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Qualitative properties of a continuum theory for thin films

Propriétés qualitatives d'une théorie de continuum pour des couches minces

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Abstract

We discuss qualitative aspects of a continuum theory for thin films rigorously derived in [B. Schmidt, On the passage from atomic to continuum theory for thin films, preprint 82/2005, Max-Planck Institut für Mathematik in den Naturwissenschaften, Leipzig]. 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 the scale of convergence used in [B. Schmidt, On the passage from atomic to continuum theory for thin films, preprint 82/2005, Max-Planck Institut für Mathematik in den Naturwissenschaften, Leipzig] is the only scale for which a limiting theory that also accounts for atomic relaxation effects is non-trivial.

Résumé

Nous discutons des aspects qualitatifs d'une théorie de continuum pour des couches minces, dérivée rigoureusement dans [B. Schmidt, On the passage from atomic to continuum theory for thin films, preprint 82/2005, Max-Planck Institut für Mathematik in den Naturwissenschaften, Leipzig]. La densité d'énergie emmagasinée est examinée pour des propriétés de convexité et comportement en limite sous des distorsions grandes et petites. Une recherche de la dépendance de la théorie à l'égard des paramètres de relaxation mène au résultat que l'échelle de la convergence employée dans [B. Schmidt, On the passage from atomic to continuum theory for thin films, preprint 82/2005, Max-Planck Institut für Mathematik in den Naturwissenschaften, Leipzig] est la seule échelle pour laquelle une théorie limite qui inclut également des effets de la relaxation atomique est non-triviale.

Keywords: Thin films; Discrete-to-continuum limits; Effective theories

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1. Introduction

The aim of this paper is to examine qualitative features of a macroscopic theory for thin films that was derived as an effective continuum theory from atomic models in [21]. Deriving thin film limits from three-dimensional elasticity is still an active area of research, see, e.g., [17–19,13,14,16] and, most recently, [15] where a whole hierarchy of different scaling limits is discussed. For the more classical developments see, e.g., [20,8]. On the other hand, by now there are also rigorous Γ-convergence results for the passage from discrete to continuum theory: for suitable pair interaction models, especially in one dimension, see [4–6]; more complicated potentials under additional assumptions as, e.g., the Cauchy–Born rule are considered in [2,3].

In [12], starting from reference configurations

$$\mathcal{L}_k = \mathbb{Z}^3 \cap [0,k] \times [0,k] \times [0,\nu-1]$$

for fixed $\nu \in \mathbb{N}$, the number of film layers, and $k \in \mathbb{N}$, a limiting continuum theory for the energy of deformations was proposed in the limit $k \to \infty$ taking into account atomistic relaxation effects. In [21], this effective theory was obtained rigorously as a variational limit of the elastic energy functional $E(y^{(k)})$ of deformations $y^{(k)} : \mathcal{L}_k \to \mathbb{R}^3$. This continuum theory was expressed in terms of the gradient of a map $u : [0,1]^2 \to \mathbb{R}^3$ and $\nu - 1$ director fields $b^i : [0,1]^2 \to \mathbb{R}^3$, $i = 1, \dots, \nu-1$:

Theorem 1.1. (*Cf.* [21]) *Under suitable assumptions on the energy function E, and for an appropriate definition of convergence of deformations, there exists $\varphi : \mathbb{R}^{3\times 2} \times (\mathbb{R}^3)^{\nu-1} \to \mathbb{R}$ such that*

$$E\big(y^{(k)}\big) \overset{\text{“}\Gamma\text{”}}{\to} \int_{[0,1]^2} \varphi\big(\nabla u, b^1, \dots, b^{\nu-1}\big) \quad \text{as } k \to \infty.$$

It is worth mentioning that the scheme described in [21] can be applied not only to thin films but to general three-dimensional bodies leading to a stored energy density φ only depending on the deformation gradient $\nabla u \in \mathbb{R}^{3\times 3}$, if one assumes sufficiently fast decay of atomic interactions. The main technical difficulty in fact stems from the non-local convergence of relative layer displacements to the family of vector fields $(b^1, \dots, b^{\nu-1})$ (cf. Definition 2.3). For the qualitative aspects examined in the present paper we will however make use of the ‘thin film structure’ as we allow atoms to explore regions perpendicular to the macroscopic film surface.

