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by

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Abstract

We derive plate theory from atomistic models in the spirit of [11] as a Γ-limit as the number of atoms tends to infinity. 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 [11], 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.

Contents

1 Introduction

The derivation of effective theories for thin elastic structures is a classical problem in elasticity theory, see, e.g., [18]. Rigorous results deriving membrane, plate or shell theories from three-dimensional elasticity have been obtained only recently (cf. [15, 16, 17, 10, 11, 12, 13]). By now there has emerged a whole hierarchy of plate theories according to different scalings of the stored energy (cf. [12]).

Another area of research concerns the passage from discrete atomic models to continuum theories. Rigorous Γ-convergence results, especially in one dimension, are proved in [3, 4, 5] for pair potentials under suitable growth assumptions on the atomic interactions. The results in [1, 2] 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.

An effective theory for thin films derived from atomistic models in the realm of membrane theory was proposed in [9] and rigorously derived in [19, 20, 21]. The aim of the present work is to derive plate theory in the regime of finite bending energies, starting from a microscopic atomic model. We assume that the energy can be decomposed into certain cell-energies similar as in [6]. 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 2, 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.

In section 3, we prove rigidity estimates for deformations in terms of their elastic energy in the spirit of [11]. 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 [11]. This is built up on [22] and [6] and generalizes two-dimensional results in [22] to higher dimensions.

Section 4 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 5, we specialize to thin films, i.e. films consisting of a fixed number $\nu+1$ of atomic layers. 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. 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 [11] from three-dimensional continuum elasticity theory. However, for 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 [11], 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.

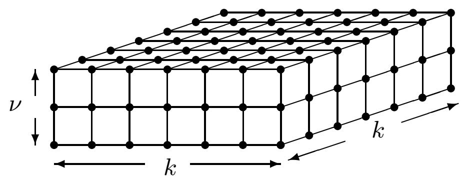
Keeping only the leading term in powers of ν, the thickness of the film, we are formally led to a continuum theory for thick films. By thick films we mean the regime $k, \nu \to \infty$, i.e. films of many atomic layers, such that still $\nu/k \to 0$. That this is indeed the correct Γ-limit in the realm of thick films, is the content of section 6. This way we obtain the functional of plate theory derived in [11] on the basis of three-dimensional elasticity rigorously as a thick film limit starting from atomistic models.

The last section 7 discusses a mass-spring model as an elementary but physically realistic example of atomic interactions to which the results in the previous sections apply.

2 The model

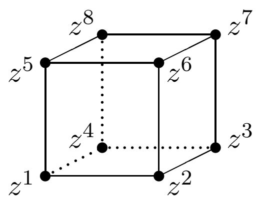
We consider films of $\nu + 1$ atomic layers, $\nu \geq 1$, whose reference configuration is given by the lattice

$$\Lambda_k = \{0, 1, \dots, k\}^2 \times \{-\nu/2, -\nu/2 + 1, \dots, \nu/2\}.$$



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 $z^1, \dots, z^8$ 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 $\vec{y}(x) = (y_1, \dots, y_8) = (y(\bar{x} + z^1), \dots, y(\bar{x} + z^8))$ and $\vec{z} = (z^1, \dots, z^8)$ 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 $W : \Lambda'_k \times (\mathbb{R}^3)^8 \to \mathbb{R}$ in the form

$$E(y) = \sum_{\bar{x} \in \Lambda'} W(\bar{x}, \vec{y}(\bar{x})) \tag{1}$$

where $W(\bar{x}, \cdot)$ splits into a bulk and a surface part

$$W(\bar{x}, \cdot) = W_{\mathrm{cell}}(\cdot) + W_{\mathrm{surface}}(\bar{x}, \cdot) \tag{2}$$

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

$$W_{\text{surface}}(\bar{x}, \vec{y}) = \begin{cases} W_{\text{surf}}(y_1, \dots, y_4) & \text{resp.} \\ W_{\text{surf}}(y_5, \dots, y_8) & \text{resp.} \\ W_{\text{surf}}(y_1, \dots, y_4) + W_{\text{surf}}(y_5, \dots, y_8) \end{cases} \tag{3}$$

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 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 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

$$T_{lmn}(x) := \text{co}(\bar{x}, \bar{x} + z^l, \bar{x} + z^m, \bar{x} + z^n)$$

for l, m, n such that $\mathcal{T} = \{T_{lmn}\}$ is a decomposition of the cube into twelve simplices, z^l, z^m, z^n on a single face of $[-1/2, 1/2]^3$. In particular, let

$$T_1 := T_{4,1,2},\ T_2 := T_{2,3,4},\ T_3 := T_{8,5,6},\ T_4 := T_{6,7,8} \in \mathcal{T}.$$

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 $w^1, \dots, w^6$ 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

$$T_{lmn}(x) := \text{co}(\bar{x}, \bar{x} + z^l, \bar{x} + z^m, \bar{x} + w^n)$$

for l, m, n such that $\mathcal{T} = \{T_{lmn}\}$ is a decomposition of the cube into 24 simplices, $|z^l - z^m| = 1$, and z^l, z^m, w^n on a single face of $[-1/2, 1/2]^3$.

In order for the deformations to be defined on common domains we also rescale defining $\tilde{y} : \Omega \to \mathbb{R}^3$ by

$$\tilde{y}(x_1, x_2, x_3) = \frac{1}{k} y(kx_1, kx_2, x_3), \quad \Omega = S \times [-\nu/2, \nu/2], \tag{4}$$

respectively

$$\tilde{y}(x_1, x_2, x_3) = \frac{1}{k} y(kx_1, kx_2, \nu x_3), \quad \Omega = S \times [-1/2, 1/2], \tag{5}$$

$S = [0, 1]^2$, 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 $L^2(S^2;\mathbb{R}^3)\oplus\ldots\oplus L^2(S^2;\mathbb{R}^3) \cong L^2(S^2\times\{-\nu/2, -\nu/2+1, \ldots, \nu/2\};\mathbb{R}^3)$.

Definition 2.1 *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

$$\frac{1}{k^2}\sum_{x\in\Lambda}\left|\tilde{y}^{(k)}(x) - \fint_{[-1/2k,1/2k]^2}\tilde{y}(x'+\xi, x_3)d\xi\right|^2 \to 0.$$

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

$$\tilde{y}^{(k)} \to \tilde{y} \quad \textit{in } L^2(\Omega;\mathbb{R}^3).$$

(ii) In the thick film regime we say $\tilde{y}^{(k)} \to \tilde{y}$ if

$$\frac{1}{k^2\nu}\sum_{x\in\Lambda}\left|\tilde{y}^{(k)}(x) - \fint_{[-1/2k,1/2k]^2\times[1/2\nu,1/2\nu]}\tilde{y}(x+\xi)d\xi\right|^2 \to 0.$$

This is equivalent to

$$\tilde{y}^{(k)} \to \tilde{y} \quad \textit{in } L^2(\Omega;\mathbb{R}^3).$$

3 Discrete geometric rigidity

As elaborated in [11], 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 [6]) and to prove lemma 3.2, a generalization to arbitrary dimensions of a result in [22]. 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

$$\bar{\nabla}y(x) := (y_1 - \bar{y}, \ldots, y_{2^n} - \bar{y}), \quad \bar{y} := \frac{1}{2^n}\sum_{i=1}^{2^n} y_i,$$

for $x \in \Lambda$, $y_i = y_i(x) = y(x+z^i)$, $z^1, \ldots, z^{2^n}$ 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 3.1 *(i)* $W_{\text{cell}} : \mathbb{R}^{n \times 2^n} \to \mathbb{R}$ *is invariant under translations and rotations, i.e. for* $\vec{y} \in \mathbb{R}^{n \times 2^n}$,

$$W_{\text{cell}}(R\vec{y} + (c, \ldots, c)) = W_{\text{cell}}(\vec{y})$$

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*

$$y_i = Rz^i + c, \quad i = 1, \ldots, 2^n.$$

(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 is positive definite on the orthogonal complement of the subspace spanned by translations* $(x_1, \ldots, x_{2^n}) \mapsto (c, \ldots, c)$ *and infinitesimal rotations* $(x_1, \ldots, x_{2^n}) \mapsto (Ax_1, \ldots, Ax_{2^n})$ *where* $A^T = -A$.

(iv) W_{cell} *grows at infinity at least quadratically on the orthogonal complement of the subspace spanned by 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

$$Q_n(v, \ldots, v) = 0, \quad Q_n(Az^1, \ldots, Az^{2^n}) = 0$$

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 [22]. For the proof also compare [6].

