ_n, φ are uniformly bounded on compact subsets of admissible matrices, we finally obtain that

$$\limsup_{k \to \infty} \left| \frac{1}{\nu k^2} \inf_{y \in \hat{\mathcal{N}}^{0,l_3}(u,\mathbf{b})} E(y) - \int_{\mathcal{S}_1} \varphi(\nabla u, \mathbf{b}) \right| \leq C(\delta^{1/5} + \sigma/\delta^3).$$

Now let $\sigma \to 0, \delta \to 0$. □

Remark: Assuming regularity for ∇u, $\mathbf{b}$, e.g., to lie in some Hölder class, the above proof gives explicit error estimates.

2.2.5 Extension to infinite pair-interactions

We will now prove theorem 2.2.4. For this paragraph we assume that proposition 2.3.1 is already proven.

Suppose E is given as in (2.15). For given δ we choose

$$E_\delta(y) = \frac{1}{2} \sum_{i \neq j} W_\delta(|y_i - y_j|) + E_0(y), \tag{2.41}$$

where $W_\delta \leq W$ satisfies the hypotheses of proposition 2.3.1, and

$$W_\delta(r) = W(r) \text{ for } r \geq \delta, \quad W_\delta(r) \geq \min_{0 < s \leq \delta} W(s) \text{ for } r \leq \delta. \tag{2.42}$$

Proposition 2.3.1 implies that E_δ is an admissible energy function. If δ is small enough, we may assume that $W(r) > 0$ for $r \leq \delta$. Note also that there exists $C = C(\delta, c)$ such that for all $z \in \mathcal{L}_k$ and y with $\|\tilde{y} - u\| \leq c/k$ (u admissible)

$$\sum_{\substack{x \in \mathcal{L}_k \\ x \neq z}} |W_\delta(|y(x) - y(z)|)| \leq C. \tag{2.43}$$

This follows from lemma 2.2.6 (with $\mathcal{K}_2 = \{z\}$) applied to the pair potential given by $|W_\delta|$.

Definition 2.2.22 *Let $\delta > 0$, and suppose y is some deformation. We call (y_i, y_j), $i \neq j$, a δ-critical bond if $|y_i - y_j| < \delta$. We say that y satisfies a minimal distance hypothesis with δ if it does not contain δ-critical bonds.*

Lemma 2.2.23 *Suppose y is a deformation with $\|\tilde{y} - u\| \leq c/k$, u admissible.*

(i) The number of atoms in a ball B of radius R is bounded by a constant $n = n(R)$.

(ii) There exists $C > 0$ such that if $(y(x), y(z))$ is 1-critical, then $|x - z| \leq C$.

Proof. (i) Suppose $y_i = y(x_i) \in B$. Choose $\delta = 2C_3/C_1$ as in the proof of lemma 2.2.6. Then for $|x-z| \geq \delta$ we have $\frac{C_1}{2}|x-z| \leq |y(x)-y(z)|$ and thus

$$|y(x)-y(z)| \leq 2R \Rightarrow |x-z| \leq \delta \text{ or } |x-z| \leq 4R/C_1.$$

So $\#\{j : y_j \in B\} \leq \#\{j : |x_i - x_j| \leq \max\{2C_3/C_1, 4R/C_1\}\} =: n(R)$.

(ii) Just note that, by lemma 2.1.2 (ii), $|x-z| \leq (|y(x)-y(z)| + C_3)/C_1$.□

We will prove theorem 2.2.4 by reducing to the case of admissible energy functions already treated. The main point is to show that we may impose an additional minimal distance hypothesis on the deformations. To this end, for given y we have to find a new configuration y' satisfying this hypothesis whose energy does not exceed $E(y)$ too much. The main difficulty comes again from the condition on local spatial averages.

Let $(A, \mathbf{b}) \in \mathcal{A}_{\text{hom}}$. As in the proof of lemma 2.2.11 we choose

$$b^0 \in \underset{b^0}{\operatorname{argmin}} \max \left\{ \max_{1 \leq i \leq \nu-1} |b^i - b^0|, |b^0| \right\} \tag{2.44}$$

and set

$$B^i = b^{i-1} - b^0,\ i = 2, \ldots, \nu, \quad B^1 = -b^0. \tag{2.45}$$

We will first assume that there is some $\theta > 0$ such that, if $|B^i|, |B^j| \geq c_0 - \theta$ and there is $z \in \mathbb{Z}^2$ with $|B^i - B^j - Az| \leq \theta$, then $i = j$ and $z = 0$.

Now suppose $y \in \hat{\mathcal{N}}_Q^{l_2,l_3}(A, \mathbf{b})$ where Q is a square of side-length $l_3 \gg 1/k$. We construct a new deformation $y' : \mathcal{L} \cap kQ \times [0,h] \to \mathbb{R}^3$ in two steps. Let

$$0 < \delta_1 < \delta_1' < \frac{\delta_2}{6n(2\delta_2)}, \quad 3\delta_2 < \delta_2' \leq \min\{1, c_1\} \tag{2.46}$$

be small enough ($n(2\delta_2)$ as in the previous lemma, $c_1 = s_1(A)$).

Step 1. We first derive an intermediate deformation from y successively moving the atoms around. At each intermediate step we are dealing with deformations $\hat{y}$ such that $\|\hat{y} - A\| \leq c_0$, so lemma 2.2.23 is applicable.

We will reorder layer by layer of the film starting with $i = 0$. Suppose the first $i-1$ layers and the first m atoms of the i-th layer $y(\cdot, i)$ have been reordered in the way described below. Let $x = (x_1, x_2, i)$ be the $(m+1)$-th atom. We reorder in the following way:

If $y(x)$ has a distance greater than or equal to δ_1 to all the other atomic positions, it remains unchanged.

Now suppose $y(x)$ takes part in a δ_1-critical bond. If there exists another atom at $y(x')$, $x' = (x_p', i)$, and a unit vector $e \in \mathbb{R}^3$ such that

$$|y(x) + re - Ax_p| \leq c_0 \quad \text{and} \quad |y(x') - re - Ax_p'| \leq c_0$$

for $0 \leq r \leq \delta_2$, then both of the atoms $y(x)$ and $y(x')$ will be moved in opposite directions. Let $L = \{y(x) + re : 0 \leq r \leq \delta_2\}$, $L' = \{y(x') - re : 0 \leq r \leq \delta_2\}$.

Claim: There are points $Y(x) \in L, Y(x') \in L'$ with

$$y(x) + y(x') = Y(x) + Y(x')$$

such that

$$|Y(x) - Y(x')|, |Y(x) - y(z)|, |Y(x') - y(z)| \geq \delta_1'$$

for all $z \in \mathcal{L}_k$, $z \neq x, x'$.

Proof of the claim: Let B, B' be balls of radius $2\delta_2$ centered at $y(x)$ resp. $y(x')$. Clearly, $\mathrm{dist}(z, \bar{z}) \geq \delta_2 > \delta_1$ if $z \in L$ and $\bar{z} \notin B$ (resp. if $z \in L'$ and $\bar{z} \notin B'$). By the preceding lemma, there are at most $n(2\delta_2)$ atoms in these balls. Consider balls B_l, resp. $B'_{l'}$ with radius δ_1' around the atoms in the balls B, resp. B'. Since by assumption $\delta_1' < \delta_2/6n(2\delta_2)$ we get ($\mathcal{H}^1$ denoting one-dimensional Hausdorff measure)

$$\mathcal{H}^1(L \setminus \bigcup_l B_l) \geq 2\delta_2/3, \quad \mathcal{H}^1(L' \setminus \bigcup_{l'} B'_{l'}) \geq 2\delta_2/3.$$

Since the mapping $L \to L'$ with $z \mapsto z'$ such that $z + z' = y(x) + y(x')$, i.e., $z' = y(x) + y(x') - z$ is isometric, we find that

$$\mathcal{H}^1(\{z \in L \setminus \bigcup_l B_l : z' \notin \bigcup_{l'} B'_{l'}\}) \geq \delta_2/3.$$

Noting that $|z - z'| \leq \delta_1' \Rightarrow |y(x) + y(x') - 2z| \leq \delta_1'$, we also get that

$$\mathcal{H}^1(\{z \in L : |z - z'| \leq \delta_1'\}) \leq \delta_1',$$

so we have shown that

$$\mathcal{H}^1(\{z \in L \setminus \bigcup_l B_l : z' \notin \bigcup_{l'} B'_{l'}, |z - z'| \geq \delta_1'\}) \geq \delta_2/3 - \delta_1' > 0.$$

In particular, there exist points $Y(x) = z \in L$, $Y(x') = z' \in L'$ as claimed.

We now update the deformation by replacing $y(x)$ by $Y(x)$ and $y(x')$ by $Y(x')$. If each atom has been considered this way we arrive at a new configuration again denoted y. We repeat the process until there are no more δ_1-critical bonds that can be removed this way. (There may still be δ_1-critical bonds left.)

Step 2. If there are no more δ_1-critical bonds, we are done. If there still are, using the new configuration constructed in step 1 (again called y), we now construct y'. Suppose $y(x)$ takes part in a δ_1-critical bond. Then it is not possible to find another atom in the same film layer and the unit vector e as described above. But then for all $x' \in \mathcal{L} \cap (kQ \times [0, h])$ with $x_3 = x_3'$,

$$|y(x') - Ax_p' - [y(x) - Ax_p]| \leq \delta_2, \tag{2.47}$$

for otherwise we could define

$$e = \frac{y(x') - Ax_p' - [y(x) - Ax_p]}{|y(x') - Ax_p' - [y(x) - Ax_p]|}.$$

In particular, there are no δ_1-critical bonds within the set $y(kQ \times \{i\})$. (If $(y(x'), y(x''))$ was critical, then, by

$$|y(x') - Ax_p' - [y(x'') - Ax_p'']| \leq 2\delta_2,$$

we had

$$|Ax'_p - Ax''_p| \le 2\delta_2 + \delta_1 < c_1$$

in contradiction to (2.46).)

Now suppose $(y(x), y(x'))$ is critical where $x' = (x'_p, i')$, $i' \ne i$. Then again, as in (2.47), for all $z_p, z'_p \in \mathbb{Z}^2 \cap kQ$,

$$\begin{aligned} |y(z_p, i) - Az_p - [y(x) - Ax_p]| &\le \delta_2 \quad \text{and} \\ |y(z'_p, i') - Az'_p - [y(x') - Ax'_p]| &\le \delta_2. \end{aligned}$$

In particular for $z'_p - z_p = x'_p - x_p$,

$$\left| y(z'_p, i') - Az'_p - [y(x') - Ax'_p] - \Big(y(z_p, i) - Az_p - [y(x) - Ax_p] \Big) \right| \le 2\delta_2,$$

so

$$\begin{aligned} |y(z'_p, i') - y(z_p, i)| &\le |y(x) - y(x') + Ax'_p - Ax_p + Az_p - Az'_p| + 2\delta_2 \\ &\le \delta_1 + 2\delta_2 \le 3\delta_2. \end{aligned}$$

Since $|x_p - x'_p| \le C$ (cf. lemma 2.2.23 (ii)), we find (up to a constant boundary layer) at least one $3\delta_2$-critical bond per atom of the i-th layer. If this case occurs, i.e., we have more than $(kl_3)^2 - Ckl_3$ $3\delta_2$-critical bonds, we reorder all the atoms in $kQ \times [0,h]$, first by placing atom x at position $V(x)$ (V such that $\tilde{V} = v$, cf. (2.9)). Now suppose δ'_2 is small enough. Then since $|B^i| < c_0 - \theta$ or $|B^j| < c_0 - \theta$ if $|B^i - B^j - Az| \le \theta$ for $i \ne j$ and some $z \in \mathbb{Z}^2$, we can eliminate all $3\delta_2$-critical bonds as in step 1, arriving at a new deformation y such that no atom in $y(kQ \times [0,h])$ takes part in a δ'_2-critical bond.

Lemma 2.2.24 *Suppose $|B^i| = |B^j| = c_0$ and $B^i - B^j \in A\mathbb{Z}^2$ only for $i = j$. (So θ as above can be chosen.) There are $0 < \delta_1, \delta'_1, \delta_2, \delta'_2$ (only depending on W, E_0, and θ) such that (2.46) holds, and (cf. (2.41)) for all $y \in \hat{\mathcal{N}}_Q^{l_2,l_3}(A, \mathbf{b})$*

$$E_{\delta_1}(y') \le E_{\delta_1}(y),$$

where y' is derived from y as described above. In fact, $y' \in \hat{\mathcal{N}}_Q^{l_2,l_3}(A, \mathbf{b})$ with $E(y') \le E_{\delta_1}(y)$.

Proof. We prove that each step of the above construction lowers energy. Assume δ'_2 is so small that $W(r) \ge 0$ on $(0, \delta'_2]$ and thus also $W_\delta \ge 0$ on $(0, \delta'_2]$ for $\delta \le \delta'_2$ (cf. (2.42)). Suppose $\hat{y}$, $\hat{y}'$ are intermediate configurations in step 1 above and $\hat{y}'$ arises from $\hat{y}$ by moving the atoms x and x'. By corollary 2.2.7, changing the position of two atoms yields an energy error in E_0 bounded by some constant C. For given (small) δ'_1 choose δ_1 so small that

$$W_{\delta_1}(r) > C + 4 \sup_{\|y - A\| \le c_0} \sup_z \sum_{z' \ne z} |W_{\delta'_1}(|y(z') - y(z)|)|$$

for all $r \leq \delta_1$ (which is possible by (2.43) and (2.42)). Now $y(x)$ having a critical bond of length $r < \delta_1$,

$$
\begin{aligned}
&E_{\delta_1}(\hat{y}) - E_{\delta_1}(\hat{y}') \\
&= \sum_{z \neq x, x'} W_{\delta_1}(|\hat{y}(z) - \hat{y}(x)|) + \sum_{z \neq x, x'} W_{\delta_1}(|\hat{y}(z) - \hat{y}(x')|) \\
&\quad - \sum_{z \neq x, x'} W_{\delta_1}(|\hat{y}'(z) - \hat{y}'(x)|) - \sum_{z \neq x, x'} W_{\delta_1}(|\hat{y}'(z) - \hat{y}'(x')|) \\
&\quad + W_{\delta_1}(|\hat{y}(x) - \hat{y}(x')|) - W_{\delta_1}(|\hat{y}'(x) - \hat{y}'(x')|) + C \\
&\geq \sum_{\substack{z \neq x, x' \\ |\hat{y}(z) - \hat{y}(x)| \geq \delta_1'}} W_{\delta_1'}(|\hat{y}(z) - \hat{y}(x)|) + \sum_{\substack{z \neq x, x' \\ |\hat{y}(z) - \hat{y}(x')| \geq \delta_1'}} W_{\delta_1'}(|\hat{y}(z) - \hat{y}(x')|) \\
&\quad - \sum_{z \neq x, x'} W_{\delta_1'}(|\hat{y}'(z) - \hat{y}'(x)|) - \sum_{z \neq x, x'} W_{\delta_1'}(|\hat{y}'(z) - \hat{y}'(x')|) \\
&\quad + W_{\delta_1}(r) - W_{\delta_1'}(|\hat{y}'(x) - \hat{y}'(x')|) - C \\
&\geq 0.
\end{aligned}
$$

Now consider the construction of y' in step 2 and suppose there are $(kl_3)^2 - Ckl_3 > (\lceil kl_3 \rceil + 1)^2/2$ $3\delta_2$-critical bonds between the i-th and i'-th layer in $y(\mathcal{L} \cap (kQ \times [0,h]))$. The energy change due to the E_0-term is bounded by $C(kl_3)^2$. So if for given δ_2', δ_1 and δ_2 are chosen such that

$$
W_{\delta_1}(r) > 2C + \sup_{\|y - A\| \leq c_0} \sup_x 2\nu \sum_{x' \neq x} |W_{\delta_2'}(|y(x') - y(x)|)|
$$

for all $r \leq 3\delta_2$, then

$$
\begin{aligned}
&E_{\delta_1}(y) - E_{\delta_1}(y') \\
&= \frac{1}{2} \sum_{x' \neq x} W_{\delta_1}(|y(x') - y(x)|) - \frac{1}{2} \sum_{x' \neq x} W_{\delta_1}(|y'(x') - y'(x)|) \\
&\quad + E_0(y) - E_0(y') \\
&\geq \frac{1}{2} \sum_{\substack{x' \neq x \\ |y(x) - y(x')| \leq 3\delta_2}} W_{\delta_1}(|y(x) - y(x')|) + \frac{1}{2} \sum_{\substack{x' \neq x \\ |y(x) - y(x')| > \delta_2'}} W_{\delta_2'}(|y(x') - y(x)|) \\
&\quad - \frac{1}{2} \sum_{x' \neq x} W_{\delta_2'}(|y'(x') - y'(x)|) + E_0(y) - E_0(y') \\
&\geq \frac{(\lceil kl_3 \rceil + 1)^2}{2} \left(2C + 2\nu \sup_{\|y - A\| \leq c_0} \sup_x \sum_{x' \neq x} |W_{\delta_2'}(|y(x') - y(x)|)| \right) \\
&\quad - \frac{1}{2} \nu (\lceil kl_3 \rceil + 1)^2 \sup_x \sum_{x' \neq x} |W_{\delta_2'}(|y(x') - y(x)|)| \\
&\quad - \frac{1}{2} \nu (\lceil kl_3 \rceil + 1)^2 \sup_x \sum_{x' \neq x} |W_{\delta_2'}(|y'(x') - y'(x)|)| - C(kl_3)^2 \\
&\geq 0.
\end{aligned}
$$

Clearly, $\|\tilde{y}' - A\|_\infty \le c_0/k$. Since step 1 leaves $⨍_Q k\Delta^i \tilde{y} d\rho$ unchanged and $k\Delta^i v = \bar{b}^i$, we have indeed $y' \in \hat{\mathcal{N}}_Q^{l_2,l_3}(A, \mathbf{b})$. By construction, y' satisfies a minimal distance hypothesis with δ_1, so $E_{\delta_1}(y') = E(y')$. $\square$

Write $\hat{\mathcal{N}}_{k,c_0}^{l_2,l_3}(u, \mathbf{b})$ to highlight the dependence of the weak neighborhoods on c_0. In the non-homogeneous setting we will need the following

Lemma 2.2.25 *Let $\delta_2 > 0$. For all $y \in \hat{\mathcal{N}}_{k,c_0-\delta_2}^{l_2,l_3}(u, \mathbf{b})$ there exists $y' \in \hat{\mathcal{N}}_{k,c_0}^{l_2,l_3}(u, \mathbf{b})$ with $E(y') \le E_{\delta_1}(y)$ if δ_1 is sufficiently small.*

Proof. Derive y' from y similarly as in step 1 of the procedure described above applied to the sets $\mathcal{L} \cap (\mathcal{D}_j \times [0, h])$ for $j = 1, \dots, N$ individually. If the unit vector e is taken to be the same for each atom to be considered, we may choose x' to be the next (the $(m+2)$-th) lattice point, resp. the first if x was the last one of the points in $k\mathcal{D}_j \cap \mathbb{Z}^2$. Clearly, $y' \in \hat{\mathcal{N}}_{k,c_0}^{l_2,l_3}(u, \mathbf{b})$. As before, we see that $E(y') \le E_{\delta_1}(y)$. $\square$

We first analyze φ. The first part of theorem 2.2.4 is contained in the following proposition.

Proposition 2.2.26 *Suppose A and $\mathbf{b}$ are admissible. Then the limit*

$$\varphi(A, \mathbf{b}) = \lim_{k\to\infty} \frac{1}{\nu k^2} \inf_{y \in \hat{\mathcal{N}}_k^{0,1}(A,\mathbf{b})} E(y)$$

exists in $(-\infty, \infty]$, φ is continuous on $\mathcal{A}_{\text{hom}}$ (as a function with values in $\mathbb{R} \cup \{\infty\}$), and $\varphi(A, \mathbf{b}) = \infty$ iff there are $z \in \mathbb{Z}^2$, $i \ne j \in \{1, \dots, \nu\}$ such that $B^i - B^j = Az$ and $|B^i| = |B^j| = c_0$. (B^i as in (2.45), (2.44).)

Furthermore, φ_δ denoting the limiting energy density corresponding to E_δ (cf. (2.41)), $\varphi_\delta \nearrow \varphi$ pointwise on $\mathcal{A}_{\text{hom}}$ as $\delta \searrow 0$.

Proof. Suppose first that $B^i - B^j \notin A\mathbb{Z}^2$ if $|B^i| = |B^j| = c_0$, $i \ne j$. By lemma 2.2.24,

$$\inf_{y \in \hat{\mathcal{N}}_k^{0,1}(A,\mathbf{b})} E(y) \le \inf_{y \in \hat{\mathcal{N}}_k^{0,1}(A,\mathbf{b})} E_{\delta_1}(y)$$

for δ_1 sufficiently small. But $E_{\delta_1} \le E$, so the reverse inequality it true, too. We may therefore replace E by E_{δ_1} and infer from theorem 2.2.2 that $\varphi(A, \mathbf{b})$ exists in $\mathbb{R}$, and φ is continuous at these $A, \mathbf{b}$.

For $0 < \theta \le 1$ given, suppose now there are $z \in \mathbb{Z}^2$ and $i \ne j$ such that $|B^i|, |B^j| \ge c_0 - \theta$, $|B^i - B^j - Az| \le \theta$. We define Y^i and $\overline{Y^i}$ as in the proof of lemma 2.2.11. There it was shown that for $|B^{i_0}| \ge c_0 - \theta$ we have (cf. (2.24) and (2.25) with $\varepsilon' = \theta$ and $\delta = 0$)

$$\left|\overline{Y^{i_0}} - B^{i_0}\right| \le C\sqrt{\theta}, \qquad \sum_{x \in \frac{1}{k}\mathbb{Z}^2 \cap \mathcal{S}_1} \left|Y^{i_0}(x) - \overline{Y^{i_0}}\right| \le Ck^2 \sqrt[4]{\theta}.$$

For $|B^i - B^j - Az| \le \theta$ this implies (modulo boundary terms)

$$\sum_{x \in \frac{1}{k}\mathbb{Z}^2 \cap \mathcal{S}_1} k\, |\tilde{y}(x, i-1) - \tilde{y}(x + z/k, j-1)|$$

$$
\begin{aligned}
&= \sum_{x\in\frac{1}{k}\mathbb{Z}^2\cap\mathcal{S}_1} \left|Y^i(x) - Y^j(x+z/k) - Az\right| \\
&\le \sum_{x\in\frac{1}{k}\mathbb{Z}^2\cap\mathcal{S}_1} \left|Y^i(x) - \overline{Y^i}\right| + \left|\overline{Y^i} - B^i\right| + \left|B^i - B^j - Az\right| \\
&\quad + \left|B^j - \overline{Y^j}\right| + \left|\overline{Y^j} - Y^j(x)\right| \\
&\le Ck^2\sqrt[4]{\theta},
\end{aligned}
$$

so the number of $4C\sqrt[4]{\theta}$-critical bonds is at least $k^2/2$. This holds for all $y \in \hat{\mathcal{N}}_k^{0,1}(A,\mathbf{b})$, so by (2.28),

$$
\varphi(A,\mathbf{b}) := \liminf_{k\to\infty} \varphi_k(A,\mathbf{b}) \ge \frac{1}{2\nu} \inf_{0<s\le 4C\sqrt[4]{\theta}} W(s) - C.
$$

Since the right hand side of this inequality converges to ∞ as $\theta \to 0$, the first part of the proposition is proven.

It remains to prove that $\varphi_\delta \nearrow \varphi$. This is clear on the set $\{\mathbf{b} : B^i - B^j \notin A\mathbb{Z}^2 \text{ for } i \ne j\}$ since there $\varphi = \varphi_\delta$ for δ sufficiently small as just shown. If $B^i - B^j \in A\mathbb{Z}^2$, then the above calculations show that

$$
\varphi(A,\mathbf{b}) \ge \varphi_\delta(A,\mathbf{b}) \ge \frac{1}{2\nu} W_\delta(0) - C \to \infty \text{ as } \delta \to 0.
$$

□

For the inhomogeneous case define

$$
\begin{aligned}
M^\theta \;:=\; &\{x \in \mathcal{S}_1 : \exists z \in \mathbb{Z}^2, i \ne j \in \{1,\dots,\nu\} \text{ s.t. } |B^i(x)|, |B^j(x)| \ge c_0 - \theta, \\
&|B^i(x) - B^j(x) - \nabla u(x) z| \le \theta\}
\end{aligned}
$$

for $(u,\mathbf{b})$ admissible, where b^0, B^i satisfy (2.44) and (2.45) pointwise.

Proof of theorem 2.2.4. By proposition 2.2.26 it remains to prove upper and lower bounds for general admissible $(u,\mathbf{b})$. This is done in four steps:

1. It is easy to get lower bounds. Since $E \ge E_{\delta_1}$, we have for $y^{(k)} \to (u,\mathbf{b})$,

$$
\liminf_{k\to\infty} \frac{1}{\nu k^2} E(y^{(k)}) \ge \liminf_{k\to\infty} \frac{1}{\nu k^2} E_{\delta_1}(y^{(k)}) \ge \int_{\mathcal{S}_1} \varphi_{\delta_1}(\nabla u, \mathbf{b})
$$

for all $\delta_1 > 0$. Now by proposition 2.2.26, $\varphi_{\delta_1} \nearrow \varphi$ pointwise as $\delta_1 \to 0$, so

$$
\liminf_{k\to\infty} \frac{1}{\nu k^2} E(y^{(k)}) \ge \int_{\mathcal{S}_1} \varphi(\nabla u, \mathbf{b})
$$

by monotone convergence.

2. First suppose that $|B^i(x)| \le c_0 - \theta$ a.e. for some $\theta > 0$. Then by lemma 2.2.25 for appropriately chosen δ_1, δ_2 small,

$$
\inf_{y\in\hat{\mathcal{N}}_{k,c_0}^{l_2,l_3}(u,\mathbf{b})} E(y) \le \inf_{y\in\hat{\mathcal{N}}_{k,c_0-\delta_2}^{l_2,l_3}(u,\mathbf{b})} E_{\delta_1}(y).
$$

Now by theorems 2.2.2 and 2.2.3 (see also corollary 2.2.20), denoting the macroscopic energy density corresponding to E_δ by φ^δ,

$$\lim_{k\to\infty} \frac{1}{\nu k^2} \inf_{y\in \hat{\mathcal{N}}^{l_2,l_3}_{k,c_0-\delta_2}(u,\mathbf{b})} E_{\delta_1}(y) = \int_{\mathcal{S}_1} \varphi^{\delta_1}_{c_0-\delta_2}(\nabla u, \mathbf{b}) \le \int_{\mathcal{S}_1} \varphi_{c_0-\delta_2}(\nabla u, \mathbf{b})$$

for $l_2, l_3 \to 0$, $kl_3 \to \infty$, and hence also

$$\limsup_{k\to\infty} \frac{1}{\nu k^2} \inf_{y\in \hat{\mathcal{N}}^{l_2,l_3}_{k,c_0}(u,\mathbf{b})} E(y) \le \int_{\mathcal{S}_1} \varphi_{c_0-\delta_2}(\nabla u, \mathbf{b}).$$

Now this holds for all δ_2, therefore

$$\limsup_{k\to\infty} \frac{1}{\nu k^2} \inf_{y\in \hat{\mathcal{N}}^{l_2,l_3}_{k,c_0}(u,\mathbf{b})} E(y) \le \int_{\mathcal{S}_1} \varphi_{c_0}(\nabla u, \mathbf{b})$$

by dominated convergence, provided $\varphi_{c_0-\delta} \to \varphi_{c_0}$ boundedly on $\{|B^i| \le c_0 - \theta\}$ as $\delta \to 0$. To see this, note first that on this set we may replace φ by φ^{δ_0} for $\delta_0 > 0$ small enough only depending on θ (see the proof of proposition 2.2.26). Now an easy consequence of lemma 2.2.11 is that $|\varphi^{\delta_0}_{k,c_0-\delta} - \varphi^{\delta_0}_{k,c_0}| \le C\delta^{1/5}$. It remains to note that $y^{(k)} \in \hat{\mathcal{N}}^{l_2,l_3}_{k,c_0}(u,\mathbf{b})$ for all k implies $y^{(k)} \to (u,\mathbf{b})$.

3. Now drop the assumption $|B^i| < c_0$, but still suppose that $|M^\theta| = 0$ for some fixed $\theta > 0$. Define approximations $\mathbf{b}_\eta \overset{\eta\to 0}{\longrightarrow} \mathbf{b}$ in L^∞ by

$$B^i_\eta = \begin{cases} B^i & \text{if } |B^i| \le c_0 - \eta, \\ (c_0 - \eta)\frac{B^i}{|B^i|} & \text{if } |B^i| > c_0 - \eta. \end{cases}$$

By continuity and boundedness of φ on $(M^\theta)^c$,

$$\lim_{\eta\to 0} \int_{\mathcal{S}_1} \varphi(\nabla u, \mathbf{b}_\eta) = \int_{\mathcal{S}_1} \varphi(\nabla u, \mathbf{b}).$$

Now choose an appropriate diagonal sequence $y^{(k)} \to (u, \mathbf{b})$ with

$$\limsup_{k\to\infty} \frac{1}{\nu k^2} E(y^{(k)}) \le \int_{\mathcal{S}_1} \varphi(\nabla u, \mathbf{b}).$$

4. For general $(u, \mathbf{b})$ we may suppose that $|M^0| = 0$ (for $|M^0| > 0$ the upper bound is trivial). For given $\mathbf{b} \in L^\infty(\mathcal{S}_1; (\mathbb{R}^3)^{\nu-1})$ we define $\mathbf{b}_\theta$ by $\mathbf{b}_\theta(x) = \mathbf{b}(x)$ if $x \notin M^\theta$, $\mathbf{b}_\theta \equiv \mathbf{0}$ else. By the previous results, $|\varphi(\nabla u(x), \mathbf{0})| \le C$. Since $\mathbf{b}_\theta \overset{*}{\rightharpoonup} \mathbf{b}$, we again find $y^{(k)} \to (u, \mathbf{b})$ such that

$$\limsup_{k\to\infty} \frac{1}{\nu k^2} E(y^{(k)}) \;\le\; \limsup_{\theta\to 0} \int_{\mathcal{S}_1} \varphi(\nabla u, \mathbf{b}_\theta) \;\le\; \int_{\mathcal{S}_1} \varphi(\nabla u, \mathbf{b})$$

by proposition 2.2.26. □

2.2.6 Extensions & variants

In the last paragraph of this section we discuss some extensions of the theory and possible changes of our set-up.

General Bravais lattices and domains

More generally, we could deal with Bravais-lattices

$$\mathcal{L} = \{x \in \mathbb{R}^3 : x = \sum_{i=1}^{3} \mu_i e_i, \mu_i \in \mathbb{Z}\},$$

where (e_1, e_2, e_3) are linearly independent in $\mathbb{R}^3$ and $\mathcal{S}_k := \{x_1 e_1 + x_2 e_2 : x_1, x_2 \in [0,k]\}$ for $k \in \mathbb{N}$. Then our reference configuration will be $\mathcal{L} \cap (\mathcal{S}_k \times [0,h]e_3)$ where $h := (\nu - 1)$, and $\Delta^i y(x_p) = y(x_p + ie_3) - y(x_p)$, $x_p \in \mathcal{S}_k$. This amounts to a simple coordinate change in the physical space $\mathbb{R}^3$.

Covering $\mathcal{S}$ with mesoscopic squares up to a negligible error at the boundary, it is not hard to see that the convergence scheme in fact applies to bounded Lipschitz domains $\mathcal{S} \subset \mathbb{R}^2$ (where φ is given as in theorem 2.2.2).

Alternative definition of convergence

In our definition of convergence $y^{(k)} \to (u, \mathbf{b})$, it is not possible to consider the limiting case of very restricted relaxation, i.e., $c_0 \to 0$, unless all b^i are zero. Instead of asking $\|\tilde{y} - u\|$ in definition 2.1.3 to be less than c_0/k one could demand that

$$\|\tilde{y} - v\| \leq c_0/k \tag{2.48}$$

where v is as in (2.9) corresponding to $u, \mathbf{b}$ with b^0 set to zero. (Condition (2.4) is not needed for this definition of convergence.) The results are analogous. Except for paragraph 3.1.3 we will not make use of this definition.

Different types of atoms

The theory developed so far may be generalized to films consisting of more than one species of atoms. Then E does not only depend on the positions y_i of the atoms but also on their type, labeled by, say, $t(i) \in \{1, \ldots, s\}$,

$$E = E(y_1, t(1), \ldots, y_N, t(N)).$$

Note that in our derivation we only made use of translational invariance of E. The theory still applies if the atoms of different type are arranged periodically on the lattice with some fixed (microscopic) period, i.e., there exist $p_1, p_2 \in \mathbb{N}$ such that for all x the atoms at (x_1, x_2, x_3), $(x_1 + p_1, x_2, x_3)$ and $(x_1, x_2 + p_2, x_3)$ are of the same type.

Distinguishable particle systems

Similarly, the convergence scheme also applies to certain systems with distinguishable particles. We will state a general result for systems with finite range interaction. The basic assumption is that only atoms that are close in the reference configuration are supposed to interact. This violates assumption 2.1.7 since the energy is not a function of atomic positions in the deformed configuration any more. It rather also depends on the reference configuration, i.e., the atoms are distinguishable. It will be clear, however, that the convergence scheme described so far still applies.

Let $a > 0$. To each $x_i \in \mathcal{L}_k$ we assign a neighborhood

$$U_{x_i} = \{x_j \in \mathcal{L} : |x_j - x_i| \leq a\} = \{x_1^i, \dots, x_{r_a}^i\},$$

where the enumeration of elements of U_{x_i} shall be such that $x_1^i = x_i$ and, if $(x_{i_1})_3 = (x_{i_2})_3$, then $x_j^{i_1} - x_{i_1} = x_j^{i_2} - x_{i_2}$ for $j = 1, \dots, r_a$.

Our goal is to study energy functions of the form

$$E_{\text{fr}}(y) = \sum_{x_i \in \mathcal{L} \cap ([a,k-a]^2 \times [0,h])} f_{x_i}(y(x_2^i) - y(x_1^i), \dots, y(x_{r_a}^i) - y(x_1^i)) + \mathcal{O}(k),$$

where $f_{x_i} : \mathbb{R}^{3(r_a-1)} \to \mathbb{R}$ are given functions representing the energy of the interactions between the i-th atom at its position $y(x_i) = y(x_1^i)$ and its neighboring atoms in their positions $y(x_2^i), \dots, y(x_{r_a}^i)$. (The term $\mathcal{O}(k)$ is introduced to compensate for boundary effects since U_{x_i} is not contained in $S_k \times [0, h]$ for x_i in a boundary layer of constant width a.)

More precisely, since we also have to consider energies of subsets of our atomic lattice, suppose the f_{x_i} are functions on $(\mathbb{R}^3 \cup \{\alpha\})^{r_a-1}$ with $\alpha \notin \mathbb{R}^3$ and $\text{dist}(\alpha, x) := 1$ for all $x \in \mathbb{R}^3$. For a subset $\mathcal{K}$ of $\mathcal{L}_k$ we define

$$E_{\text{fr}}(y(\mathcal{K})) = \sum_{x_i \in \mathcal{K}} f_{x_i}(y(x_2^i) - y(x_1^i), \dots, y(x_{r_a}^i) - y(x_1^i)) \tag{2.49}$$

with $y(x_j^i) - y(x_1^i)$ replaced by α whenever $x_j^i \notin \mathcal{K}$.

We do not assume f_{x_i} to satisfy any symmetry conditions. However, as noted earlier, we do need some periodicity, so we suppose there exist fixed $p_1, p_2 \in \mathbb{N}$ such that

$$f_{(x_1+p_1,x_2,x_3)} = f_x = f_{(x_1,x_2+p_2,x_3)} \tag{2.50}$$

for $x = (x_1, x_2, x_3) \in (\mathbb{Z}_+)^2 \times \{0, \dots, \nu - 1\}$.

Proposition 2.2.27 *Suppose E_{fr} is defined as in (2.49) and (2.50) holds. Assume that the f_{x_i} are locally Lipschitz. Then the limit φ_{fr} of theorem 2.2.2 exists, and we have*

$$\lim_{k\to\infty} \frac{1}{\nu k^2} \inf_{y \in \mathcal{W}_k^l(u,\mathbf{b})} E_{\text{fr}}(y) = \int_{\mathcal{S}_1} \varphi_{\text{fr}}(\nabla u(x), \mathbf{b}(x))dx$$

as $l \to 0$ and $kl \to \infty$.

(Adopting the notion of δ-criticality suitably (cf. definition 2.2.22), also unbounded pair-interaction parts can be treated analogously to theorem 2.2.4.)

Sketch of Proof. First note that by (2.50) there are only finitely many different functions f_x. Due to lemma 2.1.2, a bound on the distance of two atoms in the reference configuration implies a bound on their distance in the deformed state. So by a cut-off argument we may suppose that the functions f_{x_i} are uniformly bounded and have common Lipschitz constants. But each atom occurs in at most r_a summands of (2.49). This proves the desired Lipschitz property of E. As noted earlier, the remaining part of assumption 2.1.7 can be weakened to requiring that the periodicity assumption (2.50) is satisfied.

As for assumption 2.1.6, to estimate

$$|E(y(\mathcal{K}_1 \cup \mathcal{K}_2) - E(y(\mathcal{K}_1)) - E(y(\mathcal{K}_2))|$$

note that, if $x_i \in \mathcal{K}_1$ is such that $U_{x_i} \cap (\mathcal{K}_1 \cup \mathcal{K}_2) \neq U_{x_i} \cap \mathcal{K}_1$, then there exists $x' \in U_{x_i} \cap \mathcal{K}_2$, i.e., by lemma 2.1.2, $|y(x) - y(x')| \leq C$, a constant, analogously for $\mathcal{K}_1$, $\mathcal{K}_2$ interchanged. On the other hand, due to uniform boundedness of the f_{x_i}'s, the error term can be estimated by a constant (C', say) times the number (N, say) of such x_i in $\mathcal{K}_1 \cup \mathcal{K}_2$. Now if $\psi = 2C'\chi_{\{x:|x|\leq C\}}$, then indeed

$$|E(y(\mathcal{K}_1 \cup \mathcal{K}_2) - E(\mathcal{K}_1) - E(\mathcal{K}_2)| \;\leq\; C'N \;\leq \sum_{x\in\mathcal{K}_1, x'\in\mathcal{K}_2} \psi(|y(x) - y(x')|).$$

□

Remark: Dealing only with interactions whose range is bounded in the reference configuration, there is no need for a minimal strain hypothesis on u, i.e., for these interactions we might set $c_1 = 0$ in (2.3).

2.3 Examples/applications

In this section, we will investigate some examples of atomic interactions and explore under what circumstances these models fit into the theory developed in the last section. The first three models will satisfy assumptions 2.1.6 and 2.1.7 even in the more restrictive sense of assumption 2.1.8. For the last one this will be obviously false. Throughout this discussion we will assume that $u \in W^{1,\infty}(\mathcal{S}_1;\mathbb{R}^3)$, $b^i \in L^\infty(S_1;\mathbb{R}^3)$ are admissible. Applying the chain rule $\nabla f \circ g(x) = f'(g(x))\nabla g(x)$ a.e. for Lipschitz functions $f : \mathbb{R} \to \mathbb{R}$, $g : \mathbb{R}^n \to \mathbb{R}$, as usual, the right hand side is interpreted as zero whenever $\nabla g = 0$ regardless of $f'(g(x))$ being well-defined or not.

2.3.1 Pair potentials

As a first example we consider pair potentials, i.e., energy functions of the form

$$E_{\mathrm{pp}}(y) = \frac{1}{2}\sum_{i\neq j} W(|y_i - y_j|), \tag{2.51}$$

where $W : [0,\infty) \to \mathbb{R}$.

Proposition 2.3.1 *Suppose E_{pp} is defined as in (2.51). Assume that $W : [0,\infty) \to \mathbb{R}$ is Lipschitz. If there exist $M > 0$ and $q > 3$ such that for a.e. $r \geq 0$*

$$|W(r)| \leq Mr^{-q} \quad \text{and} \quad |W'(r)| \leq Mr^{-q+1},$$

then E_{pp} is admissible.

Proof. We need only check that E_{pp} satisfies assumptions 2.1.6 and 2.1.7. Clearly, E_{pp} only depends on atomic positions, is frame indifferent, and satisfies assumption 2.1.6 with $\psi(r) = |W(r)|$. Furthermore, W Lipschitz (with Lipschitz constant M', say) implies that E is Lipschitz, and we have a.e.

$$\begin{aligned} \left| \frac{\partial E}{\partial y_l}(y) \right| &= \left| \frac{1}{2} \sum_{i \neq j} W'(|y_i - y_j|) \cdot \frac{y_i - y_j}{|y_i - y_j|} \cdot (\delta_{il} - \delta_{jl}) \right| \\ &\leq \sum_{j \neq l} \left| W'(|y_l - y_j|) \right| . \end{aligned} \tag{2.52}$$

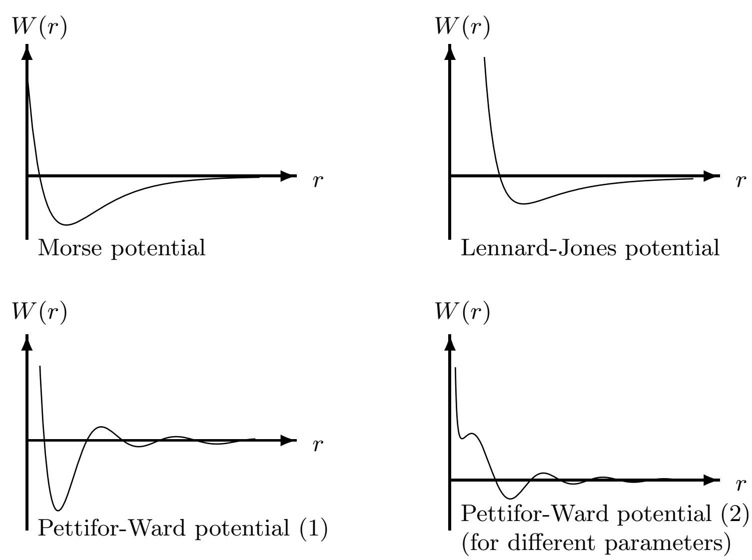
We have to find a bound on this quantity assuming $\|\tilde{y} - u\| \leq C/k$. But then as in lemma 2.1.2, y satisfies $|y(x) - y(z)| \geq C_1|x - z| - C_3$, and we can apply the technique of splitting the sum into long-range and short-range terms as in the proof of lemma 2.2.6. From $|W'(r)| \leq M'$ and $|W'(r)| \leq Mr^{-q+1}$ (if existing) for some $q > 3$, we then deduce that the right hand side of (2.52) is bounded a.e. (independently of k and l). □

An example is given by the Morse potential with interaction function

$$W_{\mathrm{M}}(r) := W_0(e^{-2a(r-r_0)} - 2e^{-a(r-r_0)})$$

for positive parameters W_0, a and r_0 (cf. [35]).

Having proven this proposition independently of theorem 2.2.4, also pair potentials with W as in (2.15) are covered by our convergence scheme, e.g., the



Lennard-Jones potential given by

$$W_{\mathrm{LJ}}(r) = W_0 \cdot \left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right),$$

$W_0 > 0$ and σ constants (cf. [35]), and the Pettifor-Ward pair potentials (cf. [37]) given by

$$W_{\mathrm{PW}}(r) = \frac{W_0}{r} \sum_{n=1}^{3} a_n \cos(k_n r + \alpha_n) e^{-\kappa_n r},$$

$W_0 > 0, a_n, k_n, \alpha_n, \kappa_n$ constants such that $\sum_n a_n \cos(\alpha_n) > 0$.