In Section 2, after introducing the model, we will recall the precise statements from [21]. Also we will collect some preparatory material that was proved in [21] and will be needed in the sequel.

The following sections are devoted to studying this continuum theory, i.e. the macroscopic energy density φ qualitatively. First, cf. Section 3, we examine the dependence of φ on the relaxation parameter c_0 (cf. Definition 2.3 and Theorems 2.7, 2.8 and 2.9) 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 a continuum theory was derived in [21] is the only scale that leads to a non-trivial limiting theory.

In the following two Sections 4 and 5, we derive the limiting behavior under large tensile and compressive strains, and explore the convexity properties and symmetries of the limiting energy functional.

Finally, in Section 6, the scaling behavior of certain systems near $O(2,3)$, i.e., $(\nabla u)^{\mathrm{T}} \nabla u \approx \mathrm{Id}_{\mathbb{R}^2}$, is examined. We still find a non-trivial energy response to compressive strains in this regime. It is, however, weaker than 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.

2. The passage from atomic to continuum theory

We give a brief account of the results obtained in [21] on the passage from atomic models to a continuum theory for thin films. For details, motivations of the concepts, and proofs of the results of this section we refer to [21].

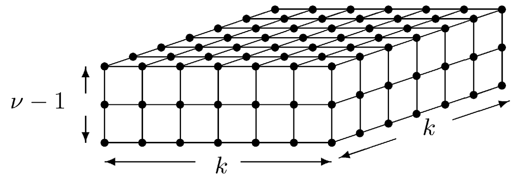

Fig. 1.

2.1. The model

2.1.1. Kinematics

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

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

where $\mathcal{S}_k := [0,k] \times [0,k]$ for $k \in \mathbb{N}$, $h := \nu - 1$ is the height of the film and, for sake of simplicity, $\mathcal{L} = \mathbb{Z}^3$ (see Fig. 1).

The deformations of this configuration will be denoted by

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

In order for y to be defined not only on the atomic positions, we will assume some interpolation between the atomic positions: for a deformation $y : \mathcal{L}_k \to \mathbb{R}^3$ let $\bar{x} = x + (1/2, 1/2)$ for $x \in \{0, \dots, k-1\}^2$ and set

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

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 $[(x, i-1), (x, i)]$. By this particular choice we guarantee that (local) averages depend only on atomic positions.

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 $\mathcal{S}_1 \times [0, h]$:

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

Considering weak*-limiting points of $\tilde{y}$ as natural variables for a continuum theory, we are led to elements u of $W^{1,\infty}([0,1]^2; \mathbb{R}^3)$ as limiting deformations. In our regime of thin films of fixed atomic height, we also introduce the quantities

$$\Delta^i \tilde{y}^{(k)}(x_p) = \tilde{y}^{(k)}(x_1, x_2, i) - \tilde{y}^{(k)}(x_1, x_2, 0), \quad i = 1, \dots, \nu - 1,$$

$x_p = (x_1, x_2)$, to measure the relative shift of the layers of our film. Also these have weak*-limits in L^∞.

As in [21] we define:

Definition 2.1. Let $u \in W^{1,\infty}(\mathcal{S}_1; \mathbb{R}^3)$ and $\mathbf{b} = (b^1, \dots, b^{\nu-1}) \in L^\infty(\mathcal{S}_1; (\mathbb{R}^3)^{\nu-1})$. 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

$$\big|u(x) - u(z)\big| \geqslant c_1 |x - z| \quad \forall x, z \in \mathcal{S}_1 \tag{1}$$

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

$$\|b^0\|_\infty, \|b^i - b^0\|_\infty \leqslant c_0, \quad i = 1, \dots, \nu - 1. \tag{2}$$

The unrescaled version of u is denoted U, i.e. $\widetilde{U} = u$. An easy consequence of our interpolation is the following

Lemma 2.2. *Suppose u is admissible and $y:\mathcal{L}_k\to\mathbb{R}^3$ some deformation with $\sup_{x\in\mathcal{L}_k}|y(x)-U(x_p)|\leqslant c$. 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) $\sup_{x\in\mathcal{S}_1\times[0,h]}|\tilde{y}(x)|\leqslant C_2$,
(ii) $C_1|x-z|-C_3\leqslant|y(x)-y(z)|\leqslant C_2|x-z|\ \forall x,z\in\mathcal{S}_k\times[0,h]$.