Lemma 3.2 *For* u *thus defined,* $Q = Q(x)$ *and* $\vec{y} = \vec{y}(x)$,

$$\int_Q dist^2(\nabla u, SO(n)) \leq C W_{\text{cell}}(\vec{y}).$$

Proof. Let $W_{\mathrm{ref}}(\vec{y}) = W_{\mathrm{ref}}(\bar{\nabla}\vec{y}) = \int_Q \mathrm{dist}^2(\nabla u, SO(n))$. Both W_{cell} and W_{ref} are invariant under rotations and translations:

$$W_{\mathrm{cell/ref}}(y_1, \ldots, y_{2^n}) = W_{\mathrm{cell/ref}}(Ry_1 + c, \ldots, Ry_{2^n} + c)$$

if $R \in SO(n)$, $c \in \mathbb{R}^n$. So it suffices to prove the claim for deformations perpendicular to the space $V_0 = \mathbb{R}^n \otimes (1, \ldots, 1)$ of infinitesimal translations $(x_1, \ldots, x_{2^n}) \mapsto (v, \ldots, v)$, $v \in \mathbb{R}^n$.

Suppose first $\vec{y} \in \mathbb{R}^{n \times 2^n}$ is given such that $\vec{y} \perp V_0$ and $\mathrm{dist}(\vec{y}, \bar{SO}(n))$ is small. Let $\bar{G}$ be the orthogonal projection of $\vec{y}$ onto $\bar{SO}(n)$. By assumption,

$$\begin{aligned} W_{\mathrm{cell}}(\vec{y}) &= W_{\mathrm{cell}}(\bar{G}) + DW_{\mathrm{cell}}(\bar{G})(\vec{y} - \bar{G}) \\ &\quad + \frac{1}{2} D^2 W_{\mathrm{cell}}(\bar{G})(\vec{y} - \bar{G}, \vec{y} - \bar{G}) + o(|\vec{y} - \bar{G}|^2) \\ &\geq c|\vec{y} - \bar{G}|^2. \end{aligned}$$

(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 $W_{\mathrm{ref}} \geq 0$ and $W_{\mathrm{ref}}(\vec{y}) = 0$ if $\bar{\nabla}\vec{y} \in \bar{SO}(n)$, we have $W_{\mathrm{ref}}(\bar{G}) = 0$, $DW_{\mathrm{ref}}(\bar{G}) = 0$, and, $\vec{y} \mapsto W_{\mathrm{ref}}(\vec{y})$ being C^2, $|\vec{y} - \bar{G}|^2 = \mathrm{dist}^2(\vec{y}, \bar{SO}(n)) \geq cW_{\mathrm{ref}}(\vec{y})$. So we have shown that, for $\vec{y}$ with $\mathrm{dist}(\vec{y}, \bar{SO}(n))$ small, indeed

$$W_{\mathrm{ref}}(\vec{y}) \leq CW_{\mathrm{cell}}(\vec{y})$$

if C is large enough.

Now if $\mathrm{dist}(\vec{y}, \bar{SO}(n))$ is not small, we only have to consider the limit $\mathrm{dist}(\vec{y}, \bar{SO}(n)) \to \infty$. Then, by continuity, the claim follows in the intermediate regime, too, since $W_{\mathrm{cell}}(\vec{y}) > 0$ for $\vec{y} \notin \bar{SO}(n)$ (and $\vec{y} \perp V_0$). But this case is clear by assumption 3.1 (iv), since $W_{\mathrm{ref}}(\vec{y})$ grows quadratically in $\vec{y} \perp V_0$. □

Theorem 3.3 *(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)

$$\int_\Omega |\nabla u - R|^2 \leq C \sum_{x \in \Lambda} W_{\mathrm{cell}}(\vec{y}(x)),$$

(ii)

$$\sum_{x \in \Lambda} |\bar{\nabla} y(x) - \bar{R}|^2 \leq C \sum_{x \in \Lambda} W_{\mathrm{cell}}(\vec{y}(x))$$

where $\bar{R} = R\vec{z}$. The constant C only depends on W_{cell} and Ω and is invariant under rescaling of Ω.

Remark. The inequality in (ii) can be rewritten as

$$\|\bar{\nabla} y - \bar{R}\|^2_{l^2(\Lambda)} \leq C \sum_{x \in \Lambda} W_{\mathrm{cell}}(\vec{y}(x)).$$

Proof. The proof of (i) is immediate from the lemma above and the following rigidity result for continuous deformations (cf. theorem 3.4). For the second part simply note that on a unit cube Q, $|\bar{\nabla} y - \bar{R}| \leq C \int_Q |\nabla u - R|$. □

Theorem 3.4 *(Continuous Rigidity, cf. [11].) 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*

$$\|\nabla v - R\|_{L^2(\Omega)} \le C(\Omega)\|\mathrm{dist}(\nabla v, SO(n))\|_{L^2(\Omega)}.$$

4 Compactness

In this section we will show that sequences having finite bending energy are precompact: there exists a subsequence that converges in the sense of definition 2.1. Form now on we will suppose assumption 3.1 is satisfied for all $W(\bar{x},\cdot)$. (Note that by (1), (2) and (3), $\{W(\bar{x},\cdot) : \bar{x} \in \Lambda'_k\}$ consists of no more than 27 functions.)

Recall the rescaling from (4) respectively (5), and for $\tilde{y} : \Omega \to \mathbb{R}^3$ set

$$\nabla_k \tilde{y} := (\nabla' \tilde{y}, k\tilde{y}_{,3}) \quad \text{resp.} \quad \nabla_{k,\nu}\tilde{y} := (\nabla'\tilde{y}, \frac{k}{\nu}\tilde{y}_{,3}) \tag{6}$$

in the thin respectively thick film regime. Also for $z \in \{-1/2, 1/2\}^3$ we define

$$\bar{\nabla}_k \tilde{y}(x)(z) \;=\; k\left(\tilde{y}(\bar{x} + (z'/k, z_3)) - \tilde{y}(\bar{x})\right) \quad \text{resp.} \tag{7}$$

$$\bar{\nabla}_{k,\nu} \tilde{y}(x)(z) \;=\; k\left(\tilde{y}(\bar{x} + (z'/k, z_3/\nu)) - \tilde{y}(\bar{x})\right) \tag{8}$$

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 $z_1, \dots, z_8$.

Theorem 4.1 *(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 relabelled) 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)

$$\bar{\nabla}_k \tilde{y}^{(k)}(x)(z) \textit{ resp. } \bar{\nabla}_{k,\nu}\tilde{y}^{(k)}(x)(z) \to (\nabla'\tilde{y}, b)(x)\cdot z \quad \textit{in } L^2(\Omega)$$

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. $E(y^{(k)}) \leq C$, by lemma 3.2 implies that

$$\int_\Omega \operatorname{dist}^2(\nabla_k \tilde{y}^{(k)}, SO(3)) = \frac{1}{k^2} \int_{kS\times(-\nu/2,\nu/2)} \operatorname{dist}^2(\nabla y^{(k)}, SO(3)) \leq \frac{C}{k^2}.$$

The first part of the theorem now directly follows from the corresponding compactness result in [11]. We recall two inequalities derived in [11] 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

$$\int_\Omega |R^{(k)}(x) - \nabla_k \tilde{y}^{(k)}(x)|^2 dx \leq C/k^2, \tag{9}$$

and, for $|\zeta| \leq c/k$ and $\Omega' = S' \times (\nu/2, \nu/2) \subset \Omega$ with $S' \subset\subset S$,

$$\int_{\Omega'} |R^{(k)}(x+\zeta) - R^{(k)}(x)|^2 dx \leq C \int_\Omega \operatorname{dist}^2(\nabla_k \tilde{y}^{(k)}(x), SO(3)) dx \leq C/k^2 \tag{10}$$

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 $T = T_{lmn}$. Choose $\varphi_k : \Omega \to \Omega$ to be the function mapping $\tilde{Q}(x)$ onto $\tilde{T}_{lmn}(x)$ isometrically when restricted to a single simplex $T_{l'm'n'}$. Since $\tilde{y}^{(k)}$ is affine on T, we have

$$\bar{\nabla}_k \tilde{y}(x)(z) = \nabla_k \tilde{y}^{(k)}(\varphi_k(x)) \cdot z,$$

$z \in \{-1/2, 1/2\}^3$. Now applying lemma A.1 with $S_1 = S$ and $S_2 = (-\nu/2, \nu/2)$, by the part already proven,

$$\lim_{k\to\infty} \bar{\nabla}_k \tilde{y}(z) = \lim_{k\to\infty} \nabla_k \tilde{y} \cdot z = (\nabla' \tilde{y}, b) \cdot z$$

strongly in L^2.