2.3.2 Pair functionals

More generally, in this paragraph we will discuss pair functionals as examples of the embedded atom method. These models have the advantage of also covering some environmental dependence of the bond strength between the nuclei at positions $\{y_i\}$ (cf. [35]). We let

$$E_{\mathrm{pf}}(y) = \frac{1}{2} \sum_{i \neq j} W(|y_i - y_j|) + \sum_i F(\rho_i), \tag{2.53}$$

where $W : [0, \infty) \to \mathbb{R}$ as above, $F : [0, \infty) \to \mathbb{R}$, and ρ_i is given by

$$\rho_i = \sum_{j \neq i} f(|y_i - y_j|), \tag{2.54}$$

$f : [0, \infty) \to [0, \infty)$.

The interpretation of such an energy function is the following (cf. [35]). As always, $\{y_i\}$ denotes the positions of the nuclei of some material. These nuclei are supposed to be embedded in some electron gas consisting of the valence electrons of the atoms of that material. Now suppose that the total energy associated with y can be split into two parts: one that describes the interaction of the various nuclei, leading to the first summand in (2.53), and the sum of the energy it costs to embed a single nucleus into an electron gas of some density ρ. Denoting this energy

$$E_{\mathrm{embedding}} = F(\rho),$$

where ρ denotes the electron density at the point the nucleus is embedded, and assuming that the electron density at y_i depends on the positions of the other nuclei through

$$\rho_i = \sum_{j \neq i} f(|y_i - y_j|),$$

this embedding energy of a single nucleus at y_i is indeed $F(\rho_i)$.

We aim at exhibiting conditions on W, F and f such that E_{pf} satisfies assumptions 2.1.6 and 2.1.7. First note that since

$$E_{\mathrm{pf}}(y) = \frac{1}{2} \sum_{i \neq j} W(|y_i - y_j|) + \sum_i F\left(\sum_{j \neq i} f(|y_i - y_j|) \right),$$

E_{pf} only depends on atomic positions and, depending in fact only on the interatomic distances, is frame indifferent.

Lemma 2.3.2 *Suppose E_{pf} is defined as in (2.53) and W is as in proposition 2.3.1 (resp. theorem 2.2.4). Assume $F : [0,\infty) \to (-\infty, 0]$ is convex and Lipschitz, $f : [0,\infty) \to [0,\infty)$ is Lipschitz and, for a.e. $r \geq 0$,*

$$|F \circ f(r)| \leq M r^{-q}, \quad |f'(r)| \leq M r^{-q+1}.$$

Then E_{pf} is admissible (resp. theorem 2.2.4 applies).

Note that – as is plausible – by the decay hypothesis and assumptions on F, necessarily $f(r) \to 0$ as $r \to \infty$ (if F is not trivial). In the following proposition we will see that F need not be Lipschitz. While the decay assumption on f' is in the spirit of the previous result, $|F \circ f(r)| \leq M r^{-q}$ poses quite severe decay conditions on f, if we take, e.g., $F(a) \sim \sqrt{a}$. This will be remedied in proposition 2.3.3.

Proof. First note $F \leq 0$ convex implies that $-F$ is subadditive. By proposition 2.3.1, it remains to verify assumptions 2.1.6 and 2.1.7 for the embedding term $E_{\text{emb}}(y) = \sum_i F(\rho_i)$. So let $\mathcal{M}$ and $\mathcal{N}$ be disjoint sets of atoms. Setting

$$\rho_v^{\mathcal{K}} = \sum_{\substack{w \in \mathcal{K} \\ w \neq v}} f(|v - w|),$$

we find

$$\begin{aligned}
&|E_{\text{emb}}(\mathcal{M} \cup \mathcal{N}) - E_{\text{emb}}(\mathcal{M}) - E_{\text{emb}}(\mathcal{N})| \\
&= \left| \sum_{v \in \mathcal{M} \cup \mathcal{N}} F(\rho_v^{\mathcal{M} \cup \mathcal{N}}) - \sum_{v \in \mathcal{M}} F(\rho_v^{\mathcal{M}}) - \sum_{v \in \mathcal{N}} F(\rho_v^{\mathcal{N}}) \right| \\
&= \left| \sum_{v \in \mathcal{M}} (F(\rho_v^{\mathcal{M} \cup \mathcal{N}}) - F(\rho_v^{\mathcal{M}})) + \sum_{v \in \mathcal{N}} (F(\rho_v^{\mathcal{M} \cup \mathcal{N}}) - F(\rho_v^{\mathcal{N}})) \right|.
\end{aligned}$$

Consider the first sum: $f \geq 0$ implies that

$$\rho_v^{\mathcal{M} \cup \mathcal{N}} = \sum_{\substack{w \in \mathcal{M} \cup \mathcal{N} \\ w \neq v}} f(|v - w|) \geq \sum_{\substack{w \in \mathcal{M} \\ w \neq v}} f(|v - w|) = \rho_v^{\mathcal{M}}.$$

So since F is decreasing (because it is convex and non-positive), we have

$$\begin{aligned}
\left| \sum_{v \in \mathcal{M}} (F(\rho_v^{\mathcal{M} \cup \mathcal{N}}) - F(\rho_v^{\mathcal{M}})) \right| &= \sum_{v \in \mathcal{M}} (-F(\rho_v^{\mathcal{M} \cup \mathcal{N}}) + F(\rho_v^{\mathcal{M}})) \\
\leq \sum_{v \in \mathcal{M}} \Bigg(\Bigg[-F\Bigg(\sum_{\substack{w \in \mathcal{M} \\ w \neq v}} f(|v - w|) \Bigg) &+ \sum_{w \in \mathcal{N}} -F(f(|v - w|)) \Bigg] + F(\rho_v^{\mathcal{M}}) \Bigg) \\
= \sum_{v \in \mathcal{M}} \sum_{w \in \mathcal{N}} -F(f(|v - w|))
\end{aligned}$$

by subadditivity of $-F$. Treating the term $|\sum_{v\in\mathcal{N}}(F(\rho_v^{\mathcal{M}\cup\mathcal{N}})-F(\rho_v^{\mathcal{N}}))|$ analogously and summing up, we have shown that

$$|E_{\rm emb}(\mathcal{M}\cup\mathcal{N})-E_{\rm emb}(\mathcal{M})-E_{\rm emb}(\mathcal{N})| \ \leq \ \sum_{\substack{v\in\mathcal{M},\\ w\in\mathcal{N}}} -2F\circ f(|v-w|),$$

so we may choose $\psi(r)=-2F\circ f(r)$. Note that since f is bounded, $F\circ f$ is bounded, too. Clearly the decay hypothesis on $\psi(r)$ as $r\to\infty$ is satisfied. This concludes the first part of the proof.

For the remaining part we again only need to consider the embedding term of the energy. (The first one is dealt with as in the proof of proposition 2.3.1.) F is Lipschitz, say $\|F'\|_\infty \leq M'$. So almost everywhere

$$\begin{aligned}
&\left|\frac{\partial}{\partial y_l}\sum_i F\left(\sum_{j\neq i} f(|y_i-y_j|)\right)\right| \\
&= \left|\sum_i\left(F'\left(\sum_{j\neq i} f(|y_i-y_j|)\right)\cdot\sum_{j\neq i} f'(|y_i-y_j|)\cdot\frac{y_i-y_j}{|y_i-y_j|}\cdot(\delta_{il}-\delta_{jl})\right)\right| \\
&\leq \ M'\left|\sum_{i\neq j} f'(|y_i-y_j|)\cdot\frac{y_i-y_j}{|y_i-y_j|}\cdot(\delta_{il}-\delta_{jl})\right| \\
&\leq \ 2M'\sum_{j\neq l}\left|f'(|y_l-y_j|)\right|. \qquad (2.55)
\end{aligned}$$

Just as before, for $\tilde{y}$ in a C/k-neighborhood of u, the decay and boundedness hypotheses on f' allow us to split this sum into long-range and short-range terms. We find a bound on this quantity independent of k and l. □

Proposition 2.3.3 *Suppose W is as in proposition 2.3.1 (resp. theorem 2.2.4). Assume now $F:[0,\infty)\to(-\infty,0]$ is convex, $f:[0,\infty)\to(0,\infty)$ is Lipschitz, and, for a.e. $r\geq 0$,*

$$|f(r)|\leq Mr^{-q}, \quad |f'(r)|\leq Mr^{-q+1}.$$

Then theorems 2.2.1, 2.2.2, and 2.2.3 (resp. 2.2.4) apply to $E_{\rm pf}$ as given in (2.53) and (2.54).

Remark: Before we prove this proposition we would like to comment on the plausability of the various assumption made. F is non-positive since placing a positively charged particle into an electron cloud yields energy. The non-negativity of f is clear since f is supposed to be a density. Strict posivity is plausible since perfect screening is not to be expected. The convexity condition on F can be understood as reflecting the fact that, due to screening, adding more electrons, i.e., raising the electron density, results in smaller and smaller effects. This seems to match experimental data (cf. [35], p. 171). A qualitatively reasonable scaling would be given by $F(a)\sim-\sqrt{a}$ as, e.g., in the Finnis-Sinclair model where $F(a) \propto -\sqrt{a}$ (cf. [35]). The remaining are decay assumptions on f as those for W.

Proof. Let y be some deformation satisfying $\|\tilde{y} - u\| \leq C/k$. Then for each $y_i = y(x_i)$, there is $y_j = y(x_j)$ with $j \neq i$ and $|y_i - y_j| \leq 2C + c_2$ (choose x_j to be a neighbor of x_i). So $\sum_{j \neq i} f(|y_i - y_j|)$ (i fixed) is bounded from below by some $\delta > 0$. Defining $\hat{F}$ suitably by

$$\hat{F}(\rho) = \begin{cases} 0 & \text{for } \rho = 0, \\ \text{linear} & \text{for } 0 \leq \rho \leq \delta, \\ F(\rho) & \text{for } \rho \geq \delta, \end{cases}$$

$\hat{F}$ is convex and Lipschitz. Furthermore, $|\hat{F} \circ f(r)| \leq \frac{|F(\delta)|}{\delta} |f(r)| \leq CMr^{-q}$. So the corresponding energy $\hat{E}_{\text{pf}}(y)$ is admissible. Since for all y with $\|\tilde{y} - u\| \leq c_0/k$

$$E_{\text{pf}}(y) = \hat{E}_{\text{pf}}(y),$$

theorems 2.2.1, 2.2.2, and 2.2.3 also apply to E. □

Remark: E_{pf} is not admissible in the usual sense since, e.g., for two atoms y_1, y_2

$$E_{\text{pf}}(y_1, y_2) = W(|y_1 - y_2|) + 2F\Big(f(|y_1 - y_2|)\Big),$$

and $F \circ f(r)$ is in general not $\mathcal{O}(r^{-q})$ for some $q > 3$.

2.3.3 Angular forces

In this paragraph we consider energy functions that may also depend on the angles between atomic bonds. For a physical motivation of such models we refer to [35]. Mathematically this leads to the consideration of potentials depending on triplets of atomic positions:

$$E_{\text{af}}(y) = \frac{1}{2} \sum_{i \neq j} W(|y_i - y_j|) + \frac{1}{6} \sum_{\substack{i,j,k \\ i \neq j \neq k \neq i}} \hat{W}(y_i, y_j, y_k) \tag{2.56}$$

where $W : [0, \infty) \to \mathbb{R}$ and $\hat{W}$ is given by

$$\begin{aligned} \hat{W}(y_i, y_j, y_k) \ &= \ h(|y_i - y_j|, |y_j - y_k|, \theta_{ijk}) + h(|y_j - y_k|, |y_k - y_i|, \theta_{jki}) \\ &\quad + h(|y_k - y_i|, |y_i - y_j|, \theta_{kij}), \end{aligned} \tag{2.57}$$

θ_{ijk} denoting the angle between $y_i - y_j$ and $y_k - y_j$, and

$$h : \begin{cases} [0, \infty) \times [0, \infty) \times \mathbb{R} \to \mathbb{R}, \\ (r_1, r_2, \theta) \mapsto h(r_1, r_2, \theta), \end{cases}$$

is 2π-periodic and symmetric in the last variable.

Again we are seeking for conditions on W and $\hat{W}$ (resp. h) such that E_{af} satisfies assumptions 2.1.6 and 2.1.7. As before, it is easy to see that $E_{\text{af}}(y)$ depending only on interatomic distances and angles is determind by atomic positions and is frame indifferent.

Proposition 2.3.4 *Suppose E_{af} is defined as in (2.56). Assume that W is as in proposition 2.3.1 (resp. theorem 2.2.4) and h is Lipschitz. Furthermore, there are bounded functions $\chi_1, \chi_2, \alpha_1, \alpha_2 : [0,\infty) \to [0,\infty)$ with*

$$\chi_\mu(r) \le Mr^{-q}, \quad \alpha_\mu(r) \le Mr^{-q+1}, \quad \mu = 1, 2$$

such that

$$|h(r_1, r_2, \theta)| \le \chi_1(r_1)\chi_2(r_2)$$

and (a.e.)

$$\left|\frac{\partial h}{\partial r_\mu}(r_1, r_2, \theta)\right| \le \alpha_1(r_1)\alpha_2(r_2), \quad \mu = 1, 2,$$

and

$$\left|\frac{\partial h}{\partial \theta}(r_1, r_2, \theta)\right| \le \alpha_1(r_1)\alpha_2(r_2)\min\{r_1, r_2\}.$$

Then E_{af} is admissible (resp. theorem 2.2.4 applicable).

Remark: Note that it is plausible to require that $\partial h/\partial\theta$ vanish as $r_1 \to 0$ or $r_2 \to 0$ since $\hat{W}(y_i, y_j, y_k)$ should depend continuously on y_i, y_j, y_k, but the angle θ_{ijk} does not when the triangle becomes degenerate.

The proof is tedious but not very hard. Splitting into long- and short-range terms, all sums occuring in the error terms can be bounded appropriately. ψ can be chosen as $\psi(r) = |W(r)| + C\max\{\chi_1(r), \chi_2(r)\}$.

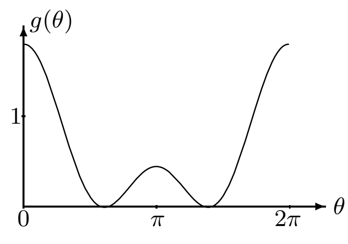
Example: If h splits into

$$h(r_1, r_2, \theta) = f_1(r_1)f_2(r_2)g(\theta),$$

as, e.g., for Stillinger-Weber-type energies (cf. [35]). Then h satisfies the conditions of proposition 2.3.4 if f_μ, f_μ' are bounded, $|f_\mu| \le Mr^{-q}$, $|f_\mu'| \le Mr^{-q+1}$ for $\mu = 1, 2$, $f_1(r_1)f_2(r_2) \le \min\{r_1, r_2\}$ and g and g' are bounded. This is satisfied, e.g., for the angular term

$$g(\theta) = (\cos(\theta) + 1/3)^2$$

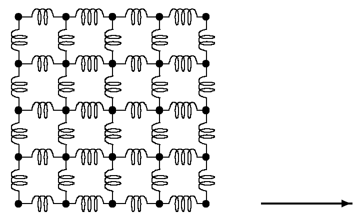
discussed in [35].



2.3.4 A simple example

Even for fairly elementary microscopic energies as, e.g., given by pair potentials, not much is known about their ground state deformations. (Some one-dimensional results in this direction can be found in [5], a recent two-dimensional result for certain pair potentials is proven in [38].) We conclude this section calculating φ explicitly for a simple nearest neighbor model. Although it lacks some physical requirements (e.g., shear resistance), it captures some realistic features as, e.g., quadratic energy growth near the reference configuration (a natural state) for pure extensions. The model consisting of two different types of bonds, the energy minimizer will not be a simple crystal. A pointwise limit would overestimate the macroscopic energy.

Suppose the atoms of our reference configuration interact only with nearest neighbors and the interaction potential is harmonic, i.e., given by springs of strength d_1 and d_2 with equilibrium at distance 1.



We assume that bonds in the reference configuration parallel to the x_2- or x_3-axes have $d_1 = 1$, while bonds parallel to the x_1 axis have alternating $d_1 = 1$ and $d_2 = 2$ as in the previous picture. So the energy is given by

$$E_{\text{nn}}(y) = \frac{1}{2} \sum_{|x_i - x_j| = 1} d_{ij}(|y_i - y_j| - 1)^2, \tag{2.58}$$

$d_{ij} = 1$ or 2 as described above.

Proposition 2.3.5 E_{nn} *is admissible in the sense of proposition 2.2.27. In particular, the limit* φ_{nn} *of theorem 2.2.2 exists for* E_{nn} *and*

$$E_{\text{nn}}(u, \mathbf{b}) = \int_{\mathcal{S}_1} \varphi_{\text{nn}}(\nabla u(x), \mathbf{b}(x))dx.$$

Furthermore (set $b^0 = 0$*), if* c_0 *is not too small,*

$$\begin{aligned} \varphi_{\text{nn}}(A, \mathbf{b}) \;=\; & \frac{4}{3}(\max\{0, |a_{\cdot 1}| - 1\})^2 + (\max\{0, |a_{\cdot 2}| - 1\})^2 \\ & + \sum_{i=1}^{\nu-1} (\max\{0, |b^i - b^{i-1}| - 1\})^2, \end{aligned}$$

where $a_{\cdot j}$ *denotes the* j^{th} *column of* A.

This is clearly a special case of (2.49) with $a = 1$ and periodicity $p_1 = 2, p_2 = 1$. So we only have to prove the representation formula for φ_{nn}.

Sketch of Proof. The main observation in the elementary but tedious proof is that the energy decouples into energies of one dimensional atomic chains

$$i \mapsto y(i, x_2, x_3), \quad \text{resp.} \quad i \mapsto y(x_1, i, x_3), \quad i = 0, \ldots, k,$$

with $k+1$ atoms ((x_2, x_3) resp. (x_1, x_3) fixed), and $\nu - 1$ chains with $(k+1)^2 + 1$ atoms whose difference of successive atoms (labeled by $0 \le x_1, x_2 \le k$) is given by $y(x_1, x_2, i) - y(x_1, x_2, i-1)$, i fixed:

$$\begin{aligned} E(y) \;=\; & \sum_{\substack{0 \le x_2 \le k \\ 0 \le x_3 \le \nu - 1}} \; \sum_{0 \le x_1 \le k-1} d(x_1)(|y(x_1+1, x_2, x_3) - y(x_1, x_2, x_3)| - 1)^2 \\ & + \sum_{\substack{0 \le x_1 \le k \\ 0 \le x_3 \le \nu - 1}} \; \sum_{0 \le x_2 \le k-1} (|y(x_1, x_2+1, x_3) - y(x_1, x_2, x_3)| - 1)^2 \\ & + \sum_{0 \le x_3 \le \nu - 2} \; \sum_{0 \le x_1, x_2 \le k} (|y(x_1, x_2, x_3+1) - y(x_1, x_2, x_3)| - 1)^2, \end{aligned}$$

where $d(x_1) = d_1 = 1$ if x_1 is even, $d(x_1) = d_2 = 2$ if x_1 is odd. Now the energy can be bounded from below by minimizing the energy of these chains separately subject to boundary conditions $\tilde{y} = v$ on $\partial S_1 \times [0, h]$ resp. $⨍ \Delta^i \tilde{y} = b^i$. Allowing for negligible error terms, these configurations can be patched together to yield the desired result. □

Chapter 3

Qualitative properties of the effective theory

3.1 The dependence of φ on the relaxation scheme

Our notion of convergence $y^{(k)} \to (u, \mathbf{b})$ of atomic deformations to macroscopic variables $u, \mathbf{b}$ depends on the constant c_0 (cf. definition 2.1.3). To keep track of this dependence, we will sometimes add c_0 as an additional subscript as, e.g., in $\hat{\mathcal{N}}^{0,1}_{k,c_0}$, φ_{k,c_0}. Our first task is to analyze this dependence of our continuum theory on the relaxation parameter c_0. It will turn out that we can not relax sending c_0 to infinity. This is due to the (physically reasonable) decay assumptions on atomic interactions. Moreover, c_0/k will prove to be the only scale which both accounts for atomistic relaxation effects and yields a non-trivial continuum theory. We start by proving the following regularity result.

Proposition 3.1.1 *Fix* $(A, \mathbf{b}) \in \mathcal{A}_{\mathrm{hom}}$. *The mapping* $c_0 \mapsto \varphi_{c_0}(A, \mathbf{b})$ *is decreasing and continuous where defined.*

Proof. Suppose $c_0 > c_0'$. By theorem 2.2.2, $\varphi_{c_0}(A, \mathbf{b}) \le \varphi_{c_0'}(A, \mathbf{b})$. Conversely, given $y \in \hat{\mathcal{N}}^{0,1}_{k,c_0}(A, \mathbf{b})$, by lemma 2.2.11 we find a deformation $y' \in \hat{\mathcal{N}}^{0,1}_{k,c_0'}(A, \mathbf{b})$ with $E(y') \le E(y) + C(c_0 - c_0')^{1/5} k^2$ provided $(A, \mathbf{b})$ is admissible for c_0' and $|c_0 - c_0'| \le 1$. Therefore, $\varphi_{c_0'}(A, \mathbf{b}) \le \varphi_{c_0}(A, \mathbf{b}) + C(c_0 - c_0')^{1/5}$. $\square$

3.1.1 The limit $c_0 \to \infty$

Suppose E is an admissible pair potential with purely attractive pair interaction $W \le 0$, $W \not\equiv 0$. Considering deformations with larger and larger periodic cells where every atom is mapped to a single point, we see that for all admissible A, $\mathbf{b}$,

$$\lim_{c_0 \to \infty} \varphi_{c_0}(A, \mathbf{b}) = -\infty.$$

In this paragraph we will show that such trivial behavior is in fact not due to this specific choice of E. Rather, the limit $c_0 \to \infty$ in general will be trivial if assumption 2.1.8 is satisfied.

Theorem 3.1.2 *Suppose E satisfies assumptions 2.1.6, 2.1.7, and 2.1.8. Define $\varphi_\infty := \lim_{c_0\to\infty} \varphi_{c_0}$. (This limit exists pointwise in $[-\infty,\infty)$ by proposition 3.1.1.) Then $\varphi_\infty(A,\mathbf{b}) = \varphi_\infty(A',\mathbf{b}')$ for all matrices A, A' of rank two and all vectors $\mathbf{b},\mathbf{b}' \in (\mathbb{R}^3)^{\nu-1}$. (Every such matrix resp. vector is admissible if c_0 is large enough.)*

Proof. Suppose first that $A' = A$. By $V_{A,\mathbf{b}}$ we denote the un-rescaled version of v (cf. (2.9)) corresponding to $u = A$ and b^0 set to zero. For $\mathbf{b}$ such that the projection of each b^i onto graph(A) has norm less than $2|A|$,

$$\begin{aligned} |V_{A,\mathbf{b}}(x) - V_{A,\mathbf{b}}(x')| &= |A(x_p - x'_p) + b^{x_3} - b^{x'_3}| \\ &\geq |A(x_p - x'_p)| - 4|A| \\ &\geq C_1|x - x'| - C_3, \end{aligned}$$

C_1, C_3 independent of $\mathbf{b}$. From assumption 2.1.8 and lemma 2.2.6 we then find a constant C such that for those $\mathbf{b}$, $E(V_{A,\mathbf{b}}) \leq Ck^2$. On the other hand, if for two vectors $\mathbf{b}_1$, $\mathbf{b}_2$ and some $i \in \{1,\dots,\nu-1\}$,

$$b_2^j = b_1^j \text{ for } j \neq i \quad \text{and} \quad b_2^i = b_1^i + Az,\ z \in \mathbb{Z}^2,$$

then $E(V_{A,\mathbf{b}_1}) = E(V_{A,\mathbf{b}_2}) + \mathcal{O}(|z|k)$. So for all $\mathbf{b}$ we obtain $\lim_{k\to\infty} \frac{1}{\nu k^2} E(V_{A,\mathbf{b}}) \leq C$, whence $\varphi_\infty(A,\cdot)$ is an upper bounded function on $\mathbb{R}^{3(\nu-1)}$ with values in $[-\infty,\infty)$. Since it is convex (by proposition 3.3.3 all $\varphi_{c_0}(A,\cdot)$ are convex), it must be constant.

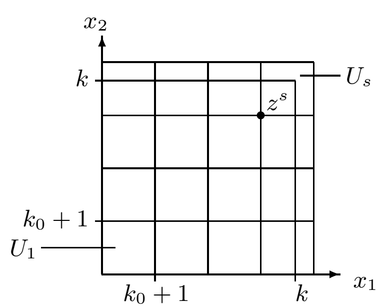
For the remaining part, it suffices to show that

$$\varphi_\infty(A',\mathbf{b}) \leq \varphi_\infty(A,\mathbf{b}).$$

We proceed similarly as in the proof of proposition 2.2.15. Fix c_0 and $\delta > 0$. Choosing k_0 large enough, by theorem 2.2.2 we find $y \in \hat{\mathcal{N}}^{0,1}_{k_0,c_0}(A,\mathbf{b})$ with

$$\frac{1}{\nu k_0^2} E(y) \leq \varphi_{c_0}(A,\mathbf{b}) + \delta/2. \tag{3.1}$$

We construct a deformation $y' : \mathcal{L}_k \to \mathbb{R}^3$, $k \gg k_0$, by patching together appropriately translated copies of y: let $U_1,\dots,U_s$ be translates of $[0,k_0+1)^2$.



Let $z_1,\dots,z_s$ denote the lower left corners of these sets, set $f^i = A'z^i$, and define

$$y'(x_1,x_2,x_3) = y(x_1 - z_1^i, x_2 - z_2^i, x_3) + f^i$$

for $x \in \mathcal{L} \cap (U_i \times [0,h])$. Then

$$\|y' - A'\| = \sup_{x \in \mathcal{L}_{k_0}} |y'(x) - A'x_p| \leq \sup_{x \in \mathcal{L}_{k_0}} |y(x)| + \sup_{x_p \in S_{k_0}} |A'x_p| =: \tilde{c_0}.$$

So $\tilde{c_0}$ depends on k_0 (and A, A') but is independent of k. Since

$$\begin{aligned}
⨍_{[0,1]^2} \left(k\Delta^i \tilde{y}' - b^i\right) d\rho &= ⨍_{\bigcup U_j} \left(k\Delta^i \tilde{y}' - b^i\right) d\rho + \mathcal{O}\left(\frac{k_0^2}{k}\right) \\
&= \frac{1}{sk_0^2} \sum_{j=1}^{s} \int_{U_j} \left(k\Delta^i \tilde{y}' - b^i\right) d\rho + \mathcal{O}\left(\frac{k_0^2}{k}\right) \\
&= \mathcal{O}\left(\frac{k_0^2}{k}\right)
\end{aligned}$$

(note $|k\Delta^i \tilde{y}'| \leq 2\tilde{c_0}$), by lemma 2.2.12 we find a deformation

$$\hat{y} \in \hat{\mathcal{N}}^{0,1}_{k,\tilde{c_0}}(A', \mathbf{b}) \tag{3.2}$$

such that

$$\left|\frac{1}{\nu k^2} E(y') - \frac{1}{\nu k^2} E(\hat{y})\right| \leq C(\tilde{c_0}) \left(\frac{k_0^2}{k}\right)^{1/5}. \tag{3.3}$$

Using lemma 2.2.8 and translational invariance, we would now like to split the energy to find that

$$\left|\frac{1}{\nu k^2} E(y'(x) : x \in \mathcal{L}_k) - \frac{1}{\nu k_0^2} E(y(x) : x \in \mathcal{L}_{k_0})\right| \leq C\left(\frac{1}{k_0} + \frac{k_0}{k}\right). \tag{3.4}$$

If this is possible, we find that by (3.4), (3.2), (3.3) and (3.1) for $k \gg k_0 \gg 1$,

$$\varphi_{k,\tilde{c_0}}(A', \mathbf{b}) \leq \frac{1}{\nu k_0^2} E(y(x) : x \in \mathcal{L}_{k_0}) + \delta/2 \leq \varphi_{c_0}(A, \mathbf{b}) + \delta.$$

Letting first $k \to \infty$, we deduce from proposition 3.1.1

$$\varphi_\infty(A', \mathbf{b}) \leq \varphi_{c_0}(A, \mathbf{b}) + \delta.$$

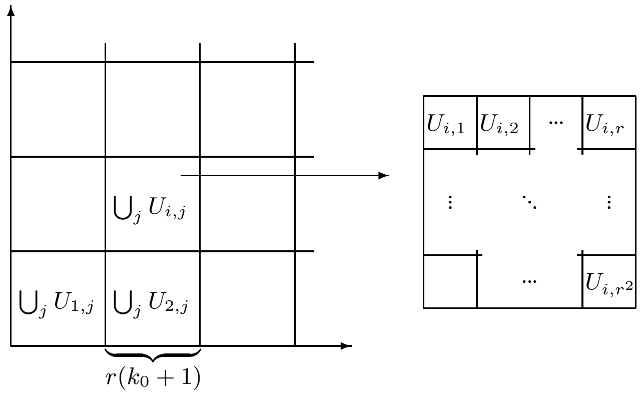
Since δ was arbitrary, we finally get sending $c_0 \to \infty$,

$$\varphi_\infty(A', \mathbf{b}) \leq \varphi_\infty(A, \mathbf{b}).$$

It remains to justify the application of lemma 2.2.8. The problem is that $\tilde{c_0}$ depends on k_0. (For nearest neighbor models as discussed in proposition 2.2.27, this splitting in (3.4) will in general not be possible: for y' as described above neglecting the bonds between sets $y(U_i \times [0,h])$ could result in neglecting an essential part of the energy.) However, as noted at the beginning of paragraph 2.2.2, if assumption 2.1.8 holds, this will be possible if we can replace y' by some y'' such that still $\|y'' - A\| \leq \tilde{c_0}$ depends only on k_0, and y'' consists of translates of $y(\mathcal{L}_{k_0})$, but in addition satisfies a far-field minimal strain hypothesis with constants C_1, C_3 independent of k_0, i.e.,

$$|y''(x_1) - y''(x_2)| \geq C_1|x_1 - x_2| - C_3. \tag{3.5}$$

We re-enumerate the squares $U_1, \ldots, U_s$ as depicted in the following diagram.



($r \in \mathbb{N}$ to be specified later.) Depending on A, A', k (and $c_0, \tilde{c_0}$), we choose a unit vector $e \in \mathbb{R}^3$ perpendicular to the graph of A' and numbers $0 < a_1 < \ldots < a_{r^2}$ (to be specified later) and define

$$y''(x_1, x_2, x_3) = y'(x_1, x_2, x_3) + a_j e$$

if $x \in \mathcal{L} \cap U_{i,j} \times [0, h]$, $j \in \{1, \ldots, r^2\}$.

We will now find C_1, C_3 independent of k_0 such that (3.5) holds. Since still on each of the sets $U_{i,j} \times [0, h]$, y'' is a translated copy of y, we may replace y' by y''. Applying (3.4) then finishes the proof.

If x_1 and x_2 lie in the same $U_{i,j} \times [0, h]$, this is clear from lemma 2.1.2 since $y \in \hat{\mathcal{N}}^{0,1}_{k_0,c_0}(A, \mathbf{b})$.

Now suppose this is not the case, but still $|x_1 - x_2|_\infty < (r-1)(k_0+1)$. Then $x_1 \in U_{i_1,j_1} \times [0, h]$, $x_2 \in U_{i_2,j_2} \times [0, h]$ with $j_1 \neq j_2$. But then

$$\begin{aligned}
|y''(x_1) - y''(x_2)| &\geq |a_{j_1} - a_{j_2}| - |y'(x_1) - y'(x_2)| \\
&\geq |a_{j_1} - a_{j_2}| - |f^{i_1,j_1} - f^{i_2,j_2}| \\
&\quad -|y(x_1 - (z^{i_1,j_1}, 0)) - y(x_2 - (z^{i_2,j_2}, 0))| \\
&\geq |a_{j_1} - a_{j_2}| - |f^{i_1,j_1} - f^{i_2,j_2}| - 2c_0 \\
&\quad -|A((x_1)_p - z^{i_1,j_1}) - A((x_2)_p - z^{i_2,j_2})| \\
&\geq |a_{j_1} - a_{j_2}| - C' r k_0 - 2c_0 - C k_0 \\
&\geq 2rk_0 \qquad \text{for } |a_{j_1} - a_{j_2}| \text{ sufficiently large} \\
&\geq |x_1 - x_2|.
\end{aligned}$$

So we assume that $|a_{j_1} - a_{j_2}|$, $j_1, j_2 \in \{1, \ldots, r^2\}$, are large enough to justify the above calculation.

Finally, let $x_1 \in U_{i_1,j_1} \times [0, h]$, $x_2 \in U_{i_1,j_2} \times [0, h]$ and $|x_1 - x_2|_\infty \geq (r-1)(k_0+1)$. Since e is perpendicular to the graph of A' and y' lies in a $\tilde{c_0}$-neighborhood of that graph, we find that for r not too small,

$$\begin{aligned}
|y''(x_1) - y''(x_2)| &= |(a_{j_1} - a_{j_2})e + y'(x_1) - y'(x_2)| \\
&\geq |(a_{j_1} - a_{j_2})e + A'(x_1 - x_2)|
\end{aligned}$$

$$
\begin{aligned}
&-|y'(x_1) - A'x_1| - |y'(x_2) - A'x_2| \\
\geq\ & |A'x_1 - A'x_2| - 2\tilde{c_0} \\
\geq\ & |y'(x_1) - y'(x_2)| - 4\tilde{c_0} \\
\geq\ & |f^{i_1,j_1} - f^{i_2,j_2}| - |y(x_1 - z^{i_2,j_1}) - y(x_2 - z^{i_2,j_2})| - 4\tilde{c_0} \\
\geq\ & |f^{i_1,j_1} - f^{i_2,j_2}| - 2c_0 - 2|A|k_0 - 4\tilde{c_0} \\
\geq\ & c|z^{i_1,j_1} - z^{i_2,j_2}| - 2c_0 - 2|A|k_0 - 4\tilde{c_0} \\
\geq\ & \frac{c}{2}|z^{i_1,j_1} - z^{i_2,j_2}| \\
\geq\ & \frac{c}{6}|x_1 - x_2|,
\end{aligned}
$$

where $c = \min_{|x|=1} |A'x|$. The last but one inequality follows from the fact that for $i_1 \neq i_2$,

$$
\frac{c}{2}|z^{i_1,j_1} - z^{i_2,j_2}| \geq \frac{c(r-1)k_0}{4} \geq 2c_0 + 2|A|k_0 + 4\tilde{c_0}
$$

for $|x_1 - x_2|_\infty > (r-1)k_0$ if we choose r sufficiently big.

Setting $\tilde{\tilde{c_0}} = \tilde{c_0} + \max_{1 \leq j \leq r^2} |a_j e|$, we furthermore have $\|y'' - A'\| \leq \tilde{\tilde{c_0}}$. So by possibly enlarging $\tilde{c_0}$ to $\tilde{\tilde{c_0}}$, we can indeed split the energy to obtain (3.4), and the proof is finished. □

For systems that do not satisfy assumption 2.1.8, φ_∞ may be nontrivial (for an example see proposition 2.3.5). In paragraph 3.3.1, we will prove that φ_∞ is quasiconvex with respect to the first variable and convex with respect to the second.

3.1.2 The limit $c_0 \to 0$

Assume that convergence of deformations is defined as in (2.48). It is not hard to calculate the limit

$$
\varphi_0(A, \mathbf{b}) := \lim_{c_0 \to 0} \varphi_{c_0}(A, \mathbf{b})
$$

which exists in $(-\infty, \infty]$ since $c_0 \mapsto \varphi_{c_0}(A, \mathbf{b})$ is decreasing.

Proposition 3.1.3 *Let $V_{A,\mathbf{b}}$ be as in (2.9) for constant $\nabla u = A$ and $\mathbf{b}$, $b^0 = 0$. Then*

$$
\varphi_0(A, \mathbf{b}) = \lim_{k \to \infty} \frac{1}{\nu k^2} E(V_{A,\mathbf{b}}(x) : x \in \mathcal{L}_k).
$$

In particular, the limit on the right hand side exists (in $\mathbb{R}$ under the usual assumptions 2.1.6 and 2.1.7, in $(-\infty, \infty]$ for energies of the form (2.15)).

Proof. Suppose first E is of the form (2.15) and there are $i \neq j \in \{0, \ldots, \nu - 1\}$ such that $b^i \in b^j + A\mathbb{Z}^2$. Then if $\|y - V_{A,\mathbf{b}}\| \leq r$,

$$
E(y) \geq \frac{k^2}{4} \inf_{0 < s \leq r} W(s) - Ck^2 \to \infty
$$

as $r \to 0$. For the remaining cases note that $E(V_{A,\mathbf{b}})$ is bounded by lemma 2.2.6 and if $\|y - V_{A,\mathbf{b}}\| \leq r$,

$$
|E(y) - E(V_{A,\mathbf{b}})| \leq L\nu k^2 r.
$$

Therefore,

$$\limsup_{k\to\infty} \sup_{y\in\hat{\mathcal{N}}_k^{0,1}(A,\mathbf{b})} \left| \frac{1}{\nu k^2} E(y) - \frac{1}{\nu k^2} E(V_{A,\mathbf{b}}) \right| \le Lc_0.$$

Now letting $c_0 \to 0$ proves the claim. $\square$

Example: For admissible pair potentials, i.e., energies of the form (2.51) with W satisfying the conditions of theorem 2.2.4, we get

$$\varphi_0(A, \mathbf{b}) = \lim_{k\to\infty} \frac{1}{2\nu k^2} \sum_{\substack{x,z\in\mathcal{L}_k \\ x\ne z}} W(|V_{A,\mathbf{b}}(x) - V_{A,\mathbf{b}}(z)|).$$

Restricting this sum to those x such that $\operatorname{dist}(x_p, \partial([0,k]^2)) > l$ where $1 \ll l \ll k$, yields an error term of order $\mathcal{O}(kl/k^2) = o(1)$. Then summing over all $z \in \mathbb{Z}^2 \times \{0, 1, \ldots, \nu - 1\}$, $z \ne x$, instead of $\mathcal{L}_k \setminus \{x\}$ gives another error term of order $\mathcal{O}(l^{2-q}) = o(1)$. This sum now being independent of x_p, we obtain

$$\begin{aligned}
\varphi_0(A, \mathbf{b}) &= \frac{1}{2\nu} \sum_{i=0}^{\nu-1} \sum_{\substack{z\in\mathcal{L}\cap(\mathbb{R}^2\times[0,h]) \\ z\ne(0,0,i)}} W(|V_{A,\mathbf{b}}(z) - V_{A,\mathbf{b}}(0,0,i)|) \\
&= \frac{1}{2\nu} \sum_{i,j=0}^{\nu-1} \sum_{\substack{z_p\in\mathbb{Z}^2 \\ (z_p,j)\ne(0,0,i)}} W(|Az_p + b^j - b^i|).
\end{aligned}$$

The corresponding macroscopic energy functional is given by

$$E(u, \mathbf{b}) = \int_{S_1} \frac{1}{2\nu} \sum_{i,j=0}^{\nu-1} \sum_{\substack{z\in\mathbb{Z}^2 \\ (z,j)\ne(0,0,i)}} W(|\nabla u(x)z + b^j(x) - b^i(x)|)dx.$$

This expression can be seen as a thin-film version with directors $b^1, \ldots, b^{\nu-1}$ of a formula derived in [7].

3.1.3 Triviality for slowly converging deformations

By our definition of convergence the effective continuum theory depends on the scale $l_1 = c_0/k$ measuring the rate of uniform convergence of $\tilde{y}^{(k)}$ to u. This paragraph serves to prove that in fact only this physically motivated choice $l_1(k) = \text{const.}/k$ yields non-trivial results in the continuum limit.

It is easy to see that for $l_1 \ll 1/k$ we reproduce the limit obtained in proposition 3.1.3. So suppose now $l_1 = l_1(k) \gg 1/k$. (Then all $\mathbf{b} \in L^\infty(\mathcal{S}_1; (\mathbb{R}^3)^{\nu-1})$ will be admissible.) In analogy to $\mathcal{W}_k^l$ (cf. theorem 2.2.3) we define

$$\mathcal{W}_k^{l_1,l_2}(u, \mathbf{b}) := \{y : \|\tilde{y} - u\| \le l_1,\ \|k\Delta^i\tilde{y} - b^i\|_{W^{-1,\infty}} \le l_2\}.$$

Theorem 3.1.4 *Suppose E satisfies assumptions 2.1.6, 2.1.7, and 2.1.8. Assume $l_1(k)$, $l_2(k)$ satisfy $kl_1(k), kl_2(k) \to \infty$. Then for all admissible u (cf. (2.3)) and all $\mathbf{b}$ the limit*

$$E = E(u, \mathbf{b}) = \lim_{k\to\infty} \frac{1}{\nu k^2} \inf_{y \in \mathcal{W}_k^{l_1,l_2}(u,\mathbf{b})} E(y)$$

exists in $[-\infty, \infty)$ and is the same for all $(u, \mathbf{b})$.

Proof. Let

$$E(u, \mathbf{b}) := \liminf_{k\to\infty} \frac{1}{\nu k^2} \inf_{y \in \mathcal{W}_k^{l_1,l_2}(u,\mathbf{b})} E(y).$$

Suppose that $\mathbf{b}, \mathbf{b}' \in L^\infty(\mathcal{S}_1; (\mathbb{R}^3)^{\nu-1})$ and u, u' are admissible. The proof follows along the lines of the proof of theorem 3.1.2, we indicate the necessary modifications. Choosing a suitable large k_0, we find $y \in \mathcal{W}_{k_0-1}^{l_1,l_2}(u, \mathbf{b})$ with

$$\frac{1}{\nu(k_0-1)^2} E(y) \le E(u, \mathbf{b}) + \delta/3$$

(resp. $\le -1/\delta$ for $E(u, \mathbf{b}) = -\infty$). In addition to the sets $U_i = z^i + [0, k_0+1)^2$ consider the subsets $\hat{U}_i = z^i + [0, k_0)^2$, and construct y' similar as in the proof of theorem 3.1.2 by

$$y'(x_1, x_2, x_3) = y(x_1 - z_1^i, x_2 - z_2^i, x_3) + U'(z^i) \quad \text{ on } \mathcal{L}_k \cap (\hat{U}_i \times [0, h]),$$

where U' denotes the unrescaled version of u'. On the remaining $(2k_0+1)\nu$ atoms of $U_i \times [0, h]$ we define y' appropriately such that

$$\fint_{U_i/k} k\Delta^i \tilde{y}' d\rho^{(k)} = \frac{1}{(k_0+1)^2} \sum_{x_p \in \mathbb{Z}^2 \cap U_i} y'(x_p, i) - y'(x_p, 0) = \fint_{U_i/k} \bar{b}'^i d\rho^{(k)}.$$

We may assume that for $x, x' \in \mathcal{L}_k$ with $x_p \in U_i \backslash \hat{U}_i$ and $x'_p \in U_i$, $|y(x) - y(x')| \ge |x_p - x'_p|$ and that $\|y' - U'\|$ is bounded in terms of k_0 independently of k.