We next define in what sense we understand deformations to converge to the limiting quantities u and $\mathbf{b}$.

Definition 2.3. 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

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

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

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

As detailed in [21], this corresponds to a relaxation scheme where the individual atoms are allowed to move in a region comparable to atomic dimensions.

2.1.2. Energy

The energy of a system of N atoms at positions $y_1,\dots,y_N\in\mathbb{R}^3$ will 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

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

The elastic energy of a deformation y, i.e. the energy of the system $(y(x):\ x\in\mathcal{L}_k)$ respectively a subsystem $\mathcal{M}=y(\mathcal{K})$, $\mathcal{K}\subset\mathcal{L}_k$, is denoted

$$E(y)=E\bigl(y(x):\ x\in\mathcal{L}_k\bigr)\quad\text{resp.}\quad E(\mathcal{M})=E\bigl(y(x):\ x\in\mathcal{K}\bigr).$$

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

The main two assumptions on E are firstly the following splitting estimate.

Assumption 2.4. Suppose u is admissible. There exists a function $\psi:[0,\infty)\to\mathbb{R}$ such that

$$|\psi|\leqslant M\quad\text{and}\quad\psi(r)\leqslant Mr^{-q}\tag{3}$$

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

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

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

Secondly, we need to assume some regularity of E:

Assumption 2.5. Let u be admissible. We assume that E is locally Lipschitz and in a C-neighborhood of U

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

where L might depend on C and on U through c_1, c_2.

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 $y(\mathcal{K})$.

For some results we will have to impose an additional restriction:

Assumption 2.6. Assume that ψ and L of Assumption 2.4 resp. 2.5 depend only on C_1 and C_3 where y satisfies $|y(x) - y(z)| \geqslant C_1|x - z| - C_3$.

2.2. Convergence theorems

Suppose E satisfies Assumptions 2.4 and 2.5, and a relaxation parameter $c_0 > 0$ is chosen. The main result of [21] is the following variational convergence result:

Theorem 2.7. *There exists a macroscopic stored energy function φ such that (in the spirit of Γ-convergence, cf.* [10]*),*

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

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

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

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

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

$$E(u, \mathbf{b}) = \int_{\mathcal{S}_1} \varphi\big(\nabla u, b^1, \ldots, b^{\nu-1}\big). \tag{4}$$

To compute φ by an associated cell problem, set

$$\widehat{\mathcal{N}}_k^{0,1}(A, \mathbf{b}) = \left\{ y : \mathcal{L}_k \to \mathbb{R}^3\colon\ \|y - A\| \leqslant c_0 \text{ and } \frac{1}{(k+1)^2} \sum_{x\in\mathbb{Z}^2\cap\mathcal{S}_k} \Delta^i y(x) = b^i \right\}. \tag{5}$$

Theorem 2.8. *The macroscopic energy density φ of Theorem* 2.9 *is given by*

$$\varphi(A, \mathbf{b}) = \lim_{k\to\infty} \varphi_k(A, \mathbf{b}) \tag{6}$$

where for later use we have introduced the quantities

$$\varphi_k(A, \mathbf{b}) = \frac{1}{\nu k^2} \inf_{y\in\widehat{\mathcal{N}}_k^{0,1}(A,\mathbf{b})} E(y). \tag{7}$$

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

Here, $\mathcal{A}_{\mathrm{hom}} \subset \mathbb{R}^{3\times2} \times (\mathbb{R}^3)^{\nu-1}$, the set of *admissible* $(A, \mathbf{b})$, is defined by

$$\mathcal{A}_{\mathrm{hom}} := \left\{ \big(A, b^1, \ldots, b^{\nu-1}\big)\colon \operatorname{rank}(A) = 2, \exists b^0 \in \mathbb{R}^3 \text{ s.t. } \big|b^0\big|, \max_{1\leqslant i\leqslant\nu-1} \big|b^i - b^0\big| \leqslant c_0 \right\}$$

for matrices $A \in \mathbb{R}^{3\times2}$ and vectors $b^1, \ldots, b^{\nu-1}$.