The reasoning for thick films is similar. We obtain a map $R^{(h)} : S \to SO(3)$ ($h := \nu/k$), piecewise constant on a partition of S into cubes of side-length h as in [11], with

$$\int_\Omega |R^{(h)}(x) - \nabla_{k,\nu} \tilde{y}^{(k)}(x)|^2 dx \leq Ch^2, \tag{11}$$

and, for $|\zeta| \leq ch$ and $\Omega' = S' \times (\nu/2, \nu/2) \subset \Omega$ with $S' \subset\subset S$,

$$\int_{\Omega'} |R^{(h)}(x+\zeta) - R^{(h)}(x)|^2 dx \leq C \int_\Omega \operatorname{dist}^2(\nabla_{k,\nu} \tilde{y}^{(k)}(x), SO(3)) dx \leq Ch^2. \tag{12}$$

For part two of the claim again apply lemma A.1, this time with $S_1 = \Omega$ and $S_2 = \{0\}$. $\square$

5 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 3.1 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. (2) and (3)) at the identity. Sufficient will be to suppose up-down-symmetry in the following sense:

Assumption 5.1 *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. (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. (2) and (3)) we require that

$$W_{\mathrm{surf}}(Py_1, Py_2, Py_3, Py_4) = W_{\mathrm{surf}}(\vec{y})$$

for all $\vec{y} \in \mathbb{R}^{3\times 4}$.

Remarks.

(i) For the quadratic forms Q_3 and Q_2 this implies

$$Q_3(Py_5, Py_6, Py_7, Py_8, Py_1, Py_2, Py_3, Py_4) = Q_3(\vec{y}) \tag{13}$$

for all $\vec{y} \in \mathbb{R}^{3\times 8}$ respectively

$$Q_2(Py_1, Py_2, Py_3, Py_4) = Q_2(\vec{y}) \tag{14}$$

for all $\vec{y} \in \mathbb{R}^{3\times 4}$.

(ii) These assumptions are satisfied for suitable mass-spring models (see section 7).

Depending on Q_3, we define a relaxed quadratic form Q_3^{rel}: for $\vec{y} = (y_1, \ldots, y_8) \in \mathbb{R}^{3\times 8}$ let

$$Q_3^{\mathrm{rel}}(\vec{y}) := \min_{v\in\mathbb{R}^3} Q_3(y_1, \ldots, y_4, y_5 + v, \ldots, y_8 + v).$$

Note that with this definition (13) remains valid when replacing Q_3 by Q_3^{rel}.

As a last preparation we introduce the following notations. For a 3×8-matrix A we denote by A_{b} its left 3×4-part, by A_{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_{p} for its left 3×2-part.

Now suppose assumption 3.1 holds for all $W(\bar{x}, \cdot)$ and W_{cell} and W_{surf} satisfy assumption 5.1. Then, in the spirit of Γ-convergence (cf. [7]), our main result for thin films is:

Theorem 5.2 *(Limiting plate theory for thin films.) For $k \to \infty$, $E = E^{(k)}$ converges to E_{thin} defined below in the following sense:*

(i) If $y^{(k)} : \Lambda \to \mathbb{R}^3$ is such that $y^{(k)} \to \tilde{y}$ (cf. definition 2.1), then

$$\liminf_{k\to\infty} E(y^{(k)}) \geq E_{\text{thin}}(\tilde{y}).$$

(ii) For all limiting deformations $\tilde{y}$ (cf. definition 2.1) there exists a sequence $y^{(k)} : \Lambda_k \to \mathbb{R}^3$ with $y^{(k)} \to \tilde{y}$ in the sense of definition 2.1 such that

$$\lim_{k\to\infty} E(y^{(k)}) = E_{\text{thin}}(\tilde{y}).$$

If $\tilde{y} \in \mathcal{A}$ (see below), the limit functional E_{thin} is given by

$$\begin{aligned} E_{\text{thin}}(\tilde{y}) \;:=\; & \int_S \Big[\frac{\nu}{8} Q_3^{\text{rel}} \left(-\text{II}_{12} M + N \cdot \vec{z}_-' \right) + \frac{\nu^3 - \nu}{24} Q_3^{\text{rel}} \left(N \cdot \vec{z}\,' \right) \\ & + \frac{1}{4} Q_2 \left(\text{II}_{12} M_{\text{b}} \right) + \frac{\nu^2}{4} Q_2 \left(N \cdot \vec{z}_{\text{b}}' \right) \Big] \, dx \end{aligned}$$

with $\vec{z}_- = (-z^1, -z^2, -z^3, -z^4, z^5, z^6, z^7, z^8)$ and

$$M = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \end{pmatrix}, \quad N = \begin{pmatrix} \text{II}_{11} & \text{II}_{12} \\ \text{II}_{21} & \text{II}_{22} \\ 0 & 0 \end{pmatrix}.$$

If $\tilde{y} \notin \mathcal{A}$, then $E_{\text{thin}}(\tilde{y}) := +\infty$. The class $\mathcal{A}$ of admissible functions consists of isometries from S into $\mathbb{R}^3$:

$$\mathcal{A} = \{ \tilde{y} \in W^{2,2}(S; \mathbb{R}^3) : |\tilde{y}_{,1}| = |\tilde{y}_{,2}| = 1, \ \tilde{y}_{,1} \cdot \tilde{y}_{,2} = 0 \},$$

and $\text{II} \in \mathbb{R}^{2\times 2}$ is the second fundamental form $\text{II}_{ij} = \tilde{y}_{,i} \cdot b_{,j}$, $b = \tilde{y}_{,1} \wedge \tilde{y}_{,2}$.

5.1 Proof of the lower bound

Suppose $y^{(k)}$ is a sequence converging to $\tilde{y}$ and has finite bending energy, so $\tilde{y}^{(k)} \to \tilde{y}$ in L^2 and, by theorem 4.1, $\nabla_k \tilde{y}^{(k)} = (\nabla' \tilde{y}^{(k)}, k\tilde{y}^{(k)}_{,3}) \to (\nabla' \tilde{y}, b) \in H^1$. Let

$$G^{(k)}(x) := k \left((R^{(k)})^T (x') \nabla_k \tilde{y}^{(k)}(x) - \text{Id} \right)$$

which is bounded in L^2 by (9), say (up to choosing a subsequence)

$$G^{(k)} \rightharpoonup G. \tag{15}$$

In [11] it is shown that

$$G_{\text{p}}(x', x_3) = G_{\text{p}}(x', 0) + x_3 N(x'). \tag{16}$$

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

$$\bar{G}^{(k)}(x) := k \left((R^{(k)})^T (x') \bar{\nabla}_k \tilde{y}^{(k)}(x', x_3) - \bar{\text{Id}} \right),$$

piecewise constant with values in $\mathbb{R}^{3\times 8}$.

Lemma 5.3 *Let G be as in (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 $\varphi_{lmn}^{(k)} : \Omega \to \Omega$ mapping $\tilde{Q}(x)$ onto $\tilde{T}_{lmn}(x)$ and $\tilde{T}_{l'm'n'}(x)$ onto $\tilde{T}_{lmn}(x)$ isometrically. By (9) for $\tilde{T}_{lmn} := \bigcup_{x\in\Omega} \tilde{T}_{lmn}(x)$,

$$\int_{\tilde{T}_{lmn}} |\nabla_k \tilde{y}^{(k)} - R^{(k)}|^2 \le \int_{\Omega} |\nabla_k \tilde{y}^{(k)} - R^{(k)}|^2 \le C/k^2.$$

So $\nabla_k \tilde{y}^{(k)} \circ \varphi_{lmn}^{(k)}$ also satisfies

$$\int_{\Omega} |\nabla_k \tilde{y}^{(k)} \circ \varphi_{lmn}^{(k)} - R^{(k)}|^2 \le C/k^2.$$

Extracting if necessary a further subsequence, it follows that $f_{lmn}^{(k)} := k((R^{(k)})^T \nabla_k \tilde{y}^{(k)} \circ \varphi_{lmn}^{(k)} - \mathrm{Id})$ converges weakly in L^2 to f_{lmn}, say. If z^i is a corner of T_{lmn}, then $f_{lmn} \cdot z^i = \bar{G}(\cdot)(z^i)$ where $\bar{G}^{(k)}(\cdot)(z^i) \rightharpoonup \bar{G}(\cdot)(z^i)$.