Choosing a scale l_3 such that $1/k \ll l_3 \ll l_2$ and applying lemmas 2.2.12 and 2.2.13 (with constants depending on k_0), we still find $\hat{y} \in \mathcal{W}_k^{l_1,l_2}(u', \mathbf{b}')$ such that for k_0 fixed

$$\left| \frac{1}{\nu k^2} E(y') - \frac{1}{\nu k^2} E(\hat{y}) \right| \to 0 \quad \text{as} \quad k \to \infty.$$

In order to show that the energy splits, again we possibly have to replace y' by y''. For the construction of y'' we can only guarantee that

$$|y''(x_1) - y''(x_2)| \ge C_1|x_1 - x_2| - C_3$$

with C_1, C_3 independent of k_0 and k for x_1 and x_2 that do not lie in the same $U_{i,j} \cap \hat{U}_i$. But lemma 2.2.8 still works in this more general case. r now might not be a fixed number, but still it only depends on k_0, the same being true for $a_1, \dots, a_{r^2}$. Also note that for the same reason and by translational invariance

$$\left| E(y'(x) : x \in \mathcal{L} \cap (U_i \times [0, h])) - E(y) \right| \le Ck_0.$$

Finally sending k to infinity gives

$$\begin{aligned}\limsup_{k\to\infty} \inf_{\hat{y}\in\mathcal{W}_k^{l_1,l_2}(u',\mathbf{b}')} E(\hat{y}) &\leq \frac{1}{\nu k_0^2}E(y)+\delta/3 \\ &\leq \frac{(k_0-1)^2}{k_0^2}(E(u,\mathbf{b})+\delta/3)+\delta/3 \\ &\leq E(u,\mathbf{b})+\delta\end{aligned}$$

if k_0, only depending on $(u,\mathbf{b})$ and δ, is sufficiently large.

Now first setting $u'=u$, $\mathbf{b}'=\mathbf{b}$, this proves that in fact

$$E(u,\mathbf{b}) = \lim_{k\to\infty} \inf_{y\in\mathcal{W}_k^{l_1,l_2}(u,\mathbf{b})} E(y).$$

Secondly, the argument shows that $E(u',\mathbf{b}') \leq E(u,\mathbf{b})$. Reversing the roles of $\mathbf{b}$ and $\mathbf{b}'$ respectively u and u', we obtain

$$E(u,\mathbf{b}) = E(u',\mathbf{b}').$$

□

3.2 Extremal strains

In this section we examine $\varphi(A,\mathbf{b})$ for A with very large (cf. paragraph 3.2.1) or small (cf. paragraph 3.2.2) singular values. Physically, the limit $A\to\infty$ is of limited relevance since (in view of the L^∞-constraint) we do not allow for fracture in our model. However, it is mathematically not difficult, so we include this discussion for the sake of completeness. The limit $A\to 0$ is more interesting. Our relaxed atomic to continuum limit leads to an intermediate energy regime between purely continuum membrane theory, for which all short maps yield zero energy, and pointwise discrete to continuum limits that assume the Cauchy-Born rule.

3.2.1 Strongly tensile deformations

Again in this paragraph we suppose that assumption 2.1.8 is satisfied.

For a system $\mathbf{y}$ of ν atoms at positions $y^0,\ldots,y^{\nu-1}\in\mathbb{R}^3$ we define $\bar{E}$ by

$$\bar{E}(\mathbf{y}) = \begin{cases} E(\mathbf{y}) & \text{for } \mathbf{y}\in B_{c_0}, \\ \infty & \text{else,}\end{cases}$$

where $B_{c_0}=\{\mathbf{y}\in(\mathbb{R}^3)^\nu : |y^i|\leq c_0\}$ is the ball of radius c_0 centered at 0 in configuration space. $\bar{E}^{**}$ denotes the convex envelope of $\bar{E}$.

Proposition 3.2.1 *The large strain limit* $\lim_{A\to\infty}\varphi(A,\mathbf{b})$ *exists, and*

$$\lim_{A\to\infty}\varphi(A,\mathbf{b}) = \frac{1}{\nu}\min_{a\in\mathbb{R}^3}\bar{E}^{**}(a,b^1+a,\ldots,b^{\nu-1}+a).$$

Here, $A\to\infty$ means that both singular values $s_1(A)$ and $s_2(A)$ of A tend to infinity.

Proof. Let $y \in \hat{\mathcal{N}}_k^{0,1}(A,\mathbf{b})$ and $\mathbf{y}_{x_p} = (y(x_p,0),\dots,y(x_p,\nu-1))$, $\Delta\mathbf{y}_{x_p} = (y(x_p,1)-y(x_p,0),\dots,y(x_p,\nu-1)-y(x_p,0))$. By lemma 2.2.5,

$$\left| E(y) - \sum_{x_p\in\mathbb{Z}^2\cap\mathcal{S}_k} E(\mathbf{y}_{x_p}) \right| \le \frac{1}{2} \sum_{x,z\in\mathcal{L}_k\,:\,x_p\neq z_p} \psi(|y(x)-y(z)|).$$

By definition of $\hat{\mathcal{N}}_k^{0,1}$, if $c_1 \le s_1(A)$, then $|y(x)-y(z)| \ge c_1|x_p-z_p| - 2c_0$ which is $\ge \frac{c_1}{2}|x_p-z_p|$ for c_1 large, $x_p \neq z_p$.

If the singular values of A tend to infinity, we may choose c_1 as large as we want and find that

$$\begin{aligned}
\left| E(y) - \sum_{x_p} E(\mathbf{y}_{x_p}) \right| &\le \frac{M}{2} \sum_{x,z\,:\,x_p\neq z_p} |y(x)-y(z)|^{-q} \\
&\le \frac{M}{2}\left(\frac{c_1}{2}\right)^{-q} \sum_{x,z\,:\,x_p\neq z_p} |x_p-z_p|^{-q} \\
&= \left(2^{q-1}M\nu^2 \sum_{x_p\neq z_p} |x_p-z_p|^{-q} \right) c_1^{-q} \\
&\le Ck^2c_1^{-q}
\end{aligned}$$

by lemma A.1, so

$$\left| \frac{1}{k^2}E(y) - \frac{1}{k^2}\sum_{x_p} E(\mathbf{y}_{x_p}) \right| \to 0$$

as $c_1 \to \infty$.

We thus have to minimize $\frac{1}{k^2}\sum_{x_p} E(\mathbf{y}_{x_p})$ subject to $y \in \hat{\mathcal{N}}_k^{0,1}(A,\mathbf{b})$. By frame indifference this is the same as minimizing

$$\frac{1}{k^2}\sum_{x_p} E(\mathbf{y}_{x_p}) \quad \text{subject to } \ \mathbf{y}_{x_p} \in B_{c_0} \text{ and } \ \frac{1}{(k+1)^2}\sum_{x_p} \Delta\mathbf{y}_{x_p} = \mathbf{b}.$$

Now the claim is an elementary consequence of Carathéodory's theorem (cf. [14] Cor. 2.9, p. 42). □

Remarks:

(i) If in definition 2.1.3 we request that $\|\tilde{y} - v_{A,\mathbf{b}}\| \le c_0/k$ instead of $\|\tilde{y} - A\| \le c_0/k$ as in (2.48), the result is analogous if we replace B_{c_0} by $B_{c_0}(\mathbf{b}) = \{\mathbf{y} \in (\mathbb{R}^3)^\nu : |y^i - b^i| \le c_0\}$ ($b^0 := 0$). Then while holding c_0 fixed, we may send $(A,\mathbf{b}) \to \infty$ in the following sense. Let $A \to \infty$ as above. If e is a unit normal to graph(A), suppose that $|\langle b^i - b^j, e\rangle| \to \infty$ for $i \neq j \in \{0,\dots,\nu-1\}$. Clearly, this leads to

$$\lim_{A,\mathbf{b}\to\infty} \varphi(A,\mathbf{b}) = 0.$$

(ii) It is necessary to require that assumption 2.1.8 be satisfied. For φ_{nn} as in proposition 2.3.5 we obviously have

$$\lim_{A\to\infty} \varphi(A,\mathbf{b}) = \lim_{A,\mathbf{b}\to\infty} \varphi(A,\mathbf{b}) = \infty.$$

3.2.2 Strongly compressive deformations

In this paragraph we consider the limiting behavior of the macroscopic energy for strongly compressive strains, in particular, if the energy diverges or remains bounded in this regime. If the energy of two particles at distance r scales like $r^{-\alpha}$ as $r \to 0$, it turns out that $\alpha = 3$ – not $\alpha = 2$ as expected from taking pointwise limits – is a critical exponent for typical values of A and $\mathbf{b}$. This is due to our allowance for atomic relaxation.

Recall the definition of $B^1, \ldots, B^\nu$ from (2.22). We consider pair potentials with interaction function W as in (2.51) satisfying the conditions of theorem 2.2.4. The main result of this paragraph is the following

Theorem 3.2.2 *Suppose $(A, \mathbf{b})$ is admissible, and let $S_p := \sqrt{A^T A} \in \mathbb{R}^{2\times 2}$.*

(i) Assume that $r^3 W(r) \to \infty$ as $r \to 0$. Then

$$\lim_{\substack{\det(S_p)\to 0 \\ |S_p|\le C<\infty}} \varphi(A, \mathbf{b}) = \infty.$$

(ii) For each $\beta < 3$ there are examples of pair potentials with pair-interaction $W(r) \sim r^{-\beta} \to \infty$ as $r \to 0$ such that

$$\limsup_{\substack{\det(S_p)\to 0 \\ |S_p|\le C<\infty}} \varphi(A, \mathbf{b}) < \infty$$

for $\mathbf{b}$ such that $|B^i| < c_0$.

We first prove two preparatory lemmas, the first is a refined version of the far field minimal strain property (cf. lemma 2.1.2). For $A \in \mathbb{R}^{3\times 2}$, in addition to $S_p = \sqrt{A^T A} \in \mathbb{R}^{2\times 2}$ we set

$$S' := \begin{pmatrix} (S_p)_{11} & (S_p)_{12} & 0 \\ (S_p)_{21} & (S_p)_{22} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \; S := \begin{pmatrix} (S_p)_{11} & (S_p)_{12} \\ (S_p)_{21} & (S_p)_{22} \\ 0 & 0 \end{pmatrix}, \; A' := \begin{pmatrix} A_{11} & A_{12} & e_1 \\ A_{21} & A_{22} & e_2 \\ A_{31} & A_{32} & e_3 \end{pmatrix},$$

where e is the unit vector perpendicular to graph(A) such that $\det(A') > 0$. By the singular value decomposition there is an orthogonal matrix $R \in SO(3)$ such that

$$A = RS, \qquad A' = RS'.$$

We will investigate the limit $\det(S_p) \to 0$ while the singular values of A, i.e., the eigenvalues of S_p, remain bounded, which we will assume for the rest of this paragraph.

Lemma 3.2.3 *Suppose $\|y - A\| \le c_0$ and $x, x' \in \mathcal{L}_k$ are such that $|y(x) - y(x')| \ge a > 0$. Then for c such that $\frac{1-c}{c} a \ge 2c_0 + 2h$:*

$$|y(x) - y(x')| \ge c|S'x - S'x'|.$$

Proof. Clear, if $|S'x - S'x'| \leq a/c$. If $|S'x - S'x'| \geq a/c$, then

$$\begin{aligned}
&|y(x) - y(x')| \\
&\geq |A'x - A'x'| - |y(x) - Ax_p| - |Ax'_p - y(x')| - |Ax_p - A'x| - |A'x' - Ax'_p| \\
&= |S'x - S'x'| - |y(x) - Ax_p| - |Ax'_p - y(x')| - |Sx_p - S'x| - |S'x' - Sx'_p| \\
&\geq |S'x - S'x'| - 2c_0 - |x_3| - |x'_3| \\
&\geq c|S'x - S'x'| + (1-c)a/c - 2c_0 - 2h \\
&\geq c|S'x - S'x'|.
\end{aligned}$$

□

In the second lemma we estimate the number of atoms that are close to other atoms.

Lemma 3.2.4 *Suppose there are N atoms at positions $y_1, \ldots, y_N$ in a bounded region $U \subset \mathbb{R}^3$. Let U_ρ, $\rho > 0$, be the ρ-neighborhood of U. Then*

$$\#\{(y_i, y_j) : i \neq j, |y_i - y_j| \leq \rho\} \geq N - \frac{6}{\pi\rho^3}|U_\rho|.$$

Proof. We place one atom after the other into U. If an atom has distance larger than ρ from all the previous atoms, it shall belong to $\mathcal{M} \subset \{y_1, \ldots, y_N\}$. Now since atoms in $\mathcal{M}$ have pairwise distances greater than ρ, we find that

$$\#\mathcal{M}\frac{4\pi}{3}\left(\frac{\rho}{2}\right)^3 \leq |U_\rho|.$$

It follows that

$$\#\{(y_i, y_j) : i \neq j, |y_i - y_j| \leq \rho\} \geq N - \#\mathcal{M} \geq N - \frac{6}{\pi\rho^3}|U_\rho|.$$

□

Proof of theorem 3.2.2. (i) If $y \in \hat{\mathcal{N}}_k^{0,1}(A, \mathbf{b})$, then all the atoms lie in the c_0-neighborhood of $A([0,k]^2)$. The volume of the r_0-neighborhood of this set is $2(c_0 + r_0)\det(S_p)k^2 + \mathcal{O}(k)$. By lemma 3.2.4 we have

$$\begin{aligned}
\#\{(y_i, y_j) : i \neq j, |y_i - y_j| \leq r_0\} &\geq \nu k^2 - \frac{6}{\pi r_0^3}(2(c_0 + r_0)\det(S_p)k^2 + \mathcal{O}(k)) \\
&\geq k^2/2,
\end{aligned}$$

provided $r_0^3 \gg \det(S_p)$ as $\det(S_p) \to 0$, and therefore (fix $a > 0$ such that W is positive on $(0, a]$ and suppose that $r_0 \leq a$)

$$\begin{aligned}
E_{\text{pp}}(y) &= \frac{1}{2}\sum_{i \neq j} W(|y_i - y_j|) \\
&\geq \frac{1}{2}\sum_{\substack{i \neq j \\ |y_i - y_j| \leq r_0}} W(|y_i - y_j|) + \frac{1}{2}\sum_{\substack{i \neq j \\ |y_i - y_j| > a}} W(|y_i - y_j|) \\
&\geq \frac{k^2}{4}\inf_{0 \leq \rho \leq r_0} W(\rho) - \frac{Ck^2}{\det(S_p)}
\end{aligned}$$

(see below). Now since $W(r) \gg r^{-3}$, we also have $\inf_{0<\rho\leq r} W(r) \gg r^{-3}$, and we may choose $r_0 \to 0$ as $\det(S_p) \to 0$ such that

$$\inf_{0\leq\rho\leq r_0} W(\rho) \gg \frac{1}{\det(S_p)} \gg r_0^{-3}.$$

Then indeed $E_{\rm pp}(y) \geq \gamma k^2$ for $\gamma = \gamma(A)$ independent of y and k with $\gamma(A) \to \infty$ as $\det(S_p) \to 0$. This proves

$$\lim_{\det(S_p)\to 0} \inf_{y\in\hat{\mathcal{N}}_k^{0,1}(A,\mathbf{b})} \frac{1}{\nu k^2} E_{\rm pp}(y) = \infty.$$

It remains to show that

$$\left| \sum_{|y(x)-y(x')|\geq a} W(|y(x)-y(x')|) \right| \leq \frac{Ck^2}{\det(S_p)}.$$

This follows from lemma 3.2.3: the left hand side can be estimated by

$$\begin{aligned}
&\sum_{\substack{|y(x)-y(x')|\geq a\\ |S'x-S'x'|\leq a}} |W|(|y(x)-y(x')|) + \sum_{\substack{|y(x)-y(x')|\geq a\\ |S'x-S'x'|>a}} |W|(|y(x)-y(x')|) \\
\leq\ & \sum_{\substack{|y(x)-y(x')|\geq a\\ |S'x-S'x'|\leq a}} Ma^{-q} + \sum_{\substack{|y(x)-y(x')|\geq a\\ |S'x-S'x'|>a}} M|y(x)-y(x')|^{-q} \\
\leq\ & \nu(k+1)^2 Ma^{-q} \#\{x\in\mathbb{Z}^3 : |S'x|\leq a\} + Mc^{-q} \sum_{|S'x-S'x'|\geq a} |S'x-S'x'|^{-q} \\
\leq\ & \frac{C\nu k^2}{\det(S')} + C\nu k^2 \sum_{|S'x|\geq a} |S'x|^{-q} \\
\leq\ & \frac{Ck^2}{\det(S')} + Ck^2 \int_{|S'x|\geq a} |S'x|^{-q} dx \\
=\ & \frac{Ck^2}{\det(S')} + Ck^2 \int_{|z|\geq a} |z|^{-q} \frac{dz}{\det(S')} \\
=\ & \frac{Ck^2}{\det(S_p)}.
\end{aligned}$$

This finishes the proof of the first part of theorem 3.2.2.

(ii) As before, e denotes a unit vector perpendicular to the graph of A. By convexity in $\mathbf{b}$ (cf. proposition 3.3.3) and $\max_i |B^i| := c_3 < c_0$, we may assume that

$$\langle b^i, e\rangle \neq \langle b^j, e\rangle$$

for $i \neq j$ and choose constants $c, l > 0$ small such that

$$\min_{i\neq j} |\langle b^i - b^j, e\rangle| \geq c \quad \text{ and } \quad c_0 \geq \sqrt{2l^2 + (c/2)^2} + c_3. \tag{3.6}$$

Consider $(k+1)^2$ points $z_{ij} = A(i,j,0)$ at positions $A(\{0,\dots,k\}^2)$. Since the singular values of S_p are bounded, for each of these points there is another one closer than d to it for d sufficiently large. Now partition the graph of A by disjoint translates of a square of side-length l such that every such point is covered. The number of those points in such a square Q is bounded by $C/\det(S_p)$.

On the other hand, if $A = RS$, each set $Q_e = \{z \in \mathbb{R}^3 : \exists \lambda \in [0, c/2] : z - \lambda e \in Q\}$ contains at least Cr^{-3} points of the lattice $rR\mathbb{Z}^3$ if r is small. Choosing r such that $r^3 = \tilde{c}\det(S_p)$, $\tilde{c}$ sufficiently small, we can move the original points z_{ij} within the sets Q_e onto distinct lattice points z'_{ij} of $rR\mathbb{Z}^3$ such that $|z_{ij} - z'_{ij}| \leq \sqrt{2l^2 + (c/2)^2}$.

Now define a deformation y by

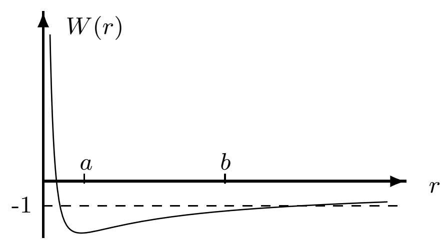
$$y(x_1, x_2, x_3) = z'_{x_1 x_2} + B^{x_3+1}.$$

By (3.6) and $|B^i| \leq c_3$, y lies in $\hat{\mathcal{N}}_k^{0,1}(A, \mathbf{b})$. y satisfies a minimal distance hypothesis with r: $|y(x) - y(x')| \geq r$ for $x \neq x'$. If $x_3 = x'_3$, this follows from the definition of y. If $x_3 \neq x'_3$ this follows from

$$\begin{aligned}
|y(x) - y(x')| &\geq |\langle y(x) - y(x'), e\rangle| \\
&= |\langle z'_{x_1x_2} + B^{x_3+1} - z'_{x'_1x'_2} - B^{x'_3+1}, e\rangle| \\
&\geq |\langle B^{x_3+1} - B^{x'_3+1}, e\rangle| - |\langle z'_{x_1x_2} - z'_{x'_1x'_2}, e\rangle| \\
&\geq |\langle b^{x_3} - b^{x'_3}, e\rangle| - c/2 \\
&\geq c/2
\end{aligned}$$

by (3.6) and construction of y.

Now suppose W is admissible and as in the picture below,



i.e., $|W(r)| \leq Cr^{-\alpha}$ with $\alpha < 3$ for $r \leq a$, and $W(r) \leq 0$ for $r \geq a$, moreover, $W(r) \leq -1$ for $a \leq r \leq b$, $0 < a < b$ given. Then for x fixed,

$$\begin{aligned}
&\sum_{x' \neq x} W(|y(x) - y(x')|) \\
&\leq \sum_{|y(x)-y(x')|\leq a} W(|y(x) - y(x')|) + \sum_{a<|y(x)-y(x')|\leq b} W(|y(x) - y(x')|) \\
&\leq C \sum_{|y(x)-y(x')|\leq a} |y(x) - y(x')|^{-\alpha} + \sum_{a<|y(x)-y(x')|\leq b} (-1) \\
&\leq C \sum_{x'\in\mathbb{Z}^3 : 0<|rx'|\leq a} |rx'|^{-\alpha} - \#\{x' : a < |y(x) - y(x')| \leq b\} \\
&= Cr^{-\alpha} \sum_{0<|x'|\leq a/r} |x'|^{-\alpha} - \#\{x' : a < |y(x) - y(x')| \leq b\} \\
&\leq Cr^{-\alpha} r^{\alpha-3} - \#\{x' : a < |y(x) - y(x')| \leq b\}.
\end{aligned}$$

Now since the singular values of S_p are bounded, the number of atoms that lie in $\{z : a < |z - y(x)| \le b\}$ is bounded below by $C(b-a)/\det(S_p)$ if $b-a$ is not too small, and we find that

$$\#\{x' : a < |y(x) - y(x')| \le b\} \ge C\frac{(b-c_0)^2 - (a+c_0)^2}{\det(S_p)} \ge C\frac{b-a}{\det(S_p)}.$$

Together with the above estimate and our choice $r^3 = \tilde{c}\det(S_p)$, this shows that

$$\sum_{x' \neq x} W(|y(x) - y(x')|) \le Cr^{-3} - \tilde{C}r^{-3}(b-a).$$

So if $b-a$ is chosen sufficiently large, this energy is negative. Now sum over all x to deduce that also the overall energy is negative. □

Remarks:

(i) It is not hard to see that, if (cf. (2.4)) b^0 is uniquely determined and there are B^i (cf. (2.22)) with $|B^i| = c_0$, then $\alpha = 2$ is the critical exponent for $\lim_{\det(S_p)\to 0} \varphi(A, \mathbf{b})$.

(ii) Part (i) of theorem 3.2.2 applies to more general energies E of the form

$$E(y) = E_{\mathrm{pp}}(y) + E_0(y)$$

where E_{pp} is an admissible pair potential with interaction function W as in (2.15) satisfying the conditions of theorem 3.2.2 (i) and $E_0 \ge -Ck^2$ independent of c_1.

3.3 Qualitative properties of φ

In this short section we discuss convexity and symmetry properties of φ. The proofs of the following results are rather elementary.

3.3.1 Convexity properties

By frame indifference of the model, convexity of φ in A is in general not to be expected (cf. [11], p. 170, also recall theorem 3.2.2 (i)). First, we show that under the usual assumptions even rank-one convexity fails in general. This is due to the restrictions made in the relaxation process. Convexity in $\mathbf{b}$ depends on the 'right' definition of convergence. Finally, for systems as in (2.49) where the c_0-relaxed energy density may be non-trivial, we show quasiconvexity resp. convexity of φ_∞ in the first resp. second component.

Loss of rank-one convexity

First recall the notion of rank-one convexity:

Definition 3.3.1 *Suppose $f : \Omega \to \mathbb{R}$, where $\Omega \subset \mathbb{R}^{m\times n}$ is a set of $m \times n$-matrices. We say that f is rank-one convex on Ω if*

$$\lambda \mapsto f(\lambda A + (1-\lambda)B), \quad \lambda \in [0,1],$$

is convex whenever $\lambda A + (1-\lambda)B \in \Omega$ for all $\lambda \in [0,1]$ and $\operatorname{rank}(A-B) = 1$.

The following result shows that φ will typically not be globally rank-one convex. Fix $\mathbf{b}$ and consider $\varphi(\cdot,\mathbf{b}) : \mathcal{A}_{\mathbf{b}} := \{A \in \mathbb{R}^{3\times 2} : \mathrm{rank}(A) = 2\} \to \mathbb{R}$.

Proposition 3.3.2 *Suppose $\varphi(\cdot,\mathbf{b})$ is rank-one convex and assumption 2.1.8 is satisfied. Then for all $A \in \mathcal{A}_{\mathbf{b}}$,*

$$\varphi(A,\mathbf{b}) \geq \lim_{A\to\infty} \varphi(A,\mathbf{b}).$$

Here, $\lim_{A\to\infty}\varphi(A,\mathbf{b})$ is the large strain limit discussed in proposition 3.2.1.

Proof. First note that φ is in fact bounded on each $\mathcal{A}_{\mathbf{b}}(c_1) := \{A \in \mathbb{R}^{3\times 2} : s_1(A) \geq c_1\}$, $c_1 > 0$, by lemma 2.2.6 and assumption 2.1.8. Let $\delta > 0$. Set

$$f(\lambda_1,\lambda_2) := \varphi(A\cdot\Lambda,\mathbf{b}), \quad \Lambda := \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}$$

for $\lambda_1,\lambda_2 \geq 1$. Note that

$$\inf_{x\neq 0} \frac{\langle A\Lambda x, A\Lambda x\rangle}{\langle x,x\rangle} \;=\; \inf_{x\neq 0} \frac{\langle Ax,Ax\rangle}{\langle \Lambda^{-1}x,\Lambda^{-1}x\rangle} \;\geq\; \min\{\lambda_1^2,\lambda_2^2\} \inf_{x\neq 0}\frac{\langle Ax,Ax\rangle}{\langle x,x\rangle}.$$

From proposition 3.2.1 we infer that for λ_1,λ_2 sufficiently large, $f(\lambda_1,\lambda_2) \geq \bar{E}^{**}(\mathbf{b}) - \delta$. Fix such λ_1,λ_2. By convexity of $\lambda \mapsto f(\lambda_1,\lambda)$ on $[1,\infty)$ we deduce that $f(\lambda_1,1) \geq \bar{E}^{**}(\mathbf{b}) - \delta$. Now convexity of $\lambda \mapsto f(\lambda,1)$ implies that $f(1,1) \geq \bar{E}^{**}(\mathbf{b}) - \delta$. ☐

Convexity in b

Discussing convexity in $\mathbf{b}$, we have to insist on $y^{(k)} \to (u,\mathbf{b})$ being defined as usual, i.e., not as proposed in (2.48) in terms of v instead of u. Then $k\Delta^i\tilde{y} \overset{*}{\rightharpoonup} \mathbf{b}$ is weak*-convergence without explicit constraints with respect to $\mathbf{b}$. So by lower semicontinuity of Γ-limits we obtain:

Proposition 3.3.3 *For A fixed, the map $\mathbf{b} \mapsto \varphi(A,\mathbf{b})$ is convex.*

A direct proof is straightforward:

Proof. $\varphi(A,\cdot)$ is continuous. Suppose $\mathbf{b} = \frac{1}{2}(\mathbf{b}_1+\mathbf{b}_2)$. Divide $\mathcal{S}_1$ into four equal squares $Q_{11},Q_{12},Q_{21},Q_{22}$, and choose $y_{ij}^{(k)} \in \hat{\mathcal{N}}_{k,Q_{ij}}^{0,1/2}(A,\mathbf{b}_j)$ satisfying

$$\frac{1}{\nu(k/2)^2} E(y_{ij}^{(k)}) \leq \varphi(A,\mathbf{b}_j) + o(1), \quad i,j = 1,2,$$

by theorem 2.2.2 and frame indifference. Defining $y^{(k)}$ by

$$y^{(k)}(x) = y_{ij}^{(k)}(x) \text{ for } x \in \mathcal{L}\cap(kQ_{ij}\times[0,h]),$$

it is easily seen that $y \in \hat{\mathcal{N}}^{0,1}(A,\mathbf{b})$ and

$$\varphi\left(A, \frac{\mathbf{b}_1+\mathbf{b}_2}{2}\right) \leq \liminf_{k\to\infty} E(y^{(k)}(x) : x \in \mathcal{L}_k) \leq \frac{1}{2}(\varphi(A,\mathbf{b}_1)+\varphi(A,\mathbf{b}_2)),$$

which concludes the proof. □

Remark: Defining convergence as in (2.48), it is not clear (and for c_0 small enough false) that y constructed in the previous proof satisfies $\|y - v_{A,\mathbf{b}}\| \leq c_0$. Consider the example from paragraph 3.1.2. For $\nu = 2$ and $A = \mathrm{Id}$,

$$\begin{aligned}\varphi_0(A,\mathbf{b}) &= \frac{1}{2\nu}\sum_{i,j=0}^{1}\sum_{\substack{z\in\mathbb{Z}^2\\(z,j)\neq(0,0,i)}} W(|Az+b^j-b^i|)\\ &= \frac{1}{2}\left(\sum_{z\in\mathbb{Z}^2\setminus\{0\}} W(|Az|)+\sum_{z\in\mathbb{Z}^2} W(|Az+b^1|)\right).\end{aligned}$$

Now if $W : [0,\infty) \to \mathbb{R}$ satisfies $W(0) > 0$ and $W(r) = 0$ for $r \geq 1$, then $\varphi_0(\mathrm{Id}_{2,3}, 0) > 0$, while $\varphi_0(\mathrm{Id}_{2,3}, (0,0,\pm1)) = 0$. Hence φ_0 is not convex in $\mathbf{b}$. Since $\varphi_0 = \lim_{c_0\to 0}\varphi_{c_0}$, convexity also fails for values of c_0 bigger than 0.

Quasiconvexity of φ_∞

For energy functions that do not satisfy assumption 2.1.8 the limit $c_0 \to \infty$ can be non-trivial. In the following proposition we examine this limit for convexity properties. As in theorem 3.1.2 we define $\varphi_\infty = \lim_{c_0\to\infty}\varphi_{c_0}$. If assumption 2.1.8 holds, the following is trivial by theorem 3.1.2. We therefore treat only finite range energies given by (2.49). By the remark after proposition 2.2.27 and (2.4), φ_∞ is defined on all of $\mathbb{R}^{3\times 2} \times (\mathbb{R}^3)^{\nu-1}$.

Recall the definition of quasiconvexity (cf., e.g., [4], p. 350):

Definition 3.3.4 *A continuous function $f : \mathbb{R}^{m\times n} \to \mathbb{R}$ is said to be quasiconvex if*

$$\fint_\Omega f(F+\nabla\zeta)dx \geq f(F)$$

for every bounded open subset $\Omega \subset \mathbb{R}^n$, $\zeta \in C_c^\infty(\Omega;\mathbb{R}^m)$, and all $F \in \mathbb{R}^{m\times n}$.

Proposition 3.3.5 *Suppose that E is of the form (2.49). Then φ_∞ is quasiconvex with respect to the first variable and convex with respect to the second.*

Remark: This reflects the fact that the full (unconstrained) Γ-limit is lower semicontinuous.

The proof is very similar to the proof of theorem 3.1.2. We indicate the modifications.

Sketch of Proof. Convexity in $\mathbf{b}$ is clear since by proposition 3.3.3 all φ_{c_0}, $c_0 > 0$, are convex. Let $f \in C_c^\infty(\mathcal{S}_1;\mathbb{R}^3)$ and set $u := A + f$. We need to show that

$$\varphi_\infty(A,\mathbf{b}) \leq \fint_{\mathcal{S}_1} \varphi_\infty(A+\nabla f,\mathbf{b})dx.$$

Let $\delta > 0$ and c_0 be given. By theorem 2.2.1, for arbitrarily large k_0 we find a deformation $y : \mathcal{L}_{k_0} \to \mathbb{R}^3$ with $\|\tilde{y} - u\| \le c_0/k_0$ and $|\fint_{[0,1]^2}(k_0\Delta^i\tilde{y} - b^i)d\rho|$ as small as we wish such that

$$\frac{1}{\nu k_0^2}E(y) \le \int_{\mathcal{S}_1} \varphi_{c_0}(\nabla u, \mathbf{b}) + \delta/3.$$

Using lemma 2.2.12, we may even assume that $\fint_{[0,1]^2}(k_0\Delta^i\tilde{y} - b^i)d\rho = 0$.

Proceeding as in theorem 3.1.2, we construct a deformation $y' : \mathcal{L}_k \to \mathbb{R}^3$ for $k \gg k_0$ by patching together appropriately translated copies of y so that

$$\sup_{x\in\mathcal{L}_k} |y'(x) - Ax_p| = \sup_{x\in\mathcal{L}_{k_0}} |y(x) - Ax_p|.$$

The crucial point to observe is that since $y \in \hat{\mathcal{N}}^{0,1}_{k_0,c_0}(u, \mathbf{b})$ and u satisfies the same boundary conditions as A, in contrast to theorem 3.1.2 the energy splitting works without further assumptions. First, since we are dealing with systems of finite range interaction, the energy error stems only from neglecting interactions between the boundary layers of the regions that were patched together. Second, since u satisfies the same boundary conditions as A, this error is negligible.

So again we find $y' \in \hat{\mathcal{N}}^{0,1}_{k,\tilde{c_0}}(A, \mathbf{b})$ ($\tilde{c_0}$ depending on f, k_0) with

$$\frac{1}{\nu k^2}E(y') \le \frac{1}{\nu k_0^2}E(y) + \delta/3$$

if k_0 and k are large enough. Taking the limit $k \to \infty$, it follows that

$$\varphi_\infty(A, \mathbf{b}) \le \varphi_{\tilde{c_0}}(A, \mathbf{b}) \le \int_{\mathcal{S}_1} \varphi_{c_0}(\nabla u, \mathbf{b}) + \delta.$$

Now sending $c_0 \to \infty$ the claim follows from monotone convergence and the arbitrariness of δ. □

3.3.2 Symmetry

In this paragraph we discuss general symmetry properties of φ and indicate – for $\nu = 1$ or 2 – their implications for a linearized theory.

By frame indifference of E,

$$\varphi(A, b^1, \dots, b^{\nu-1}) = \varphi(RA, Rb^1, \dots, Rb^{\nu-1}) \tag{3.7}$$

for all $R \in SO(3)$. So to evaluate $\varphi(A, \mathbf{b})$, we may only look at matrices

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{12} & a_{22} \\ 0 & 0 \end{pmatrix} \tag{3.8}$$

whose last row is 0 and whose top part is symmetric. Moreover, for systems of indistinguishable particles we have

Proposition 3.3.6 *φ satisfies the following symmetry properties:*

(i) If σ is a permutation of $\{1,\dots,\nu-1\}$, then

$$\varphi(A,b^1,\dots,b^{\nu-1}) = \varphi(A,b^{\sigma(1)},\dots,b^{\sigma(\nu-1)}).$$

(ii) For $1 \le j \le \nu-1$,

$$\varphi(A,b^1,\dots,b^{\nu-1}) = \varphi(A,b^1-b^j,\dots,b^{j-1}-b^j,-b^j,b^{j+1}-b^j,\dots,b^{\nu-1}-b^j).$$

(iii) If $\nu \le 2$, then for all $R \in O(3)$,

$$\varphi(A,b^1,\dots,b^{\nu-1}) = \varphi(RA,Rb^1,\dots,Rb^{\nu-1}).$$

(iv) If $R = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$, then

$$\varphi(A,b^1,\dots,b^{\nu-1}) = \varphi(AR,b^1,\dots,b^{\nu-1}).$$

(v) If $P = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, then

$$\varphi(A,b^1,\dots,b^{\nu-1}) = \varphi(AP,b^1,\dots,b^{\nu-1}).$$

Proof. Without loss of generality we may switch to the reference configuration

$$\mathcal{L} \cap ([-k/2,k/2]^2 \times [0,h]).$$

Then $(x_p,x_3) \mapsto (Px_p,x_3)$ and $(x_p,x_3) \mapsto (Rx_p,x_3)$ are lattice restoring, so (iv) and (v) follow. Also (i) is clear since this only amounts to a renumbering of the film layers, the 0-layer held fixed. Interchanging the 0^{th} and the j^{th} layer gives (ii). Finally, (iii) is trivial for $\nu = 1$, and for $\nu = 2$ it follows from (3.7) since by (ii) and (iv)

$$\varphi(A,b^1) = \varphi(AR^2,b^1) = \varphi(AR^2,-b^1) = \varphi(-A,-b^1).$$

□

Remarks:

(i) Note that the reflection P and R, rotation about 90°, span the set of symmetry operations of $[-1/2,1/2]^2$.

(ii) If $\nu \le 1$, then (i) and (ii) are trivial. For $\nu = 2$, (ii) states that

$$\varphi(A,b^1) = \varphi(A,-b^1).$$

(iii) The above statements only hold for systems of indistinguishable atoms. For situations as in (2.49) we can not permute the b^i or rotate the lattice.

Suppose now our reference configuration is a natural state. By the results in section 3.4, proposition 2.3.5 and proposition 3.3.3 we can not expect that there is a unique quadratic form approximating φ for small strains. However (as, e.g., in proposition 2.3.5), for purely tensile deformations, i.e., $s_1(A) \geq 1$, $|b^i - b^j| \geq 1$ for $i \neq j$, there can be a symmetric quadratic form Q such that for A (of the form (3.8)) and b^i with

$$A \approx \mathrm{Id}_{2,3} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{pmatrix}, \qquad b^i - b^{i-1} \approx e_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix},$$

the energy can be written as

$$E(A, \mathbf{b}) \approx Q(A - \mathrm{Id}_{2,3}, b^1 - e_3, b^2 - b^1 - e_3, \ldots, b^{\nu-1} - b^{\nu-2} - e_3).$$

Then Q is a symmetric form on $\mathbb{R}^3 \times (\mathbb{R}^3)^{\nu-1} = \mathbb{R}^{3\nu}$ leading to $(9\nu^2 + 3\nu)/2$ elastic constants. In the following, we examine the cases $\nu = 1$ and $\nu = 2$ to show how symmetry reduces this number. We only treat the case $\nu = 2$ and comment on the much easier case $\nu = 1$ thereafter. Here, $(9\nu^2 + 3\nu)/2 = 21$.

Set $b := b^1$ and let Q be given by

$$Q(\epsilon, \epsilon) = q_{ij}\epsilon_i\epsilon_j,$$

where $1 + \epsilon_1 = a_{11}$, $1 + \epsilon_2 = a_{22}$, $\epsilon_3 = a_{12}$, $\epsilon_4 = b_1$, $\epsilon_5 = b_2$ and $1 + \epsilon_6 = b_3$.

Proposition 3.3.7 *Under these hypotheses,*

$$Q = \begin{pmatrix} q_{11} & q_{12} & q_{13} & q_{14} & q_{15} & q_{16} \\ q_{21} & q_{22} & q_{23} & q_{24} & q_{25} & q_{26} \\ q_{31} & q_{32} & q_{33} & q_{34} & q_{35} & q_{36} \\ q_{41} & q_{42} & q_{43} & q_{44} & q_{45} & q_{46} \\ q_{51} & q_{52} & q_{53} & q_{54} & q_{55} & q_{56} \\ q_{61} & q_{62} & q_{63} & q_{64} & q_{65} & q_{66} \end{pmatrix} = \begin{pmatrix} q_{11} & q_{12} & 0 & 0 & 0 & q_{16} \\ q_{12} & q_{11} & 0 & 0 & 0 & q_{16} \\ 0 & 0 & q_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & q_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & q_{44} & 0 \\ q_{16} & q_{16} & 0 & 0 & 0 & q_{66} \end{pmatrix}.$$

In particular, there are only six elastic constants.

Sketch of Proof. First note that by symmetry of Q,

$$q_{ij} = q_{ji}. \tag{3.9}$$

Define

$$S = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad \tilde{P} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad \tilde{R} = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

From (iii) and (ii) of proposition 3.3.6 we get that $\varphi(A, b) = \varphi(SA, Sb) = \varphi(SA, -Sb)$ which implies

$$q_{4j} = q_{5j} = 0 \quad \text{for } j = 1, 2, 3, 6. \tag{3.10}$$

Next, from from (iii) and (v) of proposition 3.3.6 we deduce $\varphi(A,b) = \varphi(\tilde{P}AP, \tilde{P}b)$ and hence

$$q_{11} = q_{22}, \quad q_{44} = q_{55}, \quad q_{13} = q_{23}, \quad q_{16} = q_{26}. \tag{3.11}$$

Finally, by (3.7) and (iv) of proposition 3.3.6 we have $\varphi(A,b) = \varphi(\tilde{R}AR, \tilde{R}b)$ which leads to

$$q_{13} = -q_{23}, \quad q_{45} = q_{36} = 0. \tag{3.12}$$

Summarizing (3.9) – (3.12) yields the result. □

If $\nu = 1$, $(9\nu^2 + 3\nu)/2 = 6$, a similar reasoning shows that

$$Q = \begin{pmatrix} q_{11} & q_{12} & q_{13} \\ q_{21} & q_{22} & q_{23} \\ q_{31} & q_{32} & q_{33} \end{pmatrix} = \begin{pmatrix} q_{11} & q_{12} & 0 \\ q_{12} & q_{11} & 0 \\ 0 & 0 & q_{33} \end{pmatrix}.$$

In particular, there remain three elastic constants.

Remark: In general we can not expect to have less than six resp. three elastic constants. This can be seen considering suitable mass-spring models which also contain explicit angular depending terms (similar as in paragraph 3.4.2). One has to allow for bond strengths of interactions within the x_1-x_2-plane that differ from the out-of-plane interactions. The requirements of proposition 2.2.27 are satisfied, and all the assertions of proposition 3.3.6 apply.

3.4 Small strains

In this section we study the response of our continuum theory to deformations that are locally close to rigid motions. Recall the example given in paragraph 2.3.4. We could derive an explicit formula for φ which turned out to give zero energy response under contractive boundary conditions due to microscopic 'crumpling'. This model, however, lacked some physically desirable features, as already noted. Here we examine more realistic models which also include next-nearest neighbor interactions or angular-dependent terms. In particular, we find that φ shows resistance to compressive deformations which may, however, be weaker than to tensile strains. Again the crucial parameter is c_0. Still, the relevant scaling of energy with respect to $\mathrm{dist}(A, O(2,3))$ turns out to be quadratic. At first we study a one-dimensional atomic chain in detail which might be of independent interest modeling a polymer chain in a confined region. Using these results, we also obtain estimates for thin films.

3.4.1 Energy scaling of an atomic chain

Consider $L+1$ atoms at $y_0, \dots, y_L \in \mathbb{R}^3$ whose energy is given by

$$E(y) = \sum_{i=1}^{L} W_1(|y_i - y_{i-1}|) + \sum_{i=1}^{L-1} W_2(\phi_i),$$

where $\phi_i \in (-\pi, \pi]$ denotes the angle between $y_{i+1} - y_i$ and $y_i - y_{i-1}$. Assume that W_1 is locally bounded, W_2 bounded and symmetric, $W_1(1) = 0 = W_2(0)$, and there are $\alpha_1, \alpha_2 > 0$ and $\rho > 0$ such that

$$W_1(r) \geq \begin{cases} \alpha_1 (r-1)^2 & \text{for } |r-1| \leq \rho \\ \alpha_2 & \text{for } |r-1| \geq \rho \end{cases}, \quad W_2(\phi) \geq \begin{cases} \alpha_1 \phi^2 & \text{for } |\phi| \leq \rho \\ \alpha_2 & \text{for } \rho \leq |\phi| \leq \pi \end{cases}.$$

For given $a > 0$, we would like to examine

$$\varphi(a) := \lim_{L\to\infty} \frac{1}{L} \inf_{\mathcal{N}_L(a)} E(y), \quad \mathcal{N}_L(a) = \{y : |y_i - (ia, 0, 0)| \leq c_0\}. \tag{3.13}$$

($\mathcal{N}_L(a)$ is a one-dimensional version of $\hat{\mathcal{N}}_k^{0,1}$.) In particular, we are interested in the energy scaling for deformations near the zero-energy state $y_k = (k, 0, 0)$, i.e., $a \approx 1$.