We also mention the following quantitative version of Theorem 2.7:

Theorem 2.9. *Suppose $l = l(k)$ is such that $l(k) \to 0$ and $kl(k) \to \infty$ as $k \to \infty$. Let*

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

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

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

In fact, Theorems 2.7 and 2.8 also apply to the more general case where E is of the form

$$E(y) = \frac{1}{2}\sum_{i\neq j} W\big(|y_i - y_j|\big) + E_0(y) \tag{8}$$

where E_0 satisfies the usual assumptions, but $W(r)$ becomes infinitely large as r tends to zero. (In particular, the Lennard–Jones potential is covered by these energy functions.)

Theorem 2.10. *For any* $r_0 > 0$ *assume that* W *is Lipschitz on* $[r_0,\infty)$ *and there exists* $M = M(r_0)\in\mathbb{R}$ *such that for (a.e.)* $r\geqslant r_0$

$$\big|W(r)\big|\leqslant Mr^{-q},\qquad \big|W'(r)\big|\leqslant Mr^{-q+1},$$

for $r\geqslant r_0$. *Then Theorem* 2.7 *extends to energy functions of the form* (8) *where, as in Theorem* 2.8, $\varphi\colon\mathcal{A}_{\mathrm{hom}}\to(-\infty,\infty]$ *is given by* (6), *continuous as a function with values in* $\mathbb{R}\cup\{\infty\}$.

As another extension we note that the above results also apply to suitable systems of distinguishable particle systems with finite range interaction. Let $a>0$. To each $x_i\in\mathcal{L}_k$ we assign a neighborhood

$$U_{x_i} = \big\{x_j\in\mathcal{L}\colon |x_j - x_i|\leqslant a\big\} = \big\{x_1^i,\ldots,x_{r_a}^i\big\}$$

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

$$x_j^{i_1} - x_{i_1} = x_j^{i_2} - x_{i_2}\quad\text{for } j = 1,\ldots,r_a.$$

Let $\mathcal{S}_k^a = [a,k-a]^2$ and suppose the energy of a deformation y is given by

$$E_{\mathrm{fr}}(y) = \sum_{x_i\in\mathcal{L}\cap(\mathcal{S}_k^a\times[0,h])} f_{x_i}\big(y\big(x_2^i\big) - y\big(x_1^i\big),\ldots,y\big(x_{r_a}^i\big) - y\big(x_1^i\big)\big) + \mathcal{O}(k), \tag{9}$$

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 $y(x_2^i),\ldots,y(x_{r_a}^i)$. (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.) We need the following periodicity assumption: there exist fixed $p_1, p_2\in\mathbb{N}$ such that

$$f_{(x_1+p_1,x_2,x_3)} = f_x = f_{(x_1,x_2+p_2,x_3)} \tag{10}$$

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

Proposition 2.11. *Suppose* E_{fr} *is defined as in* (9) *and* (10) *holds. Assume that the* f_{x_i} *are locally Lipschitz. Then the limit* φ_{fr} *of Theorem* 2.8 *exists and we have*

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

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

Remark. For such systems we do not need to suppose that u satisfies a minimal strain hypothesis. Thus, φ is defined on all of $\mathbb{R}^{3\times 2}\times(\mathbb{R}^3)^{\nu-1}$.

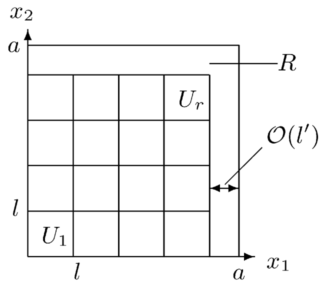

Fig. 2.