Now suppose $r \in \{-\nu/2, -\nu/2+1, \dots, \nu/2-1\}$, $r < x_3 < r+1$, and for $\varepsilon > 0$ consider the layer $\Omega_\varepsilon = S \times [r, r+\varepsilon]$. Then $G^{(k)}|_{\Omega_\varepsilon} \rightharpoonup G|_{\Omega_\varepsilon}$ by (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,

$$x' \mapsto \int_r^{r+\varepsilon} G^{(k)}(x', t)dt$$

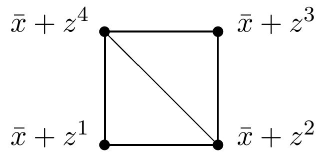
is a fine mixture of certain $f_{lmn}^{(k)}$ with volume fraction of $f_1^{(k)} = f_{412}^{(k)}$ and $f_2^{(k)} = f_{234}^{(k)}$ each $\varepsilon/2 + \mathcal{O}(\varepsilon^2)$. Sending $\varepsilon \to 0$, we deduce that

$$\frac{1}{2}(f_1 + f_2) =: H = \lim_{\varepsilon\to 0} \frac{1}{\varepsilon} \int_r^{r+\varepsilon} G(x', t)dt, \tag{17}$$

in particular,

$$\frac{1}{2}(f_1 + f_2)_{\mathrm{p}}(x', x_3) = G_{\mathrm{p}}(x', r) = G_{\mathrm{p}}(x', \bar{x}_3 - 1/2). \tag{18}$$

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

$$\bar{G}(x)(z^i) = f_1^{(k)} \cdot z^i = f_2^{(k)} \cdot z^i = H \cdot z^i. \tag{19}$$

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 $a = (0, 1/k)$. 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

$$k\left(R^T \nabla' \tilde{y}^{(k)} \circ \varphi_{1+} \cdot (z^1)' - (z^1)'\right) \tag{20}$$

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 (9) and (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 (10) and hence converges – up to subsequences – weakly to F, say. Since, by lemma A.1 and theorem 4.1, $\nabla_k \tilde{y}^{(k)} \circ \varphi_{1+} \to (\nabla' \tilde{y}, b)$ 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

$$k\left(R^T \nabla' \tilde{y}^{(k)} \circ \varphi_{1+} \cdot (z^1)' - (z^1)'\right) \rightharpoonup (f_1)_{\mathrm{p}} (z^1)' - (\nabla' \tilde{y}, b)_{,2}^T \nabla' \tilde{y} \cdot (z^1)' \quad \text{in } L^1. \tag{21}$$

On the other hand, note

$$\begin{aligned} \nabla' \tilde{y}^{(k)} \circ \varphi_{1+} \cdot (z^1)' \;=\; & \frac{1}{2}\left(\nabla' \tilde{y}^{(k)} \circ \varphi_{1+} + \nabla' \tilde{y}^{(k)} \circ \varphi_{2+}\right) \cdot (z^2)' + \nabla' \tilde{y}^{(k)} \circ \varphi_2 \cdot (z^1)' \\ & + \frac{1}{2}\left(\nabla' \tilde{y}^{(k)} \circ \varphi_1 + \nabla' \tilde{y}^{(k)} \circ \varphi_2\right) \cdot (z^4)' \end{aligned}$$

and by, (18),

$$\begin{aligned} k\left(R^T \nabla' \tilde{y}^{(k)} \circ \varphi_2 \cdot (z^1)' - (z^1)'\right) \;&\rightharpoonup\; (f_2)_{\mathrm{p}} \cdot (z^1)', \\ k\left(R^T \frac{\nabla' \tilde{y}^{(k)} \circ \varphi_1 + \nabla' \tilde{y}^{(k)} \circ \varphi_2}{2} \cdot (z^4)' - (z^4)'\right) \;&\rightharpoonup\; G_{\mathrm{p}}(x', \bar{x}_3 - 1/2) \cdot (z^4)', \\ k\left(R^T \frac{\nabla \tilde{y}^{(k)} \circ \varphi_1 + \nabla' \tilde{y}^{(k)} \circ \varphi_2}{2} \cdot (z^2)' - (z^2)'\right) \;&\rightharpoonup\; G_{\mathrm{p}}(x', \bar{x}_3 - 1/2) \cdot (z^2)' \end{aligned}$$

in L^2. Since $(z^2)' + (z^4)' = 0$, it follows that

$$k\left(R^T \nabla' \tilde{y}^{(k)} \circ \varphi_{1+} \cdot (z^1)' - (z^1)'\right) \rightharpoonup (f_2)_{\mathrm{p}} \cdot (z^1)' + g \tag{22}$$

in L^2 where g is the L^2-weak limit of

$$g^{(k)} := kR^T \left(\frac{\nabla'\tilde{y}^{(k)} \circ \varphi_{1+} + \nabla'\tilde{y}^{(k)} \circ \varphi_{2+}}{2} - \frac{\nabla'\tilde{y}^{(k)} \circ \varphi_{1} + \nabla'\tilde{y}^{(k)} \circ \varphi_{2}}{2} \right) \cdot (z^2)'.$$

To calculate g, note 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. Again restricting to Ω_ε, we see that the limit of $R^{(k)}g^{(k)}$ equals (up to $\mathcal{O}(\varepsilon)$ since $\|\bar{\nabla}_k \tilde{y}^{(k)} \circ \varphi_{lmn} - \bar{\nabla}_k \tilde{y}^{(k)} \circ \varphi_{l'm'n'}\|_{L^2} \leq C\|\nabla_k \tilde{y}^{(k)} - R\|_{L^2} \leq C/k$) the limit of

$$k\nabla'\tilde{y}^{(k)}(x+a) \cdot (z^2)' - k\nabla'\tilde{y}^{(k)}(x) \cdot (z^2)'$$

as $k \to \infty$. Using that the $\tilde{y}^{(k)}$ are Lipschitz mappings we can write

$$\tilde{y}^{(k)}(x+a) - \tilde{y}^{(k)}(x) = \int_0^1 \frac{d}{dt}\tilde{y}^{(k)}(x+ta)dt = \int_0^1 \nabla'\tilde{y}^{(k)}(x+ta) \cdot a dt$$

for a.e. x. But $\int_0^1 \nabla'\tilde{y}^{(k)}(x+ta) \to \nabla'\tilde{y}(x)$ in L^2 and $ka \equiv (0,1)$, so

$$\nabla' \left(k \int_0^1 \nabla'\tilde{y}^{(k)}(x+ta) a dt \right) \cdot (z^2)' \rightharpoonup (\nabla')^2 \tilde{y}(x)((0,1),(z^2)') \quad \text{in } W^{-1,2}.$$

Sending $\varepsilon \to 0$, it follows that

$$g = \frac{1}{2}(\nabla'\tilde{y}, b)^T (\nabla')^2 \tilde{y}((0,1),(1,-1)) = \frac{1}{2}(\nabla'\tilde{y}, b)^T \left(\tilde{y}_{,21} - \tilde{y}_{,22}\right).$$

Together with (21) and (22) this shows that

$$(f_1)_{\mathrm{p}} \cdot (z^1)' - (\nabla'\tilde{y}, b)^T_{,2} \nabla'\tilde{y} \cdot (z^1)' = (f_2)_{\mathrm{p}} \cdot (z^1)' + \frac{1}{2}(\nabla'\tilde{y}, b)^T \left(\tilde{y}_{,21} - \tilde{y}_{,22}\right). \quad (23)$$

Since $S \subset\subset S$ was arbitrary, this equality holds in all of Ω.

Now elementary calculations for $(\nabla'\tilde{y}, b) \in SO(3)$, $\tilde{y} \in W^{2,2}$, show that $(\nabla'\tilde{y}, b)^T (\tilde{y}_{,21} - \tilde{y}_{,22}) = (0,0,-\mathrm{II}_{21} + \mathrm{II}_{22})^T$ 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 (23) reduces to

$$(f_1 - f_2) \cdot z^1 = \begin{pmatrix} 0 \\ 0 \\ -\mathrm{II}_{12} \end{pmatrix}.$$

Together with (17) it follows that

$$f_1 \cdot z^1 = \frac{1}{2}\left((f_1 + f_2) \cdot z^1 + (f_1 - f_2) \cdot z^1\right) = H \cdot z^1 - \frac{1}{2} \begin{pmatrix} 0 \\ 0 \\ \mathrm{II}_{12} \end{pmatrix} \quad (24)$$

and

$$\begin{aligned} f_2 z^3 &= \frac{1}{2}\left((f_2 + f_1) \cdot z^3 + (f_2 - f_1) \cdot z^3\right) \\ &= H \cdot z^3 + \frac{1}{2}(f_1 - f_2) \cdot z^1 = H \cdot z^3 - \frac{1}{2} \begin{pmatrix} 0 \\ 0 \\ \mathrm{II}_{12} \end{pmatrix}. \quad (25) \end{aligned}$$

Summarizing (17), (18), (19), (24) and (25), the lemma is proven for $i = 1, 2, 3, 4$. Replacing z^i by z^{i+4}, $\fint_r^{r+\varepsilon}$ by $\fint_{r+1-\varepsilon}^{r+1}$ 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 5.2:

Proof of theorem 5.2 (i). Following [11], 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 $W_{\rm cell}$ is C^2 in a neighborhood of $\bar{\rm Id}$, there is $\omega(t) \ge 0$ such that for $\bar{A} \in \mathbb{R}^{3\times 8}$

$$W_{\rm cell}(\bar{\rm Id} + \bar{A}) \ge \frac{1}{2} Q_3(\bar{A}) - \omega(|\bar{A}|)$$

and $\omega(t)/t^2 \to 0$ as $t \to 0$. Analogously, if $\bar{x}$ lies in the top or bottom film layer,

$$W_{\rm surf}(\bar{x}, \bar{\rm Id}_{\rm b/t} + \bar{A}_{\rm b/t}) \ge \frac{1}{2} Q_2(\bar{A}_{\rm b/t}) - \omega(|\bar{A}|).$$