Lemma 3.4.1 *For each $a > 0$ the limit in (3.13) exists.*

Proof. This is just an easy one-dimensional special case of theorem 2.2.2. We include a proof for the sake of completeness. First note that since W_1, restricted to $[0, 2c_0 + a]$, and W_2 are bounded, say by $C > 0$, we have $|E(y)/L| \leq 2C$, so

$$\varphi(a) := \liminf_{L\to\infty} \frac{1}{L} \inf_{y\in\mathcal{N}_L(a)} E$$

exists in $\mathbb{R}$. For $\varepsilon > 0$ choose L_0 such that

$$\frac{1}{L_0} \inf_{y\in\mathcal{N}_{L_0}(a)} E(y) \leq \varphi(a) + \varepsilon \quad \text{and} \quad \frac{1}{L} \inf_{y\in\mathcal{N}_L(a)} E(y) \geq \varphi(a) - \varepsilon \ \forall L \geq L_0.$$

Then choose $y^0 \in \mathcal{N}_{L_0}(a)$ such that

$$\frac{1}{L_0} E(y^0) \leq \varphi(a) + 2\varepsilon.$$

We may assume that $y_0^0 = (0, 0, 0)$ and $y_{L_0}^0 = (L_0 a, 0, 0)$ if L_0 is large enough. For $L \geq L_0$ we can break the atomic chain into pieces of length L_0 plus a remaining part of length smaller than L_0 and define y by $(0 \leq r < L_0)$

$$y_{kL_0+r} = (kL_0 a, 0, 0) + y_r^0.$$

Clearly, y is in $\mathcal{N}_L(a)$, and by translational invariance,

$$E(y_0, \ldots, y_L) \leq \lfloor L/L_0 \rfloor E(y_0^0, \ldots, y_{L_0}^0) + 2CL_0 + 2C\lfloor L/L_0 \rfloor.$$

So dividing by L and choosing L_0 large enough, this shows that for L sufficiently large indeed

$$\varphi(a) - \varepsilon \leq \frac{1}{L} E(y_0, \ldots, y_L) \leq \varphi(a) + 3\varepsilon.$$

□

It is easy to get upper bounds for $\varphi(a)$:

Lemma 3.4.2 *Suppose that in addition there exists $\alpha_3 \geq \alpha_1$ such that $W_1(r) \leq \alpha_3(r-1)^2$ if $|r-1| \leq \rho$, and $W_2(0) = 0$. Then for $|a-1| \leq \rho$*

$$\varphi(a) \leq \alpha_3(a-1)^2.$$

Proof. Just insert the Cauchy-Born state $y_k = (ka, 0, 0)$ and let $L \to \infty$. □

We will now prove lower bounds for φ. Suppose first $1 \leq a \leq 2$. Noting that imposing the additional constraints $y_0 = 0$ and $y_L = La$ only leads to negligible energy errors (of order $\mathcal{O}(1/L)$), we define E_L by

$$E_L(a) = \inf\{E(y) : |y_i - (ia, 0, 0)| \leq c_0 \text{ and } y_0 = 0, y_L = (La, 0, 0)\}.$$

But if $|y_i - (ia, 0, 0)| \leq c_0$, then $|y_{i+1} - y_i| \leq a + 2c_0 \leq 2(c_0 + 1)$, so we have

$$E_L(a) \;\geq\; \inf\left\{\sum_{i=1}^{L} f(z_i) : z_1, \ldots, z_L \in \mathbb{R}^3 \text{ and } z_1 + \ldots + z_L = (La, 0, 0)\right\},$$

where $f : \mathbb{R}^3 \to \mathbb{R} \cup \{\infty\}$ is given by

$$f(z) = \begin{cases} W_1(|z|) & \text{for } |z| \leq 2c_0 + 2, \\ \infty & \text{for } |z| > 2c_0 + 2. \end{cases}$$

Now clearly there exists $\alpha_4 > 0$ such that

$$f^{**}(z) \geq \begin{cases} 0 & \text{for } |z| \leq 1, \\ \alpha_4(|z| - 1)^2 & \text{for } 1 < |z| \leq 2c_0 + 2, \\ \infty & \text{for } |z| > 2c_0 + 2. \end{cases}$$

It follows that

$$\varphi(a) = \lim_{L\to\infty} \frac{1}{L} E_L(a) \geq \lim_{L\to\infty} f^{**}(a, 0, 0) \geq \alpha_4(a-1)^2. \tag{3.14}$$

Suppose now $a < 1$. Since the inter-atomic distances $|y_i - y_{i-1}|$ remain bounded, by rescaling E, we may assume that

$$W_1(r) \geq (r-1)^2, \qquad W_2(\phi) \geq \phi^2.$$

If y is any deformation with $E(y) \leq \delta$, then

$$\sum_{i=1}^{L} (|y_i - y_{i-1}| - 1)^2 \leq \delta, \quad \sum_{i=1}^{L-1} \phi_i^2 \leq \delta,$$

and hence by Cauchy-Schwarz,

$$\sum_{i=1}^{L} ||y_i - y_{i-1}| - 1| \leq \sqrt{L}\sqrt{\delta}, \quad \sum_{i=1}^{L-1} |\phi_i| \leq \sqrt{L-1}\sqrt{\delta}.$$

Noting that the absolute value of the angle between $y_i - y_{i-1}$ and $y_j - y_{j-1}$ is bounded by $\sum_{k=1}^{L-1} |\phi_k|$, we find that for $\delta L \le 1$,

$$\begin{aligned}
|y_L - y_0|^2 &= \left| \sum_{i=1}^{L} y_i - y_{i-1} \right|^2 \\
&= \sum_{\substack{1\le i\le L \\ 1\le j\le L}} \langle y_i - y_{i-1}, y_j - y_{j-1} \rangle \\
&\ge \sum_{\substack{1\le i\le L \\ 1\le j\le L}} |y_i - y_{i-1}||y_j - y_{j-1}| \cos(\sqrt{L\delta}) \\
&= \left(\sum_{1\le i\le L} |y_i - y_{i-1}| \right)^2 \cos(\sqrt{L\delta}) \\
&\ge \left(L - \sqrt{L\delta} \right)^2 (1 - L\delta),
\end{aligned}$$

in particular, choosing $\delta = \delta(L) = L^{-3}$, we obtain

$$|y_L - y_0|^2 \ge L^2(1 - 3L^{-2}). \tag{3.15}$$

If y satisfies $|y_i - (ia, 0, 0)| \le c_0$ for $i = 0, \dots, L$, then $La - 2c_0 \le (y_L)_1 - (y_0)_1 \le La + 2c_0$. So for $|a - a'| \le 2c_0/L$ we define E_L depending on two parameters a, a' by

$$\mathcal{N}_L(a, a') := \{ y \in \mathcal{N}_L(a) : (y_L)_1 - (y_0)_1 = La' \}$$

and

$$E_L(a, a') = \inf_{\mathcal{N}_L(a,a')} E(y).$$

Also let $m = \left\lceil \sqrt{3 + 4c_0^2} + 1 \right\rceil$ and define $a_0, a_1, \dots$ and $L_0, L_1, \dots$ by

$$1 - a_n = 4^{-1-n} \quad \text{and} \quad L_n = \frac{4m}{\sqrt{1 - a_n}} = 2^{3+n} m.$$

Lemma 3.4.3 *There exists $c > 0$ such that for all $k \in \mathbb{N}$,*

$$\frac{1}{kL_n} E_{kL_n}(a, a') \ge c(1 - a')^2 \quad \forall\ a' \in [3/4, a_n],\ |a - a'| \le \frac{2c_0}{kL_n}.$$

Proof. The lemma is proven by induction on n. The case $n = 0$ directly follows from the following claim which will be proven later.

Claim. There exists $C > 0$ such that for all $k \in \mathbb{N}$,

$$\frac{1}{kL_0} E_{kL_0}(a, a') \ge C \quad \forall\ a' \in [1/2, a_0],\ |a - a'| \le \frac{2c_0}{kL_0}.$$

Suppose the lemma is proven for n and choose $c = \min\{(4m)^{-4}, C\}$.

$$L_n = \frac{4m}{\sqrt{1-a_n}} = \frac{m}{\sqrt{1-a_{n+2}}} \geq \frac{m}{\sqrt{1-a'}}$$

for $a' \leq a_{n+2}$ implies

$$L_n^2(1-a') > 3 + (2c_0)^2,$$

and thus

$$(L_n a')^2 + (2c_0)^2 < L_n^2(1 - 3L_n^{-2}).$$

But if $y \in \mathcal{N}_{L_n}(a, a')$, then $|y_{L_n} - y_0|^2 \leq (L_n a')^2 + (2c_0)^2$, so (3.15) can not hold. It follows that

$$\frac{1}{L_n} E(y) \geq \frac{\delta(L_n)}{L_n} = L_n^{-4} \quad \forall y \in \mathcal{N}_{L_n}(a, a'),\ 0 < a' \leq a_{n+2}. \tag{3.16}$$

Now let $3/4 \leq a' \leq a_{n+1}$, $|a - a'| \leq \frac{2c_0}{kL_{n+1}}$. Considering the first components of the atoms $y_0, y_{L_n}, \ldots, y_{2kL_n}$ for deformations $y \in \mathcal{N}_{kL_{n+1}}$ (note that $L_{n+1}/L_n = 2$), we deduce

$$E_{kL_{n+1}}(a, a') \geq \sum_{i=1}^{2k} E_{L_n}(a, x_i),$$

where $x_1 + \ldots + x_{2k} = 2ka'$ and $x_i > 1/2$ because

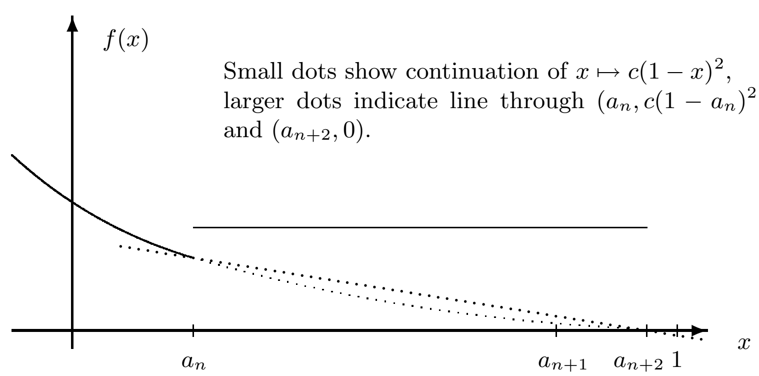
$$L_n x_i \geq L_n a - 2c_0 \geq L_n a' - L_n \frac{2c_0}{kL_{n+1}} - 2c_0 \geq 3L_n/4 - 3c_0 > L_n/2.$$

So if $f : \mathbb{R} \to \mathbb{R} \cup \{\infty\}$ is defined by

$$f(x) = \begin{cases} \infty & \text{for } x \leq 1/2, \\ c(1-x)^2 & \text{for } 1/2 < x \leq a_n, \\ L_n^{-4} & \text{for } a_n < x \leq a_{n+2}, \\ 0 & \text{for } a_{n+2} < x, \end{cases}$$

we have by (3.16), the above claim (note that $C \geq c(1/2)^2$) and induction hypothesis,

$$\frac{1}{kL_{n+1}} E_{kL_{n+1}}(a, a') \geq \frac{1}{2k} \sum_{i=1}^{2k} \frac{1}{L_n} E_{L_n}(a, x_i) \geq \frac{1}{2k} \sum_{i=1}^{2k} f(x_i) \geq f^{**}(a').$$



Now since $L_n^{-4} = (4m)^{-4}(1-a_n)^2 \geq c(1-a_n)^2$, $1-a_n = 16(1-a_{n+2})$ and $-2c(1-a_n) < -\frac{16}{15}c(1-a_n)$, f^{**} is given by

$$f^{**}(x) = \begin{cases} \infty & \text{for } x \leq 1/2, \\ c(1-x)^2 & \text{for } 1/2 < x \leq a_n, \\ \frac{c(1-a_n)}{15}(16(1-x)-(1-a_n)) & \text{for } a_n < x \leq a_{n+2}, \\ 0 & \text{for } a_{n+2} < x. \end{cases}$$

So for $a' \leq a_n$ we are done. But also for $a' \in [a_n, a_{n+1}]$,

$$f^{**}(a') = \frac{c(1-a_n)}{15}(16(1-a')-(1-a_n)) \geq c(1-a')^2.$$

(Set $1-a' = \lambda(1-a_n)$, then this is equivalent to $\frac{1}{15}(16\lambda - 1) \geq \lambda^2$ which in turn is equivalent to $\lambda \in [1/15, 1]$. This is guaranteed by $a' \in [a_n, a_{n+1}]$.)

The claim at the beginning of the proof can now be shown by analogous arguments: $y \in \mathcal{N}_{L_0}(a, a')$ implies

$$\frac{1}{L_0}E(y_0, \dots, y_{L_0}) \geq \frac{\delta(L_0)}{L_0} = L_0^{-4} \quad \text{for } 0 \leq a' \leq a_1.$$

For $1/2 \leq a' \leq a_0$ again considering the first components of the atomic sites $y_0, y_{L_0}, \dots, y_{kL_0}$, $x_1 + \ldots + x_k = ka'$, $x_i > 0$, we deduce

$$\frac{1}{kL_0}E_{kL_0}(a, a') \geq \frac{1}{k}\sum_{i=1}^{k}\frac{1}{L_0}E_{L_0}(a, x_i) \geq \frac{1}{k}\sum_{i=1}^{k} f(x_i) \geq f^{**}(a') \geq C > 0,$$

where now $f : \mathbb{R} \to \mathbb{R} \cup \{\infty\}$ is defined by

$$f(x) = \begin{cases} \infty & \text{for } x \leq 0, \\ L_0^{-4} & \text{for } 0 < x \leq a_1, \\ 0 & \text{for } a_1 < x. \end{cases}$$

□

We can now state the main result of our one-dimensional model problem:

Proposition 3.4.4 *There exist $\delta, c > 0$ such that for all $1-\delta \leq a \leq 1+\delta$*

$$\varphi(a) \geq c(1-a)^2.$$

If in addition W_1 and W_2 are bounded from above as in lemma 3.4.2, then there are $C, c > 0$ such that

$$c(1-a)^2 \leq \varphi(a) \leq C(1-a)^2.$$

Proof. The upper bound is immediate from lemma 3.4.2. The lower bound for $a \geq 1$ was established in (3.14). The additional constraint in $\mathcal{N}(a, a')$ is negligible, so the lower bound for $a < 1$ follows by choosing n such that

$a = a' \leq a_n$ and letting $k \to \infty$ in lemma 3.4.3 noting that, by lemma 3.4.1, it suffices to consider a subsequence in (3.13). □

So the energy scales quadratically with the distance of a to 1. The following examples show that, even for quadratic energy wells

$$W_1(r) = \alpha_1 (r-1)^2 \quad \text{resp.} \quad W_2(\phi) = \alpha_2 \phi^2, \tag{3.17}$$

φ will not be C^2 at $a = 1$.

Examples: 1. Let W_1, W_2 be as in (3.17). If $a \geq 1$, then as in the derivation of (3.14) we see that the Cauchy-Born state $y_k = (ka, 0, 0)$ is asymptotically optimal, leading to

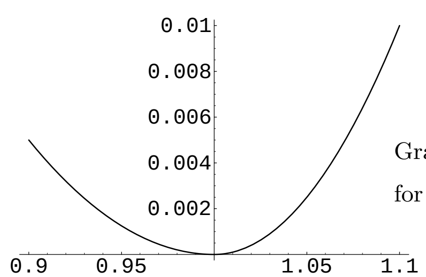
$$\varphi(a) = \alpha_1 (1-a)^2.$$

For $0 < a < 1$ consider the spiral deformation $y_k := (ka, c_0 \cos(k\psi), c_0 \sin(k\psi))$, $k = 0, \dots, L$, with $|\psi|$ small. Then $|y_{k+1} - y_k|^2$ and ϕ_k are independent of k. An elementary calculation shows that $\phi_k^2 = c_0^2 \psi^4 / a^2 + \mathcal{O}(\psi^6)$. Choosing ψ such that $c_0^2 \psi^2 / (2a) = \kappa(1-a)$ and minimizing the corresponding energy with respect to κ, we find $\psi_{\min}$ with energy

$$E_{\min} = \frac{\alpha_1 \alpha_2}{\alpha_2 + \alpha_1 c_0^2/4} (1-a)^2 + \mathcal{O}((1-a)^3).$$

This is by a c_0-dependent factor smaller than the Cauchy-Born minimizer $y_k = (ka, 0, 0)$ which has mean energy $\alpha_1 (1-a)^2$.

Also this shows that the minimal energy is not twice differentiable in a at $a = 1$ since for $a \geq 1$ the Cauchy-Born state is optimal. Note that for $c_0 \to \infty$ this expression converges to 0, reflecting the fact that without this constraint we would expect energy responses to compressions that occur only at lower energy scales.



Graph of $a \mapsto \begin{cases} E_{\min}(a) & \text{if } a \leq 1 \\ \alpha_1(1-a)^2 & \text{if } a \geq 1 \end{cases}$ for $\alpha_1 = \alpha_2 = 1, c_0 = 2$.

2. To extend this observation to thin films, we also study the following two dimensional deformation (E as in the preceding example). Consider a piece of a circle in the x_1-x_3-plane with radius R (large):

$$\gamma \mapsto (R \sin(\gamma), 0, R(1 - \cos(\gamma)) - d)$$

for $0 \leq \gamma \leq \gamma_{\max}$, $\gamma_{\max}$ given by $R(1 - \cos(\gamma_{\max})) = d$. We place atoms on this curve starting at $\gamma = 0$ with distances 1 between neighboring atoms:

$$y_k = (R \sin(k\Phi/L), 0, R(1 - \cos(k\Phi/L)) - d), \quad k = 0, \dots, L, \tag{3.18}$$

where $2R\sin(\Phi/2L) = 1$ and $\Phi \leq \gamma_{\max}$, $\Phi + \Phi/L > \gamma_{\max}$. Now for given $a < 1$ (near 1), we choose R so big that

$$\sin(\gamma_{\max}) = a\gamma_{\max}.$$

An elementary analysis proves that for $d < c_0$ and a sufficiently close to 1, $y \in \mathcal{N}_L(a)$ and $\Phi/L = 3(1-a)/d + \mathcal{O}((1-a)^2)$. For later use, we mention that in powers of $(1-a)$,

$$\Phi \approx \sqrt{6}(1-a)^{1/2}, \quad R \approx \frac{d}{3}(1-a)^{-1}, \quad L \approx \frac{\sqrt{2}d}{\sqrt{3}}(1-a)^{-1/2}.$$

The mean energy of y is thus

$$\frac{1}{L}E(y) = \alpha_2 \left(\frac{\Phi}{L}\right)^2 = \frac{9\alpha_2}{d^2}(1-a)^2 + \mathcal{O}((1-a)^3).$$

Now patching together appropriately translated and reflected copies of this configuration, leads to y in $\mathcal{N}_L(a)$ with arbitrarily large L and mean energy $\approx \frac{9\alpha_2}{d^2}(1-a)^2$. Finally, set $y' = \bar{a}y \in \mathcal{N}_L(a\bar{a})$ for $\bar{a} \leq 1$ near 1, and for given $x \leq 1$ near 1 minimize $E(y')$ subject to $a\bar{a} = x$. It follows that

$$\varphi(x) \leq \frac{9\alpha_1\alpha_2}{d^2\alpha_1 + 9\alpha_2}(1-x)^2 + \mathcal{O}((1-x)^3).$$

Again, this is is preferable to the Cauchy-Born energy $\alpha_1(1-x)^2$.

Remark: In terms of scaling with large c_0, the lower and upper bound for $\varphi(a)$ derived in the preceding examples respectively in proposition 3.4.4 do not match: the factors of $(1-a)^2$ scale like c_0^{-2} respectively $c \sim m^{-4} \sim c_0^{-4}$ (cf. lemma 3.4.3). In fact, the lower bound can be improved as we shall now detail.

Fix c_0, and let $k \in \mathbb{N}$. Suppose $y \in \mathcal{N}_{kL,kc_0}(a)$ (c_0 is replaced by kc_0), and consider the corresponding k-step chain $Y = (Y_0, \ldots, Y_L)$ defined by $Y_j = y_{kj}$. For the corresponding angles we obtain

$$|\Phi_j| \leq \sum_{i=k(j-1)+1}^{k(j+1)-1} |\phi_i|.$$

To estimate $|Y_j - Y_{j-1}|$, let $\bar{\Phi}_j = \sum_{i=k(j-1)+1}^{kj-1} |\phi_i|$. Then if $\bar{\Phi} \leq 1$, similarly as on page 80 we obtain

$$|Y_j - Y_{j-1}| = \left| \sum_{i=k(j-1)+1}^{kj} (y_i - y_{i-1}) \right| \geq \sum_{i=k(j-1)+1}^{kj} |y_i - y_{i-1}|(1 - \bar{\Phi}_j^2).$$

On the other hand, clearly $|Y_j - Y_{j-1}| \leq \sum_{i=k(j-1)+1}^{kj} |y_i - y_{i-1}|$, so setting $\gamma k := \sum_{i=k(j-1)+1}^{kj} |y_i - y_{i-1}|$,

$$\begin{aligned}
(|Y_j - Y_{j-1}| - k)^2 &\leq \max\left\{(\gamma k - k)^2, \left(\gamma k - k - \gamma k\bar{\Phi}_j^2\right)^2\right\} \\
&\leq 2(\gamma k - k)^2 + 2\left(\gamma k\bar{\Phi}_j^2\right)^2 \\
&\leq 10(\gamma k - k)^2 + 2\left(2k\bar{\Phi}_j\right)^2.
\end{aligned}$$

(If $\gamma \le 2$, this is clear. If $\gamma \ge 2$, it follows from $10(\gamma-1)^2 \ge 2(\gamma-1)^2 + 2\gamma^2$ and $\bar{\Phi}_j^2 \le 1$. If $\bar{\Phi}_j \ge 1$, we get such an estimate even easier:

$$(|Y_j - Y_{j-1}| - k)^2 \le 2((2c_0 + a)k)^2 + 2k^2 \le Ck^2\bar{\Phi}_j^2.$$

Now let $y' := Y/k$. Then clearly $y' \in \mathcal{N}_{L,c_0}(a)$. Considering lower bounds for φ, without loss of generality we may assume there exists α_3 as in lemma 3.4.2. By Cauchy-Schwarz,

$$\begin{aligned}
E_L(y') &\le \alpha_3 \sum_{j=1}^{L} (|y'_j - y'_{j-1}| - 1)^2 + \alpha_3 \sum_{j=1}^{L-1} \Phi_j^2 \\
&= \frac{\alpha_3}{k^2} \sum_{j=1}^{L} (|Y_j - Y_{j-1}| - k)^2 + \alpha_3 \sum_{j=1}^{L-1} \Phi_j^2 \\
&\le \alpha_3 \sum_{j=1}^{L} \left(10\,(\gamma-1)^2 + C\bar{\Phi}_j^2\right) + \alpha_3 \sum_{j=1}^{L-1} \Phi_j^2 \\
&\le \alpha_3 \sum_{j=1}^{L} \left(\frac{10}{k^2} k \sum_{i=k(j-1)+1}^{kj} (|y_i - y_{i-1}| - 1)^2\right) \\
&\quad + \alpha_3 \sum_{j=1}^{L-1} \left(Ck \sum_{i=k(j-1)+1}^{k(j+1)-1} |\phi_i|^2\right) \\
&\le C\left(\frac{1}{k} \sum_{i=1}^{Lk} (|y_i - y_{i-1}| - 1)^2 + k \sum_{i=1}^{Lk-1} |\phi_i|^2\right).
\end{aligned}$$

It follows that

$$\frac{1}{L} E_L(y') \le \frac{Ck^2}{Lk} E_{Lk}(y),$$

and since $y \in \mathcal{N}_{kL,kc_0}(a)$ was arbitrary, letting $L \to \infty$ in fact yields

$$\varphi_{kc_0}(a) \ge c(c_0)k^{-2}\varphi_{c_0}(a).$$

This proves that also the lower bound scales like c_0^{-2}. □

Application: a polymer chain in a confined region

The atomic chain described above can serve as a model of a polymer confined to a tubular region about itself, e.g., by neighboring chains. The above considerations suggest that its energy, at least for small strains a, can be described by a Hamiltonian

$$H(a) = \begin{cases} \alpha_1(1-a)^2 & \text{for } a \le 1, \\ \alpha_2(1-a)^2 & \text{for } a \ge 1, \end{cases}$$

where $0 < \alpha_1 < \alpha_2$. The corresponding Boltzmann distribution of statistical mechanics is

$$d\mathbb{P}_\beta(a) = \frac{1}{Z_\beta} e^{-\beta H(a)} da,$$

$\beta = 1/kT > 0$, where k is Boltzmann's constant and T temperature. For large β, i.e., sufficiently low temperature, we may take this as an approximation for all a.

It is elementary to see that the partition function Z_β is given by

$$Z_\beta = \frac{1}{2}\sqrt{\frac{\pi}{\beta}}\left(\sqrt{\frac{1}{\alpha_1}} + \sqrt{\frac{1}{\alpha_2}}\right).$$

The mean of this distribution, i.e., the preferred elongation of the atomic chain, can also be calculated explicitly:

$$\int a d\mathbb{P}_\beta(a) = 1 - \frac{1}{\sqrt{\pi\beta}}\left(\sqrt{\frac{1}{\alpha_1}} - \sqrt{\frac{1}{\alpha_2}}\right).$$

Since $\alpha_2 > \alpha_1$, this is strictly less than 1 and increasing in β, reflecting thermal contraction as expected for polymers (cf. [41]).

3.4.2 Energy scaling of a film near O(2,3)

Taking into account only next neighbor interactions, leads to zero energy response to compressions, as noted earlier (see proposition 2.3.5). Using the results of the previous paragraph, we will now examine the energy scaling near the zero energy set $O(2,3)$ of a thin film. To simplify the discussion, we consider two related models of nearest and next nearest neighbor interaction resp. nearest neighbor and angular interaction. We also add an additional energy penalty for two atoms getting too close to each other, as is physically not unreasonable.

Suppose $W_1, W_1' : [0,\infty) \to \mathbb{R}$, $W_2 : \mathbb{R} \to \mathbb{R}$ are continuous, W_2 is 2π-periodic, $W_1(1) = W_1'(\sqrt{2}) = W_2(0) = 0$, and there is an $\alpha > 0$ such that

$$W_1(r) \geq \alpha(r-1)^2, \quad W_1'(r) \geq \alpha(r-\sqrt{2})^2, \quad W_2(\phi) \geq \alpha\phi^2$$

for r in a neighborhood of 1 resp. $\sqrt{2}$ and ϕ in a neighborhood of 0.

Let $\delta > 0$, and define the energy function E_{an} by

$$\begin{aligned} E_{\text{an}}(y) &= \frac{1}{2}\sum_{|x_i - x_j| = 1} W_1(|y_i - y_j|) + \frac{\delta}{2}\sum_{|x_i - x_j| = 2} \chi_{[0,r_0)}(|y_i - y_j|) \\ &\quad + \frac{1}{2}\sum |y_i - y_k||y_j - y_k| W_2(|\theta_{ikj}| - \pi/2) \end{aligned} \tag{3.19}$$

where the third sum runs over all k and all i,j such that $x_i - x_k$ and $x_j - x_k$ are perpendicular and of norm 1. The next-nearest neighbor interaction is given by

$$\begin{aligned} E_{\text{nnn}}(y) &= \frac{1}{2}\sum_{|x_i - x_j| = 1} W_1(|y_i - y_j|) + \frac{1}{2}\sum_{|x_i - x_j| = \sqrt{2}} W_1'(|y_i - y_j|) \\ &\quad + \frac{\delta}{2}\sum_{|x_i - x_j| = 2} \chi_{[0,r_0)}(|y_i - y_j|). \end{aligned} \tag{3.20}$$

Proposition 3.4.5 *Both E_{an} and E_{nnn} are admissible energy functions leading to continuum stored energy functions φ_{an} resp. φ_{nnn}. For $\nu \geq 2$ there exist $\delta, c > 0$ such that for* $\mathrm{dist}(A, O(2,3)) \leq \delta$,

$$\varphi_{\mathrm{an}}(A, \mathbf{b}), \varphi_{\mathrm{nnn}}(A, \mathbf{b}) \geq c \ \mathrm{dist}^2(A, O(2,3)).$$

Clearly, E_{an} and E_{nnn} are admissible energy functions (see proposition 2.2.27). It remains to prove the lower bound on φ in terms of $\mathrm{dist}^2(A, O(2,3))$. To give a detailed proof is cumbersome, we mention the main ideas.

Sketch of proof. The film contains various atomic chains. For $\nu \geq 2$, the film energy can be bounded from below, e.g., by the energies of the chains $y(j, x_2, x_3)$, $j = 0, \ldots, k$, where these chain energies also contain angular terms as in the previous paragraph due to the angular resp. next nearest neighbor part in E. Similar this holds for the diagonal chains. Since the deviation of A from $O(2,3)$ for A in the vicinity of $O(2,3)$ can be estimated by the deviation of $|A(1,0)|$ and $|A(0,1)|$ from 1 and the deviation of $|A(1,1)|$ and $|A(1,-1)|$ from $\sqrt{2}$, applying proposition 3.4.4 gives the result. □

Remarks:

(i) Proposition 3.4.5 is false for $\nu = 1$, i.e., films consisting of only one single layer. (This can be seen by considering folded configurations.)

(ii) Define $\bar{\varphi}(A) := \inf_{\mathbf{b}} \varphi(A, \mathbf{b})$. For $\nu \geq 2$, this result implies that $\bar{\varphi}$ (defined on $\mathbb{R}^{3\times 2}$, cf. the remark below proposition 2.2.27) is not rank-one convex. This is because φ vanishes on $O(2,3)$, but not on its rank-one convex hull $\{A \in \mathbb{R}^{3\times 2} : s_2(A) \leq 1\}$ (see [16], page 50, corollary 2.3.2).

In the rest of this paragraph we will see that $\bar{\varphi}$ is not twice differentiable at $A = \mathrm{Id}$. For the sake of simplicity, we assume that c_0 is not too small.

Recall the construction (3.18) for the atomic chain. Let R, L and Φ be the same as in (3.18). Set $R(x_3) = R + \frac{\nu-1}{2} - x_3$. We define a film deformation patching together appropriately cylindrical configurations

$$y(x_1, x_2, x_3) = (R(x_3)\sin(x_1\Phi/L), x_2, R(x_3)(1 - \cos(x_1\Phi/L)) - d),$$

for $x \in \{0, \ldots, L\} \times \{0, \ldots, k\} \times \{0, \ldots, \nu - 1\}$. The nearest neighbor, next nearest neighbor lengths and bond angles in the x_3-layer resp. between the x_3- and $(x_3 + 1)$-layer are approximately

$$1 + \frac{1}{R}\left(\frac{\nu-1}{2} - x_3\right), \quad \sqrt{2} + \frac{1}{\sqrt{2}R}\left(\frac{\nu-1}{2} - x_3\right) - \frac{1}{2\sqrt{2}}\frac{\Phi}{L}, \quad \pm\frac{\pi}{2} \pm \frac{\Phi}{2L},$$

respectively. Since $\Phi/L \approx R^{-1} \approx 3(1-a)/d$, this implies that, similar as in (3.18), for $A = (ae_1, e_2)$, $a \leq 1$ near 1,

$$\bar{\varphi}(A) \leq \frac{\mathrm{const.}}{c_0^2}(1-a)^2,$$

provided there exists $\beta > 0$ such that, in a neighborhood of 1 resp. $\sqrt{2}$ resp. 0, $W_1(r) \leq \beta(r-1)^2$, $W_1'(r) \leq \beta(r - \sqrt{2})^2$, $W_2(\phi) \leq \beta\phi^2$. For $a \geq 1$, however, it is not hard to prove that $\bar{\varphi}(A) \geq \alpha_1(1-a)^2$. (This can be seen considering the one dimensional atomic chains $i \mapsto y(i, x_2, x_3)$.) □

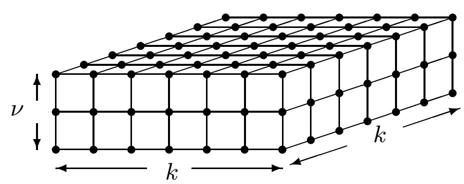
Chapter 4

A derivation of continuum nonlinear plate theory from atomistic models

4.1 The model

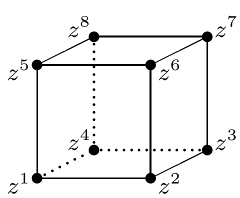
For bending dominated configurations it is convenient to choose the reference configuration symmetric with respect to the x_1-x_2-plane. Also the results of this chapter will only be interesting for films consisting of at least two atomic layers. We therefore consider films of $\nu+1$ atomic layers, $\nu \geq 1$, whose reference configuration is given by the lattice

$$\Lambda_k = \{0, 1, \ldots, k\}^2 \times \{-\nu/2, -\nu/2+1, \ldots, \nu/2\}.$$



The lattice of centers of unit-cubes with corners in Λ_k is denoted by Λ'_k. If $x \in [0,k]^2 \times [-\nu/2, \nu/2]$, we denote by $\bar{x}$ an element of Λ'_k closest to x. The unit cell corresponding to x is $Q(x) = \bar{x} + (-1/2, 1/2)^3$.

Deformations of this film are mappings $y : \Lambda_k \to \mathbb{R}^3$. We define eight vectors $z^1, \ldots, z^8$ by



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

and view $\vec{y}(x) = (y_1, \ldots, y_8) = (y(\bar{x}+z^1), \ldots, y(\bar{x}+z^8))$ and $\vec{z} = (z^1, \ldots, z^8)$ as elements of $\mathbb{R}^{3\times 8}$.

Our basic assumption is that the energy of a deformation y can be expressed by cell energies $W : \Lambda'_k \times \mathbb{R}^{3\times 8} \to \mathbb{R}$ in the form

$$E(y) = \sum_{\bar{x}\in\Lambda'} W(\bar{x}, \vec{y}(\bar{x})), \tag{4.1}$$

where $W(\bar{x}, \cdot)$ splits into a bulk and a surface part

$$W(\bar{x}, \cdot) = W_{\text{cell}}(\cdot) + W_{\text{surface}}(\bar{x}, \cdot) \tag{4.2}$$

with $W_{\text{surface}}(\bar{x}, \cdot) = 0$ if $\bar{x}$ does not lie in a boundary cube. We assume that $W_{\text{surface}}(\bar{x}, \vec{y})$ depends on $\bar{x}$ only through the number of boundary faces and the direction of their outward normals, and, if $Q(\bar{x})$ does not contain a lateral boundary face, can be written as

$$W_{\text{surface}}(\bar{x}, \vec{y}) = \begin{cases} W_{\text{surf}}(y_1, \ldots, y_4) & \text{resp.} \\ W_{\text{surf}}(y_5, \ldots, y_8) & \text{resp.} \\ W_{\text{surf}}(y_1, \ldots, y_4) + W_{\text{surf}}(y_5, \ldots, y_8) \end{cases} \tag{4.3}$$

for $\bar{x}_3 = -(\nu - 1)/2$ resp. $\bar{x}_3 = (\nu - 1)/2$ resp. $\nu = 1$.

Our goal being to prove a Γ-convergence result for the limit $k \to \infty$, we have to make precise what convergence of deformations means. We will study two distinct regimes:

- Thin films: Let $k \to \infty$ with $\nu \in \mathbb{N}$ fixed.
- Thick films: Let $k \to \infty$ and $\nu \to \infty$ such that $\nu/k \to 0$.

When proving compactness and the lower bound in the following Γ-convergence results, it will be convenient to choose particular interpolations of the lattice deformations.

To interpolate y on $Q(x)$ in the thin film regime, set $y(\bar{x}) = \frac{1}{8}\sum_{i=1}^{8} y(\bar{x}+z^i)$ and interpolate linearly on

$$T_{lmn}(x) := \bar{x} + T_{lmn}, \quad T_{lmn} := \text{co}(0, z^l, z^m, z^n),$$

for l, m, n such that $\mathcal{T} = \{T_{lmn}\}$ is a decomposition of $[-1/2, 1/2]^3$ into twelve simplices, z^l, z^m, z^n on a single face of the cube. In particular, let

$$T_1 := T_{412},\ T_2 := T_{234},\ T_3 := T_{856},\ T_4 := T_{678} \in \mathcal{T}.$$

In the thick film regime we again set $y(\bar{x}) = \frac{1}{8}\sum_{i=1}^{8} y(\bar{x}+z^i)$, and in addition we let $y(\bar{x} + w^i) = \frac{1}{4}\sum_j y(\bar{x} + z^j)$, where $w^1, \ldots, w^6$ are the centers of faces of $[-1/2, 1/2]^3$ and the summation runs over j such that z^j are the corners of the cube face centered at w^i. Now interpolate linearly on

$$T_{lmn}(x) := \bar{x} + T_{lmn}, \quad T_{lmn} := \text{co}(0, z^l, z^m, w^n),$$

for l, m, n such that $\mathcal{T} = \{T_{lmn}\}$ is a decomposition of $[-1/2, 1/2]^3$ into 24 simplices, $|z^l - z^m| = 1$, and z^l, z^m, w^n on a single face of the cube.

In order for the deformations to be defined on common domains, we also rescale, defining $\tilde{y} : \Omega \to \mathbb{R}^3$ by

$$\tilde{y}(x_1, x_2, x_3) = \frac{1}{k} y(kx_1, kx_2, x_3), \quad \Omega = S \times [-\nu/2, \nu/2], \tag{4.4}$$

respectively

$$\tilde{y}(x_1, x_2, x_3) = \frac{1}{k} y(kx_1, kx_2, \nu x_3), \quad \Omega = S \times [-1/2, 1/2], \tag{4.5}$$

$S = [0,1]^2$, for thin respectively thick films. By $\tilde{\Lambda}_k, \tilde{\Lambda}_k' \subset \Omega$ we denote the correspondingly rescaled lattices.

We now make precise in what sense we understand deformations $\tilde{y}^{(k)}$ to converge to some limiting deformation $\tilde{y}$. While for thick films a natural function space to consider is $L^2(\Omega, \mathbb{R}^3)$, for thin films the limiting deformations are elements of $L^2(S;\mathbb{R}^3) \oplus \ldots \oplus L^2(S;\mathbb{R}^3) \cong L^2(S \times \{-\nu/2, -\nu/2+1, \ldots, \nu/2\}; \mathbb{R}^3)$.

Definition 4.1.1 *Elements of these spaces will be called limiting deformations. Suppose $\tilde{y}$ is a limiting deformation (extended by zero outside Ω). By $x' = (x_1, x_2)$ denote the planar components of $x \in \mathbb{R}^3$.*

(i) In the thin film regime we say $\tilde{y}^{(k)} \to \tilde{y}$ if

$$\frac{1}{k^2} \sum_{x \in \tilde{\Lambda}_k} \left| \tilde{y}^{(k)}(x) - \fint_{[-1/2k, 1/2k]^2} \tilde{y}(x' + \xi, x_3) d\xi \right|^2 \to 0.$$

Interpolating $\tilde{y}$ linearly in x_3 on intervals $[i, i+1]$, $i = -\frac{\nu}{2}, \ldots, \frac{\nu}{2} - 1$, this is equivalent to

$$\tilde{y}^{(k)} \to \tilde{y} \quad \text{in } L^2(\Omega; \mathbb{R}^3).$$

(ii) In the thick film regime we say $\tilde{y}^{(k)} \to \tilde{y}$ if

$$\frac{1}{k^2 \nu} \sum_{x \in \tilde{\Lambda}_k} \left| \tilde{y}^{(k)}(x) - \fint_{[-1/2k, 1/2k]^2 \times [-1/2\nu, 1/2\nu]} \tilde{y}(x + \xi) d\xi \right|^2 \to 0.$$

This is equivalent to

$$\tilde{y}^{(k)} \to \tilde{y} \quad \text{in } L^2(\Omega; \mathbb{R}^3).$$

More precisely, in the thick film regime we are dealing with sequences of deformations $\tilde{y}^{(k,\nu)} : \tilde{\Lambda}_{k,\nu} \to \mathbb{R}^3$ such that $k, \nu \to \infty$ and $\nu/k \to 0$. For simplicity of notation, the ν-dependency is suppressed.

4.2 Discrete geometric rigidity

As elaborated in [21], the main tool to derive plate theory from three-dimensional elasticity is a quantitative rigidity estimate for deformations near $SO(3)$. In our setting we need such an estimate for discrete lattice deformations. The main point of this section is to state the relevant assumptions on the cell energies (compare [13]) and to prove lemma 4.2.2, a generalization to arbitrary dimensions of a result in [39]. The results of this section actually hold in any dimension $n \in \mathbb{N}$.

Suppose $\Omega \subset \mathbb{R}^n$ is a domain consisting of translated unit cubes and y some lattice deformation:

$$\Omega = \bigcup_{x \in \Lambda} x + [-1/2, 1/2]^n, \quad \Lambda \subset a + \mathbb{Z}^n \text{ finite, } a \in \mathbb{R}^n,$$

and

$$y : \bigcup_{x \in \Lambda} x + \{-1/2, 1/2\}^n \to \mathbb{R}^n.$$

The discrete deformation gradient is defined to be

$$\bar{\nabla} y(x) := (y_1 - \bar{y}, \dots, y_{2^n} - \bar{y}), \quad \bar{y} := \frac{1}{2^n} \sum_{i=1}^{2^n} y_i,$$

for $x \in \Lambda$, $y_i = y_i(x) = y(x + z^i)$, $z^1, \dots, z^{2^n}$ some enumeration of $\{-1/2, 1/2\}^n$. Also let

$$\bar{SO}(n) := \{\bar{\nabla}(x \mapsto Rx) = R\vec{z} : R \in SO(n)\}.$$

The energy of y shall be of the form

$$E(y) = \sum_{x \in \Lambda} W_{\text{cell}}(\vec{y}(x)),$$

where $\vec{y}(x) = (y(x + z) : z \in \{-1/2, 1/2\}^n)$ and W_{cell} satisfies the following

Assumption 4.2.1 *(i)* $W_{\text{cell}} : \mathbb{R}^{n \times 2^n} \to \mathbb{R}$ *is invariant under translations and rotations, i.e., for* $\vec{y} \in \mathbb{R}^{n \times 2^n}$*,*

$$W_{\text{cell}}(R\vec{y} + (c, \dots, c)) = W_{\text{cell}}(\vec{y})$$

for all $R \in SO(n)$*,* $c \in \mathbb{R}^n$*.*

(ii) $W_{\text{cell}}(\vec{y})$ *is minimal (*$= 0$*) if and only if there exists* $R \in SO(n)$ *and* $c \in \mathbb{R}^n$ *such that*

$$y_i = Rz^i + c, \quad i = 1, \dots, 2^n.$$

(iii) W_{cell} *is* C^2 *in a neighborhood of* $\bar{SO}(n)$*, and the Hessian* $Q_n = D^2 W_{\text{cell}}$ *at the identity* $\bar{\text{Id}} = \vec{z}$ *is positive definite on the orthogonal complement of the subspace spanned by infinitesimal translations* $(c, \dots, c)$*,* $c \in \mathbb{R}^n$*, and infinitesimal rotations* $(Az^1, \dots, Az^{2^n})$ *where* $A^T = -A \in \mathbb{R}^{n \times n}$*.*

(iv) W_{cell} *grows at infinity at least quadratically on the orthogonal complement of the subspace spanned by infinitesimal translations, i.e.,*

$$\liminf_{|\bar{\nabla} y| \to \infty} \frac{W_{\text{cell}}(\bar{\nabla} y)}{|\bar{\nabla} y|^2} > 0.$$

Remark: For Q_n, the Hessian of W_{cell} at the identity, these assumptions imply

$$Q_n(v,\dots,v)=0,\quad Q_n(Az^1,\dots,Az^{2^n})=0$$

for all $v\in\mathbb{R}^n$ and $A\in\mathbb{R}^{n\times n}$ with $A^T=-A$.