2.3. Technical results

We now collect some of the technical results obtained in [21] that will be useful in the following sections.

Consider deformations $y : k\Omega \times [0,h] \to \mathbb{R}^3$ for $\Omega \subset [0,1]^2$.

Lemma 2.12. *Let y be a deformation satisfying $|\tilde{y} - u| \leqslant c/k$ 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*

$$\left|E\big(y(x)\colon x \in \mathcal{K}\big) - E\big(y(x)\colon x \in \mathcal{K}_1\big)\right| \leqslant C\#\mathcal{K}_2.$$

Suppose $Q = [0,a)^2$, $a \leqslant 1$, is partitioned by squares $U_1, \ldots, U_r$ of side-length l where $c_0/k \leqslant l \leqslant a$ plus some rest R with $|R| = \mathcal{O}(a \cdot l')$, $l' \ll a$, as in Fig. 2. (Then $r \sim (a/l)^2$.)

Set $\mathcal{M} := \{y(x)\colon x \in \mathcal{L} \cap (kQ \times [0,h])\}$, $\mathcal{M}_i := \{y(x)\colon x \in \mathcal{L} \cap (kU_i \times [0,h])\}$.

Lemma 2.13. *Suppose $y : kQ \times [0,h] \to \mathbb{R}^3$ satisfies $|\tilde{y} - u| \leqslant c/k$ for some admissible u. Then there exists $C > 0$ such that*

$$\left|E(\mathcal{M}) - \sum_{i=1}^{r} E(\mathcal{M}_i)\right| \leqslant C\left(\frac{ka^2}{l} + k^2 a l'\right).$$

Remark. In both of the previous lemmas, C will only depend on C_1 and C_3 provided Assumption 2.6 is satisfied.

To measure local spatial averages, we define the measure $\rho = \rho(k) = \sum_{x \in \mathbb{Z}^2} \delta_{x/k}$ where $\delta_{x/k}$ is the Dirac measure at x/k. Also set (after extending b^i boundedly outside $\mathcal{S}_1$ (constantly if b^i is constant))

$$\bar{b}^i(x) = \fint_{x + [-1/2k, 1/2k]^2} b^i(z)\,\mathrm{d}z. \tag{11}$$

Let b^0 as in (2) be given. For later use we introduce the deformations $v = v^{(k)}$, defined by (interpolation of)

$$v(x_1, x_2, i) = \begin{cases} u(x_1, x_2) - \frac{1}{k}\bar{b}^0(x_1, x_2) & \text{for } i = 0, \\ u(x_1, x_2) + \frac{1}{k}(\bar{b}^i(x_1, x_2) - \bar{b}^0(x_1, x_2)) & \text{for } 1 \leqslant i \leqslant \nu - 1 \end{cases} \tag{12}$$

for $(x_1, x_2) \in \frac{1}{k}\mathbb{Z}^2 \cap \mathcal{S}_1$. Clearly, $v^{(k)} \to (u, \mathbf{b})$. Its un-rescaled version will be denoted V, i.e. $\tilde{V} = v$.

Lemma 2.14. *Suppose y is a deformation with*

$$\|y - U\| \leqslant c_0 + \delta_1 \quad \textit{and} \quad \left|\ \fint_{[0,1]^2} \big(k\Delta^i \tilde{y} - \bar{b}^i\big)\,\mathrm{d}\rho\right| \leqslant \delta_2,$$

$\delta_1, \delta_2 \leqslant 1$. *Then there exists $y' : \mathcal{L}_k \to \mathbb{R}^3$ with*

$$\|y' - U\| \leqslant c_0, \qquad \fint_{[0,1]^2} k\Delta^i \tilde{y}'\,\mathrm{d}\rho = \bar{b}^i,$$

and

$$\left|E(y)-E(y')\right| \leqslant C\left(\delta_1^{1/5}+\delta_2^{1/5}\right)k^2.$$

(This combines Lemmas 3.11 and 3.13 in [21].)