Therefore summing over those cubes that do not have lateral boundary faces ($\Omega_k = S_k \times (-\nu/2, \nu/2)$, $S_k = \{x \in S : \operatorname{dist}(x', \partial S) \ge 1/k)$,

$$\begin{aligned}
E(y^{(k)}) &\ge \sum_{\bar{x}} W(\bar{x}, \vec{y}^{(k)}(x)) \\
&= \sum_{\bar{x}} W\left(\bar{x}, (R^{(k)})^T(\bar{x}) \bar{\nabla}_k \tilde{y}^{(k)}(\bar{x})\right) \\
&\ge k^2 \int_{\Omega_k} \chi_k W_{\rm cell}\left(\bar{\rm Id} + \frac{1}{k}\bar{G}^{(k)}(x)\right) dx \\
&\quad + k^2 \int_{S_k} \chi_k W_{\rm surf}\left(\bar{\rm Id}_{\rm t} + \frac{1}{k}\bar{G}^{(k)}_{\rm t}(x', \nu/2)\right) dx' \\
&\quad + k^2 \int_{S_k} \chi_k W_{\rm surf}\left(\bar{\rm Id}_{\rm b} + \frac{1}{k}\bar{G}^{(k)}_{\rm b}(x', -\nu/2)\right) dx' \\
&\ge \frac{1}{2} \int_{\Omega_k} Q_3\left(\chi_k \bar{G}^{(k)}\right) - k^2 \chi_k \omega\left(\left|\frac{1}{k}\bar{G}^{(k)}\right|\right)\, dx \\
&\quad + \frac{1}{2} \int_{S_k} Q_2\left(\chi_k \bar{G}^{(k)}_{\rm t}(x', \nu/2)\right) - k^2 \chi_k \omega\left(\left|\frac{1}{k}\bar{G}^{(k)}(x', \nu/2)\right|\right)\, dx' \\
&\quad + \frac{1}{2} \int_{S_k} Q_2\left(\chi_k \bar{G}^{(k)}_{\rm b}(x', -\nu/2)\right) - k^2 \chi_k \omega\left(\left|\frac{1}{k}\bar{G}^{(k)}(x', -\nu/2)\right|\right)\, dx'.
\end{aligned}$$

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 $A \mapsto Q_3(A)$ and $A \mapsto Q_3(A) + Q_2(A_{\rm b/t})$, respectively $A \mapsto Q_3(A) + Q_2(A_{\rm b}) + Q_2(A_{\rm t})$ if $\nu = 1$, are positive semidefinite. So from lower semicontinuity we deduce

$$\begin{aligned}
\liminf_{k\to\infty} E(y^{(k)}) &\ge \frac{1}{2} \int_\Omega Q_3(\bar{G}) + \frac{1}{2} \int_S Q_2(\bar{G}_{\rm t}(\cdot, \nu/2)) + Q_2(\bar{G}_{\rm b}(\cdot, -\nu/2)) \\
&\ge \frac{1}{2} \int_\Omega Q_3^{\rm rel}(\bar{G}) + \frac{1}{2} \int_S Q_2(\bar{G}_{\rm t}(\cdot, \nu/2)) + Q_2(\bar{G}_{\rm b}(\cdot, -\nu/2)). \qquad (26)
\end{aligned}$$

Now by lemma 5.3 and (16), $\bar{G}(x)(z^i) = H(x, z_3^i) \cdot z^i - \frac{1}{2}\mathrm{II}_{12}M(z^i)$ with $H_\mathrm{p}(x, z_3^i) = G_\mathrm{p}(x', 0) + (\bar{x}_3 + z_3^i)N$. So by assumptions on Q_3 and definition of Q_3^rel,

$$Q_3^\mathrm{rel}(\bar{G}(x)(\vec{z})) = Q_3^\mathrm{rel}(G_\mathrm{p}^0(x', 0) \cdot \vec{z}\,' + (\bar{x}_3 + z_3)N \cdot \vec{z}\,' - \frac{1}{2}\mathrm{II}_{12}M)$$

where $z_3 N \cdot \vec{z}\,'$ is understood as $(-\frac{1}{2}N\vec{z}_\mathrm{b}', \frac{1}{2}N\vec{z}_\mathrm{t}')$ and G_p^0 denotes the matrix G_p whose last row is replaced by $(0, 0)$. Integrating over x_3 we obtain

$$\begin{aligned}
\int_{-\nu/2}^{\nu/2} Q_3^\mathrm{rel}(\bar{G}(x)(\vec{z}))dx_3 &= \nu Q_3^\mathrm{rel}\left(G_\mathrm{p}'(x', 0) \cdot \vec{z}\,' - \frac{1}{2}\mathrm{II}_{12}M + z_3 N \cdot \vec{z}\,'\right) \\
&\quad + \sum_{\bar{x}_3 = -\nu/2+1/2}^{\nu/2-1/2} \bar{x}_3^2 Q_3^\mathrm{rel}\left(N \cdot \vec{z}\,'\right) \\
&= \nu Q_3^\mathrm{rel}\left(G_\mathrm{p}(x', 0) \cdot \vec{z}\,' - \frac{1}{2}\mathrm{II}_{12}M + \frac{1}{2}N \cdot \vec{z}_-'\right) \\
&\quad + \frac{\nu^3 - \nu}{12} Q_3^\mathrm{rel}\left(N \cdot \vec{z}\,'\right). \qquad (27)
\end{aligned}$$

By up-down-symmetry, $Q_3^\mathrm{rel}(G_\mathrm{p}^0(x', 0) \cdot \vec{z}\,' + M) = Q_3^\mathrm{rel}(G_\mathrm{p}^0(x', 0) \cdot \vec{z}\,' - M)$ and $Q_3^\mathrm{rel}(G_\mathrm{p}^0(x', 0) \cdot \vec{z}\,' + N \cdot \vec{z}_-') = Q_3^\mathrm{rel}(G_\mathrm{p}^0(x', 0) \cdot \vec{z}\,' - N \cdot \vec{z}_-')$, so the first term of the last expression equals

$$\nu Q_3^\mathrm{rel}\left(G_\mathrm{p}^0(x', 0) \cdot \vec{z}\right) + \nu Q_3^\mathrm{rel}\left(-\frac{\mathrm{II}_{12}}{2}M + \frac{1}{2}N \cdot \vec{z}_-'\right). \qquad (28)$$

For the surface terms we obtain

$$Q_2(\bar{G}_\mathrm{t/b}(\cdot, \pm\nu/2)) = Q_2(G_\mathrm{p}^0(x', 0)\vec{z}_\mathrm{t/b}' \pm \frac{\nu}{2}N \cdot \vec{z}_\mathrm{t/b}' - \frac{1}{2}\mathrm{II}_{12}M_\mathrm{t/b})$$

and therefore (note $M_\mathrm{t} = M_\mathrm{b}$ and $\vec{z}_\mathrm{t}' = \vec{z}_\mathrm{b}'$)

$$\begin{aligned}
&Q_2(\bar{G}_\mathrm{t}(\cdot, \nu/2)) + Q_2(\bar{G}_\mathrm{b}(\cdot, -\nu/2)) \\
&= 2Q_2\left(G_\mathrm{p}^0(x', 0)\vec{z}_\mathrm{b}' - \frac{1}{2}\mathrm{II}_{12}M_\mathrm{b}\right) + \frac{\nu^2}{2}Q_2\left(N \cdot \vec{z}_\mathrm{b}'\right) \\
&= 2Q_2\left(G_\mathrm{p}^0(x', 0)\vec{z}_\mathrm{b}'\right) + 2Q_2\left(\frac{1}{2}\mathrm{II}_{12}M_\mathrm{b}\right) + \frac{\nu^2}{2}Q_2\left(N \cdot \vec{z}_\mathrm{b}'\right) \qquad (29)
\end{aligned}$$

where the last step again follows from assumption 5.1.

Dropping the non-negative term $\nu Q_3(G_\mathrm{p}^0(x', 0) \cdot \vec{z}\,') + 2Q_2(G_\mathrm{p}^0(x', 0)\vec{z}_\mathrm{b}')$ we deduce from (26), (27), (28) and (29)

$$\begin{aligned}
\liminf_{k\to\infty} E(y^{(k)}) \;\geq\; &\int_S \frac{\nu^3 - \nu}{24} Q_3^\mathrm{rel}\left(N \cdot \vec{z}\,'\right) + \frac{\nu}{8}Q_3^\mathrm{rel}\left(-\mathrm{II}_{12}M + N \cdot \vec{z}_-'\right) \\
&+ \int_S Q_2\left(\frac{1}{2}\mathrm{II}_{12}M_\mathrm{b}\right) + \frac{\nu^2}{4}Q_2\left(N \cdot \vec{z}_\mathrm{b}'\right).
\end{aligned}$$

□

5.2 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

$$\underline{f}(x) = \fint_{(0,1/k)^2} f(\mu(x_0 + \xi))d\xi = \fint_{\mu x_0 + (0,\mu/k)^2} f(\xi)d\xi \tag{30}$$

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 5.4 and 5.5 is straight forward.