Now choose an appropriate interpolation u of y: partition the cubes $Q(x)=x+[-1/2,1/2]^n$ into simplices with corners in $x+\{-1/2,1/2\}^n$ and interpolate linearly, or analogously to the previous section: first define y at the cube center resp. face centers as appropriate averages and interpolate piecewise linearly on a partition into simplices having one corner at x resp. one corner at x and one corner at a face center.

The following lemma generalizes to higher dimension a lemma in [39]. For the proof also compare [13].

Lemma 4.2.2 *For u thus defined, $Q=Q(x)$ and $\vec{y}=\vec{y}(x)$,*

$$\int_Q \operatorname{dist}^2(\nabla u, SO(n))\le CW_{\text{cell}}(\vec{y}).$$

Proof. Let $W_{\text{ref}}(\vec{y})=W_{\text{ref}}(\bar{\nabla}\vec{y})=\int_Q\operatorname{dist}^2(\nabla u,SO(n))$. Both W_{cell} and W_{ref} are invariant under rotations and translations:

$$W_{\text{cell/ref}}(y_1,\dots,y_{2^n})=W_{\text{cell/ref}}(Ry_1+c,\dots,Ry_{2^n}+c)$$

if $R\in SO(n)$, $c\in\mathbb{R}^n$. So it suffices to prove the claim for deformations perpendicular to the space $V_0=\mathbb{R}^n\otimes(1,\dots,1)$ of infinitesimal translations.

Suppose first $\vec{y}\in\mathbb{R}^{n\times 2^n}$ is given such that $\vec{y}\perp V_0$ and $\operatorname{dist}(\vec{y},\bar{SO}(n))$ is small. Let $\bar{G}$ be the orthogonal projection of $\vec{y}$ onto $\bar{SO}(n)$. By assumption,

$$\begin{aligned}W_{\text{cell}}(\vec{y}) &= W_{\text{cell}}(\bar{G})+DW_{\text{cell}}(\bar{G})(\vec{y}-\bar{G})\\ &\quad+\frac{1}{2}D^2W_{\text{cell}}(\bar{G})(\vec{y}-\bar{G},\vec{y}-\bar{G})+o(|\vec{y}-\bar{G}|^2)\\ &\ge c|\vec{y}-\bar{G}|^2.\end{aligned}$$

(Note that $\vec{y}-\bar{G}\perp T_{\bar{G}}\bar{SO}(n)$ and $\vec{y}-\bar{G}\perp V_0$ since $\bar{R}\perp V_0$ for all $\bar{R}\in\bar{SO}(n)$.)

On the other hand, since $W_{\text{ref}}\ge 0$ and $W_{\text{ref}}(\vec{y})=0$ if $\bar{\nabla}\vec{y}\in\bar{SO}(n)$, we have $W_{\text{ref}}(\bar{G})=0$, $DW_{\text{ref}}(\bar{G})=0$, and, $\vec{y}\mapsto W_{\text{ref}}(\vec{y})$ being C^2 in a neighborhood of $\bar{SO}(n)$, $|\vec{y}-\bar{G}|^2=\operatorname{dist}^2(\vec{y},\bar{SO}(n))\ge cW_{\text{ref}}(\vec{y})$. So we have shown that for $\vec{y}$ with $\operatorname{dist}(\vec{y},\bar{SO}(n))$ small indeed

$$W_{\text{ref}}(\vec{y})\le CW_{\text{cell}}(\vec{y})$$

if C is large enough.

Now if $\operatorname{dist}(\vec{y},\bar{SO}(n))$ is not small, we only have to consider the limit $\operatorname{dist}(\vec{y},\bar{SO}(n))\to\infty$. Then by continuity the claim follows in the intermediate regime, too, since $W_{\text{cell}}(\vec{y})>0$ for $\vec{y}\notin\bar{SO}(n)$ (and $\vec{y}\perp V_0$). But this case is clear by assumption 4.2.1 (iv) since $W_{\text{ref}}(\vec{y})$ grows quadratically in $\vec{y}\perp V_0$. □

Theorem 4.2.3 *(Discrete Rigidity.) Suppose y is some lattice deformation, and let $u:\Omega\to\mathbb{R}^n$ be the associated interpolation (on the unit cubes $Q(x)$ as above). Then there exists a rotation $R\in SO(n)$ such that*

(i)

$$\int_\Omega |\nabla u - R|^2 \le C \sum_{x\in\Lambda} W_{\rm cell}(\vec{y}(x)),$$

(ii)

$$\sum_{x\in\Lambda} |\bar\nabla y(x) - \bar R|^2 \le C \sum_{x\in\Lambda} W_{\rm cell}(\vec{y}(x))$$

where $\bar R = R\vec{z}$. The constant C only depends on $W_{\rm cell}$ and Ω and is invariant under rescaling of Ω.

Proof. The proof of (i) is immediate from the lemma above and the following rigidity result for continuous deformations (cf. theorem 4.2.4). For the second part simply note that on a unit cube Q, $|\bar\nabla y - \bar R| \le C \int_Q |\nabla u - R|$. $\square$

Theorem 4.2.4 *(Continuous Rigidity, cf. [21].) Suppose $\Omega \subset \mathbb{R}^n$ is a Lipschitz domain. Then there exists a constant $C(\Omega)$, invariant under rescaling of Ω, such that for all $v \in W^{1,2}(\Omega;\mathbb{R}^n)$ there is a rotation $R \in SO(n)$ with*

$$\|\nabla v - R\|_{L^2(\Omega)} \le C(\Omega)\|{\rm dist}(\nabla v, SO(n))\|_{L^2(\Omega)}.$$

4.3 Compactness

In this section we will show that certain rescaled (discrete) gradients of sequences having finite bending energy are precompact in L^2. From now on we will suppose assumption 4.2.1 is satisfied for all $W(\bar x,\cdot)$. (Note that by (4.2) and (4.3), $\{W(\bar x,\cdot) : \bar x \in \Lambda'_k\}$ consists of no more than 27 functions.)

Recall the rescaling from (4.4) respectively (4.5), and for $\tilde y : \Omega \to \mathbb{R}^3$ set

$$\nabla_k \tilde y := (\nabla'\tilde y, k\tilde y_{,3}) \quad \text{resp.} \quad \nabla_{k,\nu}\tilde y := (\nabla'\tilde y, \frac{k}{\nu}\tilde y_{,3}) \tag{4.6}$$

in the thin respectively thick film regime. Also, for $z \in \{-1/2, 1/2\}^3$ we define

$$\bar\nabla_k \tilde y(x)(z) := k\left(\tilde y(\bar x + (z'/k, z_3)) - \tilde y(\bar x)\right) \quad \text{resp.} \tag{4.7}$$

$$\bar\nabla_{k,\nu} \tilde y(x)(z) := k\left(\tilde y(\bar x + (z'/k, z_3/\nu)) - \tilde y(\bar x)\right) \tag{4.8}$$

for $x \in \tilde Q(x)$, a rescaled unit cube with center $\bar x$. We view $\bar\nabla_k \tilde y$ and $\bar\nabla_{k,\nu}\tilde y$ as mappings from Ω to $\mathbb{R}^{3\times 8}$, where the columns of the image are labeled by $z^1, \ldots, z^8$.

Theorem 4.3.1 *(Compactness.) Suppose a sequence $y^{(k)} : \Lambda_k \to \mathbb{R}^3$ has finite bending energy, i.e.,*

$$\limsup_{k\to\infty} E(y^{(k)}) < \infty \quad \textit{resp.} \quad \limsup_{k,\nu\to\infty} \frac{1}{\nu^3} E(y^{(k)}) < \infty.$$

Then $\nabla_k \tilde y^{(k)}$ resp. $\nabla_{k,\nu}\tilde y^{(k)}$ is precompact in $L^2(\Omega)$: there exists a subsequence (not relabeled) such that

$$\nabla_k \tilde y^{(k)} \textit{ resp. } \nabla_{k,\nu}\tilde y^{(k)} \to (\nabla'\tilde y, b) \quad \textit{in } L^2(\Omega)$$

with $(\nabla'\tilde{y}, b) \in SO(3)$ *a.e. Furthermore,* $(\nabla'\tilde{y}, b)$ *is independent of* x_3 *and* $(\nabla'\tilde{y}, b) \in H^1(\Omega)$.

The piecewise constant mappings of lattice gradients satisfy (for the same subsequence)

$$\bar{\nabla}_k \tilde{y}^{(k)}(x)(z) \text{ resp. } \bar{\nabla}_{k,\nu} \tilde{y}^{(k)}(x)(z) \to (\nabla'\tilde{y}, b)(x) \cdot z \quad \text{in } L^2(\Omega)$$

where $z \in \{-1/2, 1/2\}^3$.

Proof. Consider thin films first. As noted at the beginning of this section, there are at most 27 functions $W(\bar{x}, \cdot)$ as $\bar{x}$ runs through Λ'_k. Therefore, finite bending energy, i.e., $E(y^{(k)}) \le C$, by lemma 4.2.2 implies that

$$\int_\Omega \operatorname{dist}^2(\nabla_k \tilde{y}^{(k)}, SO(3)) = \frac{1}{k^2} \int_{kS\times(-\frac{\nu}{2},\frac{\nu}{2})} \operatorname{dist}^2(\nabla y^{(k)}, SO(3)) \le \frac{C}{k^2}.$$

The first part of the theorem now directly follows from the corresponding compactness result in [21]. We recall two inequalities derived in [21] that will be used in the sequel. Applying the geometric rigidity estimate (in un-rescaled variables) to the sets

$$\left(\bar{x}' + (-1/2, 1/2)^2\right) \times (-\nu/2, \nu/2)$$

yields a piecewise constant map $R^{(k)} : S \to SO(3)$ with

$$\int_\Omega |R^{(k)}(x) - \nabla_k \tilde{y}^{(k)}(x)|^2 dx \le C/k^2, \tag{4.9}$$

and for $|\zeta| \le c/k$ and $\Omega' = S' \times (-\nu/2, \nu/2) \subset \Omega$ with $S' \subset\subset S$,

$$\int_{\Omega'} |R^{(k)}(x+\zeta) - R^{(k)}(x)|^2 dx \le C \int_\Omega \operatorname{dist}^2(\nabla_k \tilde{y}^{(k)}(x), SO(3)) dx \le C/k^2 \tag{4.10}$$

such that $R^{(k)} \to R$ in L^2, $R = (\nabla'\tilde{y}, b) \in H^1$, $b = \tilde{y}_{,1} \wedge \tilde{y}_{,2}$.

For the second part let z be a corner of T_{lmn}. Choose $\varphi^{(k)}_{lmn} : \Omega \to \Omega$ to be the function mapping $\tilde{Q}(x)$ onto $\tilde{T}_{lmn}(x)$, isometrically when restricted to a single simplex $T_{l'm'n'}(x)$. Since $\tilde{y}^{(k)}$ is affine on $T_{lmn}(x)$, we have

$$\bar{\nabla}_k \tilde{y}^{(k)}(x)(z) = \nabla_k \tilde{y}^{(k)}(\varphi^{(k)}_{lmn}(x)) \cdot z,$$

$z \in \{-1/2, 1/2\}^3$. Now applying lemma A.3 with $S_1 = S$ and $S_2 = (-\nu/2, \nu/2)$, by the part already proven

$$\lim_{k\to\infty} \bar{\nabla}_k \tilde{y}^{(k)}(z) = \lim_{k\to\infty} \nabla_k \tilde{y}^{(k)} \cdot z = (\nabla'\tilde{y}, b) \cdot z$$

strongly in L^2.

The reasoning for thick films is similar. We obtain a map $R^{(k,\nu)} : S_h \to SO(3)$, piecewise constant on a partition of $S_h \subset S$ into squares of side-length $h := \nu/k$ as in [21], with $\{x \in S : \operatorname{dist}(x, \partial S) \ge h\} \subset S_h \subset S$,

$$\int_{S_h\times(-\frac{1}{2},\frac{1}{2})} |R^{(k,\nu)}(x) - \nabla_{k,\nu} \tilde{y}^{(k)}(x)|^2 dx \le Ch^2, \tag{4.11}$$

and for $|\zeta| \leq ch$ and $\Omega' = S' \times (-1/2, 1/2) \subset \Omega$ with $S' \subset\subset S$,

$$\int_{\Omega'} |R^{(k,\nu)}(x+\zeta) - R^{(k,\nu)}(x)|^2 dx \leq C \int_{\Omega} \mathrm{dist}^2(\nabla_{k,\nu}\tilde{y}^{(k)}(x), SO(3)) dx \leq Ch^2. \tag{4.12}$$

For part two of the claim again apply lemma A.3, this time with $S_1 = \Omega$ and $S_2 = \{0\}$. □

4.4 Limiting plate theory for thin films

In this section we will derive a continuum plate theory for thin films in the bending energy regime $E(y^{(k)}) \sim 1$ from our discrete model. (This corresponds to the well known fact that for the rescaled expression $\frac{1}{k^3} E(y^{(k)})$ which leads to finite energy per volume, bending energies scale cubically in the film thickness, i.e., aspect ratio ν/k.) As before we will assume that assumption 4.2.1 is satisfied for all $W(\bar{x}, \cdot)$. The Hessian of $W(\bar{x}, \cdot)$ at the identity $\bar{\mathrm{Id}}$ is denoted $Q_3(\bar{x}, \cdot)$. In addition, we will need some decoupling property of Q_3 and Q_2, the Hessians of W_{cell} resp. W_{surf} (cf. (4.2) and (4.3)) at $\bar{\mathrm{Id}}$ resp. the right or left 3×4-part of $\bar{\mathrm{Id}}$. Sufficient will be to suppose up-down-symmetry in the following sense:

Assumption 4.4.1 *Both W_{cell} and W_{surface} are C^2 in a neighborhood of $\bar{SO}(3)$. Let P be the reflection $P(x', x_3) = (x', -x_3)$. For the bulk part of the energy (cf. (4.2)), we assume that*

$$W_{\mathrm{cell}}(Py_5, Py_6, Py_7, Py_8, Py_1, Py_2, Py_3, Py_4) = W_{\mathrm{cell}}(\vec{y})$$

for all $\vec{y} \in \mathbb{R}^{3\times 8}$. For the surface part (cf. (4.2) and (4.3)) we require that W_{surf} is translational invariant and

$$W_{\mathrm{surf}}(Py_1, Py_2, Py_3, Py_4) = W_{\mathrm{surf}}(\vec{y})$$

for all $\vec{y} \in \mathbb{R}^{3\times 4}$.

Remarks:

(i) For the quadratic forms Q_3 and Q_2 this implies

$$Q_3(Py_5, Py_6, Py_7, Py_8, Py_1, Py_2, Py_3, Py_4) = Q_3(\vec{y}) \tag{4.13}$$

for all $\vec{y} \in \mathbb{R}^{3\times 8}$ respectively

$$Q_2(Py_1, Py_2, Py_3, Py_4) = Q_2(\vec{y}) \tag{4.14}$$

for all $\vec{y} \in \mathbb{R}^{3\times 4}$.

(ii) These assumptions are satisfied for suitable mass-spring models (see section 4.6).

Depending on Q_3, we define a relaxed quadratic form $Q_3^{\rm rel}$: for $\vec{y} \in \mathbb{R}^{3\times 8}$ let

$$Q_3^{\rm rel}(\vec{y}) := \min_{v\in\mathbb{R}^3} Q_3(y_1,\dots,y_4,y_5+v,\dots,y_8+v).$$

Note that with this definition (4.13) remains valid when replacing Q_3 by $Q_3^{\rm rel}$.

As a last preparation we introduce the following notations. For a 3×8-matrix A we denote by $A_{\rm b}$ its left 3×4-part, by $A_{\rm t}$ its right 3×4-part. If A is any $3\times n$-matrix, we write A' for its upper $2\times n$-part and, for $n=3$, $A_{\rm p}$ for its left 3×2-part.

Now suppose assumption 4.2.1 holds for all $W(\bar{x},\cdot)$ and $W_{\rm cell}$ and $W_{\rm surf}$ satisfy assumption 4.4.1. Then, in the spirit of Γ-convergence (cf. [15]), our main result for thin films is:

Theorem 4.4.2 *(Limiting plate theory for thin films.) For $k\to\infty$, $E=E^{(k)}$ converges to $E_{\rm thin}$ defined below in the following sense:*

(i) If $y^{(k)}:\Lambda_k\to\mathbb{R}^3$ is such that $y^{(k)}\to\tilde{y}$ (cf. definition 4.1.1), then

$$\liminf_{k\to\infty} E(y^{(k)}) \ge E_{\rm thin}(\tilde{y}).$$

(ii) For all limiting deformations $\tilde{y}$ (cf. definition 4.1.1) there exists a sequence $y^{(k)}:\Lambda_k\to\mathbb{R}^3$ with $y^{(k)}\to\tilde{y}$ in the sense of definition 4.1.1 such that

$$\lim_{k\to\infty} E(y^{(k)}) = E_{\rm thin}(\tilde{y}).$$

If $\tilde{y}\in\mathcal{A}$ (see below), the limit functional $E_{\rm thin}$ is given by

$$E_{\rm thin}(\tilde{y}) := \int_S \Big[\frac{\nu}{8}Q_3^{\rm rel}\left(-\mathrm{II}_{12}M + N\cdot\vec{z}_-{}'\right) + \frac{\nu^3-\nu}{24}Q_3^{\rm rel}\left(N\cdot\vec{z}\,'\right) + \frac{1}{4}Q_2\left(\mathrm{II}_{12}M_{\rm b}\right) + \frac{\nu^2}{4}Q_2\left(N\cdot\vec{z}_{\rm b}'\right)\Big]\,dx$$

with $\vec{z}_- = (-z^1,-z^2,-z^3,-z^4,z^5,z^6,z^7,z^8)$ and

$$M = \begin{pmatrix} 0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0\\ 1&0&1&0&1&0&1&0 \end{pmatrix}, \quad N = \begin{pmatrix} \mathrm{II}_{11} & \mathrm{II}_{12}\\ \mathrm{II}_{21} & \mathrm{II}_{22}\\ 0 & 0\end{pmatrix}.$$

If $\tilde{y}\notin\mathcal{A}$, then $E_{\rm thin}(\tilde{y}) := +\infty$. The class $\mathcal{A}$ of admissible functions consists of isometries from S into $\mathbb{R}^3$ (viewed as functions on Ω independent of x_3):

$$\mathcal{A} = \{\tilde{y}\in W^{2,2}(S;\mathbb{R}^3) : |\tilde{y}_{,1}| = |\tilde{y}_{,2}| = 1,\ \tilde{y}_{,1}\cdot\tilde{y}_{,2} = 0\},$$

and $\mathrm{II}\in\mathbb{R}^{2\times 2}$ is the second fundamental form $\mathrm{II}_{ij} = \tilde{y}_{,i}\cdot b_{,j}$, $b = \tilde{y}_{,1}\wedge\tilde{y}_{,2}$.

4.4.1 Proof of the lower bound

Suppose $y^{(k)}$ is a sequence converging to a limiting deformation $\tilde{y}$ and has finite bending energy, so $\tilde{y}^{(k)} \to \tilde{y}$ in L^2 and, by theorem 4.3.1, $\nabla_k \tilde{y}^{(k)} = (\nabla' \tilde{y}^{(k)}, k\tilde{y}^{(k)}_{,3}) \to (\nabla' \tilde{y}, b) \in H^1$. Let

$$G^{(k)}(x) := k\left((R^{(k)})^T(x')\nabla_k \tilde{y}^{(k)}(x) - \mathrm{Id}\right)$$

which is bounded in L^2 by (4.9), say (up to choosing a subsequence)

$$G^{(k)} \rightharpoonup G. \tag{4.15}$$

In [21] it is shown that

$$G_{\mathrm{p}}(x', x_3) = G_{\mathrm{p}}(x', 0) + x_3 N(x'). \tag{4.16}$$

For our discrete system this will, however, not be sufficient to describe the deviations of these deformations from rigid motions. We also need to consider

$$\bar{G}^{(k)}(x) := k\left((R^{(k)})^T(x')\bar{\nabla}_k \tilde{y}^{(k)}(x', x_3) - \bar{\mathrm{Id}}\right),$$

piecewise constant with values in $\mathbb{R}^{3\times 8}$.

Lemma 4.4.3 *Let G be as in (4.15). Then (for a subsequence)*

$$\bar{G}^{(k)}(x)(z^i) \rightharpoonup H(x, z_3^i)\cdot z^i - \frac{1}{2}\,\mathrm{II}_{12}(x')M(z^i)$$

in L^2 where $H(x, z_3^i) \in \mathbb{R}^{3\times 3}$ with $H_{\mathrm{p}}(x, z_3^i) = G_{\mathrm{p}}(x', \bar{x}_3 + z_3^i)$.

Proof. As before, we define $\varphi^{(k)}_{lmn} : \Omega \to \Omega$ mapping $\tilde{Q}(x)$ onto $\tilde{T}_{lmn}(x)$ and $\tilde{T}_{l'm'n'}(x)$ onto $\tilde{T}_{lmn}(x)$ isometrically. By (4.9) for $\tilde{T}_{lmn}(\Omega) := \bigcup_{x\in\Omega} \tilde{T}_{lmn}(x)$,

$$\int_{\tilde{T}_{lmn}(\Omega)} |\nabla_k \tilde{y}^{(k)} - R^{(k)}|^2 \le \int_\Omega |\nabla_k \tilde{y}^{(k)} - R^{(k)}|^2 \le C/k^2.$$

So $\nabla_k \tilde{y}^{(k)} \circ \varphi^{(k)}_{lmn}$ also satisfies

$$\int_\Omega |\nabla_k \tilde{y}^{(k)} \circ \varphi^{(k)}_{lmn} - R^{(k)}|^2 \le C/k^2.$$

Extracting, if necessary, a further subsequence, it follows that $f^{(k)}_{lmn} := k((R^{(k)})^T \nabla_k \tilde{y}^{(k)} \circ \varphi^{(k)}_{lmn} - \mathrm{Id})$ converges weakly in L^2 to f_{lmn}, say. If z^i is a corner of T_{lmn}, then $f^{(k)}_{lmn}\cdot z^i = \bar{G}^{(k)}(\cdot)(z^i)$, whence $\bar{G}^{(k)}(\cdot)(z^i)$ converges to $\bar{G}(\cdot)(z^i)$, say, and $f_{lmn}\cdot z^i = \bar{G}(\cdot)(z^i)$.

Now suppose $r \in \{-\nu/2, -\nu/2+1, \ldots, \nu/2-1\}$, $r < x_3 < r+1$, and for $\varepsilon > 0$ consider the layer $\Omega_\varepsilon = S \times [r, r+\varepsilon]$. Then $G^{(k)}|_{\Omega_\varepsilon} \rightharpoonup G|_{\Omega_\varepsilon}$ by (4.15), and hence

$$\int_r^{r+\varepsilon} G^{(k)}(x', t)dt \rightharpoonup \int_r^{r+\varepsilon} G(x', t)dt \quad \text{ on } S.$$

On the other hand,

$$x' \mapsto \int_r^{r+\varepsilon} G^{(k)}(x', t) dt$$

is a fine mixture of certain $f_{lmn}^{(k)}$ with volume fraction of $f_1^{(k)} = f_{412}^{(k)}$ and $f_2^{(k)} = f_{234}^{(k)}$ each $\varepsilon/2 + \mathcal{O}(\varepsilon^2)$. Sending $\varepsilon \to 0$, we deduce that

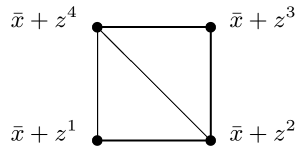
$$\frac{1}{2}(f_1 + f_2) =: H = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \int_r^{r+\varepsilon} G(x', t) dt, \tag{4.17}$$

in particular,

$$\frac{1}{2}(f_1 + f_2)_{\mathrm{p}}(x', x_3) = G_{\mathrm{p}}(x', r) = G_{\mathrm{p}}(x', \bar{x}_3 - 1/2) \tag{4.18}$$

(well-defined by (4.16)).

Consider the corners $\bar{x} + z^i$, $i = 1, \dots, 4$, of $Q(x)$ lying in Ω_ε.



The reasoning so far suffices to determine $\bar{G}(x)(z^i)$ for $i = 2, 4$ since then

$$\bar{G}(x)(z^i) = f_1 \cdot z^i = f_2 \cdot z^i = H \cdot z^i. \tag{4.19}$$

In order to calculate $\bar{G}(z^1) = f_1 z^1$ and $\bar{G}(z^3) = f_2 z^3$, we only have to consider the first two columns of $f_{1,2}$ since $f_1 \cdot (0,0,1)^T = f_2 \cdot (0,0,1)^T$. The following considerations are valid on any subset $\Omega' = S' \times (-\nu/2, \nu/2) \subset \Omega$ with $S' \subset\subset S$. Define $\varphi_1 = \varphi_{412}^{(k)}$ mapping $\tilde{Q}$ onto $\tilde{T}_1 = \tilde{T}_{412}$ and $\varphi_2 = \varphi_{234}^{(k)}$ mapping $\tilde{Q}$ onto $\tilde{T}_2 = \tilde{T}_{234}$ as before, and let $a = (0, 1/k, 0)$. Also set $\varphi_{i+}(x) = \varphi_i(x) + a$, $R_+(x) = R_+^{(k)}(x) = R(x+a) = R^{(k)}(x+a)$. We determine the limit of

$$k\left(R^T \nabla' \tilde{y}^{(k)} \circ \varphi_{1+} \cdot (z^1)' - (z^1)'\right) \tag{4.20}$$

in two different ways. (The limit exists – up to subsequences – weakly in L^2 since $f_{lmn}^{(k)}$ is bounded and $\|kR^T(\nabla_k \tilde{y}^{(k)} \circ \varphi_{1+} - \nabla_k \tilde{y}^{(k)} \circ \varphi_1)\| \le Ck\|\nabla_k \tilde{y}^{(k)} - R^{(k)}\| + k\|R_+^{(k)} - R^{(k)}\| \le C$ by (4.9) and (4.10).)

On the one hand,

$$R^T \nabla' \tilde{y}^{(k)} \circ \varphi_{1+} = R_+^T \nabla' \tilde{y}^{(k)} \circ \varphi_{1+} + (R^T - R_+^T) \nabla' \tilde{y}^{(k)} \circ \varphi_{1+},$$

where

$$k\left(R_+^T \nabla' \tilde{y}^{(k)} \circ \varphi_{1+} - \mathrm{Id}_{\mathrm{p}}\right) \rightharpoonup (f_1)_{\mathrm{p}} \quad \text{in } L^2.$$

For the second term note that $k(R_+ - R)$ is bounded in L^2 by (4.10) and hence converges – up to subsequences – weakly to F, say. Since by lemma A.3 and theorem 4.3.1 $\nabla_k \tilde{y}^{(k)} \circ \varphi_{1+} \to (\nabla' \tilde{y}, b)$ in L^2, we obtain

$$k(R^T - R_+^T) \nabla' \tilde{y}^{(k)} \circ \varphi_{1+} \rightharpoonup -F^T \nabla' \tilde{y} \quad \text{in } L^1.$$

Furthermore, since $R^{(k)} \to (\nabla' \tilde{y}, b)$, $F = (\nabla' \tilde{y}, b)_{,2}$. It follows that

$$k\left(R^T \nabla' \tilde{y}^{(k)} \circ \varphi_{1+} \cdot (z^1)' - (z^1)'\right) \rightharpoonup (f_1)_{\mathrm{p}} \cdot (z^1)' - (\nabla' \tilde{y}, b)_{,2}^T \nabla' \tilde{y} \cdot (z^1)' \quad \text{in } L^1. \tag{4.21}$$

On the other hand, note

$$\begin{aligned}\nabla'\tilde{y}^{(k)}\circ\varphi_{1+}\cdot(z^1)' &= \nabla'\tilde{y}^{(k)}\circ\varphi_{1+}\cdot(z^2)' + \nabla'\tilde{y}^{(k)}\circ\varphi_2\cdot(z^1)' \\ &\quad + \nabla'\tilde{y}^{(k)}\circ\varphi_1\cdot(z^4)'\end{aligned}$$

and by (4.18)

$$\begin{aligned}k\left(R^T\nabla'\tilde{y}^{(k)}\circ\varphi_2\cdot(z^1)'-(z^1)'\right) &\rightharpoonup (f_2)_{\mathrm{p}}\cdot(z^1)', \\ k\left(R^T\nabla'\tilde{y}^{(k)}\circ\varphi_1\cdot(z^i)'-(z^i)'\right) &\rightharpoonup G_{\mathrm{p}}(x',\bar{x}_3-1/2)\cdot(z^i)', \quad i=2,4\end{aligned}$$

in L^2. Since $(z^2)'+(z^4)'=0$, it follows that

$$k\left(R^T\nabla'\tilde{y}^{(k)}\circ\varphi_{1+}\cdot(z^1)'-(z^1)'\right)\rightharpoonup(f_2)_{\mathrm{p}}\cdot(z^1)'+g \tag{4.22}$$

in L^2 where g is the L^2-weak limit of

$$g^{(k)} := kR^T\left(\nabla'\tilde{y}^{(k)}\circ\varphi_{1+}-\nabla'\tilde{y}^{(k)}\circ\varphi_1\right)\cdot(z^2)'.$$

To calculate g, note first that since $R^{(k)}\to(\nabla'\tilde{y},b)$ boundedly in measure,

$$R^{(k)}g^{(k)}\rightharpoonup(\nabla'\tilde{y},b)g$$

in L^2. Then by lemma A.3 and theorem 4.3.1 $\nabla'\tilde{y}^{(k)}\circ\varphi_1\to\nabla'\tilde{y}$ in L^2 and therefore,

$$k\left(\nabla'\tilde{y}^{(k)}\circ\varphi_{1+}-\nabla'\tilde{y}^{(k)}\circ\varphi_1\right)=k\left(\nabla'\tilde{y}^{(k)}\circ\varphi_1(\cdot+a)-\nabla'\tilde{y}^{(k)}\circ\varphi_1\right)\rightharpoonup(\nabla'\tilde{y})_{,2}.$$

It follows that

$$g=(\nabla'\tilde{y},b)^T(\nabla'\tilde{y})_{,2}\cdot(z^2)'=\frac{1}{2}(\nabla'\tilde{y},b)^T\left(\tilde{y}_{,21}-\tilde{y}_{,22}\right).$$

Together with (4.21) and (4.22) this shows that

$$(f_1)_{\mathrm{p}}\cdot(z^1)'-(\nabla'\tilde{y},b)^T_{,2}\nabla'\tilde{y}\cdot(z^1)'=(f_2)_{\mathrm{p}}\cdot(z^1)'+\frac{1}{2}(\nabla'\tilde{y},b)^T\left(\tilde{y}_{,21}-\tilde{y}_{,22}\right). \tag{4.23}$$

Since $S\subset\subset S$ was arbitrary, this equality holds in all of Ω.

Now elementary calculations using $(\nabla'\tilde{y},b)\in SO(3)$ and $\tilde{y}\in W^{2,2}$, show that $(\nabla'\tilde{y},b)^T\left(\tilde{y}_{,21}-\tilde{y}_{,22}\right)=(0,0,-\mathrm{II}_{21}+\mathrm{II}_{22})^T$ and $(\nabla'\tilde{y},b)^T_{,2}\nabla'\tilde{y}\cdot(z^1)'=\frac{1}{2}(0,0,-\mathrm{II}_{12}-\mathrm{II}_{22})^T$. Furthermore, as noted before, $(f_1-f_2)(0,0,1)^T=0$. So (4.23) reduces to

$$(f_1-f_2)\cdot z^1=\begin{pmatrix}0\\0\\-\mathrm{II}_{12}\end{pmatrix}.$$

Together with (4.17) it follows that

$$f_1\cdot z^1=\frac{1}{2}\left((f_1+f_2)\cdot z^1+(f_1-f_2)\cdot z^1\right)=H\cdot z^1-\frac{1}{2}\begin{pmatrix}0\\0\\\mathrm{II}_{12}\end{pmatrix} \tag{4.24}$$

and

$$\begin{aligned} f_2 z^3 &= \frac{1}{2}\left((f_2+f_1)\cdot z^3 + (f_2-f_1)\cdot z^3\right) \\ &= H\cdot z^3 + \frac{1}{2}(f_1-f_2)\cdot z^1 \;=\; H\cdot z^3 - \frac{1}{2}\begin{pmatrix} 0 \\ 0 \\ \mathrm{II}_{12} \end{pmatrix}. \end{aligned} \tag{4.25}$$

Summarizing (4.17), (4.18), (4.19), (4.24) and (4.25), the lemma is proven for $i = 1, 2, 3, 4$. Replacing z^i by z^{i+4}, $⨍_r^{r+\varepsilon}$ by $⨍_{r+1-\varepsilon}^{r+1}$ and $\bar{x}_3 - 1/2$ by $\bar{x}_3 + 1/2$, analogous arguments yield the remaining part $i = 5, \ldots, 8$. $\square$

We can now prove the first part of theorem 4.4.2:

Proof of theorem 4.4.2 (i). Following [21], we estimate the energy of $\tilde{y}$ in terms of $\bar{G}$ by a careful Taylor expansion of $W(\bar{x}, \cdot)$. Let χ_k be the characteristic function of $\{|\bar{G}^{(k)}| \le k^{1/2}\}$. Since W_{cell} is C^2 in a neighborhood of $\bar{\mathrm{Id}}$, there is $\omega(t) \ge 0$ such that for $\bar{A} \in \mathbb{R}^{3\times 8}$,

$$W_{\mathrm{cell}}(\bar{\mathrm{Id}} + \bar{A}) \ge \frac{1}{2} Q_3(\bar{A}) - \omega(|\bar{A}|)$$

and $\omega(t)/t^2 \to 0$ as $t \to 0$. Analogously, if $\bar{x}$ lies in the top or bottom film layer,

$$W_{\mathrm{surf}}(\bar{x}, \bar{\mathrm{Id}}_{\mathrm{b/t}} + \bar{A}_{\mathrm{b/t}}) \ge \frac{1}{2} Q_2(\bar{A}_{\mathrm{b/t}}) - \omega(|\bar{A}|).$$

Therefore summing over those cubes that do not have lateral boundary faces (set $\Omega_k = S_k \times (-\nu/2, \nu/2)$, $S_k = \{x \in S : \mathrm{dist}(x', \partial S) \ge 1/k\}$ and, for $\nu \ge 2$, $\Omega_k^- = S_k \times (-\nu/2, -\nu/2+1)$, $\Omega_k^0 = S_k \times (-\nu/2+1, \nu/2-1)$, $\Omega_k^+ = S_k \times (\nu/2-1, \nu/2)$),

$$\begin{aligned} E(y^{(k)}) &\ge \sum_{\bar{x}} W(\bar{x}, \vec{y}^{(k)}(x)) \;=\; \sum_{\bar{x}} W\left(\bar{x}, (R^{(k)})^T(\bar{x})\bar{\nabla}_k \tilde{y}^{(k)}(\bar{x})\right) \\ &\ge k^2 \int_{\Omega_k} \chi_k W\left(\bar{x}, \bar{\mathrm{Id}} + \frac{1}{k}\bar{G}^{(k)}(x)\right) dx \\ &\ge \frac{1}{2}\left(\int_{\Omega_k^-} + \int_{\Omega_k^0} + \int_{\Omega_k^+}\right) Q_3\left(\bar{x}, \chi_k \bar{G}^{(k)}\right) - k^2 \chi_k \omega\left(\left|\frac{1}{k}\bar{G}^{(k)}\right|\right)\, dx. \end{aligned}$$

The second terms in the integrals converge to zero, because $\bar{G}^{(k)}$ is bounded in L^2 and $|\bar{G}^{(k)}|/k \le k^{-1/2}$ on $\{\chi_k \ne 0\}$, whence $|\bar{G}^{(k)}|^2 \omega(|\bar{G}^{(k)}|/k)/|\bar{G}^{(k)}/k|^2$ is a product of a bounded sequence in L^1 and a sequence tending to zero in L^∞. For the first terms note that since $\chi_{S_k}\chi_k \to 1$ boundedly in measure, $\chi_{S_k}\chi_k \bar{G}^{(k)} \rightharpoonup \bar{G}$ weakly in L^2. By assumption, the quadratic forms $A \mapsto Q_3(\bar{x}, A)$ are positive semidefinite. So from lower semicontinuity we deduce

$$\liminf_{k\to\infty} E(y^{(k)}) \ge \frac{1}{2}\int_\Omega Q_3(\bar{x}, \bar{G}). \tag{4.26}$$

Now by lemma 4.4.3 and (4.16), $\bar{G}(x)(z^i) = H(x, z_3^i)\cdot z^i - \frac{1}{2}\mathrm{II}_{12} M(z^i)$ with $H_{\mathrm{p}}(x, z_3^i) = G_{\mathrm{p}}(x', 0) + (\bar{x}_3 + z_3^i)N$. Using (4.26) to estimate the energies, we will from now on assume that the last row of $G_{\mathrm{p}}(x',0)$ is $(0,0)$. This is no loss of generality (see the remark after assumption 4.2.1). By definition of Q_3^{rel},

$$\liminf_{k\to\infty} E(y^{(k)}) \geq \frac{1}{2}\int_\Omega Q_3^{\mathrm{rel}}(\bar{G}) + \frac{1}{2}\int_S Q_2(\bar{G}_{\mathrm{t}}(\cdot,\nu/2)) + Q_2(\bar{G}_{\mathrm{b}}(\cdot,-\nu/2)) \quad (4.27)$$

with

$$Q_3^{\mathrm{rel}}(\bar{G}(x)) = Q_3^{\mathrm{rel}}(G_{\mathrm{p}}(x',0)\cdot\vec{z}\,' + (\bar{x}_3+z_3)N\cdot\vec{z}\,' - \frac{1}{2}\mathrm{II}_{12}M),$$

where $z_3N\cdot\vec{z}\,'$ is understood as $(-\frac{1}{2}N\vec{z}_{\mathrm{b}}\,', \frac{1}{2}N\vec{z}_{\mathrm{t}}\,')$. Integrating over x_3, we obtain

$$\begin{aligned}\int_{-\nu/2}^{\nu/2} Q_3^{\mathrm{rel}}(\bar{G}(x))dx_3 &= \nu Q_3^{\mathrm{rel}}\left(G_{\mathrm{p}}(x',0)\cdot\vec{z}\,' - \frac{1}{2}\mathrm{II}_{12}M + z_3N\cdot\vec{z}\,'\right)\\ &\quad + \sum_{\bar{x}_3=-\nu/2+1/2}^{\nu/2-1/2} \bar{x}_3^2 Q_3^{\mathrm{rel}}\left(N\cdot\vec{z}\,'\right)\\ &= \nu Q_3^{\mathrm{rel}}\left(G_{\mathrm{p}}(x',0)\cdot\vec{z}\,' - \frac{1}{2}\mathrm{II}_{12}M + \frac{1}{2}N\cdot\vec{z}_-\,'\right)\\ &\quad + \frac{\nu^3-\nu}{12}Q_3^{\mathrm{rel}}\left(N\cdot\vec{z}\,'\right). \end{aligned} \quad (4.28)$$

By up-down-symmetry, $Q_3^{\mathrm{rel}}(G_{\mathrm{p}}(x',0)\cdot\vec{z}\,'+M) = Q_3^{\mathrm{rel}}(G_{\mathrm{p}}(x',0)\cdot\vec{z}\,'-M)$ and $Q_3^{\mathrm{rel}}(G_{\mathrm{p}}(x',0)\cdot\vec{z}\,'+N\cdot\vec{z}_-\,') = Q_3^{\mathrm{rel}}(G_{\mathrm{p}}(x',0)\cdot\vec{z}\,'-N\cdot\vec{z}_-\,')$, so the first term of the last expression equals

$$\nu Q_3^{\mathrm{rel}}\left(G_{\mathrm{p}}(x',0)\cdot\vec{z}\right) + \nu Q_3^{\mathrm{rel}}\left(-\frac{\mathrm{II}_{12}}{2}M + \frac{1}{2}N\cdot\vec{z}_-\,'\right). \quad (4.29)$$

For the surface terms we obtain

$$Q_2\left(\bar{G}_{\mathrm{t/b}}(x',\pm\nu/2)\right) = Q_2\left(G_{\mathrm{p}}(x',0)\vec{z}_{\mathrm{t/b}}\,' \pm \frac{\nu}{2}N\cdot\vec{z}_{\mathrm{t/b}}\,' - \frac{1}{2}\mathrm{II}_{12}M_{\mathrm{t/b}}\right)$$

and therefore (note $M_{\mathrm{t}} = M_{\mathrm{b}}$ and $\vec{z}_{\mathrm{t}}\,' = \vec{z}_{\mathrm{b}}\,'$)

$$\begin{aligned}&Q_2(\bar{G}_{\mathrm{t}}(\cdot,\nu/2)) + Q_2(\bar{G}_{\mathrm{b}}(\cdot,-\nu/2))\\ &= 2Q_2\left(G_{\mathrm{p}}(x',0)\vec{z}_{\mathrm{b}}\,' - \frac{1}{2}\mathrm{II}_{12}M_{\mathrm{b}}\right) + \frac{\nu^2}{2}Q_2\left(N\cdot\vec{z}_{\mathrm{b}}\,'\right)\\ &= 2Q_2\left(G_{\mathrm{p}}(x',0)\vec{z}_{\mathrm{b}}\,'\right) + 2Q_2\left(\frac{1}{2}\mathrm{II}_{12}M_{\mathrm{b}}\right) + \frac{\nu^2}{2}Q_2\left(N\cdot\vec{z}_{\mathrm{b}}\,'\right), \end{aligned} \quad (4.30)$$

where the last step again follows from assumption 4.4.1.

Dropping the non-negative term $\nu Q_3(G_{\mathrm{p}}(x',0)\cdot\vec{z}\,') + 2Q_2(G_{\mathrm{p}}(x',0)\vec{z}_{\mathrm{b}}\,')$, we deduce from (4.27), (4.28), (4.29) and (4.30)

$$\begin{aligned}\liminf_{k\to\infty} E(y^{(k)}) &\geq \int_S \frac{\nu^3-\nu}{24}Q_3^{\mathrm{rel}}\left(N\cdot\vec{z}\,'\right) + \frac{\nu}{8}Q_3^{\mathrm{rel}}\left(-\mathrm{II}_{12}M + N\cdot\vec{z}_-\,'\right)\\ &\quad + \int_S \frac{1}{4}Q_2\left(\mathrm{II}_{12}M_{\mathrm{b}}\right) + \frac{\nu^2}{4}Q_2\left(N\cdot\vec{z}_{\mathrm{b}}\,'\right). \end{aligned}$$

□

4.4.2 Proof of the upper bound

For $f \in L^2(S)$ we denote by $\underline{f} = \underline{f}^{(k)} \in L^2(\mu^{-1}S)$, $\mu = k/(k+1)$, the function defined by

$$\underline{f}(x) = \fint_{(0,1/k)^2} f(\mu(x_0+\xi))d\xi = \fint_{\mu x_0+(0,\mu/k)^2} f(\xi)d\xi \tag{4.31}$$

whenever $x \in x_0 + [0,1/k)^2$, $x_0 \in \frac{1}{k}\mathbb{Z}^2 \cap S$.

It will be convenient to split the proof into several lemmas. The proofs of lemma 4.4.4 and 4.4.5 are straightforward.

Lemma 4.4.4 *Let $a = (1,0), (0,1),$ or $(1,1)$.*

(i) If $f, f_k \in L^2$, $f_k \to f$ in L^2, then

$$\underline{f_k} \to f \quad \text{in } L^2(S)$$

and thus (extending f by zero outside S), the $\underline{f_k}$ being piecewise constant,

$$\frac{1}{k^2} \sum_{x \in \frac{1}{k}\mathbb{Z}^2 \cap S} \left| \underline{f_k}(x) - \fint_{x+(-1/2k,1/2k)^2} f(\xi)d\xi \right|^2 \to 0.$$

(ii) If $f, f_k \in W^{1,2}$, $f_k \to f$ in $W^{1,2}$, then

$$k\left(\underline{f_k}(x+a/k) - \underline{f_k}(x)\right) \to \nabla f(x)\cdot a \quad \text{in } L^2(S).$$

.