Instead of b^i, it is sometimes more convenient to work with the quantities B^i defined by choosing $\bar{b}^0$ minimizing

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

and setting

$$B^i := \bar{b}^{i-1}-\bar{b}^0 \quad \text{for } i=2,\dots,\nu, \qquad B^1 := -\bar{b}^0. \tag{13}$$

3. 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 2.3). (To keep track of this dependence, we will sometimes add c_0 as an additional subscript as e.g. in $\widehat{\mathcal{N}}^{0,1}_{k,c_0}$, 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 cannot 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. *Fix $(A,\mathbf{b}) \in \mathcal{A}_{\mathrm{hom}}$. The mapping $c_0 \mapsto \varphi_{c_0}(A,\mathbf{b})$ is decreasing and continuous.*

Proof. Suppose $c_0 > c_0'$. By Theorem 2.8, $\varphi_{c_0}(A,\mathbf{b}) \leqslant \varphi_{c_0'}(A,\mathbf{b})$. Conversely, given $y \in \widehat{\mathcal{N}}^{0,1}_{k,c_0}(A,\mathbf{b})$, by Lemma 2.14 we find a deformation $y' \in \widehat{\mathcal{N}}^{0,1}_{k,c_0'}(A,\mathbf{b})$ with $E(y') \leqslant E(y) + C(c_0-c_0')^{1/5}k^2$ provided $(A,\mathbf{b})$ is admissible for c_0' and $|c_0-c_0'| \leqslant 1$. Therefore $\varphi_{c_0'}(A,\mathbf{b}) \leqslant \varphi_{c_0}(A,\mathbf{b}) + C(c_0-c_0')^{1/5}$. $\square$

3.1. The limit $c_0 \to \infty$

Suppose E is an admissible pair potential with purely attractive pair interaction $W \leqslant 0$, $W \not\equiv 0$. 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 the limit $c_0 \to \infty$ in general will be trivial if Assumption 2.6 is satisfied.

Theorem 3.2. *Suppose E satisfies Assumptions* 2.4, 2.5, *and* 2.6. *Define $\varphi_\infty := \lim_{c_0\to\infty}\varphi_{c_0}$. (This limit exists pointwise in $[-\infty,\infty)$ by Proposition* 3.1.*) 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. (12)) 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 $2|A|$,

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

C_1, C_3 independent of $\mathbf{b}$. From Assumption 2.6 and Lemma 2.12 we then find a constant C such that for those $\mathbf{b}$, $E(V_{A,\mathbf{b}}) \leqslant Ck^2$. On the other hand, if for two vectors $\mathbf{b}_1, \mathbf{b}_2$ and some $i \in \{1,\dots,\nu-1\}$,

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

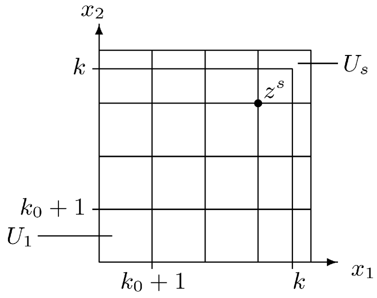

Fig. 3.

then $E(V_{A,\mathbf{b}_1}) = E(V_{A,\mathbf{b}_2}) + \mathcal{O}(|z|k)$. So for all $\mathbf{b}$ we obtain $\lim_{k\to\infty} \frac{1}{\nu k^2} E(V_{A,\mathbf{b}}) \leqslant C$, 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 5.3 all $\varphi_{c_0}(A,\cdot)$ are convex), it must be constant.

For the remaining part it suffices to show that

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

We proceed similarly as in the proof of Proposition 3.16 of the existence of φ under homogeneous conditions in [21].

Fix c_0 and $\delta > 0$. Choosing k_0 large enough we find by Theorem 2.8 $y \in \widehat{\mathcal{N}}^{0,1}_{k_0,c_0}(A,\mathbf{b})$ with

$$\frac{1}{\nu k_0^2} E(y) \leqslant \varphi_{c_0}(A,\mathbf{b}) + \frac{\delta}{2}. \tag{14}$$

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 $[0,k_0+1)^2$ as in Fig. 3.