Lemma 5.4 *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*) by piecewise constancy of* $\underline{f_k}$,

$$\frac{1}{k^2} \sum_{x \in \frac{1}{k}\mathbb{Z}^2 \cap S} \left| \underline{f_k}(x) - \fint_{x + (-1/2k, 1/2k)^2} f(\xi)d\xi \right|^2 \to 0.$$

(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

$$\frac{1}{k^2}\sum_{x_0} \left| \fint_{(0,1/k)^2} k^2 \Big(f_k(\mu(x_0 + a/k + \xi)) - f_k(\mu(x_0 + \xi)) \right.$$
$$\left. - \frac{1}{k}\nabla f_k(\mu(x_0 + \xi)) \cdot a \Big) - \frac{1}{2}\nabla^2 f(\mu(x_0 + \xi))(a,a)\ d\xi \right|^2 \to 0$$

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., [23]). The claim then follows from lemma A.2. $\square$

For $\tilde{y} \notin \mathcal{A}$ the upper bound is trivial, so assume $\tilde{y} \in \mathcal{A}$ and set $b = \tilde{y}_{,1} \wedge \tilde{y}_{,2}$. As shown in [11] (cf. page 1484), we may choose approximations $\tilde{y}^\lambda \in W^{2,\infty}$ and $b^\lambda \in W^{1,\infty}$ 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

$$S^\lambda = \{x \in \mathbb{R}^2 : \tilde{y}(x) \neq \tilde{y}^\lambda(x) \text{ or } b(x) \neq b^\lambda(x)\} \quad \text{and} \quad \omega(\lambda) \to 0 \text{ as } \lambda \to \infty.$$

Furthermore, as shown in [11]:

$$\|\operatorname{dist}((\nabla' \tilde{y}^\lambda, b^\lambda), SO(3))\|_{L^\infty} \le C\sqrt{\omega(\lambda)}. \tag{31}$$

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 5.5 *With this choice of λ we have:*

(i) $\|\tilde{y}^\lambda - \tilde{y}\|_{W^{2,2}(S)},\ \|b^\lambda - b\|_{W^{1,2}(S)} \to 0,$

(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

$$\|\tilde{y}^\lambda - \tilde{y}\|^2_{W^{2,2}} \le C \int_{\{\tilde{y}^\lambda \neq \tilde{y}\}} |\nabla^2 \tilde{y}^\lambda - \nabla^2 \tilde{y}|^2 \le C \int_{S^\lambda} |\nabla^2 \tilde{y}|^2 + \omega(\lambda) \to 0.$$

The same argument shows $\|b^\lambda - b\|_{W^{1,2}} \to 0$.

Now since both $(\nabla' \tilde{y}, b)$ and $(\nabla' \tilde{y}^\lambda, b^\lambda)$ are bounded (cf. (31)), we have

$$\|\underline{(\nabla' \tilde{y}, b)} - \underline{(\nabla' \tilde{y}^\lambda, b^\lambda)}\|^2_{L^2} \le \mu^{-2}\|(\nabla' \tilde{y}, b) - (\nabla' \tilde{y}^\lambda, b^\lambda)\|^2_{L^2} \le C|S^\lambda| = o(1/k^2).$$

$\square$

Before defining our upper bound trial function, we prove one more preparatory lemma.

Lemma 5.6 *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 $\|\operatorname{dist}(f, SO(3))\|_{L^\infty} \le C\sqrt{\omega(\lambda)}$ by (31), 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 all x.

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 by 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 5.5, 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. $\square$

Now let $d \in C^1(\overline{\Omega})$ and consider the trial function

$$\tilde{y}^{(k)}(x', x_3) = \underline{\tilde{y}^\lambda}(x') + \frac{1}{k}x_3\underline{b^\lambda}(x') + \frac{1}{k^2}d(x', x_3). \tag{32}$$

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 5.2 (ii). First note that by lemma 5.5 (i) and lemma 5.4 (i), $\tilde{y}^{(k)} \to \tilde{y}$ in the sense of definition 2.1.

Instead of $\bar{\nabla}_k\tilde{y}^{(k)}$, it is more convenient to calculate the discrete gradient

$$\bar{D}_k\tilde{y}^{(k)}(x)(a) = k\left(y(\hat{x} + (a'/k, a_3)) - y(\hat{x})\right)$$

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 5.4, 5.5 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.3 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 $\|\underline{f}\|_{L^\infty} \le \|f\|_{L^\infty}$). 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 5.6, 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 we can proceed:

$$\begin{aligned} E(\tilde{y}^{(k)}) &= k^2\int_\Omega W(\bar{x}, \bar{D}_k\tilde{y}^{(k)}) = k^2\int_\Omega W(\bar{x}, U^T\bar{D}_k\tilde{y}^{(k)}) \\ &= k^2\int_\Omega W\left(\bar{x}, \bar{\mathrm{Id}} + U^T\frac{1}{k}F^{(k)}\right) \end{aligned}$$

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 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

$$0, \quad -\frac{1}{2}\mathrm{II}_{11}, \quad -\frac{1}{2}\left(\mathrm{II}_{11} + \mathrm{II}_{12} + \mathrm{II}_{21} + \mathrm{II}_{22}\right), \qquad \text{resp.} \qquad -\frac{1}{2}\mathrm{II}_{22}.$$

For the remaining part we obtain, with $z = a - (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})^T$,

$$\begin{aligned}
&(\nabla'\tilde{y}, b)^T(x')\Big((\bar{x}_3 + z_3)\nabla' b(x')((1/2, 1/2)^T + z') + d(x', \hat{x}_3 + \zeta_3) - d(x', \hat{x}_3)\Big) \\
&\quad = \ (\bar{x}_3 + z_3)N \cdot z' + z_3 N \cdot (1/2, 1/2)^T + (\nabla' y, b)^T e(x', \bar{x}_3)
\end{aligned}$$

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 $\beta_1 = \mathrm{II}_{12} + \mathrm{II}_{11}$, $\beta_2 = \mathrm{II}_{12} + \mathrm{II}_{22}$, $\beta_3 = \frac{\mathrm{II}_{11} + \mathrm{II}_{22}}{4}$, $v = (\nabla' y, b)^T \bar{x}_3 \nabla' b(x') \cdot (1/2, 1/2)^T$. After some elementary calculations we obtain

$$\begin{aligned}
&B(x)(z^i) + (\nabla'\tilde{y}, b)^T(x')F(x)(z^i) \\
&\quad = \ \frac{-\mathrm{II}_{12}}{2} M(z^i) + (\bar{x}_3 + z_3)N \cdot (z^i)' + (\nabla' y, b)^T\left(d(x', \hat{x}_3 + \zeta_3) - d(x', \hat{x}_3)\right).
\end{aligned}$$

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 $m = (0,0,0,0,1,1,1,1)^T \in \mathbb{R}^8$)

$$\begin{aligned}
E(\tilde{y}^{(k)}) \ \to \ \int_\Omega \frac{1}{2} Q_3\Big(&\bar{x}, \frac{-\mathrm{II}_{12}}{2} M + \frac{1}{2} N \cdot \vec{z}_-' + (\nabla' y, b)^T d^1 \otimes m \\
&+ \bar{x}_3 N \cdot \vec{z}' + \bar{x}_3 (\nabla' y, b)^T d^2 \otimes m\Big)
\end{aligned}$$

$$
\begin{aligned}
= \int_S \Bigg[& \frac{\nu}{8} Q_3 \Big(-\mathrm{II}_{12} M + N \cdot \vec{z}_-' + 2(\nabla' y, b)^T d^1 \otimes m \Big) \\
& + \frac{\nu^3 - \nu}{24} Q_3 \Big(N \cdot \vec{z}\,' + (\nabla' y, b)^T d^2 \otimes m \Big) \\
& + \frac{1}{2} Q_2 \left(-\frac{\mathrm{II}_{12}}{2} M_\mathrm{t} + \frac{\nu}{2} N \vec{z}_\mathrm{t}' \right) + \frac{1}{2} Q_2 \left(-\frac{\mathrm{II}_{12}}{2} M_\mathrm{b} - \frac{\nu}{2} N \vec{z}_\mathrm{b}' \right) \Bigg].
\end{aligned}
$$

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

$$
d^1_{\min} := \operatorname{argmin} Q_3 \Big(-\mathrm{II}_{12} M + N \cdot \vec{z}_-' + 2(\nabla' y, b)^T d^1 \otimes m \Big) \in L^2
$$

resp.

$$
d^2_{\min} := \operatorname{argmin} Q_3 \Big(N \cdot \vec{z}\,' + (\nabla' y, b)^T d^2 \otimes m \Big) \in L^2.
$$

This finishes the proof. □

6 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 5.2 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 3.1 and 5.1.