(iii) If $f, f_k \in W^{2,2}$, $f_k \to f$ in $W^{2,2}$, then

$$k^2\left(\underline{f_k}(x+a/k) - \underline{f_k}(x) - \frac{1}{k}\underline{\nabla f_k}(x)\cdot a\right) \to \frac{1}{2}\nabla^2 f(x)(a,a) \quad \text{in } L^2(S).$$

Proof. (i) is clear if f is continuous and $f_k \equiv f$. It follows for general $f_k \to f$ by approximation. (Note $\|\underline{f} - \underline{g}\|_{L^2} \le \mu^{-1}\|f-g\|_{L^2}$ by Jensen's inequality.)

We only prove (iii), (ii) is even easier. Since $\underline{\nabla^2 f} \to \nabla^2 f$ in L^2 by (i), we have to prove that

$$\frac{1}{k^2}\sum_{x_0} \left| \fint_{(0,1/k)^2} k^2\Big(f_k(\mu(x_0+a/k+\xi)) - f_k(\mu(x_0+\xi)) - \frac{1}{k}\nabla f_k(\mu(x_0+\xi))\cdot a\Big) - \frac{1}{2}\nabla^2 f(\mu(x_0+\xi))(a,a)\, d\xi \right|^2 \to 0,$$

where the sum runs over $x_0 \in \frac{1}{k}\mathbb{Z}^2$ with $x_0 + [0,1/k]^2 \subset S$. By Jensen's inequality, pulling the square inside the averaged integral and changing variables, this is implied by

$$\mu^{-2}\int_{\mu S} \left| k^2\left(f_k(x+a/k) - f_k(x) - \frac{1}{k}\nabla f_k(x)\cdot a\right) - \frac{1}{2}\nabla^2 f(x)(a,a)\right|^2 \, dx \to 0.$$

Since S has Lipschitz boundary, we may extend f, f_k to all of $\mathbb{R}^n$ such that f_k has compact support and $f_k \to f \in W^{2,2}(\mathbb{R}^n)$ (cf., eg., [42]). The claim then follows from lemma A.4. □

For $\tilde{y} \notin \mathcal{A}$, the upper bound in theorem 4.4.2 is trivial. So assume $\tilde{y} \in \mathcal{A}$, and set $b = \tilde{y}_{,1} \wedge \tilde{y}_{,2}$. As shown in [21] (cf. page 1484), we may choose approximations $\tilde{y}^\lambda \in W^{2,\infty}$ and $b^\lambda \in W^{1,\infty}$ to $\tilde{y}$ and b (extended to maps in $W^{2,2}(\mathbb{R}^2, \mathbb{R}^3)$) for $\lambda > 0$ such that

$$\|\nabla^2 \tilde{y}^\lambda\|_{L^\infty},\ \|\nabla b^\lambda\|_{L^\infty} \le \lambda, \qquad |S^\lambda| \le \frac{\omega(\lambda)}{\lambda^2},$$

where

$$S^\lambda = \{x \in \mathbb{R}^2 : \tilde{y}(x) \ne \tilde{y}^\lambda(x) \text{ or } b(x) \ne b^\lambda(x)\} \quad \text{and} \quad \omega(\lambda) \to 0 \text{ as } \lambda \to \infty.$$

Furthermore, as shown in [21]:

$$\|\operatorname{dist}((\nabla' \tilde{y}^\lambda, b^\lambda), SO(3))\|_{L^\infty(S)} \le C\sqrt{\omega(\lambda)}. \tag{4.32}$$

Here, we will let $\lambda = \alpha k \to \infty$ where $\alpha = \alpha(k) \to 0$ as $k \to \infty$ so slowly that

$$\frac{\omega(\lambda)}{\lambda^2} = \frac{\omega(\alpha k)}{\alpha^2 k^2} = o(1/k^2).$$

Lemma 4.4.5 *With this choice of λ we have:*

(i) $\|\tilde{y}^\lambda - \tilde{y}\|_{W^{2,2}(\mathbb{R}^2)},\ \|b^\lambda - b\|_{W^{1,2}(\mathbb{R}^2)} \to 0,$

(ii) $k\|\underline{(\nabla' \tilde{y}, b)} - \underline{(\nabla' \tilde{y}^\lambda, b^\lambda)}\|_{L^2(S)} \to 0.$

Proof. By continuity of measures and $\|\nabla^2 \tilde{y}^\lambda\|_{L^\infty} \le \lambda$, we have

$$\|\tilde{y}^\lambda - \tilde{y}\|^2_{W^{2,2}} \le C \int_{\{\tilde{y}^\lambda \ne \tilde{y}\}} |\nabla^2 \tilde{y}^\lambda - \nabla^2 \tilde{y}|^2 \le C \int_{S^\lambda} |\nabla^2 \tilde{y}|^2 + \omega(\lambda) \to 0.$$

The same argument shows $\|b^\lambda - b\|_{W^{1,2}} \to 0$.

Now since the $(\nabla' \tilde{y}^\lambda, b^\lambda)$ are uniformly bounded on S (cf. (4.32)), we have

$$\|\underline{(\nabla' \tilde{y}, b)} - \underline{(\nabla' \tilde{y}^\lambda, b^\lambda)}\|^2_{L^2} \le \mu^{-2} \|(\nabla' \tilde{y}, b) - (\nabla' \tilde{y}^\lambda, b^\lambda)\|^2_{L^2} \le C|S^\lambda| = o(1/k^2).$$

□

Before defining our upper bound trial function, we prove one more preparatory lemma.

Lemma 4.4.6 *Let $U = U(x') \in SO(3)$ be the projection of $\underline{(\nabla' \tilde{y}^\lambda, b^\lambda)}$ onto $SO(3)$. Then*

(i) $\underline{(\nabla' \tilde{y}^\lambda, b^\lambda)} - U \to 0$ *in* $L^\infty(S)$,

(ii) $k\left(\underline{(\nabla' \tilde{y}^\lambda, b^\lambda)} - U\right) \to 0$ *in* $L^2(S)$.

Proof. Set $f = (\nabla' \tilde{y}^\lambda, b^\lambda)$. First note that

$$\|f - \underline{f}\|_{L^\infty} \le \frac{2\sqrt{2}}{k} \|\nabla f\|_{L^\infty} \le C\lambda/k.$$

Since furthermore $\|\mathrm{dist}(f, SO(3))\|_{L^\infty} \le C\sqrt{\omega(\lambda)}$ by (4.32), we have

$$|\underline{f} - U|, \ |f - U| \to 0 \quad \text{in } L^\infty.$$

This proves (i).

Write $g(x) = f(x) - U(\mu^{-1}x) = g^\perp(x) + g^\parallel(x)$ as a sum with $g^\perp$ perpendicular and $g^\parallel$ tangential to $SO(3)$ at $U(x)$. Then $\underline{g^\perp} = \underline{f} - U$ and $\underline{g^\parallel} = 0$. Therefore, $|g^\parallel(x)| \le C\lambda/k = C\alpha$ for a.e. x. (On the squares $\mu x_0 + [0, \mu/k)^2$, $U(\mu^{-1}\cdot)$ is constant and $|\nabla g^\parallel| \le |\nabla g| = |\nabla f|$.)

Now for given $\varepsilon > 0$, if k is large enough, we have $|g^\perp(x)| \le \varepsilon |g^\parallel(x)|$ if $x \notin S^\lambda$ (because $f(x) \in SO(3)$). Set $V = x_0 + (0, 1/k)^2$, $x_0 \in \frac{1}{k}\mathbb{Z}^2$. Since $g|_{\mu V} \in W^{1,\infty}$, we may apply Poincaré's inequality to obtain for $x \in V$,

$$\begin{aligned}
\left|\underline{f} - U\right|^2(x) &= \left(\fint_{\mu V} g^\perp \right)^2 \le \fint_{\mu V} |g^\perp|^2 \\
&\le \varepsilon^2 \fint_{\mu V} |g^\parallel|^2 + \frac{k^2}{\mu^2} \int_{\mu V \cap S^\lambda} |g|^2 \\
&\le \varepsilon^2 \frac{C}{k^2} \fint_{\mu V} |\nabla g^\parallel|^2 + \frac{k^2}{\mu^2} |\mu V \cap S^\lambda| \fint_{\mu V \cap S^\lambda} |g|^2 \\
&\le \varepsilon^2 \frac{C}{k^2} \fint_{\mu V} |\nabla f|^2 + \frac{k^2}{\mu^2} |\mu V \cap S^\lambda| \, \|g\|_{L^\infty}^2.
\end{aligned}$$

Since $\|\nabla f\|_{L^2}$ is bounded by lemma 4.4.5, summing over all such $V \subset S$ yields

$$\begin{aligned}
\|\underline{f} - U\|_{L^2}^2 &= \sum_V \frac{1}{k^2} \left| \underline{f}|_V - U|_V \right|^2 \\
&\le \sum_V \frac{C}{k^2} \varepsilon^2 \mu^{-2} \int_{\mu V} |\nabla f|^2 + \mu^{-2} \sum_V |\mu V \cap S^\lambda| \, \|f - U(\mu^{-1}\cdot)\|_{L^\infty}^2 \\
&\le \frac{C\varepsilon^2}{k^2} \int_S |\nabla f|^2 + \mu^{-2} |S^\lambda| \, \|f - U(\mu^{-1}\cdot)\|_{L^\infty}^2.
\end{aligned}$$

So in fact $\|k(\underline{f} - U)\|_{L^2} \le C\varepsilon + o(1)$, i.e., (ii) holds. □

Now let $d \in C^1(\overline{\Omega})$ and consider the trial function

$$\tilde{y}^{(k)}(x', x_3) = \underline{\tilde{y}^\lambda}(x') + \frac{1}{k} x_3 \underline{b^\lambda}(x') + \frac{1}{k^2} d(x', x_3). \tag{4.33}$$

We will not re-interpolate linearly on simplices in $\mathcal{T}$ as before but rather evaluate $\tilde{y}^{(k)}$ only at atomic lattice sites.

Proof of theorem 4.4.2 (ii). First note that by lemma 4.4.5 (i) and lemma 4.4.4 (i), $\tilde{y}^{(k)} \to \tilde{y}$ in the sense of definition 4.1.1.

Instead of $\bar{\nabla}_k \tilde{y}^{(k)}$, it is more convenient to calculate the discrete gradient

$$\bar{D}_k \tilde{y}^{(k)}(x)(a) := k\left(\tilde{y}^{(k)}(\hat{x} + (a'/k, a_3)) - \tilde{y}^{(k)}(\hat{x})\right),$$

where $\hat{x} = \frac{1}{k}(\lfloor kx_1 \rfloor, \lfloor kx_2 \rfloor, \lfloor x_3 \rfloor)$, $a^i = \frac{1}{2}(1,1,1)^T + z^i \in \{0,1\}^3$. Let $\zeta = (a'/k, a_3)$. For $x \in \hat{x} + (0, 1/k)^2 \times (0,1) \subset \Omega$ we compute:

$$\begin{aligned} D\tilde{y}^{(k)}(x)(a) &= k\left(\tilde{y}^{(k)}(\hat{x}+\zeta) - \tilde{y}^{(k)}(\hat{x})\right) \\ &= k\left(\underline{\tilde{y}^\lambda}(x'+\zeta') - \underline{\tilde{y}^\lambda}(x')\right) + (\hat{x}_3+\zeta_3)\underline{b^\lambda}(x'+\zeta') - \hat{x}_3\underline{b^\lambda}(x') \\ &\quad + \frac{1}{k}\left(d(\hat{x}+\zeta) - d(\hat{x})\right). \end{aligned}$$

By lemmas 4.4.4, 4.4.5 and continuity of d,

$$\begin{aligned} k^2\left(\underline{\tilde{y}^\lambda}(x'+\zeta') - \underline{\tilde{y}^\lambda}(x') - \underline{\nabla'\tilde{y}^\lambda}(x')a'/k\right) &\to \frac{1}{2}\nabla'^2\tilde{y}(x')(a',a'), \\ k\left((\hat{x}_3+\zeta_3)\underline{b^\lambda}(x'+\zeta') - \hat{x}_3\underline{b^\lambda}(x') - \zeta_3\underline{b^\lambda}(x')\right) &\to (\hat{x}_3+\zeta_3)\nabla' b(x')a', \\ d(\hat{x}+\zeta) - d(\hat{x}) &\to d(x', \hat{x}_3+\zeta_3) - d(x', \hat{x}_3) \end{aligned}$$

in L^2. By lemma A.5 also

$$\begin{aligned} k\left(\underline{\tilde{y}^\lambda}(x'+\zeta') - \underline{\tilde{y}^\lambda}(x') - \underline{\nabla'\tilde{y}^\lambda}(x')a'/k\right) &\to 0, \\ (\hat{x}_3+\zeta_3)\underline{b^\lambda}(x'+\zeta') - \hat{x}_3\underline{b^\lambda}(x') - \zeta_3\underline{b^\lambda}(x') &\to 0, \\ \frac{1}{k}\left(d(\hat{x}+\zeta) - d(\hat{x})\right) &\to 0 \end{aligned}$$

in L^∞ (note $\|\underline{f}\|_{L^\infty} \leq \|f\|_{L^\infty}$ and recall lemma 4.4.5 (i)). Therefore,

$$\begin{aligned} & k\left(\bar{D}\tilde{y}^{(k)}(x)(a) - \underline{(\nabla'\tilde{y}^\lambda, b^\lambda)}(x') \cdot a\right) \\ &= k^2\left(\underline{\tilde{y}^\lambda}(x'+\zeta') - \underline{\tilde{y}^\lambda}(x') - \underline{\nabla'\tilde{y}^\lambda}(x')a'/k\right) \\ &\quad + k\left((\hat{x}_3+\zeta_3)\underline{b^\lambda}(x'+\zeta') - \hat{x}_3\underline{b^\lambda}(x') - \zeta_3\underline{b^\lambda}(x')\right) \\ &\quad + d(\hat{x}+\zeta) - d(\hat{x}) \\ &\to \frac{1}{2}\nabla'^2\tilde{y}(x')(a',a') + (\hat{x}_3+\zeta_3)\nabla' b(x')a' \\ &\quad + d(x', \hat{x}_3+\zeta_3) - d(x', \hat{x}_3) \end{aligned}$$

in L^2 and

$$\bar{D}\tilde{y}^{(k)}(x)(a) - \underline{(\nabla'\tilde{y}^\lambda, b^\lambda)}(x') \cdot a \to 0$$

in L^∞.

Now as shown in lemma 4.4.6, there exists a piecewise constant mapping U with values in $SO(3)$ such that $\|k(\underline{(\nabla'\tilde{y}^\lambda, b^\lambda)} - U)\|_{L^2} \to 0$, $\|\underline{(\nabla'\tilde{y}^\lambda, b^\lambda)} - U\|_{L^\infty} \to 0$. Then

$$\begin{aligned} E(\tilde{y}^{(k)}) &= k^2\int_\Omega W(\bar{x}, \bar{D}_k\tilde{y}^{(k)}) = k^2\int_\Omega W(\bar{x}, U^T\bar{D}_k\tilde{y}^{(k)}) \\ &= k^2\int_\Omega W\left(\bar{x}, \vec{a} + U^T\frac{1}{k}F^{(k)}\right) \end{aligned}$$

with $\frac{1}{k}F^{(k)} \to 0$ in L^∞ and $F^{(k)} \to F$ in L^2, where

$$F(a) := \frac{1}{2}\nabla'^2\tilde{y}(x')(a',a') + (\hat{x}_3+\zeta_3)\nabla' b(x')a' + d(x',\hat{x}_3+\zeta_3) - d(x',\hat{x}_3).$$

Since $U \to (\nabla'\tilde{y}, b)$ boundedly in measure, it follows

$$E(\tilde{y}^{(k)}) \;\to\; \int_\Omega \frac{1}{2}Q_3\left(\bar{x}, (\nabla'\tilde{y}, b)^T(x')F(x)\right),$$

where $Q_3(\bar{x},\cdot)$ is the Hessian of $W(\bar{x},\cdot)$ at $\bar{\mathrm{Id}}$.

Consider the term $(\nabla'\tilde{y}, b)^T(x')F(x)(a)$. For $a' = (0,0)$, $(1,0)$, $(1,1)$, resp. $(0,1)$, the first two components of $\frac{1}{2}(\nabla'\tilde{y}, b)^T(x')\nabla'^2\tilde{y}(x')(a',a')$ are zero while the third equals

$$0, \quad -\frac{1}{2}\mathrm{II}_{11}, \quad -\frac{1}{2}\left(\mathrm{II}_{11}+\mathrm{II}_{12}+\mathrm{II}_{21}+\mathrm{II}_{22}\right), \quad \text{resp.} \quad -\frac{1}{2}\mathrm{II}_{22}.$$

For the remaining part we obtain with $z = a - (\frac{1}{2},\frac{1}{2},\frac{1}{2})^T$,

$$\begin{aligned}
&(\nabla'\tilde{y}, b)^T(x')\Big((\bar{x}_3+z_3)\nabla' b(x')((1/2,1/2)^T + z') + d(x',\hat{x}_3+\zeta_3) - d(x',\hat{x}_3)\Big)\\
&= (\bar{x}_3+z_3)N\cdot z' + z_3 N\cdot(1/2,1/2)^T + (\nabla'\tilde{y}, b)^T e(x',\bar{x}_3),
\end{aligned}$$

where

$$e(x',\bar{x}_3) = d(x',\hat{x}_3+\zeta_3) - d(x',\hat{x}_3) + \bar{x}_3\nabla' b(x')\cdot(1/2,1/2)^T.$$

Without changing the value of $Q(\bar{x},\cdot)$, we may add the term $B(x) \in \mathbb{R}^{3\times 8}$ defined as

$$\frac{1}{2}\begin{pmatrix} 0 & 0 & -\beta_1\\ 0 & 0 & -\beta_2\\ \beta_1 & \beta_2 & 0\end{pmatrix}\cdot\vec{z} + \beta_3\begin{pmatrix} 0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0\\ 1&1&1&1&1&1&1&1\end{pmatrix} - \begin{pmatrix} v & v & v & v & v & v & v & v\end{pmatrix},$$

where $\beta_1 = \mathrm{II}_{12}+\mathrm{II}_{11}$, $\beta_2 = \mathrm{II}_{12}+\mathrm{II}_{22}$, $\beta_3 = \frac{\mathrm{II}_{11}+\mathrm{II}_{22}}{4}$, $v = (\nabla'\tilde{y}, b)^T\bar{x}_3\nabla' b(x')\cdot(1/2,1/2)^T$. After some elementary calculations we obtain

$$\begin{aligned}
&B(x)(z^i) + (\nabla'\tilde{y}, b)^T(x')F(x)(z^i)\\
&= \frac{-\mathrm{II}_{12}}{2}M(z^i) + (\bar{x}_3+z_3)N\cdot(z^i)' + (\nabla'\tilde{y}, b)^T\left(d(x',\hat{x}_3+\zeta_3) - d(x',\hat{x}_3)\right).
\end{aligned}$$

Now choosing d such that

$$d((x',\hat{x}_3+\zeta_3) - d((x',\hat{x}_3)) = \zeta_3 d^1(x') + \zeta_3\bar{x}_3 d^2(x'),$$

yields (with $m = (0,0,0,0,1,1,1,1)^T \in \mathbb{R}^8$)

$$\begin{aligned}
E(\tilde{y}^{(k)}) \;\to\; \int_\Omega \frac{1}{2}Q_3\Big(&\bar{x}, \frac{-\mathrm{II}_{12}}{2}M + \frac{1}{2}N\cdot\vec{z}'_- + (\nabla'\tilde{y}, b)^T d^1\otimes m\\
&+\bar{x}_3 N\cdot\vec{z}' + \bar{x}_3(\nabla'\tilde{y}, b)^T d^2\otimes m\Big)
\end{aligned}$$

$$
\begin{aligned}
= \int_S \Bigg[& \frac{\nu}{8} Q_3 \Big(- \mathrm{II}_{12} M + N \cdot \vec{z}_-' + 2(\nabla'\tilde{y}, b)^T d^1 \otimes m \Big) \\
& + \frac{\nu^3 - \nu}{24} Q_3 \Big(N \cdot \vec{z}' + (\nabla'\tilde{y}, b)^T d^2 \otimes m \Big) \\
& + \frac{1}{2} Q_2 \left(-\frac{\mathrm{II}_{12}}{2} M_\mathrm{t} + \frac{\nu}{2} N \vec{z}_\mathrm{t}' \right) + \frac{1}{2} Q_2 \left(-\frac{\mathrm{II}_{12}}{2} M_\mathrm{b} - \frac{\nu}{2} N \vec{z}_\mathrm{b}' \right) \Bigg].
\end{aligned}
$$

By density of C^1 in L^2 and continuity of the above term in d^i in L^2, we may replace d^1 resp. d^2 by

$$
d^1_{\min} := \operatorname{argmin} Q_3 \Big(- \mathrm{II}_{12} M + N \cdot \vec{z}_-' + 2(\nabla'\tilde{y}, b)^T d^1 \otimes m \Big) \in L^2
$$

resp.

$$
d^2_{\min} := \operatorname{argmin} Q_3 \Big(N \cdot \vec{z}' + (\nabla'\tilde{y}, b)^T d^2 \otimes m \Big) \in L^2.
$$

This finishes the proof. □

4.5 Limiting plate theory for thick films

For thick films the scaling of bending energies is determined by $\frac{1}{k^3} E(y^{(k)}) \sim (\frac{\nu}{k})^3$. It is suggestive to divide the limiting expression derived in theorem 4.4.2 by ν^3 and let $\nu \to \infty$. That this actually leads to the correct thick film Γ-limit in the bending energy regime is the content of the following theorem. We again suppose that E satisfies assumptions 4.2.1 and 4.4.1.

Theorem 4.5.1 *(Limiting plate theory for thick films.) For $k \to \infty$ and $\nu \to \infty$ such that $\nu/k \to 0$, $\frac{1}{\nu^3} E^{(k)}$ converges to E_thick defined below in the following sense:*

(i) If $y^{(k)} : \Lambda_k \to \mathbb{R}^3$ is such that $\tilde{y}^{(k)} \to \tilde{y}$ in the sense of definition 4.1.1, then

$$
\liminf_{k \to \infty} E(y^{(k)}) \geq E_\mathrm{thick}(\tilde{y}).
$$

(ii) For all $\tilde{y} \in L^2(\Omega)$ there exists a sequence $y^{(k)} : \Lambda_k \to \mathbb{R}^3$ with $\tilde{y}^{(k)} \to \tilde{y}$ in the sense of definition 4.1.1 such that

$$
\lim_{k \to \infty} E(y^{(k)}) = E_\mathrm{thick}(\tilde{y}).
$$

The limit functional E_thick is given by

$$
E_\mathrm{thick}(\tilde{y}) := \begin{cases} \int_S \frac{1}{24} Q_3^\mathrm{rel} (N \cdot \vec{z}')\, dx & \text{for } \tilde{y} \in \mathcal{A}, \\ \infty & \text{for } \tilde{y} \notin \mathcal{A}, \end{cases}
$$

where the matrix N and the class $\mathcal{A}$ of admissible functions are as in theorem 4.4.2.

More precisely, in (ii) we will show that for any choice of $k_n, \nu_n \to \infty$ such that $\nu_n/k_n \to 0$ there exists a sequence $\tilde{y}^{(k_n,\nu_n)} \to \tilde{y}$ such that

$$\lim_{n\to\infty} E(y^{(k_n,\nu_n)}) = E_{\text{thick}}(\tilde{y}).$$

Remark: In [13] it is shown that the Cauchy-Born rule holds near $SO(3)$ for bulk material if assumption 4.2.1 is satisfied for the bulk energy W_{cell}. This justifies defining a macroscopic energy density by $W_{\text{macro}}(A) := W_{\text{cell}}(A \cdot \vec{z})$. Letting $Q_{\text{macro}}(F) = \frac{\partial^2 W_{\text{macro}}}{\partial F^2}(\text{Id})(F,F)$ and defining a relaxed quadratic form $Q^{\text{rel}}_{\text{macro}}$ on $\mathbb{R}^{2\times 2}$ by

$$Q^{\text{rel}}_{\text{macro}}(F) = \min_{c\in\mathbb{R}^3} Q_{\text{macro}}(\hat{F} + c \otimes e_3),$$

where $\hat{F}$ is the 3×3-matrix $\sum_{i,j=1}^2 F_{ij} e_i \otimes e_j$, i.e., $Q^{\text{rel}}_{\text{macro}} = Q_2$ in the language of [21], we recover the formula of nonlinear bending energy derived in [21] from $Q^{\text{rel}}_3(N \cdot \vec{z}\,') = Q^{\text{rel}}_{\text{macro}}(\text{II})$.

Again we will split the proof into deriving the lower bound (i) and finding a recovery sequence (ii) into the following two subsections.

4.5.1 Proof of the lower bound

Let $h := \frac{\nu}{k}$. Analogously to paragraph 4.4.1 we consider $G^{k,\nu} : \Omega \to \mathbb{R}^{3\times 3}$ with

$$G^{(k,\nu)} = \frac{1}{h}(R^T \nabla_{k,\nu} \tilde{y}^{(k)} - \text{Id}) \quad \text{on } S_h \times (-\nu/2, \nu/2),$$

$R = R^{(k,\nu)}$, extended by zero, and the piecewise constant mapping $\bar{G}^{k,\nu} : \Omega \to \mathbb{R}^{3\times 8}$ defined by

$$\bar{G}^{(k,\nu)} = \frac{1}{h}(R^T \bar{\nabla}_{k,\nu} \tilde{y}^{(k)} - \bar{\text{Id}}) \quad \text{on } S_h \times (-\nu/2, \nu/2),$$

extended by zero, where $\nabla_{k,\nu}\tilde{y}^{(k)}$ and $\bar{\nabla}_{k,\nu}\tilde{y}^{(k)}$ are defined as in (4.6) and (4.8). As before (see the proof of lemma 4.4.3 resp. (4.11)) we see that $G^{k,\nu}$ and $\bar{G}^{k,\nu}$ are bounded in L^2, say $G^{k,\nu} \rightharpoonup G$ and $\bar{G}^{k,\nu} \rightharpoonup \bar{G}$ in L^2 for a suitable subsequence, and G_{p} is as in (4.16).

Lemma 4.5.2 *There is $v \in L^2(\Omega; \mathbb{R}^3)$ such that for $i = 1, \dots, 8$,*

$$\bar{G}(x)(z^i) = \bar{G}(z^1) + (G_{\text{p}}|v) \cdot (z^i - z^1).$$

Assuming this lemma is proven, we immediately can prove the first part of theorem 4.5.1:

Proof of theorem 4.5.1 (i). Simply note that by a similar reasoning as before,

$$\begin{aligned}
\liminf_{\nu,k\to\infty} \frac{1}{\nu^3} E(y^{(k)}) &= \liminf_{\nu,k\to\infty} \frac{1}{\nu^3} k^2 \nu h^2 \int_{S\times(\frac{-\nu+2}{2\nu},\frac{\nu-2}{2\nu})} \frac{1}{2} Q_3(\bar{G}^{(k,\nu)}(x))\, dx \\
&\geq \frac{1}{2} \int_\Omega Q^{\text{rel}}_3(G_{\text{p}}(x',0) \cdot \vec{z}\,' + x_3 N \cdot \vec{z}\,') \\
&\geq \frac{1}{24} \int_S Q^{\text{rel}}_3(N \cdot \vec{z}\,'),
\end{aligned}$$

because subtracting $\bar{G}(z^1)$ in each column does not alter the value of Q_3. $\square$

Proof of lemma 4.5.2. Let $i \in \{1,2,3,4\}$, and set $a = (z^i - z^1)/k$, $x_+ = x + a$. Suppose $\bar{x} \in \tilde{\Lambda}'$ and $Q = \bar{x} + (-1/2k, 1/2k)^2 \times (-1/2\nu, 1/2\nu)$. Then

$$\begin{aligned} & k\left(\tilde{y}^{(k)}(\bar{x} + ((z^i)'/k, z_3^i/\nu)) - \tilde{y}^{(k)}(\bar{x})\right) - \fint_Q \nabla'\tilde{y}^{(k)}(\xi)d\xi \cdot (z^i)' \\ = \ & k\left(\tilde{y}^{(k)}(\bar{x}_+ + ((z^1)'/k, z_3^1/\nu)) - \tilde{y}^{(k)}(\bar{x}_+)\right) - \fint_Q \nabla'\tilde{y}^{(k)}(\xi)d\xi \cdot (z^1)' \\ & +k\left(\tilde{y}^{(k)}(\bar{x}_+) - \tilde{y}^{(k)}(\bar{x})\right) + \fint_Q \nabla'\tilde{y}^{(k)}(\xi)d\xi \cdot (z^1 - z^i)'. \end{aligned} \tag{4.34}$$

Since by our interpolation for thick films,

$$\begin{aligned} k\left(\tilde{y}^{(k)}(\bar{x}_+) - \tilde{y}^{(k)}(\bar{x})\right) &= k\fint_Q \left(\tilde{y}^{(k)}(\xi_+) - \tilde{y}^{(k)}(\xi)\right)d\xi \\ &= k\fint_Q \int_0^1 \nabla\tilde{y}^{(k)}(\xi + ta)\cdot a \ dtd\xi \\ &= \fint_Q \int_0^1 \nabla\tilde{y}^{(k)}(\xi + ta)dtd\xi \cdot (z^i - z^1), \end{aligned}$$

i.e.,

$$\begin{aligned} & k\left(\tilde{y}^{(k)}(\bar{x}_+) - \tilde{y}^{(k)}(\bar{x})\right) + \fint_Q \nabla'\tilde{y}^{(k)}(\xi)d\xi \cdot (z^1 - z^i)' \\ = \ & \fint_Q \int_0^1 \left(\nabla'\tilde{y}^{(k)}(\xi + ta) - \nabla'\tilde{y}^{(k)}(\xi)\right) dtd\xi \cdot (z^i - z^1)' \\ =: \ & f(x)\cdot(z^i - z^1)' \end{aligned}$$

for $f = f^{(k,\nu)} : \Omega \to \mathbb{R}^{3\times 2}$ piecewise constant on the rescaled unit cubes $\tilde{Q}(x)$, (4.34) can be rewritten as

$$\bar{\nabla}_{k,\nu}\tilde{y}^{(k)}(x)(z^i) - \bar{\nabla}_{k,\nu}\tilde{y}^{(k)}(x_+)(z^1) = \fint_{\tilde{Q}(x)} \nabla'\tilde{y}^{(k)}(\xi)\cdot(z^i - z^1)' + f(x)\cdot(z^i - z^1)'. \tag{4.35}$$

Now let $\varphi \in C_c^\infty(\Omega;\mathbb{R}^{3\times 2})$ and set $r(x) = \varphi(x) - \overline{\varphi}(x)$, $\overline{\varphi}(x) := \fint_{\tilde{Q}(x)} \varphi$. Then

$$\begin{aligned} \int_\Omega \frac{1}{h} f(x) : \varphi(x)dx \ &= \ \sum_{x\in\tilde{\Lambda}'} |\tilde{Q}(x)| \frac{1}{h} f(x) : \overline{\varphi}(x) \\ = \ & \sum_{x\in\tilde{\Lambda}'} |\tilde{Q}(x)| \fint_{\tilde{Q}(x)} \left(\int_0^1 \frac{\nabla'\tilde{y}^{(k)}(\xi + ta) - \nabla'\tilde{y}^{(k)}(\xi)}{h}\right) dt : \overline{\varphi}(\xi)d\xi \\ = \ & \int_0^1 \int_\Omega \left(\frac{\nabla'\tilde{y}^{(k)}(x + ta) - \nabla'\tilde{y}^{(k)}(x)}{h} : (\varphi(x) - r(x))\right) dxdt. \end{aligned}$$

For the term not involving r use partial integration to obtain

$$-\int_0^1 \int_\Omega \left(\frac{\tilde{y}^{(k)}(x + ta) - \tilde{y}^{(k)}(x)}{h} \cdot \operatorname{div}\varphi\right) dxdt$$

$$\begin{aligned} &= -\int_0^1 \int_\Omega \left(\tilde{y}^{(k)}(x) \cdot \frac{\operatorname{div}\varphi(x-ta) - \operatorname{div}\varphi(x)}{h} \right) dxdt \\ &\to 0 \end{aligned}$$

as $h \to 0$ since $|a| \ll h$. But also the remaining term tends to zero, because $r \to 0$ uniformly and $\frac{1}{h}(\nabla' \tilde{y}^{(k)}(x+ta) - \nabla' \tilde{y}^{(k)}(x))$ is bounded in L^2 uniformly in $t \in (0,1)$ by (4.11) and – note that φ has compact support – (4.12). Summarizing, this proves that $\frac{1}{h} f \to 0$ in distributions.

Define

$$\bar{G}_+^{(k,\nu)}(x) = \frac{1}{h}\left(R^T(x') \bar{\nabla}_{k,\nu} \tilde{y}^{(k)}(x_+) - \bar{\mathrm{Id}} \right).$$

Then from

$$\frac{1}{h}\left(R^T(x'_+) \bar{\nabla}_{k,\nu} \tilde{y}^{(k)}(x_+) - \bar{\mathrm{Id}} \right) \rightharpoonup \bar{G} \quad \text{in } L^2$$

and

$$\frac{1}{h}\left(R^T(x'_+) - R^T(x') \right) \bar{\nabla}_{k,\nu} \tilde{y}^{(k)}(x_+) \rightharpoonup 0 \quad \text{in } L^2$$

it follows

$$\bar{G}_+^{(k,\nu)} \rightharpoonup \bar{G} \quad \text{in } L^2 \tag{4.36}$$

on $\Omega' = S' \times (-\nu/2, \nu/2) \subset \Omega$ with $S' \subset\subset S$. (Note that $R^{(k,\nu)}$ being constant on squares of side-length h implies

$$\begin{aligned} \left\| \frac{1}{h}(R^T(x'_+) - R^T(x')) \right\|_{L^2}^2 &\le \frac{C/k}{h} \left\| \frac{1}{h} \max_{|\zeta| \le 2h} |R^T(x'+\zeta) - R^T(x')| \right\|_{L^2}^2 \\ &\le \frac{C}{\nu} \quad \text{(by (4.12))} \\ &\to 0.) \end{aligned}$$

Now by (4.35), the fact that $\frac{1}{h} f \to 0$ in distributions, and $(z^i - z^1)_3 = 0$, we have

$$\begin{aligned} & R\left(\bar{G}^{(k,\nu)}(z^i) - \bar{G}_+^{(k,\nu)}(z^1) - \frac{1}{h}\left(R^T \fint_{\tilde{Q}(x)} \nabla \tilde{y}^{(k)}(\xi) - \mathrm{Id} \right) \cdot (z^i - z^1) \right) \\ &= \frac{1}{h}\left(R(h\bar{G}^{(k,\nu)}(z^i) + z^i) - R(h\bar{G}_+^{(k,\nu)}(z^1) + z^1) - \fint_{\tilde{Q}(x)} \nabla \tilde{y}^{(k)}(\xi) \cdot (z^i - z^1) \right) \\ &= \frac{1}{h}\left(\bar{\nabla}_{k,\nu}(x) \tilde{y}^{(k)}(z^i) - \bar{\nabla}_{k,\nu} \tilde{y}^{(k)}(x_+)(z^1) - \fint_{\tilde{Q}(x)} \nabla' \tilde{y}^{(k)}(\xi) \cdot (z^i - z^1)' \right) \\ &= \frac{1}{h} f(x) \cdot (z^i - z^1)' \\ &\to 0 \end{aligned}$$

in distributions.

On the other hand, we have for the individual terms $R^{(k,\nu)} \to (\nabla' y, b)$ boundedly in measure, $\bar{G}^{(k)}, \bar{G}_+^{(k)} \rightharpoonup \bar{G}$ in $L^2(\Omega')$ by (4.36), and

$$\frac{1}{h}\left(R^T \fint_{Q(x)} \nabla \tilde{y}^{(k)}(\xi) - \mathrm{Id} \right) \rightharpoonup G(x) \quad \text{in } L^2(\Omega'),$$

because, up to negligible errors if $k/\nu \notin \mathbb{N}$, the left hand side equals $\fint_{Q(x)} G^{(k,\nu)}$ which converges to $G(x)$ weakly in L^2. It follows that in all of Ω

$$(\nabla' y, b)\left(\bar{G}(z^i) - \bar{G}(z^1) - G \cdot (z^i - z^1)\right) = 0,$$

i.e., $\bar{G}(z^i) - \bar{G}(z^1) = G \cdot (z^i - z^1)$ for $i = 1, 2, 3, 4$.

An analogous argument with z^1 replaced by z^5 shows that $\bar{G}(z^i) - \bar{G}(z^5) = G \cdot (z^i - z^5)$, $i = 5, 6, 7, 8$. Setting $v = \bar{G}(z^5) - \bar{G}(z^1)$, we have shown that

$$\bar{G}(z^i) = \bar{G}(z^1) + (G_{\mathrm{p}}|v) \cdot (z^i - z^1)$$

for $i \in \{1, \ldots, 8\}$. □

4.5.2 Proof of the upper bound

For $\tilde{y} \notin \mathcal{A}$ the upper bound is trivial, so assume $\tilde{y} \in \mathcal{A}$, $b = \tilde{y}_{,1} \wedge \tilde{y}_{,2}$. Again choose $\tilde{y}^\lambda \in W^{2,\infty}(\mathbb{R}^2)$, $b^\lambda \in W^{1,\infty}(\mathbb{R}^2)$ such that

$$\|\nabla^2 \tilde{y}^\lambda\|_{L^\infty},\ \|\nabla b^\lambda\|_{L^\infty} \le \lambda, \qquad |S^\lambda| \le \frac{\omega(\lambda)}{\lambda^2},$$

where

$$S^\lambda = \{x \in \mathbb{R}^2 : \tilde{y}(x) \neq \tilde{y}^\lambda(x) \text{ or } b(x) \neq b^\lambda(x)\}, \qquad \omega(\lambda) \to 0 \text{ as } \lambda \to \infty.$$

For thick films we let $\lambda = \alpha/h = \alpha k/\nu \to \infty$ where $\alpha = \alpha(h) \to 0$ as $h \to \infty$ so slowly that

$$\frac{\omega(\lambda)}{\lambda^2} = \frac{\omega(\alpha(h)/h)}{\alpha^2(h)h^{-2}} = o(h^2)$$

and consider the trial function

$$\tilde{y}^{(k)}(x', x_3) = \underline{\tilde{y}^\lambda}(x') + hx_3\underline{b^\lambda}(x') + h^2 d(x', x_3).$$

for $d \in C^1(\overline{\Omega})$. (Recall the definition of $\underline{f}$ from (4.31).)

As before, we define $U = U(x') \in SO(3)$ to be the projection of $\underline{(\nabla'\tilde{y}^\lambda, b^\lambda)}$ onto $SO(3)$. The analogue of lemma 4.4.5 and 4.4.6 for thick films is the following

Lemma 4.5.3 *(i)* $\|\tilde{y}^\lambda - \tilde{y}\|_{W^{2,2}(\mathbb{R}^2)},\ \|b^\lambda - b\|_{W^{1,2}(\mathbb{R}^2)} \to 0.$

(ii) $h^{-1}\|\underline{(\nabla'\tilde{y}, b)} - \underline{(\nabla'\tilde{y}^\lambda, b^\lambda)}\|_{L^2(S)} \to 0.$

(iii) $\underline{(\nabla'\tilde{y}^\lambda, b^\lambda)} - U \to 0$ *in* $L^\infty(S)$.

(iv) $h^{-1}\left(\underline{(\nabla'\tilde{y}^\lambda, b^\lambda)} - U\right) \to 0$ *in* $L^2(S)$.

The proof is similar to the proofs of lemma 4.4.5 and lemma 4.4.6. The necessary modifications are straightforward.

We can now estimate the energy of our trial function:

Proof of theorem 4.5.1 (ii). By lemmas 4.4.4 and 4.5.3, $y^{(k)} \to \tilde{y}$. Again we calculate the discrete gradient

$$\begin{aligned} D\tilde{y}^{(k)}(x)(a) &= k\left(\tilde{y}^{(k)}(\hat{x}+\zeta) - \tilde{y}^{(k)}(\hat{x})\right) \\ &= k\left(\underline{\tilde{y}^\lambda}(x'+\zeta') - \underline{\tilde{y}^\lambda}(x')\right) + kh\left((\hat{x}_3+\zeta_3)\underline{b^\lambda}(x'+\zeta') - \hat{x}_3\underline{b^\lambda}(x')\right) \\ &\quad +kh^2\left(d(\hat{x}+\zeta) - d(\hat{x})\right) \end{aligned}$$

for $x \in \hat{x} + (0, 1/k)^2 \times (0, 1/\nu) \subset \Omega$, $\hat{x} \in \tilde{\Lambda}_k$, $\zeta = (a'/k, a_3/\nu)$, and $a \in \{0,1\}^3$ as before.

Now using lemmas 4.4.4, 4.5.3 and the fact that d lies in C^1, we obtain

$$\begin{aligned} \frac{k}{h}\left(\underline{\tilde{y}^\lambda}(x'+\zeta') - \underline{\tilde{y}^\lambda}(x') - \underline{\nabla'\tilde{y}^\lambda}(x')a'/k\right) &\to 0, \\ k\left((\hat{x}_3+\zeta_3)\underline{b^\lambda}(x'+\zeta') - \hat{x}_3\underline{b^\lambda}(x') - \zeta_3\underline{b^\lambda}(x')\right) &\to x_3\nabla' b(x')a', \\ \nu\left(d(\hat{x}+\zeta) - d(\hat{x})\right) &\to \begin{cases} 0 & \text{for } a_3 = 0, \\ d_{,3}(x', x_3) & \text{for } a_3 = 1 \end{cases} \end{aligned}$$

in L^2 since $1 \ll \nu \ll k$. By lemma A.5 (with $h = 1/k$, $\tilde{h} = \nu/k$) also

$$\begin{aligned} k\left(\underline{\tilde{y}^\lambda}(x'+\zeta') - \underline{\tilde{y}^\lambda}(x') - \underline{\nabla'\tilde{y}^\lambda}(x')a'/k\right) &\to 0, \\ kh\left((\hat{x}_3+\zeta_3)\underline{b^\lambda}(x'+\zeta') - \hat{x}_3\underline{b^\lambda}(x') - \zeta_3\underline{b^\lambda}(x')\right) &\to 0, \\ h\nu\left(d(\hat{x}+\zeta) - d(\hat{x})\right) &\to 0 \end{aligned}$$

in L^∞ (note $\|\underline{f}\|_{L^\infty} \le \|f\|_{L^\infty}$). Therefore,

$$\begin{aligned} &\frac{1}{h}\left(\bar{D}\tilde{y}^{(k)}(x)(a) - \underline{(\nabla'\tilde{y}^\lambda, b^\lambda)}(x') \cdot a\right) \\ &= \frac{k}{h}\left(\underline{\tilde{y}^\lambda}(x'+\zeta') - \underline{\tilde{y}^\lambda}(x') - \underline{\nabla'\tilde{y}^\lambda}(x')a'/k\right) \\ &\quad +k\left((\hat{x}_3+\zeta_3)\underline{b^\lambda}(x'+\zeta') - \hat{x}_3\underline{b^\lambda}(x') - \zeta_3\underline{b^\lambda}(x')\right) \\ &\quad +kh\left(d(\hat{x}+\zeta) - d(\hat{x})\right) \\ &\to x_3\nabla' b(x')a' + d_{,3}(x', x_3)\delta_{a_3 1} \end{aligned}$$

in L^2 and

$$\bar{D}\tilde{y}^{(k)}(x)(a) - \underline{(\nabla'\tilde{y}^\lambda, b^\lambda)}(x') \cdot a \to 0$$

in L^∞.