Theorem 6.1 *(Limiting plate theory for thick films.) For $k \to \infty$, $\nu \to \infty$ 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 $y^{(k)} \to \tilde{y}$ in the sense of definition 2.1, then

$$
\liminf_{k \to \infty} E(y^{(k)}) \ge E_\mathrm{thick}(\tilde{y}).
$$

(ii) For all $\tilde{y} \in L^2(\Omega)$ there exists a sequence $y^{(k)} : \Lambda_k \to \mathbb{R}^3$ with $y^{(k)} \to \tilde{y}$ in the sense of definition 2.1 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 5.2.

Remark. In [6] it is shown that the Cauchy-Born rule holds near $SO(3)$ for bulk material if assumption 3.1 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 [11], we recover the formula of nonlinear bending energy derived in [11] 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.

6.1 Proof of the lower bound

Let $h := \frac{\nu}{k}$. Analogously to subsection 5.1, we consider $G^{k,\nu} : \Omega \to \mathbb{R}^{3\times 3}$ with

$$G^{k,\nu} = \frac{1}{h}((R^{(k)})^T \nabla_{k,\nu} \tilde{y}^{(k)} - \text{Id})$$

and the piecewise constant mapping $\bar{G}^{k,\nu} : \Omega \to \mathbb{R}^{3\times 8}$ defined by

$$\bar{G}^{k,\nu} = \frac{1}{h}((R^{(k)})^T \bar{\nabla}_{k,\nu} \tilde{y}^{(k)} - \bar{\text{Id}})$$

where $\nabla_{k,\nu}\tilde{y}^{(k)}$ and $\bar{\nabla}_{k,\nu}\tilde{y}^{(k)}$ are defined as in (6) and (8). As before (cf. theorem 3.3 resp. (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 (16).

Lemma 6.2 *There is $v \in L^2(\Omega;\mathbb{R}^3)$ such that for $i = 1,\ldots,8$,*

$$\bar{G}(x)(z^i) = \bar{G}(z^1) + (G_{\text{p}}|v) \cdot (z^i - z^1).$$

Having proven this lemma, we immediately can prove the first part of theorem 6.1:

Proof of theorem 6.1 (i). Simply note that by a similar reasoning as before,

$$\begin{aligned}
\liminf_{\nu,k\to\infty} \frac{1}{\nu^3} E(y^{(k)}) &= \liminf_{\nu,k\to\infty} \frac{1}{\nu^3} k^2 \nu h^2 \Bigg(\int_\Omega \frac{1}{2} Q_3(\bar{G}) \\
&\qquad + \int_S \Bigg(\int_{\frac{1}{2}-\frac{1}{\nu}}^{\frac{1}{2}} \frac{1}{2} Q_2(\bar{G}_{\text{t}}) + \int_{\frac{1}{2}}^{\frac{1}{2}+\frac{1}{\nu}} \frac{1}{2} Q_2(\bar{G}_{\text{b}}) \Bigg) \Bigg) \\
&\geq \frac{1}{2} \int_\Omega Q^{\text{rel}}_3(G_{\text{p}}(x',0) \cdot \vec{z}\,' + x_3 N \cdot \vec{z}\,') \\
&\geq \frac{1}{24} \int_S Q^{\text{rel}}_3(N \cdot \vec{z}\,')
\end{aligned}$$

because subtracting $\bar{G}(z^1)$ in each column does not alter the value of Q_3. $\square$

Proof of lemma 6.2. 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

$$\begin{aligned}
& k\left(\tilde{y}^{(k)}(\bar{x} + ((z^i)'/k, z_3^i/\nu)) - \tilde{y}^{(k)}(\bar{x})\right) - \fint_Q \nabla'\tilde{y}^{(k)}(\xi)d\xi \cdot (z^i)' \\
&= k\left(\tilde{y}^{(k)}(\bar{x}_+ + ((z^1)'/k, z_3^1/\nu)) - \tilde{y}^{(k)}(\bar{x}_+)\right) - \fint_Q \nabla'\tilde{y}^{(k)}(\xi)d\xi \cdot (z^1)' \\
&\quad + k\left(\tilde{y}^{(k)}(\bar{x}_+) - \tilde{y}^{(k)}(\bar{x})\right) + \fint_Q \nabla'\tilde{y}^{(k)}(\xi)d\xi \cdot (z^1 - z^i)'. \qquad (33)
\end{aligned}$$

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 $\tilde{Q}(x)$, (33) can be rewritten as

$$\bar{\nabla}_{k,\nu}\tilde{y}^{(k)}(x)(z^i) - \bar{\nabla}_{k,\nu}\tilde{y}^{(k)}(x_+)(z^1) = \fint_{\tilde{Q}(x)} \nabla'\tilde{y}^{(k)}(\xi) \cdot (z^i - z^1)' + f(x) \cdot (z^i - z^1)'. \qquad (34)$$

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 (11) and – note that φ has compact support – (12). Summarizing, this proves that $\frac{1}{h}f \to 0$ in distributions.

Define

$$\bar{G}_+^{(k)}(x) = \frac{1}{h}\left(R^T(x')\bar{\nabla}_{k,\nu}\tilde{y}^{(k)}(x_+) - \bar{\mathrm{Id}} \right).$$

Then from

$$\frac{1}{h}\left(R^T(x'_+)\bar{\nabla}_{k,\nu}\tilde{y}^{(k)}(x_+) - \bar{\mathrm{Id}} \right) \rightharpoonup \bar{G}$$

and

$$\frac{1}{h}\left(R^T(x'_+) - R^T(x') \right) \bar{\nabla}_{k,\nu}\tilde{y}^{(k)}(x_+) \rightharpoonup 0,$$

it follows

$$\bar{G}_+^{(k)} \rightharpoonup \bar{G} \tag{35}$$

on $\Omega' = S' \times (\nu/2, \nu/2) \subset \Omega$ with $S' \subset\subset S$. (Note that $R^{(k)}$ being constant on squares of side-length h implies

$$\begin{aligned} \left\| \frac{1}{h}(R^T(x'_+) - R^T(x')) \right\|_{L^2}^2 &\le \frac{C/k}{h} \left\| \frac{1}{h} \max_{|\zeta| \le 2h} |R^T(x'+\zeta) - R^T(x')| \right\|_{L^2}^2 \\ &\le \frac{C}{\nu} \quad \text{(by (10))} \\ &\to 0.) \end{aligned}$$

Now by (34), the fact that $\frac{1}{h}f \to 0$ in distributions, and $(z^i - z^1)_3 = 0$, we have

$$\begin{aligned} & R^{(k)}\left(\bar{G}^{(k)}(z^i) - \bar{G}_+^{(k)}(z^1) - \frac{1}{h}\left((R^{(k)})^T \fint_{\tilde{Q}(x)} \nabla\tilde{y}^{(k)}(\xi) - \mathrm{Id} \right) \cdot (z^i - z^1) \right) \\ &= \frac{1}{h}\left(R^{(k)}(h\bar{G}^{(k)}(z^i) + z^i) - R^{(k)}(h\bar{G}_+^{(k)}(z^1) + z^1) - \fint_{\tilde{Q}(x)} \nabla\tilde{y}^{(k)}(\xi) \cdot (z^i - z^1) \right) \\ &= \frac{1}{h}\left(\bar{\nabla}_{k,\nu}(x)\tilde{y}^{(k)}(z^i) - \bar{\nabla}_{k,\nu}\tilde{y}^{(k)}(x_+)(z^1) - \fint_{\tilde{Q}(x)} \nabla'\tilde{y}^{(k)}(\xi) \cdot (z^i - z^1)' \right) \\ &= \frac{1}{h}f(x) \cdot (z^i - z^1)' \\ &\to 0 \end{aligned}$$

in distributions.

On the other hand, we have for the individual terms $R^{(k)} \to (\nabla'y, b)$ boundedly in measure, $\bar{G}^{(k)}, \bar{G}_+^{(k)} \rightharpoonup \bar{G}$ in $L^2(\Omega')$ by (35), and

$$\frac{1}{h}\left((R^{(k)})^T \fint_{Q(x)} \nabla\tilde{y}^{(k)}(\xi) - \mathrm{Id} \right) = \fint_{Q(x)} G^{(k)} \rightharpoonup G(x) \quad \text{in } L^2.$$

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 $i \in \{1,\dots,8\}$. $\square$

6.2 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 $\tilde{y}^\lambda \in W^{2,\infty}(S)$, $b^\lambda \in W^{1,\infty}(S)$ 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 (30).)

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 5.5 and 5.6 for thick films is the following

Lemma 6.3 *(i)* $\|\tilde{y}^\lambda - \tilde{y}\|_{W^{2,2}},\ \|b^\lambda - b\|_{W^{1,2}} \to 0$.

(ii) $h^{-1}\|\underline{(\nabla'\tilde{y}, b)} - \underline{(\nabla'\tilde{y}^\lambda, b^\lambda)}\|_{L^2} \to 0$.