As before, by lemma 4.5.3 we may replace $\underline{(\nabla'\tilde{y}^\lambda, b^\lambda)}$ by U and find

$$E(\tilde{y}^{(k)}) = k^2\nu \int_\Omega W(\bar{x}, U^T \bar{D}_k \tilde{y}^{(k)}) = k^2\nu \int_\Omega W\left(\bar{x}, \vec{a} + U^T h F^{(k)}\right)$$

with $hF^{(k)} \to 0$ in L^∞ and $F^{(k)} \to F$ in L^2, where

$$F(a) := x_3\nabla' b(x')a' + d_{,3}(x', x_3)\delta_{a_3 1}.$$

It follows (note $U \to (\nabla' \tilde{y}, b)$ boundedly in measure and $\frac{1}{\nu^3} k^2 \nu h^2 = 1$)

$$\begin{aligned}
\frac{1}{\nu^3} E(\tilde{y}^{(k)}) \;\to\; & \int_\Omega \frac{1}{2} Q_3\Big((\nabla' \tilde{y}, b)^T (x') F(x) \Big) \\
& + \lim_{\nu,k\to\infty} \int_S \Bigg(\int_{\frac{1}{2}-\frac{1}{\nu}}^{\frac{1}{2}} \frac{1}{2} Q_2((\nabla' \tilde{y}, b)^T (x') F_{\mathrm{t}}^{(k)}(x)) \\
& \qquad + \int_{-\frac{1}{2}}^{-\frac{1}{2}+\frac{1}{\nu}} \frac{1}{2} Q_2((\nabla' \tilde{y}, b)^T (x') F_{\mathrm{b}}^{(k)}(x)) \Bigg),
\end{aligned}$$

where the surface terms vanish since $Q_2((\nabla' \tilde{y}, b)^T F_{\mathrm{b/t}}^{(k)})$ converges in L^1. Choosing $d(x) = \frac{1}{2} x_3^2 d(x')$ and setting $m = (0,0,0,0,1,1,1,1)^T$ yields

$$\begin{aligned}
\frac{1}{\nu^3} E(\tilde{y}^{(k)}) \;\to\; & \int_\Omega \frac{1}{2} Q_3\Big(x_3 \Big(N \cdot \vec{a}\,' + (\nabla' \tilde{y}, b)^T (x') d(x') \otimes m \Big)\Big) \\
= \; & \frac{1}{24} \int_S Q_3 \Big(N \cdot \vec{z}\,' + (\nabla' \tilde{y}, b)^T (x') d(x') \otimes m \Big)
\end{aligned}$$

because adding $(N \cdot (\frac{1}{2}, \frac{1}{2})^T) \otimes (1, \ldots, 1)$ does not change the value of Q_3.

By density of $C^1(\bar{S})$ in $L^2(S)$ and continuity of the above term in d in L^2, we may replace d by

$$d_{\min} := \operatorname{argmin} Q_3 \Big(N \cdot \vec{z}\,' + (\nabla' \tilde{y}, b)^T d \otimes m \Big) \in L^2.$$

This finishes the proof. □

4.6 Example: a mass-spring model

In this section we give an example of an atomic interaction to which the results of the previous sections apply. Motivated by the investigations in [25], we examine mass-spring models: lattices of atoms whose energy is given by springs between nearest and next nearest neighbors.

For a deformation $y : \Lambda_k \to \mathbb{R}^3$ let

$$\begin{aligned}
E_{\mathrm{ms}}(y) \;=\; & \frac{1}{2} \sum_{\substack{x_1, x_2 \in \Lambda_k \\ |x_1 - x_2| = 1}} \frac{K_1}{2} (|y(x_1) - y(x_2)| - 1)^2 \\
& + \frac{1}{2} \sum_{\substack{x_1, x_2 \in \Lambda_k \\ |x_1 - x_2| = \sqrt{2}}} \frac{K_2}{2} (|y(x_1) - y(x_2)| - \sqrt{2})^2 + \sum_{\bar{x} \in \Lambda'_k} \chi(\vec{y}(\bar{x})).
\end{aligned}$$

The non-negative term χ is needed to assure that deformations are locally orientation preserving and assumption 4.2.1 (ii) is satisfied. We choose χ invariant under rotations and translations such that (see assumption 4.4.1) $\chi(Py(P\vec{z})) = \chi(y(\vec{z}))$, χ is zero in a neighborhood of $\bar{SO}(3) + \mathbb{R} \otimes (1, \ldots, 1)$ and positive ($\geq c > 0$) in a neighborhood of $\bar{O}(3) \setminus \bar{SO}(3) + \mathbb{R} \otimes (1, \ldots, 1)$. E.g., set $\chi(\vec{y}) := c$ for $\operatorname{dist}(\vec{y}, \bar{O}(3) \setminus \bar{SO}(3) + \mathbb{R} \otimes (1, \ldots, 1)) \leq \varepsilon$, some $\varepsilon > 0$, $\chi(\vec{y}) := 0$ else.

Proposition 4.6.1 *For any values of $K_1, K_2 \in (0,\infty)$, $E_{\rm ms}$ is an admissible energy function, i.e., satisfies assumptions 4.2.1 and 4.4.1.*

Proof. To see that E_{ms} can be written in the form (4.1), for $\vec{y} = y(\vec{z})$ we define the cell energy

$$\begin{aligned} W_{\rm cell}(\vec{y}) &= \frac{1}{8} \sum_{|z^j - z^i| = 1} \frac{K_1}{2}(|y(z^j) - y(z^i)| - 1)^2 \\ &+ \frac{1}{4} \sum_{|z^j - z^i| = \sqrt{2}} \frac{K_2}{2}(|y(z^j) - y(z^i)| - \sqrt{2})^2 + \chi(\vec{y}) \end{aligned}$$

and the surface energy

$$\begin{aligned} W_{\rm surf}(y_1, \ldots, y_4) &= \frac{1}{4} \sum_{\substack{1 \le i \le 4 \\ j = i+1 \mod 4}} \frac{K_1}{2}(|y_j - y_i| - 1)^2 \\ &+ \frac{1}{2} \sum_{\substack{1 \le i \le 2 \\ j = i+2}} \frac{K_2}{2}(|y_j - y_i| - \sqrt{2})^2. \end{aligned}$$

For cubes with lateral boundary faces, $W_{\rm surface}$ is defined appropriately.

Now assumption 4.4.1 on $W_{\rm cell}$ and $W_{\rm surf}$ and assumptions 4.2.1 (i) and (iv) on $W(\bar{x}, \cdot)$ are easily seen to be satisfied. Also $W(\bar{x}, \cdot) \ge 0$ being C^2 in a neighborhood of $\bar{SO}(3)$ and $W(\bar{x}, \bar{\rm Id}) = 0$ is clear. The remaining part can be first checked for $W_{\rm cell}$. The claim then follows from noting that $W_{\rm surface} \ge 0$ vanishes on rotations and translations. $\square$

Chapter 5

Minimal energy configurations of strained multi-layers

5.1 Bending energy for strained multi-layers

Assume that $\Omega_h = S \times (-h/2, h/2) \subset \mathbb{R}^3$, $S \subset \mathbb{R}^2$ a bounded Lipschitz domain, is the reference configuration of a thin film. If the material is homogeneous, the elastic energy of a deformation $v : \Omega_h \to \mathbb{R}^3$ is given by

$$\int_{\Omega_h} W(\nabla v(z))dz.$$

Here, $W : \mathbb{R}^{3\times 3} \to \mathbb{R}$ is the stored energy function which shall satisfy the following hypotheses:

(i) W is continuous, C^2 in a neighborhood of $SO(3)$.

(ii) W is frame indifferent: $W(F) = W(RF)$ for all $F \in \mathbb{R}^{3\times 3}$ and all $R \in SO(3)$.

(iii) $W(F) \geq C\text{dist}^2(F, SO(3))$ for all $F \in \mathbb{R}^{3\times 3}$, $W(F) = 0$ if $F \in SO(3)$.

For strained thin films we will consider potentials varying in x_3-direction:

$$\int_{\Omega_h} W(z_3, \nabla v(z))dz.$$

In detail, we are interested in the following two regimes:

$$W(x_3, F) := W_0\left(\frac{1}{a(x_3)}F\right) \tag{5.1}$$

for $a : (-\delta, \delta) \to \mathbb{R}$ differentiable at 0 and

$$W(x_3, F) := W^{(h)}(x_3, F) := W_0\left(\frac{1}{1 + hf(x_3/h)}F\right) \tag{5.2}$$

for $f \in L^\infty((-1/2, 1/2); \mathbb{R})$ where W_0 satisfies the above hypotheses (i)-(iii). Here, (5.1) serves as a model of a thermally strained film of a single material, whereas (5.2) describes films consisting of different layers, internally stressed due to mismatching energy wells. In order to avoid stretching energies in the reference configurations, we assume that $a(0) = 1$ resp. $f \in L^\infty((-1/2, 1/2); \mathbb{R})$ satisfies $\int_{-1/2}^{1/2} f(t)dt = 0$.

To treat both cases simultaneously, we will from on – slightly more generally – assume that W is of the form

$$W(x_3, F) := W^{(h)}(x_3, F) := W_0\left(\frac{1}{1 + hf^{(h)}(x_3/h)}F\right) \tag{5.3}$$

with $f^{(h)}(t) = f(t) + o(1)$ for $f(t) = a'(0)t$, a as in (5.1), resp. f as in (5.2). Changing variables $y(x', x_3) = v^{(h)}(x', hx_3)$, the 3-dimensional energy functional is

$$\begin{aligned} E^{(h)}(v^{(h)}) &= \int_{\Omega_h} W(x_3, \nabla v^{(h)}(x))dx \\ &= h\int_{\Omega_1} W(hx_3, \nabla' y(x), \frac{1}{h}y_{,3}(x))dx \ =: \ hI^{(h)}(y) \end{aligned} \tag{5.4}$$

for $y \in W^{1,2}(\Omega_1, \mathbb{R}^3)$.

The following compactness result is proven in [21] in case $W = W_0$.

Theorem 5.1.1 *(Compactness) Let the energy be of the form (5.4) with W as in (5.3). Suppose a sequence $y^{(h)} \subset W^{1,2}(\Omega; \mathbb{R}^3)$ has finite bending energy, i.e.,*

$$\limsup_{h\to\infty} \frac{1}{h^2}\int_{\Omega_1} W\left(hx_3, \nabla' y^{(h)}(x), \frac{1}{h}y^{(h)}_{,3}(x)\right)dx < \infty.$$

Then $\nabla_h y^{(h)} = (\nabla' y^{(h)}, \frac{1}{h}y_3^{(h)})$ is precompact in $L^2(\Omega)$ as $h \to 0$: there exists a subsequence (not relabeled) such that

$$\nabla_h y^{(h)} \to (\nabla' y, b) \in L^2(\Omega),$$

$(\nabla' y, b) \in SO(3)$ a.e. Furthermore, $(\nabla' y, b) \in H^1(\Omega)$ is independent of x_3.

Proof. This follows directly from the homogeneous case (cf. [21]) since

$$\limsup_{h\to\infty} \frac{1}{h^2}\int_{\Omega_1} \mathrm{dist}^2\left(\nabla_h y^{(h)}, SO(3)\right)dx < \infty :$$

By hypothesis (iii) on W_0, $\mathrm{dist}^2(F, SO(3))$ is bounded by

$$\begin{aligned} &2\mathrm{dist}^2\left(\frac{1}{1+hf^{(h)}(x_3)}F, SO(3)\right) + 2\left|F - \frac{1}{1+hf^{(h)}(x_3)}F\right|^2 \\ \le\ &\frac{2}{C}W(hx_3, F) + 2\left(\frac{1}{1+hf^{(h)}(x_3)} - 1\right)^2 |F|^2 \end{aligned}$$

for all $x_3 \in (-1/2, 1/2)$. Noting that $(\frac{1}{1+hf^{(h)}(x_3)} - 1)^2 = \mathcal{O}(h^2)$ and $|F| \le C(1 + \mathrm{dist}(F, SO(3)))$ implies $\mathrm{dist}^2(F, SO(3)) \le C'\left(W(hx_3, F) + h^2\right)$. $\square$

The main result of this section is the following derivation of limiting bending energies by Γ-convergence. As in the previous chapter, for a deformation $y \in$

$W^{2,2}(S,\mathbb{R}^3)$, we denote by II its second fundamental form: $\mathrm{II}_{ij} = y_{,i} \cdot b_{,j}$, $b = y_{,1} \wedge y_{,2}$. The set of $W^{2,2}$-isometric immersions is denoted

$$\mathcal{A} := \{y \in W^{2,2}(S;\mathbb{R}^3) : |y_{,1}| = |y_{,2}| = 1, y_{,1} \cdot y_{,2} = 0\}$$

(viewed as a set of functions in $W^{2,2}(\Omega_1;\mathbb{R}^3)$ independent of x_3 whenever convenient). To be consistent with the notation used in [21], in this chapter we denote by Q_3 the Hessian of W_0 at the identity and define the relaxed quadratic form on 2×2-matrices by

$$Q_2(F) = \min_{c \in \mathbb{R}^3} Q_3(\hat{F} + c \otimes e_3)$$

where $\hat{F}$ is the 3×3-matrix $\sum_{i,j=1}^{2} F_{ij} e_i \otimes e_j$.

Theorem 5.1.2 *(Γ-limit) The functionals $\frac{1}{h^2} I^{(h)}$ Γ-converge to I^0 in $W^{1,2}$ as $h \to 0$. The two-dimensional limiting energy functional is given by*

$$\begin{aligned} I^0(y) &= \begin{cases} \frac{1}{24}\int_S Q_2(\mathrm{II} - a_1 \mathrm{Id}) - a_2 \, dx & \text{for } y \in \mathcal{A}, \\ \infty & \text{else,} \end{cases} \qquad \text{where} \\ a_1 &= 12 \int_{-1/2}^{1/2} t f(t) dt \qquad \text{and} \\ a_2 &= \left(6 \left(\int_{-1/2}^{1/2} t f(t) dt \right)^2 - \frac{1}{2} \int_{-1/2}^{1/2} f^2(t) dt \right) Q_2(\mathrm{Id}). \end{aligned}$$

If W is as in (5.1), this reads

$$I^0(y) = \begin{cases} \frac{1}{24}\int_S Q_2(\mathrm{II} - a'(0)\mathrm{Id}) dx & \text{for } y \in \mathcal{A}, \\ \infty & \text{else.} \end{cases}$$

Proof. The proof closely follows the proof of theorem 6.1 in [21] (also see the proofs of the last chapter).

(i) *Lower bound.* For sequences $(y^{(h)})$ with bounded energy converging to y, it is shown in [21] that one can construct a piecewise constant approximation $R^{(h)} : S'_h \subset S \to \mathbb{R}^{3\times3}$ to $\nabla_h y^{(h)}$ such that (for a subsequence)

$$G^{(h)}(x', x_3) = \frac{R^{(h)}(x')^T \nabla_h y^{(h)}(x', x_3) - \mathrm{Id}}{h},$$

extended by zero outside $S'_h \times (-1/2, 1/2)$ converges weakly in L^2 to some G. If G' denotes the 2×2-matrix obtained by omitting the third row and third column, it is further shown that

$$G'(x', x_3) = G'(x', 0) + x_3 \mathrm{II}(x'), \quad \mathrm{II} = (\nabla' y)^T \nabla' b, \tag{5.5}$$

and

$$\chi_h G^{(h)} \rightharpoonup G \quad \text{in } L^2(\Omega),$$

where χ_h is the characteristic function of the set $S'_h \cap \{|G^{(h)}(x)| \leq h^{-1/2}\}$.

It remains to estimate the energy in terms of G. This is done in analogy to [21] by a careful Taylor expansion of W_0 around the identity: $W_0(\mathrm{Id}+A) = \frac{1}{2}Q_3(A) + \eta(A)$ with $\eta(A)/|A|^2 \to 0$ as $|A| \to 0$. Set $\omega(t) := \sup_{|A|\le t} |\eta(A)|$.

Frame indifference leads to

$$\begin{aligned}
\frac{1}{h^2}\int_\Omega W(hx_3, \nabla_h y^{(h)})dx &\geq \frac{1}{h^2}\int_\Omega \chi_h W_0\left(\frac{1}{1+hf^{(h)}(x_3)}(R^{(h)})^T\nabla_h y^{(h)}\right)dx \\
&= \frac{1}{h^2}\int_\Omega \chi_h W_0\left(\mathrm{Id} + hA^{(h)}\right)dx \\
&\geq \int_\Omega \frac{1}{2}\chi_h Q_3\left(A^{(h)}\right) - \frac{1}{h^2}\chi_h \omega\left(|hA^{(h)}|\right)dx,
\end{aligned}$$

where

$$A^{(h)} = \frac{\frac{1}{1+hf^{(h)}} - 1}{h}\mathrm{Id} + \frac{1}{1+hf^{(h)}}G^{(h)}, \quad \chi_h A^{(h)} \rightharpoonup -f(x_3)\mathrm{Id} + G \text{ in } L^2(\Omega).$$

Using lower semicontinuity of Q_3, $h\chi_h A^{(h)} \to 0$ in L^∞ and $Q_3(F) \geq Q_2(F')$, as in [21] we find that

$$\liminf_{h\to 0}\frac{1}{h^2}\int_\Omega W(hx_3, \nabla_h y^{(h)})dx \geq \frac{1}{2}\int_\Omega Q_2\left(G'(x',0) + x_3\mathrm{II}(x') - f(x_3)\mathrm{Id}'\right).$$

Because of $\int_{-1/2}^{1/2} x_3 dx_3 = \int_{-1/2}^{1/2} f(x_3)dx_3 = 0$, integrating over x_3 yields

$$\begin{aligned}
&\liminf_{h\to 0}\frac{1}{h^2}\int_\Omega W(hx_3, \nabla_h y^{(h)})dx \\
&\geq \frac{1}{24}\int_S Q_2(\mathrm{II}(x))dx - c_1\int_S Q_2(\mathrm{II}(x), \mathrm{Id})dx + \frac{c_2}{2}\int_S Q_2(\mathrm{Id})dx \\
&= \frac{1}{24}\int_S Q_2(\mathrm{II}(x) - 12c_1\mathrm{Id})dx - \left(6c_1^2 - \frac{1}{2}c_2\right)Q_2(\mathrm{Id})dx,
\end{aligned}$$

where $c_1 = \int_{-1/2}^{1/2} x_3 f(x_3)dx_3$, $c_2 = \int_{-1/2}^{1/2} f^2(x_3)dx_3$.

(ii) *Attainment of the lower bound.* Let $y \in \mathcal{A}$. As in [21] (and chapter 4), we choose approximations y^λ and b^λ to y and $b = y_{,1} \wedge y_{,2}$ (extended to maps in $W^{2,2}(\mathbb{R}^2, \mathbb{R}^3)$ resp. $W^{1,2}(\mathbb{R}^2, \mathbb{R}^3)$) such that

$$\|\nabla^2 y^\lambda\|_{L^\infty}, \|\nabla b^\lambda\|_{L^\infty} \leq \lambda, \quad |S^\lambda| \leq \frac{\omega(\lambda)}{\lambda^2},$$

where

$$S^\lambda = \{x \in \mathbb{R}^2 : y(x) \neq y^\lambda(x) \text{ or } b(x) \neq b^\lambda(x)\}, \quad \omega(\lambda) \to 0 \text{ as } \lambda \to \infty.$$

Let $\lambda_h = c/h$. More generally than in [21] we define test functions

$$y^{(h)}(x', x_3) = y^{\lambda_h}(x') + hx_3 b^{\lambda_h}(x') + h^2 D(x', x_3)$$

for $D(x',x_3) = \int_0^{x_3} d(x',t)dt$, $d \in C^1(\overline{\Omega}_1;\mathbb{R}^3)$. (If W is as in (5.1), we can use trial functions with $D(x',x_3) = \frac{1}{2}x_3^2 D(x')$ as in [21].) Furthermore, denote $R(x') := (\nabla' y(x'), b(x'))$ and

$$\begin{aligned} R^T\left(\nabla' y^{(h)}, \frac{1}{h}y^{(h)}_{,3}\right) &= R^T\Big((\nabla' y^{\lambda_h}, b^{\lambda_h}) + h(x_3\nabla' b^{\lambda_h}, d) + h^2(\nabla' D, 0)\Big) \\ &=: \mathrm{Id} + B^{(h)}. \end{aligned}$$

Similar as above let

$$A^{(h)} = \left(\frac{1}{1+hf^{(h)}(x_3)} - 1\right)\mathrm{Id} + \frac{1}{1+hf^{(h)}(x_3)}B^{(h)}.$$

On the good set $S \setminus S^{\lambda_h}$ we have $R^T(\nabla' y^{\lambda_h}, b^{\lambda_h}) = \mathrm{Id}$ and

$$|B^{(h)}| \le C(h\lambda_h + h + h^2) \le C(c + h_0 + h_0^2) \quad \text{for all } h \le h_0.$$

An analogous estimate holds for $|A^{(h)}|$. Choosing c small enough and using that $W_0(\mathrm{Id}+A) \le C\mathrm{dist}^2(\mathrm{Id}+A, SO(3))$ in a neighborhood of $SO(3)$ (and letting χ_h denote the characteristic function of $S \setminus S^{\lambda_h}$), we obtain for all $h \le h_0$

$$\begin{aligned} \frac{1}{h^2}\chi_h W_0(\mathrm{Id}+A^{(h)}) &\le \frac{C}{h^2}\chi_h|A^{(h)}|^2 \\ &\le \frac{2C}{h^2}\chi_h\left(3\left(\frac{1}{1+hf^{(h)}(x_3)} - 1\right)^2 + \left|\frac{1}{1+hf^{(h)}(x_3)}B^{(h)}\right|^2\right) \\ &\le C\left(\left(\frac{\frac{1}{1+hf^{(h)}(x_3)} - 1}{h}\right)^2 + \frac{|(\nabla' b, d)|^2 + h^2|\nabla' D|^2}{|1+hf^{(h)}(x_3)|^2}\right) \\ &\le C(1 + |(\nabla' b, d)|^2 + h_0^2|\nabla' D|^2) \in L^1(\Omega). \end{aligned}$$

Furthermore,

$$\frac{1}{h^2}\chi_h W_0(\mathrm{Id}+A^{(h)}) \to \frac{1}{2}Q_3(-f(x_3) + R^T(x_3\nabla' b, d))dx$$

in measure. So by dominated convergence

$$\begin{aligned} \frac{1}{h^2}\int_\Omega \chi_h W\left(x_3, \nabla' y^{(h)}, \frac{1}{h}y^{(h)}_{,3}\right)dx &= \frac{1}{h^2}\int_\Omega \chi_h W_0(\mathrm{Id}+A^{(h)})dx \\ &\to \frac{1}{2}\int_\Omega Q_3(-f(x_3) + R^T(x_3\nabla' b, d))dx. \end{aligned}$$

On the bad set S^{λ_h}, as shown in [21], $\mathrm{dist}(\mathrm{Id}+B^{(h)}, SO(3)) \le C$ for arbitrarily small $C > 0$, thus also $\mathrm{dist}(\mathrm{Id}+A^{(h)}, SO(3)) \le C$. So

$$\frac{1}{h^2}\int_\Omega (1-\chi_h)W\left(x_3, \nabla' y^{(h)}, \frac{1}{h}y^{(h)}_{,3}\right)dx \le C\frac{|S^{\lambda_h}|}{h^2} \;\to\; 0 \quad (h \to 0).$$

Together with our previous estimate we find

$$\frac{1}{h^2}\int_\Omega W\left(x_3, \nabla' y^{(h)}, \frac{1}{h}y^{(h)}_{,3}\right)dx \to \frac{1}{2}\int_\Omega Q_3(-f(x_3) + R^T(x_3\nabla' b, d))dx.$$

To finish the proof as in [21], it suffices to note that

$$d_{\min}(x', x_3) := \text{argmin } Q_3(-f(x_3) + R^T(x_3\nabla' b, d)) \in L^2$$

and

$$Q_3(-f(x_3) + R^T(x_3\nabla' b, d_{\min})) = Q_2(-f(x_3) + x_3\mathrm{II}) :$$

(ii) then follows by a standard approximation procedure. □

Remarks:

(i) Appropriate body forces and boundary conditions can be included in the above analysis. By standard arguments in Γ-convergence, the above results imply (subsequential) convergence of (almost) minimizers.

(ii) Due to the assumptions made on W_0, Q_3 is positive semidefinite and positive definite when restricted to symmetric matrices. It is not hard to see that this implies that Q_2 is positive definite on symmetric 2×2-matrices.

(iii) Consider deformations of Euler-Bernoulli type. Suppose $S = (0, L) \times (0, w)$ and we are only considering deformations y in the $x_1 - x_3$ plane, i.e., $y(x_1, x_2) = (f_1(x_1), x_2, f_2(x_1))$. The class of isometric deformations can then be described by the curve $\gamma \in W^{2,2}((0, L); \mathbb{R}^2)$, $\gamma(t) = (f_1(t), f_2(t))$, where $|\frac{d\gamma}{dt}| \equiv 1$. The second fundamental form is given by $\mathrm{II}_{ij} = -\kappa$ for $i = j = 1$ and $\mathrm{II}_{ij} = 0$ else. Here, κ is the curvature of the curve γ. This leads to a limiting energy

$$E(\gamma) = \alpha_1 \int_0^L (\kappa(t) - \alpha_2)^2 + \alpha_3 \; dt \tag{5.6}$$

for constants $\alpha_1 > 0, \alpha_2, \alpha_3 \in \mathbb{R}$.

5.2 Minimal energy configurations in 3D

As seen in the previous section, thin strained multi-layers deformed by $y : S \subset \mathbb{R}^2 \to \mathbb{R}^3$ have bending energy

$$E(y) = \begin{cases} \int_S Q(\mathrm{II} - c_0\mathrm{Id}) + c_0' \; dx & \text{for } y \in \mathcal{A}, \\ \infty & \text{else} \end{cases} \tag{5.7}$$

for some Q, positive definite on symmetric 2×2-matrices, $c_0, c_0' \in \mathbb{R}$. In the following we will address the question what one can say about the set of energy minimizers of (5.7)

$$\mathcal{M} = \{u \in W^{2,2}(S; \mathbb{R}^3) : E(u) = \min_{y \in W^{2,2}(S;\mathbb{R}^3)} E(y)\}.$$

Note that energy minimizers in general will be non-unique. For isotropic material, e.g., every winding direction will be equally well suited to reduce energy.

We will, slightly more general, only assume that Q is any positive semidefinite quadratic form on symmetric 2×2-matrices. We start with the following observation.

Lemma 5.2.1 *Let* $\mathcal{N} := \operatorname{argmin}\{Q(F - c_0\mathrm{Id}) : F$ *singular and symmetric*$\}$. *Then* $u \in \mathcal{M}$ *if and only if* $\mathrm{II} \in \mathcal{N}$ *a.e. In particular,* $\mathcal{M}$ *contains cylinders.*

Proof. Any u of finite energy is an $W^{2,2}$-isometry, so $\det(\mathrm{II}) = 0$ (see [34]). Since the set of symmetric singular 2×2-matrices is $\mathbb{R} \cdot \{n \otimes n : n \in \mathbb{R}^2, |n| = 1\}$, which is just the set of (constant) fundamental forms of cylinders, we can – and therefore have to – minimize E in (5.7) by minimizing the integrand pointwise subject to II being singular and symmetric. Choosing u to be a cylinder with $\mathrm{II} \equiv F_0 \in \mathcal{N}$ constant, u lies in $\mathcal{M}$. □

In the following we will identify a symmetric matrix $F = (F_{ij})$ with the vector $(F_{11}, F_{22}, F_{12})^T \in \mathbb{R}^3$. Accordingly, Q will be viewed as a positive semidefinite quadratic form on $\mathbb{R}^3$ with $\operatorname{rank}(Q)$ denoting the rank of the corresponding symmetric 3×3-matrix. The cone of singular symmetric matrices is denoted $\mathcal{C} := \{m \in \mathbb{R}^3 : m_1 m_2 - m_3^2 = 0\}$, and we set $c = (c_0, c_0, 0)^T$ for c_0 is as in (5.7). (Note that c lies on the symmetry axis of $\mathcal{C}$.)

As noted, $u \in \mathcal{M}$ iff $\mathrm{II} \in \mathcal{N}$ a.e. It is therefore interesting to examine $\mathcal{N}$ in more detail. Depending on the rank of Q, $\mathcal{N}$ is the intersection of $\mathcal{C}$ with an ellipsoid centered at c and touching $\mathcal{C}$ from inside, with a straight line through c, or with a plane containing c.

Suppose $c_0 \neq 0$. Then it is elementary to see that if $\operatorname{rank}(Q) = 2$, $\mathcal{N}$ consists of at most two points, in case $\operatorname{rank}(Q) = 1$ and $Q(\mathrm{Id}) \neq 0$, $\mathcal{N}$ is a non-degenerate conic, and for $\operatorname{rank}(Q) = 1$ and $Q(\mathrm{Id}) = 0$, $\mathcal{N} = \mathbb{R}N^{(1)} \cup \mathbb{R}N^{(2)}$, where $N^{(1)}_{ij} \geq 0$ and $N^{(2)}_{11} = N^{(1)}_{22}$, $N^{(2)}_{22} = N^{(1)}_{11}$, $N^{(2)}_{12} = -N^{(1)}_{12}$. Except for this last case, any two elements of $\mathcal{N}$ are linearly independent.

If $c_0 = 0$, we either have $\mathcal{N} = \{0\}$, or $\operatorname{rank}(Q) \leq 2$ and $\mathcal{N} = \mathbb{R}N$, or $\operatorname{rank}(Q) = 1$ and $\mathcal{N} = \mathbb{R}N^{(1)} \cup \mathbb{R}N^{(2)}$ for some $N, N^{(1)}, N^{(2)} \in \mathcal{C}$, $N^{(1)}, N^{(2)}$ linearly independent.

Claim. If $\operatorname{rank}(Q) = 3$, then $\#\mathcal{N} = 1$, $\#\mathcal{N} = 2$, or $\mathcal{N}$ is a circle. In every case, if $F^{(1)}, F^{(2)} \in \mathcal{N}$, then $\operatorname{trace}(F^{(1)}) = \operatorname{trace}(F^{(2)})$.

Proof. The proof is completely elementary; we indicate the main steps. If $\min\{Q(m - c) : m \in \mathcal{C}\} = q_0$, then $\mathcal{N} = \mathcal{C} \cap \mathcal{E}$ for $\mathcal{E} = \{Q(m - c) = q_0\}$, an ellipsoid touching $\mathcal{C}$ from inside. If $\#\mathcal{N} \geq 2$, choose $a, b \in \mathcal{N}$, $a \neq b$, and consider a plane $\mathcal{P}$ through a, b, c. On $\mathcal{P}$ choose a coordinate system (x_1, x_2) with origin at c such that the x_2-axis is an axis of symmetry of the conic $\mathcal{C} \cap \mathcal{P}$. In these coordinates let $a = (a_1, a_2)$ and $b = (b_1, b_2)$. Since the ellipsoid $\mathcal{E}$ touches $\mathcal{C}$ from inside, a_2 and b_2 have the same sign, say $a_2, b_2 < 0$. Now suppose $a_2 \neq b_2$, and note that also $\mathcal{E} \cap \mathcal{P}$ touches $\mathcal{C} \cap \mathcal{P}$ from inside. Reflection about the x_2-axis shows that a_1 and b_1 (can be chosen to) have the same sign, say $a_1, b_1 < 0$.

We now rescale the x_2-axis such that in case $\mathcal{C} \cap \mathcal{P}$ is compact, we obtain an ellipse touching a circle from inside, and in case $\mathcal{C} \cap \mathcal{P}$ is not compact, we obtain a sufficiently flat ellipse touching a hyperbola or parabola from inside at a and b. The normals to the outer conic at a and b intersect at the circle center resp. at some (d_1, d_2) with $d_1 > 0$ and d_2 sufficiently large. In each case this leads to a contradiction when viewed as normals to the inner ellipse. The claim now easily follows. □

Also note that in case $\mathcal{N}$ is a circle, Q is of the form

$$Q(m_1, m_2, m_3) = \alpha\left(\frac{m_1+m_2}{2}\right)^2 + \beta\left(\frac{m_1-m_2}{2}\right)^2 + \beta m_3^2$$

for some $\alpha > 0, \beta \geq 0$, hence Q is isotropic:

$$Q(\mathrm{II}) = \frac{\beta}{2}|\mathrm{II}|^2 + \frac{\alpha-\beta}{4}(\mathrm{trace}(\mathrm{II}))^2 = \frac{\alpha+\beta}{4}|\mathrm{II}|^2,$$

where the last equality followed from $\det(\mathrm{II}) = 0$. Furthermore, if Q describes a material with cubic symmetry, then $Q(R^TMR) = Q(M)$ for all symmetric M and $R = e_2 \otimes e_1 - e_1 \otimes e_2 \in \mathbb{R}^{2\times 2}$. Straightforward calculations for $Q(m_1, m_2, m_3) = \sum_{1\leq i,j\leq 3} q_{ij}m_im_j$ with $q_{ij} = q_{ji}$ lead to

$$(q_{ij})_{ij} = \begin{pmatrix} q_{11} & q_{12} & q_{13} \\ q_{12} & q_{11} & -q_{13} \\ q_{13} & -q_{13} & q_{33} \end{pmatrix}.$$

Then $\mathbb{R}c$ is a principal axis for every ellipsoid $\{Q(m_1, m_2, m_3) = \mathrm{const.}\}$. So if Q is not isotropic, i.e., $q_{13} \neq 0$ or $q_{11} - q_{12} - q_{33}/2 \neq 0$, $\mathcal{N} = \{n^{(1)} \otimes n^{(1)}, n^{(2)} \otimes n^{(2)}\}$ with $|n^{(1)}| = |n^{(2)}|$ and $n^{(1)} \perp n^{(2)}$ as expected.

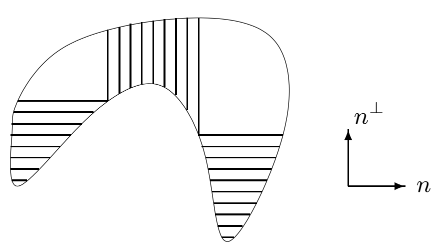
The following theorem gives a complete description of the minimizers of E.

Theorem 5.2.2 *Suppose $u \in \mathcal{M}$ and $c_0 \neq 0$. If* $\mathrm{rank}(Q) = 2$ *or* 3*, or if* $\mathrm{rank}(Q) = 1$ *and* $Q(\mathrm{Id}) \neq 0$*, then u is a cylinder. If* $\mathrm{rank}(Q) = 1$ *and* $Q(\mathrm{Id}) = 0$*, then there exists a unique normal vector $n \in \mathbb{R}^2$ with $n_1 > 0, n_2 \geq 0$ such that u is locally of Euler-Bernoulli type w.r.t. n or $n^\perp = (-n_2, n_1)^T$.*

Here, we say that a deformation $y : S \to \mathbb{R}^3$ is of *Euler-Bernoulli type* (w.r.t. $n \in \mathbb{R}^2$) if there is a plane $\mathcal{P} \in \mathbb{R}^3$ with normal ν and a function $f : \mathbb{R} \supset I \to \mathcal{P}$ such that

$$u(x) = f(x \cdot n) + (x \cdot n^\perp)\nu.$$

In the last case we obtain a decomposition of S (as in the following picture) into stripes parallel to $n^\perp$ resp. n on which u is of Euler-Bernoulli type w.r.t. n resp. $n^\perp$ and a rest where $\mathrm{II} = 0$, i.e., u is rigid. These stripes can meet only at the boundary ∂S.



The proof of this theorem will also show that in case $c_0 = 0$, depending on the structure of $\mathcal{N}$ (cf. page 121), minimizers will be (flat) cylinders or of Euler-Bernoulli type or locally of Euler-Bernoulli type.

Lemma 5.2.3 *Let $n \in \mathbb{R}^2$. Suppose $y \in \mathcal{A}$ with $\mathrm{II}(x) = \mu(x) n \otimes n$. Then y is locally of Euler-Bernoulli type w.r.t. n.*

Proof. Elementary calculations using $\nabla y \in O(2,3)$ a.e. show that $\nabla_{n^\perp} u(x) =: \nu$ is constant. Applying $\nabla y \in O(2,3)$ again, the claim follows. □

Proof of theorem 5.2.2. In [34] it is shown that (locally on convex subdomains) $u \in \mathcal{A}$ implies that u is a developable ruled surface. Moreover, there exists $f_u \in W^{1,2}(S, \mathbb{R}^2)$ such that $\nabla f_u = \mathrm{II}$, and the connected components of the pre-images of f_u are the segments (or neighborhoods of points) on which u is affine. We may choose coordinates (s,t) such that

$$u(\gamma(t) + s\nu(t)) = \tilde{\gamma}(t) + s v(t),$$

where, in the regions where f_u is not constant, $\gamma \in W^{2,\infty}$ (parameterized by arclength) is orthogonal to the inverse images of f_u, and $\nu = (\gamma')^\perp$. (γ is a 'leading curve' in the terminology of [34], and the coordinate change $(t,s) \mapsto \gamma(t) + s\nu(t)$ is locally bi-Lipschitz.) By κ we denote the curvature of γ, i.e., $\gamma'' = \kappa\nu$.

As in [34], note that $\Gamma(t) = f_u(\gamma(t) + s\nu(t))$ is independent of s. Since both rows of ∇f_u are parallel to γ' and $d\Gamma/dt = \nabla f_u(\gamma(t) + s\nu(t))(\gamma'(t) + s\nu'(t)) = \nabla f_u(\gamma(t) + s\nu(t))(1 - s\kappa)\gamma'(t)$, we can write

$$\nabla f_u(\gamma(t) + s\nu(t)) = \mu(s,t)(\nu(t))^\perp \otimes (\nu(t))^\perp = \frac{\mu(t)}{1 - s\kappa}(\nu(t))^\perp \otimes (\nu(t))^\perp.$$

In case $\mathrm{rank}(Q) = 1$ and $Q(\mathrm{Id}) = 0$, since ν is continuous, it follows from $\mathrm{II} \in \mathcal{N}$ that ν is locally constant, and hence u is locally of Euler-Bernoulli type by lemma 5.2.3. In the remaining cases, the elements of $\mathcal{N}$ are pairwise linearly independent, whence in fact $\kappa = 0$ a.e. But then $\nu' = 0$, i.e., $\nu(t) \equiv \nu(t_0)$ and $\mathrm{II} = \mu(t_0)(\nu(t_0))^\perp \otimes (\nu(t_0))^\perp$. Now II being constant on every convex subdomain, it must be constant on S. □

In case II is smooth we give an alternative proof of the above result not using developability. Note that this is in fact sufficient for the case $\mathrm{rank}(Q) = 3$ which is interesting in elasticity theory: by the reasoning above there is a constant r_0 such that for all $\mathrm{II} \in \mathcal{N}$, $\mathrm{II}_{11} + \mathrm{II}_{22} = r_0$. Also in [34] (cf. lemma 2.6) it is proven that the Codazzi-Mainardi-equations $\mathrm{II}_{11,2} = \mathrm{II}_{12,1}$ and $\mathrm{II}_{12,2} = \mathrm{II}_{22,1}$ hold in distributions. But then locally there exists $f \in W^{1,2}$ such that $\nabla f = \mathrm{II}$. It follows

$$0 = \mathrm{div}\ \mathrm{cof}\ \nabla f = \mathrm{div} \begin{pmatrix} \mathrm{II}_{22} & -\mathrm{II}_{21} \\ -\mathrm{II}_{12} & \mathrm{II}_{11} \end{pmatrix} = \mathrm{div} \begin{pmatrix} -\mathrm{II}_{11} & -\mathrm{II}_{12} \\ -\mathrm{II}_{21} & -\mathrm{II}_{22} \end{pmatrix},$$

i.e., $\Delta f = \mathrm{div}\ \nabla f = 0$. But then f and hence II is smooth and we can proceed as follows.

Write $\mathrm{II}(x) = \pm n(x) \otimes n(x)$, $n \in \mathbb{R}^2$. Up to a discrete exceptional set we can solve the relation $\mathrm{II} \in \mathcal{N}$ locally in matrix space, w.l.o.g. for n_2: $n_2 = f(n_1)$, f analytic. Inserting this into the Codazzi-Mainardi-equations $(n_1^2)_{,2} = (n_1 n_2)_{,1}$ and $(n_2^2)_{,1} = (n_1 n_2)_{,2}$ leads to

$$\begin{aligned} 2n_1 n_{1,2} &= (f(n_1) + n_1 f'(n_1)) n_{1,1}, \\ 2f(n_1) f'(n_1) n_{1,1} &= (f(n_1) + n_1 f'(n_1)) n_{1,2}, \end{aligned}$$

a linear system for ∇n_1 which has non-trivial solutions if and only if

$$0 = \det \begin{pmatrix} (f(n_1) + n_1 f'(n_1)) & -2n_1 \\ -2f(n_1)f'(n_1) & (f(n_1) + n_1 f'(n_1)) \end{pmatrix} = (f(n_1) - n_1 f'(n_1))^2.$$

Now if $\nabla n_1 \neq 0$ on some open set (and hence the image of n_1 not discrete), we have

$$f(t) - tf'(t) = 0 \quad \Rightarrow \quad f(t) = Ct.$$

Hence $n(x) = \mu(x)\,(1, C)^T =: \mu(x) n_0$. As before this implies that u is locally of Euler-Bernoulli type resp. a cylinder due to the structure of $\mathcal{N}$. $\square$

5.3 Minimal energy configurations in 2D

In this section we consider thin strained multi-layers of Euler Bernoulli type. As noted at the end of section 5.1, these objects are described by a planar curve γ tracing the position of the middle fiber of a two-dimensional film section. In this setting the determination of energy minimizers of the two-dimensional energy functional (5.7), (5.6) becomes trivial. However, considering films of finite thickness $h > 0$, in the regime $L \sim 1/h$, a non-interpenetration condition will lead to non-trivial geometric behavior globally.

Consider a curve $\gamma \subset \mathbb{R}^2$ of length $|\gamma| = L$. Let t be arclength, $\gamma : [0, L] \to \mathbb{R}^2$, $e_1 = d\gamma/dt$, $e_2 = e_1^{\perp}$. The film of thickness h associated to γ is

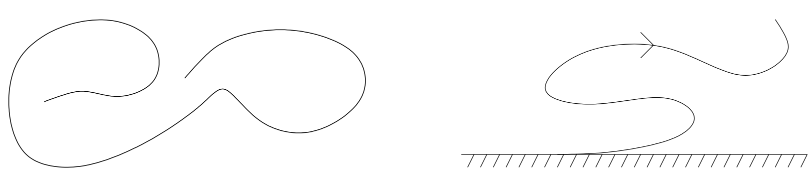
$$\{\gamma(t) + se_2(t) : 0 \leq t \leq L, -h/2 < s < h/2\}.$$

Note that – to first order in h – this is a reasonable model for a film of thickness $0 < h \ll 1$ motivated by the shape of our test functions in the proof of theorem 5.1.2. We will impose the following non-interpenetration condition (on the precise representative of γ):

$$\gamma(t_1) + s_1 e_2(t_1) = \gamma(t_2) + s_2 e_2(t_2) \Longrightarrow t_1 = t_2 \text{ and } s_1 = s_2. \tag{5.8}$$

Seeking for energy minimizers among such curves, we will speak of curves with two free ends.

It will be interesting to also consider curves γ in the upper half plane, where one end is attached to the x_1-axis (curves with one free end).