(iii) $\underline{(\nabla'\tilde{y}^\lambda, b^\lambda)} - U \to 0$ *in* L^∞.

(iv) $h^{-1}\left(\underline{(\nabla'\tilde{y}^\lambda, b^\lambda)} - U\right) \to 0$ *in* L^2.

The proof is similar to the proofs of lemma 5.5 and lemma 5.6. The necessary modifications are straight forward.

We can now estimate the energy of our trial function:

Proof of theorem 6.1 (ii). By lemmas 5.4 and 6.3, $y^{(k)} \to \tilde{y}$. 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 $x \in \hat{x} + (0,1/k)^2 \times (0,1/\nu) \subset \Omega$, $\zeta = (a'/k, a_3/\nu)$, and $a \in \{0,1\}^3$ as before.

Now using lemmas 5.4, 6.3 and 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.3 (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,

$$\begin{aligned} &\frac{1}{h}\left(\bar{D}\tilde{y}^{(k)}(x)(a) - \underline{(\nabla'\tilde{y}^{\lambda}, b^{\lambda})}(x')\cdot a\right) \\ &\quad = \frac{k}{h}\left(\underline{\tilde{y}^{\lambda}}(x'+\zeta') - \underline{\tilde{y}^{\lambda}}(x') - \underline{\nabla'\tilde{y}^{\lambda}}(x')a'/k\right) \\ &\qquad +k\left((\hat{x}_3+\zeta_3)\underline{b^{\lambda}}(x'+\zeta') - \hat{x}_3\underline{b^{\lambda}}(x') - \zeta_3\underline{b^{\lambda}}(x')\right) \\ &\qquad +kh\left(d(\hat{x}+\zeta) - d(\hat{x})\right) \\ &\quad \to x_3\nabla'b(x')a' + d_{,3}(x',x_3)\delta_{a_3 1} \end{aligned}$$

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 6.3 we may replace $\underline{(\nabla'\tilde{y}^{\lambda}, b^{\lambda})}$ by U and find

$$E(\tilde{y}^{(k)}) = k^2\nu\int_\Omega W(\bar{x}, U^T\bar{D}_k\tilde{y}^{(k)}) = k^2\nu\int_\Omega W\left(\bar{x}, \bar{\mathrm{Id}} + U^ThF^{(k)}\right)$$

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 $C^1(\overline{S})$ in $L^2(S)$ and continuity of the above term in d in L^2, we may replace d by

$$
d_{\min} := \operatorname{argmin} Q_3 \Big(N \cdot \vec{z}\,' + (\nabla' y, b)^T d \otimes m \Big) \in L^2.
$$

This finishes the proof. □

7 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 [14] 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 $\chi(\vec{y})$ is assumed to be non-zero only for deformations which are not locally orientation preserving, in particular it is zero in a neighborhood of $\bar{SO}(3)$ and positive ($\geq c > 0$) on $\bar{O}(3) \setminus \bar{SO}(3)$.

Proposition 7.1 *For any values of $K_1, K_2 \in (0, \infty)$, E_{ms} is an admissible energy function, i.e. satisfies assumptions 3.1 and 5.1.*

Proof. To see that E_{ms} can be written in the form (1), for $\vec{y} = y(\vec{z})$ we define the cell energy

$$\begin{aligned} W_{\rm cell}(\vec{y}) &= \frac{1}{8} \sum_{|z^j - z^i| = 1} \frac{K_1}{2} (|y(z^j) - y(z^i)| - 1)^2 \\ &\quad + \frac{1}{4} \sum_{|z^j - z^i| = \sqrt{2}} \frac{K_2}{2} (|y(z^j) - y(z^i)| - \sqrt{2})^2 + \chi(\vec{y}) \end{aligned}$$

and the surface energy

$$\begin{aligned} W_{\rm surf}(y_1, \ldots, y_4) &= \frac{1}{4} \sum_{\substack{1 \le i \le 4 \\ j = i+1 \mod 4}} \frac{K_1}{2} (|y_j - y_i| - 1)^2 \\ &\quad + \frac{1}{2} \sum_{\substack{1 \le i \le 2 \\ j = i+2}} \frac{K_2}{2} (|y_j - y_i| - \sqrt{2})^2. \end{aligned}$$

For cubes with lateral boundary faces, $W_{\rm surface}$ is defined appropriately.

Now assumption 5.1 on $W_{\rm cell}$ and $W_{\rm surf}$ and assumptions 3.1 (i) and (iv) on $W(\bar{x}, \cdot)$ are easily seen to be satisfied. Also $W(\bar{x}, \cdot) \ge 0$ being C^2 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 $W_{\rm surface} \ge 0$ is zero on rotations and translations. □

A Analytical lemmas

For ease of reference we state here three analytical lemmas in the particular form they were used in the previous sections. The content of these lemmas is standard, for sake of completeness we include their (rather short) proofs.

Lemma A.1 *Suppose $S_1 \subset \mathbb{R}^{n_1}$, $S_2 \subset \mathbb{R}^{n_2}$ are 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 $\varphi_k : S_1 \times S_2 \to S_1 \times S_2$ 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 density $d\varphi_k(\lambda)/d\lambda$ is 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 $\|f_k - f\|_{L^2} \le \varepsilon/4\sqrt{C}$. Then also

$$\begin{aligned} \|f_k \circ \varphi_k - f^\varepsilon \circ \varphi_k\|_{L^2} &= \left(\int_{S_1 \times S_2} |f_k(\varphi_k(x)) - f^\varepsilon(\varphi_k(x))|^2 d\lambda \right)^{1/2} \\ &= \left(\int_{\varphi_k(S_1 \times S_2)} |f_k(x) - f^\varepsilon(x)|^2 d\varphi_k(\lambda) \right)^{1/2} \\ &\le \sqrt{C} \left(\int_{S_1 \times S_2} |f_k(x) - f^\varepsilon(x)|^2 d\lambda \right)^{1/2} \\ &\le \varepsilon/2. \end{aligned}$$

If necessary enlarging k, it follows that

$$\|f_k \circ \varphi_k - f\|_{L^2} \le \varepsilon/2 + \|f^\varepsilon \circ \varphi_k - f^\varepsilon\|_{L^2} + \varepsilon/4 \le \varepsilon.$$

$\square$

Lemma A.2 *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. $f, f_h \in H^2(\mathbb{R}^n)$, $f_h \to f$ 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

$$A_h f(x) \to \frac{1}{2}\nabla^2 f(x)(a,a) \quad \text{uniformly} \tag{36}$$

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,

$$\int_{R^n} |A_h f(x) - A_h g(x)|^2 dx \le \frac{1}{3}\|\nabla^2 f(a,a) - \nabla^2 g(a,a)\|_{L^2}^2. \tag{37}$$

By approximation this estimate holds for all $f, g \in H^2$.

Now given $f \in H^2$ choose g smooth with $\|f-g\|_{H^2} \le \varepsilon$. Choosing h sufficiently small, we have $\|\nabla^2 f_h - \nabla^2 f\|_{L^2} \le \varepsilon$ and, by (36), $\|A_h g - \frac{1}{2}\nabla^2 g(a,a)\| \le \varepsilon$. By (37) then

$$\begin{aligned} \|A_h f_h - \frac{1}{2}\nabla^2 f\| &\le \|A_h f_h - A_h g\| + \|A_h g - \frac{1}{2}\nabla^2 g(a,a)\| \\ &\quad + \frac{1}{2}\|\nabla^2 g(a,a) - \nabla^2 f(a,a)\| \\ &\le 3\varepsilon. \end{aligned}$$

$\square$

Lemma A.3 *In addition to the hypotheses of the previous lemma suppose that*

$$\tilde{h}\|\nabla f_h\|_{L^\infty} \to 0 \qquad \textit{resp.} \qquad \tilde{h}\|\nabla^2 f_h\|_{L^\infty} \to 0$$

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 $f_h \in W^{1,\infty}$,

$$\frac{\tilde{h}}{h}\left|f_h(x+ha) - f(x)\right| \le \frac{\tilde{h}}{h}\|\nabla f_h\|_{L^\infty}|ha| \to 0.$$

For $f_h \in W^{2,\infty} \subset C^1$ we calculate

$$\begin{aligned}
|\tilde{h} A_h^2 f_h(x)| &\le \frac{\tilde{h}}{h^2}\left|\int_0^1 \nabla f_h(x+tha)\cdot ha\,dt - h\nabla f_h(x)\cdot a\right| \\
&\le \frac{\tilde{h}}{h}\int_0^1 \left|\nabla f_h(x+tha)\cdot a - \nabla f_h(x)\cdot a\right|\,dt \\
&\le \frac{\tilde{h}}{h}\int_0^1 \|\nabla^2 f_h\|_{L^\infty}|ha|\,|a|dt \\
&\to 0.
\end{aligned}$$

□

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