More precisely, in the second case we demand that $\gamma : [0, L] \to \mathbb{R} \times [-h/2, \infty)$, $\gamma(0) = (0, -h/2)$ and $((-\infty, 0] \times \{-h/2\}) \cup \gamma$ satisfy the non-intersection condition (5.8).

According to (5.6), we define the energy of γ by

$$E(\gamma) = \int_0^L (\kappa(t) - \kappa_0)^2,$$

where $\kappa(t)$ denotes the curvature of γ at t, and $\kappa_0 \geq 0$ is a fixed constant. By definition, κ satisfies

$$\frac{d^2\gamma}{dt^2} = \frac{de_1}{dt} = \kappa(t)e_2.$$

The corresponding admissible classes of curves are

$$\mathcal{A}_1 := \{\gamma \in W^{2,2}(0,L;\mathbb{R}^2) : |\gamma'| \equiv 1 \text{ and (5.8) holds}\},$$

respectively

$$\mathcal{A}_2 := \{\gamma \in W^{2,2}(0,L;\mathbb{R}^2) : |\gamma'| \equiv 1, \gamma(0) = (0,-h/2) \text{ and } \\ \text{(5.8) holds for } ((-\infty,0] \times \{-h/2\}) \cup \gamma\}.$$

Since the non-intersection condition (5.8) implies $|\kappa(t)| \leq 2/h$, in fact for fixed L and h the elements of $\mathcal{A}_i$, $i = 1,2$, are uniformly bounded in $W^{2,\infty}$.

Using the direct method of the calculus of variations, it is easy to show existence of minimizers.

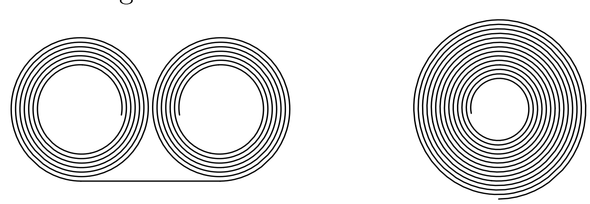
Proposition 5.3.1 *(Existence of minimizers) There exist $u_i \in \mathcal{A}_i$, $i = 1,2$, such that $E(u_i) = \min_{u \in \mathcal{A}_i} E(u)$.*

Proof. For a minimizing sequence $\gamma^{(n)}$ we may assume that $\gamma^{(n)}(0) = (0,-h/2)$, $e_1^{(n)}(0) = (1,0)$ for all n, and $\gamma^{(n)} \overset{*}{\rightharpoonup} \gamma$ in $W^{2,\infty}$. Then $\gamma^{(n)} \to \gamma$ in $W^{1,\infty}$, and by lower semicontinuity $E(\gamma) = \inf_{u \in \mathcal{A}_i} E(u)$. It only remains to check that γ (resp. $((-\infty,0] \times \{-h/2\}) \cup \gamma$) satisfies our non-intersection condition. Suppose not, i.e., $\gamma(t_1) + s_1 e_2(t_1) = p = \gamma(t_2) + s_2 e_2(t_2)$ for some $t_1, t_2 \in (0,L)$, $s_1, s_2 \in (-h/2, h/2)$ with $(t_1, s_1) \neq (t_2, s_2)$. Choosing n large enough, we find neighborhoods U_i of t_i and V_i of s_i with $U_1 \cap U_2 = \emptyset$ or $V_1 \cap V_2 = \emptyset$ such that

$$p \in \{\gamma^{(n)}(t) + s e_2^{(n)}(t) : t \in U_i, s \in V_i\}, \quad i = 1,2,$$

which contradicts our non-intersection assumption on $\gamma^{(n)}$. □

As energy minimizers for the curve with only one free end we expect a spiral deformation. A moments thought shows that, in case the curve has two free ends, we can do better by joining two spirals by a straight line, the energy of which is negligible for large L.



In the following we will determine the minimal mean energy $\frac{1}{L}E(\gamma)$ up to $\mathcal{O}(h)$ in the limit $L \to \infty$, $h \to 0$. The result turns out to depend only on $a := Lh$. The proof will also show that minimizing configurations (to leading order) are in fact of the shape described above.

Upper Bounds

To obtain upper bounds for the energy minimizers, we consider a specific example. Let (in polar coordinates)

$$\gamma(t) = (r(t) = r_0 + h\varphi(t)/2\pi, \varphi(t)),$$

where $\varphi(0) = 0$ and $\varphi' = 1/\sqrt{(h/2\pi)^2 + r^2} > 0$, so t is arclength. Up to an error of order $\mathcal{O}(1)$, $E(\gamma)$ is the sum of the energies of nested circles with distances h, the smallest of radius r_0, the largest of radius R_0, where $\pi R_0^2 - \pi r_0^2 = Lh = a$. Up to $\mathcal{O}(1)$ this energy is

$$\frac{1}{h}\int_{r_0}^{R_0} 2\pi r \left(\frac{1}{r} - \kappa_0\right)^2 dr.$$

Now minimizing this energy expression with respect to $\pi R_0^2 - \pi r_0^2 = a$ for fixed a yields r_0 and R_0 uniquely given in terms of a and κ_0 by

$$\pi R_0^2 - \pi r_0^2 = a \quad \text{and} \quad 1/r_0 - \kappa_0 = \kappa_0 - 1/R_0. \tag{5.9}$$

Setting

$$E_2(a) = \frac{2\pi}{a}\Big[\log(r) - 2\kappa_0 r + \kappa_0^2 r^2/2\Big]_{r_0}^{R_0} \tag{5.10}$$

for r_0, R_0 as in (5.9), we see that the energy of γ satisfies

$$\frac{1}{L}E(\gamma) = E_2(a) + \mathcal{O}(h). \tag{5.11}$$

In case the film has two free ends, we get an upper bound on the minimal energy by considering a bi-spiral γ whose energy $E(\gamma)$ is, up to $\mathcal{O}(1)$, the energy of two (equal) single spirals:

$$\frac{1}{L}E(\gamma) = E_1(a) + \mathcal{O}(h), \quad E_1(a) = E_2(a/2). \tag{5.12}$$

In theorem 5.3.4 we will see that indeed

$$\min_{\gamma\in\mathcal{A}_i} \frac{1}{L}E(\gamma) = E_i(a) + \mathcal{O}(h), \quad i = 1, 2, \quad a = Lh.$$

Spirals as minimizers

Consider the case of curves in $\mathcal{A}_2$ (with one end fixed) first.

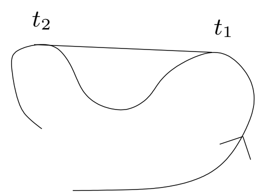
Proposition 5.3.2 *Let $\gamma \in \mathcal{A}_2$. If $\kappa < 0$ on a set of positive measure, then there exists another curve in $\mathcal{A}_2$ having less energy than γ.*

The idea of the proof is to show that the contact set of γ with its convex envelope connected.

Proof. Let $\mathrm{co}(\gamma)$ be the convex hull of γ. Clearly $\gamma(0) \in \partial\mathrm{co}(\gamma)$. Let t_1 be the last time such that $\gamma(t) \in \partial\mathrm{co}(\gamma|_{[t,L]})$ for all $t \leq t_1$. There exists $t_2 > t_1$ such that $\gamma(t_2) \in \partial\mathrm{co}(\gamma|_{[t_1,L]})$ and $\gamma \cap (\gamma(t_1), \gamma(t_2)) = \emptyset$. We obtain three cases:

$$e_1(t_2) = e_1(t_1) \quad \text{or} \quad e_1(t_2) = -e_1(t_1) \quad \text{or} \quad e_1(t_2) \neq \pm e_1(t_1).$$

Case 1: Replace $\gamma|_{[t_1,t_2]}$ by a straight line connecting $\gamma(t_1)$ and $\gamma(t_2)$.



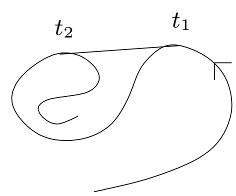
Since by strict convexity of the energy functional

$$E(\gamma|_{[t_1,t_2]}) > \kappa_0^2(t_2 - t_1),$$

this yields an amount of energy larger than $\kappa_0^2(t_2 - t_1 - |[\gamma(t_1), \gamma(t_2)]|)$, while it makes the film $t_2 - t_1 - |[\gamma(t_1), \gamma(t_2)]|$ units shorter. Note that this procedure does not enlarge the convex hull of $\gamma|_{[t_1,L]}$, so the new configuration is admissible. Now add the segment $[(-t_2 + t_1 + |[\gamma(t_1), \gamma(t_2)]|, -h/2), (0, -h/2)]$ to this new configuration and shift to the right.

Case 3: If $e_1(t_2) \neq \pm e_1(t_1)$, then $t_2 = L$, and we replace γ by $\gamma|_{[0,t_1]} \cup [(-t_2 + t_1, -h/2), (0, -h/2)]$ and shift to the right. As in case 1, one sees that this lowers energy noting that $\int_{t_1}^{t_2} \kappa(t)dt < 0$.

Case 2:



γ on $[t_1, t_2]$, together with the line segment $[\gamma(t_2), \gamma(t_1)]$, forms a closed curve such that $\gamma(t)$ lies in its interior Ω for $t > t_2$ and in its exterior $\overline{\Omega}^c$ for $t < t_1$.

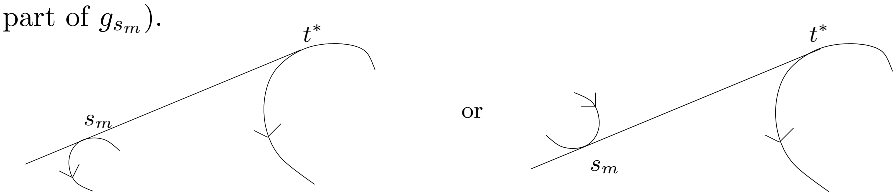
For $s \geq t_2$ we define g_s to be the shortest curve in $\overline{\Omega}$ that connects $\gamma(t_1)$ to $\gamma(s)$. (Note that g_s is unique since Ω is simply connected. Furthermore, $g_s \setminus \gamma$ consists of intervals where g_s is a straight line, and – as does γ – g_s lies in $W^{2,\infty}$.) By $I \subset [t_2, L]$ we denote the set of those s for which $g_s \cap \gamma|_{[t_2,L]} = \{\gamma(s)\}$. Let $t^{(s)}$ be arclength of g_s, $e_1^{(s)} = dg_s/dt^{(s)}$ and $\kappa^{(s)}$ the curvature of g_s.

Claim. Suppose $s \in I$. If $\gamma(t) = g_s(t^{(s)}) \in \gamma|_{[t_1,t_2)} \cap g_s$, then $e_1(t) = e_1^{(s)}(t^{(s)})$. Furthermore, $\kappa^{(s)} \geq 0$ a.e.

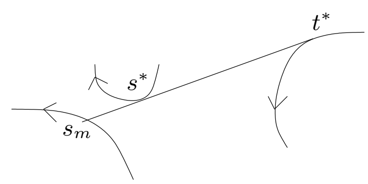
Proof of the claim. Clearly, for small $t^{(s)} > 0$ with $g_s(t^{(s)}) \in \gamma([t_1, t_2))$, $(e_1^{(s)})^\perp$ points outside Ω. Assuming one of the statements of the claim is not satisfied, there are points $g_s(t^{(s)})$ on $\gamma|_{[t_1,t_2)}$ such that $(e_1^{(s)}(t^{(s)}))^\perp$ points inside Ω. Choose $t_2^{(s)}$ minimal with this property, and suppose $t_1^{(s)} < t_2^{(s)}$ is maximal with $g_s(t_1^{(s)}) \in \gamma|_{[t_1,t_2)}$, $(e_1^{(s)}(t_1^{(s)}))^\perp$ pointing outside Ω (recall (5.8)). But then the union of $g_s([t_1^{(s)}, t_2^{(s)}])$ and $\gamma([\gamma^{-1}(g_s(t_1^{(s)})), \gamma^{-1}(g_s(t_2^{(s)}))])$ is the graph of a closed curve with $\gamma(s)$ lying in its interior and $\gamma(t_2)$ in the exterior. This contradicts the fact that this curve does not intersect $\gamma|_{[t_2,L]}$ due to $s \in I$. $\square$

Define $s_m := \sup I \ (> t_2)$, $t^* := \min\{t \in [t_1, t_2) : [\gamma(t), \gamma(s_m)] \subset g_{s_m}\}$. Our aim is as in case 1 to connect some $\gamma(t)$, $t \in [t_1, t_2)$, to some $\gamma(s)$, $s \in [t_2, L]$, by a straight line.

Suppose first $s_m < L$. If $s_m \in I$, set $s^* = s_m$. Then $e_1(s^*) = e_1(t^*)$, and in a neighborhood of s^*, γ lies on one side of its tangent at s^* (which contains the last part of g_{s_m}).



If $s_m \notin I$, then g_{s_m} intersects $\gamma|_{[t_2,L]}$ before s_m due to the definition of s_m, and we choose s^* such that $s^* \in I$ and $\gamma(s^*) \in g_{s_m}$. Note that there is a sequence $s^{(n)} \in I$, $s^{(n)} \to s_m$, such that $g_{s^{(n)}}$ converges to g_{s_m} uniformly, in particular, $e_1(s^*)$ is parallel to $e_1(t^*)$, γ lies on one side of g_{s_m} in a neighborhood of s^* and $\gamma(s^*) \in [\gamma(t^*), \gamma(s_m)]$.



Indeed we must have $e_1(s^*) = e_1(t^*)$, for else consider the closed curve $\gamma|_{[s^*,s_m]} \cup [\gamma(s_m), \gamma(s^*)]$. For ε small enough this curve would have to be intersected by $\gamma|_{[t_2,s^*-\varepsilon]}$ which is not possible.

Now we have to take care of our non-intersection condition (5.8). Let $B = B_1 \cup B_2$ where

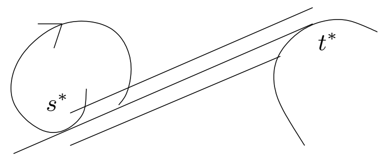
$$\begin{aligned} B_1 &= \{\tau\gamma(t^*) + (1-\tau)\gamma(s^*) + \sigma e_2(t^*) : 0 < \tau < 1, 0 \le \sigma < h\}, \\ B_2 &= \{\tau\gamma(t^*) + (1-\tau)\gamma(s^*) + \sigma e_2(t^*) : 0 < \tau < 1, -h < \sigma < 0\}. \end{aligned}$$

First note that $\gamma|_{[t_1,t^*]}$ does not intersect B: extend g_{s_m} after s_m straightly until it hits $\gamma|_{[t_1,t_2)}$ at $\gamma(t')$. Then note that $\gamma|_{[t_1,t^*]}$ does not enter $\{\gamma(t) + \sigma e_2(t) : t^* < t \le t', 0 \le \sigma < h\}$ nor $[\gamma(t^*), \gamma(t')]$, hence $\gamma|_{[t_1,t^*]} \cap B_1 = \emptyset$.

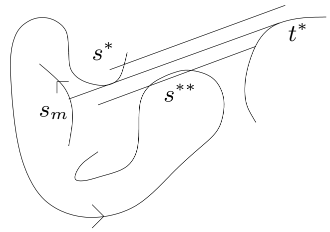
To see that $\gamma|_{[t_1,t^*]}$ does not intersect B_2, note $(\gamma(t^*), \gamma(s^*)]$ lies in the interior of $g_{s_m}|_{[0,g_{s_m}^{-1}(\gamma(t^*))]} \cup \gamma|_{[t^*,t_2]} \cup [\gamma(t_2), \gamma(t_1)]$. If $\gamma|_{[t_1,t^*]}$ intersected B_2, then also $g_{s_m}|_{[0,g_{s_m}^{-1}(\gamma(t^*))]}$ would have to intersect B_2. But this is impossible since $\kappa^{(s_m)} \ge 0$ a.e. due to our claim above.

If also $\gamma|_{(s^*,L]}$ does not intersect B, then replacing $\gamma|_{[t^*,s^*]}$ by the straight line $[\gamma(t^*), \gamma(s^*)]$ leads to a configuration satisfying (5.8).

Suppose now $\gamma|_{(s^*,L]}$ intersects B. This intersection can not take place on the same side of g_{s_m} as γ lies in a neighborhood of s^* since then $s^* - \varepsilon$ could not be connected to t_2.



For $s_m = s^*$ the intersection can not take place on the other side of g_{s_m} either due to maximality of s_m, and we are done. Now consider the remaining case. Note that if $\gamma(s) \in B$, $s > s^*$, then $s \leq s_m$ since $\gamma(s)$ lies in the interior of $\gamma|_{[s^*,s_m]} \cup [\gamma(s_m), \gamma(s^*)]$ for $s > s_m$ and $\langle e_1(s), e_1(t^*)\rangle > 0$ (else t_2 can not be connected to s_m).



Let $s^{**} \in (s^*, s_m]$ be such that $\gamma(s^{**}) \in B$ is closest to $[\gamma(t^*), \gamma(s^*)]$. Now shift $\gamma|_{[s^{**},L]}$ (by an amount $< h$) perpendicular to $\gamma(s^*) - \gamma(t^*)$ such that $\gamma(s^{**})$ lies on (the old) g_{s_m} and connect $\gamma(t^*)$ to $\gamma(s^{**})$. This does not violate our non-intersection condition since $\gamma|_{[t^*,s^{**}]}$ is removed.

As in the previous cases we add a suitable line segment $[(-l, -h/2), (0, -h/2)]$ so that our new configuration has length L and shift to the right. As before, this reduces energy: note that $\int_{t^*}^{s^*} \kappa(t)dt$ and $\int_{t^*}^{s^{**}} \kappa(t)dt$ are equal to 0 or -2π.

Now if $s_m = L$, we proceed as above replacing $\gamma|_{[t^*,s_m]}$ by $[\gamma(t^*), \gamma(s_m)]$, adding a suitable segment and shifting. Note that here $\int_{t^*}^{s^*} \kappa(t)dt \leq 0$. □

Minimal Energy Estimates for Spirals

We consider the subclass of spirals in $\mathcal{A}_2$: $\mathcal{A}_2^{\mathrm{sp}} = \{\gamma \in \mathcal{A}_2 : \kappa(t) \geq 0 \text{ a.e.}\}$.

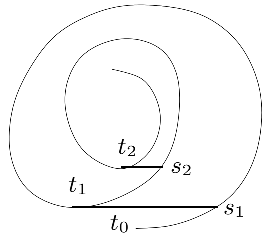
Lemma 5.3.3 *Define $E_2(a)$ as in (5.9), (5.10). There exists a constant C depending on h and L only through $a = hL$ such that for each $\gamma \in \mathcal{A}_2^{\mathrm{sp}}$,*

$$\frac{1}{L}E(\gamma) \geq E_2(a) - Ch.$$

Proof. Choose $t_0 = 0 < t_1 < t_2, \ldots, t_N \leq L$ such that $\int_{t_{n-1}}^{t_n} \kappa(t)dt = 2\pi$ and $\int_{t_N}^{L} \kappa(t)dt < 2\pi$. By convexity,

$$\begin{aligned} E(\gamma) &= \int_0^L (\kappa(t) - \kappa_0)^2 dt \;\geq\; \sum_{n=1}^{N} \int_{t_{n-1}}^{t_n} (\kappa(t) - \kappa_0)^2 dt \\ &\geq \sum_{n=1}^{N} (t_n - t_{n-1}) \left(\frac{2\pi}{t_n - t_{n-1}} - \kappa_0 \right)^2 . \end{aligned} \tag{5.13}$$

Now consider the following closed curves: For $n = 1, \ldots, N$ choose s_n minimal such that $\gamma(s_n)$ lies on the half line starting at $\gamma(t_n)$ with direction $e_1(t_n)$. Define γ^n to be the closed curve $[\gamma(t_n), \gamma(s_n)] \cup \gamma|_{[s_n,t_n]}$.



Recall the definition of r_0 and R_0 from (5.9) and assume first that $r_0/6 \leq |\gamma^n| \leq 8\pi R_0$ for all n. (Then also $L - t_N$ is bounded for w.l.o.g. $N \geq 1$.) Also suppose that $|\gamma(t_1) - \gamma(t_0)| \leq 4\pi R_0$.

Since γ^n are nested closed and convex curves with mutual distance $\geq h$, we deduce from lemma A.6 that

$$|\gamma^n| \geq |\gamma^{n+1}| + 2\pi h.$$

Also note that there exists C independent of N such that

$$\left| \sum_{k=1}^{n} |\gamma^k| - \sum_{k=1}^{n} (t_k - t_{k-1}) \right| \leq C \qquad \forall n \in \{1, \ldots, N\}. \tag{5.14}$$

To see this, note that in components $\gamma = (\gamma_1, \gamma_2)$,

$$\sum_{k=1}^{n} (t_k - t_{k-1}) - |\gamma^k| = \sum_{k=1}^{n} (s_k - t_{k-1}) - (\gamma_1(s_k) - \gamma_1(t_k))$$

with $\gamma_1(s_k) - \gamma_1(t_{k-1}) \leq s_k - t_{k-1} \leq \gamma_1(s_k) - \gamma_1(t_{k-1}) + \gamma_2(s_k) - \gamma_2(t_{k-1})$, i.e.,

$$s_k - t_{k-1} - (\gamma_1(s_k) - \gamma_1(t_k)) \begin{cases} \geq \gamma_1(t_k) - \gamma_1(t_{k-1}) \\ \leq \gamma_1(t_k) - \gamma_1(t_{k-1}) + \gamma_2(t_k) - \gamma_2(t_{k-1}). \end{cases}$$

Summing over k, we get lower and upper bounds by evaluating telescoping sums which are bounded since the spiral occupies a bounded region.

By lemma A.9 we may therefore replace $t_n - t_{n-1}$ in (5.13) by $|\gamma^n|$ and obtain

$$E(\gamma) \geq \sum_{n=1}^{N} |\gamma^n| \left(\frac{2\pi}{|\gamma^n|} - \kappa_0 \right)^2 + \mathcal{O}(1).$$

Now this is exactly the energy of N nested circles (annuli) of length $|\gamma^n|$. Since for two such annuli of different size enlarging the smaller one and shortening the bigger one by the same amount yields energy, we may assume that the annuli touch (i.e., have distances h). Since by (5.14) $\sum_{k=1}^{N} |\gamma^k| = t_N + \mathcal{O}(1) = L + \mathcal{O}(1)$, the previous calculation of the upper bound (cf. (5.11)) applies to this configuration, and we find that

$$\frac{1}{L} E(\gamma) \geq E_2(a) - Ch.$$

Now if $|\gamma^n| \geq 8\pi R_0$ for $n \leq N_1$, $|\gamma^n| \leq r_0/6$ for $n \geq N_2$ and $r_0/6 \leq |\gamma^n| \leq 8\pi R_0$ else, we apply the above reasoning to $\gamma|_{[t_{N_1}, t_{N_2}]}$ replacing the middle part of γ by nested circles of optimal energy leading to inner and outer radii $\bar{r}_0 \geq r_0$ and $\bar{R}_0 \leq R_0$, respectively.

Consider $\gamma|_{[t_{N_2},L]}$. If $L - t_{N_2} \leq r_0$, this part is negligible. If not, we proceed as follows: Since $\gamma|_{[t_{N_2},L]}$ is contained in the domain bounded by γ^{N_2} of diameter $\leq r_0/12$, by lemma A.7 we have $\int_{t_{N_2}}^{L} \kappa(t)dt \geq \lfloor (L - t_{N_2})/(r_0/3) \rfloor \geq 2(L - t_{N_2})/r_0$. By convexity we may lower energy replacing $\gamma|_{[t_{N_2},L]}$ by a curve of constant curvature $2/r_0$. The energy can be reduced further by replacing this part by nested touching annuli whose biggest radius is $\bar{r}_0 - h$. (Note that curvature is reduced pointwise since, by the isoperimetric inequality, $(L - t_{N_2})h \leq \pi(r_0/12\pi)^2 + \mathcal{O}(h) < \pi r_0^2(1 - 1/4)$.)

For the first part of the curve observe that since $\gamma|_{[0,t_{N_1}]}$ lies outside the domain Ω bounded by γ^{N_1} which has perimeter $\geq 8\pi R_0$, $t_n - t_{n-1} \geq 4\pi R_0$ for $n \leq N_1$. (Apply lemma A.8 with $p = \gamma(t_{n-1})$ and $q = \gamma(t_n)$.) As in (5.13), replacing this part of the curve by annuli of circumference $t_n - t_{n-1}$ yields energy. Similar as in the case just treated, we may reduce the energy even further replacing these by nested annuli whose smallest radius is $\bar{R}_0 + h$. $\square$

We summarize the above results in the following

Theorem 5.3.4 *Let $a = Lh$, E_1, E_2 as in (5.12), resp. (5.10). Then*

(i)
$$\inf_{\gamma \in \mathcal{A}_2} \frac{1}{L} E(\gamma) = \min_{\gamma \in \mathcal{A}_2} \frac{1}{L} E(\gamma) = \min_{\gamma \in \mathcal{A}_2^{\mathrm{sp}}} \frac{1}{L} E(\gamma) = E_2(a) + \mathcal{O}(h),$$

(ii)
$$\inf_{\gamma \in \mathcal{A}_1} \frac{1}{L} E(\gamma) = \min_{\gamma \in \mathcal{A}_1} \frac{1}{L} E(\gamma) = E_1(a) + \mathcal{O}(h).$$

Proof. It only remains to prove $\frac{1}{L}E(\gamma) \geq E_1(a) - Ch$ for $\gamma \in \mathcal{A}_1$. Let $\mathrm{co}(\gamma)$ be the convex hull of γ. If there exists $t_0 \in [0, L]$ with $\gamma(t_0) \in \partial\mathrm{co}(\gamma)$ such that $e_2(t_0)$ is not an outward normal of $\mathrm{co}(\gamma)$, we consider $\gamma|_{[0,t_0]}$ and $\gamma|_{[t_0,L]}$ separately. This reduces (up to $\mathcal{O}(h)$) to the spiral case (i) already treated. For $a_1 = t_0 h$, $a_2 = (L - t_0)h$ we see that

$$\frac{1}{L} E(\gamma) \geq \frac{1}{L} \left(t_0 E_2(a_1) + (L - t_0) E_2(a_2) \right) - Ch \geq E_2(a/2) - Ch.$$

If such a t_0 does not exist, find $t_1 < t_2$ with $\gamma(t_1), \gamma(t_2) \in \partial\mathrm{co}(\gamma)$ such that $\int_{t_1}^{t_2} \kappa(t)dt = -2\pi$. Now let $t_1' \leq t_1$ (resp. $t_2' \geq t_2$) be the largest (resp. smallest) time such that $\partial\mathrm{co}(\gamma|_{[0,t_1']}) \cap \gamma|_{[0,t_1']}$ (resp. $\partial\mathrm{co}(\gamma|_{[t_2',L]}) \cap \gamma|_{[t_2',L]}$) contains a point $\gamma(t)$ with $e_2(t)$ not an outward normal. Choose $t_1'' \in [0, t_1']$ maximal with this property ($t_2'' \in [t_2', L]$ minimal). Now treat $\gamma|_{[0,t_1'']}$ and $\gamma|_{[t_2'',L]}$ as in the spiral case. Observe that $\int_{t_1''}^{t_1'} \kappa, \int_{t_2'}^{t_2''} \leq \pi$, so replacing $[t_1'', t_2'']$ by a straight line yields energy. Now add this straight line to one of the two spirals to obtain two spirals with lower energy. As above it follows that $\frac{1}{L}E(\gamma) \geq E_2(a/2) - Ch$. $\square$

Remarks:

(i) The proof shows that the minimal energy configurations are (up to $\mathcal{O}(h)$) indeed of the form depicted on page 125.

(ii) In fact, $Lh \sim 1$ is the only interesting regime for the mean energy $\frac{1}{L}E$. Considering $E_i(a)$ in the limits $a \to 0$ and $a \to \infty$, it follows that, for $h \ll L^{-1} \ll 1$,

$$\lim_{\substack{h\to 0\\ L\to\infty}} \inf_{\gamma\in\mathcal{A}_i} \frac{1}{L}E(\gamma) = 0,$$

whereas for $L^{-1} \ll h \ll 1$,

$$\lim_{\substack{h\to 0\\ L\to\infty}} \inf_{\gamma\in\mathcal{A}_i} \frac{1}{L}E(\gamma) = \kappa_0^2,$$

the mean energy of a straight line.

Appendix A

Some analytical lemmas

For ease of reference we state here some analytical lemmas in the particular form they were used in the previous chapters.

Lemma A.1 *Let $d \in \mathbb{N}$, $q > d$. In addition suppose $c > 0$. Then there is a constant C (depending on c) such that for $a > 0$*

$$\sum_{\substack{x \in \mathbb{Z}^{d+1},\ 0 \le x_{d+1} \le c \\ |x| \ge a}} |x|^{-q} \le C a^{d-q}.$$

The proof is standard.

Lemma A.2 *Let $\Omega \subset \mathbb{R}^n$ be of finite measure, $v_k : \Omega \to K$, $k = 1, 2, \ldots$, measurable, K some compact subset of $\mathbb{R}^m$, and $f_k : K \to \mathbb{R}$ such that $f_k \circ v_k$ is integrable. Furthermore suppose that $\Omega_k \subset \Omega$ is measurable with $|\Omega \setminus \Omega_k| \to 0$ as $k \to \infty$. If $f_k \to f$ uniformly on K, $f : K \to \mathbb{R}$ continuous and $v_k \to v$ in measure, then*

$$\lim_{k \to \infty} \int_{\Omega_k} f_k(v_k) = \int_{\Omega} f(v).$$

The proof of this lemma is a straightforward $\varepsilon/4$-argument.

Lemma A.3 *Suppose $S_1 \subset \mathbb{R}^{n_1}$, $S_2 \subset \mathbb{R}^{n_2}$ are bounded domains, $f, f_k \in L^2(S_1 \times S_2)$ with $f_k \to f$ in $L^2(S_1 \times S_2)$ and $f(x, y)$ being independent of $y \in S_2$. Assume $\varphi_k : S_1 \times S_2 \to S_1 \times S_2$ measurable are such that $\|P \circ \varphi_k - P\|_{L^\infty} \to 0$, P the projection of $S_1 \times S_2$ onto S_1, and the densities $d\varphi_k(\lambda)/d\lambda$ of the image measures exist and are bounded uniformly in k (λ denoting Lebesgue-measure). Then*

$$f_k \circ \varphi_k \to f \quad \text{in } L^2(S_1 \times S_2).$$

Proof. If f is uniformly continuous and $f_k \equiv f$, then even $f_k \circ \varphi_k \to f$ uniformly. For general $f \in L^2$, $f_k \to f$, $\varepsilon > 0$ given, choose f^ε uniformly continuous such that $f^\varepsilon(x, y)$ depends only on $x \in S_1$ with $\|f - f^\varepsilon\|_{L^2} \le \min\{\varepsilon/4\sqrt{C}, \varepsilon/4\}$ and

k so large that $\|f_k - f\|_{L^2} \leq \varepsilon/4\sqrt{C}$ where $\|d\varphi_k(\lambda)/d\lambda\|_{L^\infty} \leq C$. Then also

$$\begin{aligned}
\|f_k \circ \varphi_k - f^\varepsilon \circ \varphi_k\|_{L^2} &= \left(\int_{S_1 \times S_2} |f_k(\varphi_k(x)) - f^\varepsilon(\varphi_k(x))|^2 d\lambda\right)^{1/2} \\
&= \left(\int_{\varphi_k(S_1 \times S_2)} |f_k(x) - f^\varepsilon(x)|^2 d\varphi_k(\lambda)\right)^{1/2} \\
&\leq \sqrt{C}\left(\int_{S_1 \times S_2} |f_k(x) - f^\varepsilon(x)|^2 d\lambda\right)^{1/2} \\
&\leq \varepsilon/2.
\end{aligned}$$

If necessary enlarging k, it follows that

$$\|f_k \circ \varphi_k - f\|_{L^2} \leq \varepsilon/2 + \|f^\varepsilon \circ \varphi_k - f^\varepsilon\|_{L^2} + \varepsilon/4 \leq \varepsilon.$$

□

Lemma A.4 *Let $a \in \mathbb{R}^n$ and define $A_h^{1,2}$ by*

$$\begin{aligned}
A_h^1 f(x) &:= \frac{1}{h}\left(f(x+ha) - f(x)\right) \qquad \textit{resp.} \\
A_h^2 f(x) &:= \frac{1}{h^2}\left(f(x+ha) - f(x) - h\nabla f(x)\cdot a\right)
\end{aligned}$$

for $f \in L^2(\mathbb{R}^n)$ resp. $H^1(\mathbb{R}^n)$. If $f, f_h \in H^1(\mathbb{R}^n)$ resp. $f, f_h \in H^2(\mathbb{R}^n)$ and $f_h \to f$ in $H^1(\mathbb{R}^n)$ resp. $H^2(\mathbb{R}^n)$, then

$$A_h^1 f_h \to \nabla f(\cdot)\cdot a \qquad \textit{resp.} \qquad A_h^2 f_h \to \frac{1}{2}\nabla^2 f(\cdot)(a,a)$$

in L^2 as $h \to 0$.

Proof. We only consider $A_h = A_h^2$, the other case is easier. If f is compactly supported and smooth, then

$$A_h f(x) \to \frac{1}{2}\nabla^2 f(x)(a,a) \quad \text{uniformly,} \tag{A.1}$$

which proves the claim for $f \in C_c^\infty(\mathbb{R}^n)$ and $f_h \equiv f$.

Now if $f, g \in C_c^\infty(\mathbb{R}^n)$, then

$$A_h f(x) - A_h g(x) = \int_0^1 \int_0^1 \nabla\left(\nabla(f-g)(x+stha)\cdot a\right)\cdot ta\; dsdt,$$

so by Jensen's inequality

$$\int_{\mathbb{R}^n} |A_h f(x) - A_h g(x)|^2 dx \leq \frac{1}{3}\|\nabla^2 f(a,a) - \nabla^2 g(a,a)\|_{L^2}^2. \tag{A.2}$$

By approximation this estimate holds for all $f, g \in H^2$.

Now given $f \in H^2$, choose g smooth with $\|f-g\|_{H^2} \leq \varepsilon$. Choosing h sufficiently small, we have $\|\nabla^2 f_h - \nabla^2 f\|_{L^2} \leq \varepsilon$ and, by (A.1), $\|A_h g - \frac{1}{2}\nabla^2 g(a,a)\| \leq \varepsilon$. By (A.2) then

$$\begin{aligned}\|A_h f_h - \frac{1}{2}\nabla^2 f(a,a)\|_{L^2} &\leq \|A_h f_h - A_h g\|_{L^2} + \|A_h g - \frac{1}{2}\nabla^2 g(a,a)\|_{L^2} \\ &\quad + \frac{1}{2}\|\nabla^2 g(a,a) - \nabla^2 f(a,a)\|_{L^2} \\ &\leq 2\varepsilon + \varepsilon + \varepsilon = 4\varepsilon.\end{aligned}$$

□

Lemma A.5 *In addition to the hypotheses of the previous lemma suppose that*

$$\tilde{h}\|\nabla f_h\|_{L^\infty} \to 0 \quad \textit{resp.} \quad \tilde{h}\|\nabla^2 f_h\|_{L^\infty} \to 0$$

for $\tilde{h} = \tilde{h}(h) \to 0$ *as* $h \to 0$. *Then*

$$\tilde{h} A_h^{1,2} f_h \to 0$$

in L^∞ *as* $h \to 0$.

Proof. The claim for A_h^1 is trivial: Since $f_h \in W^{1,\infty}$,

$$\frac{\tilde{h}}{h}\,|f_h(x+ha) - f(x)| \leq \frac{\tilde{h}}{h}\|\nabla f_h\|_{L^\infty}|ha| \to 0.$$

For $f_h \in W^{2,\infty} \subset C^1$ we calculate

$$\begin{aligned}|\tilde{h} A_h^2 f_h(x)| &\leq \frac{\tilde{h}}{h^2}\left|\int_0^1 \nabla f_h(x+tha)\cdot ha\,dt - h\nabla f_h(x)\cdot a\right| \\ &\leq \frac{\tilde{h}}{h}\int_0^1 |\nabla f_h(x+tha)\cdot a - \nabla f_h(x)\cdot a|\;dt \\ &\leq \frac{\tilde{h}}{h}\int_0^1 \|\nabla^2 f_h\|_{L^\infty}|ha|\,|a|dt \;\to\; 0.\end{aligned}$$

□

The next three lemmas collect more or less elementary facts for curves resp. domains in $\mathbb{R}^2$.

Lemma A.6 *Suppose* $\Omega_1, \Omega_2 \subset \mathbb{R}^2$ *are convex domains with* $\Omega_1 \subset \Omega_2$ *and* $\operatorname{dist}(\partial\Omega_1, \partial\Omega_2) \geq h$. *Then*

$$|\partial\Omega_2| \geq |\partial\Omega_1| + 2\pi h,$$

and equality holds iff $\Omega_2 = \Omega_1^h := \{x \in \mathbb{R}^2 : \operatorname{dist}(x, \Omega_1) < h\}$.

Proof. Suppose first $\partial\Omega_1, \partial\Omega_2$ are C^2, and parameterize $\partial\Omega_1$ by $[t_1, t_2] \ni t \mapsto \gamma(t)$ where t is arclength, oriented such that $e_2 = e_1^\perp$ is the inner normal to $\partial\Omega_1$, $e_1 = d\gamma/dt$, and $\kappa = d^2\gamma/dt^2 \cdot e_2 \geq 0$. Then $\partial\Omega_2$ can be parameterized by $\tilde{\gamma}(t) = \gamma(t) - f(t)e_2(t)$, $f \geq h$. Since $de_2/dt = de_1^\perp/dt = \kappa e_2^\perp = -\kappa e_1$, we can calculate:

$$\begin{aligned}
|\partial\Omega_2| &= \int_{t_1}^{t_2} \left| \frac{d}{dt}\tilde{\gamma} \right| dt = \int_{t_1}^{t_2} \left| \frac{d\gamma}{dt} - \frac{df}{dt}e_2 - f\frac{de_2}{dt} \right| dt \\
&= \int_{t_1}^{t_2} \left| e_1 - \frac{df}{dt}e_2 + f\kappa e_1 \right| dt \geq \int_{t_1}^{t_2} |1 + \kappa f| dt \\
&= \int_{t_1}^{t_2} (1 + \kappa f) dt \geq t_2 - t_1 + h \int_{t_1}^{t_2} \kappa dt \\
&= |\partial\Omega_1| + 2\pi h
\end{aligned}$$

with equality everywhere iff $f \equiv h$, i.e., $\Omega_2 = \Omega_1^h$. For general Ω_1, Ω_2 approximate by convex domains having smooth boundary.

(Alternatively assume that Ω_1 has polygonal boundary (else approximate). Projecting (i.e., contracting) Ω_2 onto $\overline{\Omega_1^h}$ yields $|\partial\Omega_2| \geq |\partial\Omega_1^h| = |\partial\Omega_1| + 2\pi h$ with equality iff $\Omega_2 = \Omega_1^h$. This argument also shows that we do not have to require that Ω_2 be convex.) □

Lemma A.7 *Suppose $\Omega \subset \mathbb{R}^2$ is a domain of diameter d, $\gamma : [0, l] \to \Omega$ a curve (parameterized by arclength) in Ω. Then*

$$\int_0^l |\kappa|(t) dt \geq \frac{1}{2} \left\lfloor \frac{l}{2d} \right\rfloor,$$

$\lfloor l/2d \rfloor$ denoting the integer part of $l/2d$.

Proof. W.l.o.g. $l > 2d$. Since for $0 \leq t_1 < t_2 \leq l$,

$$d \geq |\gamma(t_2) - \gamma(t_1)| = \left| \int_{t_1}^{t_2} \left(\frac{d\gamma}{dt}(t_1) + \int_{t_1}^{t} \frac{d^2\gamma}{dt^2}(s) ds \right) dt \right|,$$

we have

$$\begin{aligned}
\left| (t_2 - t_1)\frac{d\gamma}{dt}(t_1) \right| &\leq d + \int_{t_1}^{t_2} \int_{t_1}^{t_2} \left| \frac{d^2\gamma}{dt^2}(s) \right| ds dt \\
&= d + (t_2 - t_1) \int_{t_1}^{t_2} |\kappa(t)| dt.
\end{aligned}$$

Therefore $\int_{t_1}^{t_2} |\kappa(t)| dt \geq 1 - d/(t_2 - t_1)$. In particular, if $t_2 - t_1 = 2d$, then $\int_{t_1}^{t_2} |\kappa(t)| dt \geq 1/2$. Cutting γ into $\lfloor l/2d \rfloor$ pieces of length $2d$, we thus find that

$$\int_0^l |\kappa|(t) dt \geq \frac{1}{2} \left\lfloor \frac{l}{2d} \right\rfloor.$$

□

Lemma A.8 *Suppose $\Omega \subset \mathbb{R}^2$ is a convex domain, $p, q \in \mathbb{R}^2$ separated (not necessarily strictly) from Ω by some hyper-plane. Then any domain Ω' (with sufficiently smooth boundary) containing Ω, p, q satisfies*

$$|\partial\Omega'| \geq |p - q| + \frac{1}{2}|\partial\Omega|.$$

Proof. W.l.o.g. assume that Ω' is the convex hull of Ω, p and q. Reducing $|\partial\Omega'| - |p - q|$, we may also assume that p and q lie on the separating hyperplane, even that the image of the orthogonal projection of Ω to this line is (p, q). But then $|p - q| \leq |\partial\Omega|/2$, so the claim follows from $|\partial\Omega'| \geq |\partial\Omega|$ because of $\Omega' \supset \Omega$ (cf. lemma A.6). □

Finally, we needed the following estimate for convex functions on the line.

Lemma A.9 *Let $I \subset \mathbb{R}$ be an interval and $f : I \to \mathbb{R}$ be convex. Let $x_1, \ldots, x_N$, $y_1, \ldots, y_N \in I$ such that $y_1 \leq y_2, \ldots \leq y_N$. Assume that there is a constant c such that $|\sum_{k=1}^n x_k - \sum_{k=1}^n y_k| \leq c$ for all $n \in \{1, \ldots, N\}$. Then there exists $C > 0$ only depending on c, $f'(y_1)$ and $f'(y_N)$ such that*

$$\sum_{k=1}^{N} f(x_k) \geq \sum_{k=1}^{N} f(y_k) - C.$$

(By $f'(x)$ we denote any element in the subdifferential of f at x.)

Proof. Let $a_n := f'(y_n) - f'(y_{n-1})$ if $n \geq 2$, $a_1 := f'(y_1)$, $b_n := x_n - y_n$, and set $A_n = a_1 + \ldots + a_n$, $B_n = b_1 + \ldots + b_n$. By convexity and partial summation,

$$\begin{aligned}
\sum_{n=1}^{N} f(x_n) - \sum_{n=1}^{N} f(y_n) &\geq \sum_{n=1}^{N} f'(y_n)(x_n - y_n) = \sum_{n=1}^{N} A_n b_n \\
&= A_N B_N - \sum_{n=2}^{N} a_n B_{n-1} \\
&= f'(y_N) \sum_{n=1}^{N} (x_n - y_n) - \sum_{n=2}^{N} a_n B_{n-1} \\
&\geq -|f'(y_N)|c - \max_{1 \leq n \leq N-1} |B_n| \sum_{n=2}^{N} a_n \\
&\geq C(f'(y_N), f'(y_1), c).
\end{aligned}$$

(Note that by convexity and (y_n) being increasing, $a_n \geq 0$ for $n \geq 2$.) □

Of course this lemma also applies to $y_1 \geq y_2, \ldots \geq y_N$. Just note that

$$\left|\sum_{k=n}^{N} x_k - y_k\right| = \left|\sum_{k=1}^{N} x_k - y_k - \sum_{k=1}^{n-1} x_k - y_k\right| \leq 2c.$$

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