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

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

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

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

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

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

(note $|k\Delta^i \tilde{y}'| \leqslant 2\widetilde{c_0}$), by Lemma 2.14 we find a deformation

$$\hat{y} \in \widehat{\mathcal{N}}^{0,1}_{k,\widetilde{c_0}}(A',\mathbf{b}) \tag{15}$$

such that

$$\bigg|\frac{1}{\nu k^2} E(y') - \frac{1}{\nu k^2} E(\hat{y})\bigg| \leqslant C(\widetilde{c_0}) \bigg(\frac{k_0^2}{k}\bigg)^{1/5}. \tag{16}$$

Using Lemma 2.13 and translational invariance, we would now like to split the energy to find that

$$\bigg|\frac{1}{\nu k^2} E\big(y'(x)\colon x \in \mathcal{L}_k\big) - \frac{1}{\nu k_0^2} E\big(y(x)\colon x \in \mathcal{L}_{k_0}\big)\bigg| \leqslant C\bigg(\frac{1}{k_0} + \frac{k_0}{k}\bigg). \tag{17}$$

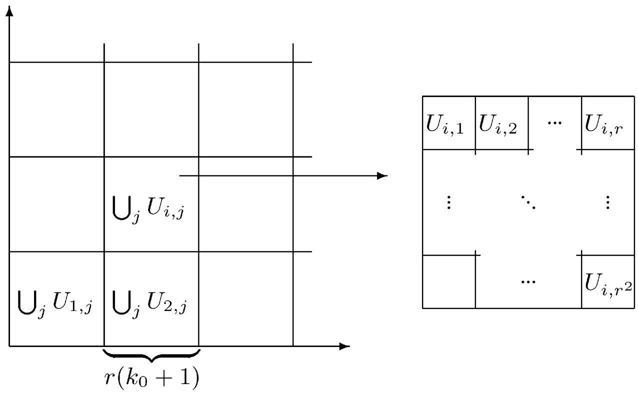

Fig. 4.

If this is possible, we find that by (17), (15), (16) and (14) for $k \gg k_0 \gg 1$

$$\begin{aligned}\varphi_{k,\widetilde{c_0}}(A', \mathbf{b}) &\leqslant \frac{1}{\nu k^2} E\big(\hat{y}(x)\colon x \in \mathcal{L}_k\big)\\ &\leqslant \frac{1}{\nu k_0^2} E\big(y(x)\colon x \in \mathcal{L}_{k_0}\big) + \frac{\delta}{2}\\ &\leqslant \varphi_{c_0}(A, \mathbf{b}) + \delta.\end{aligned}$$

Letting first $k \to \infty$, we deduce from Proposition 3.1

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

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

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

It remains to justify the application of Lemma 2.13. The problem is that $\widetilde{c_0}$ depends on k_0. (For nearest neighbor models as discussed in Proposition 2.11, this splitting in (17) 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.) By the remark after Lemma 2.13, however, this will be possible if we can replace y' by some y'' such that still $\|y'' - A\| \leqslant \widetilde{c_0}$ 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.

$$\big|y''(x_1) - y''(x_2)\big| \geqslant C_1 |x_1 - x_2| - C_3. \tag{18}$$

We re-enumerate the squares $U_1, \ldots, U_s$ as depicted in Fig. 4. ($r \in \mathbb{N}$ to be specified later.) Depending on A, A', k (and $c_0, \widetilde{c_0}$) we choose a unit vector $e \in \mathbb{R}^3$ perpendicular to the graph of A' and numbers $0 < a_1 < \cdots < a_{r^2}$ (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 (18) 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 (17) 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 2.2 since $y \in \widehat{\mathcal{N}}^{0,1}_{k_0,c_0}(A, \mathbf{b})$.

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

$$\begin{aligned}\big|y''(x_1) - y''(x_2)\big| &\geqslant |a_{j_1} - a_{j_2}| - \big|y'(x_1) - y'(x_2)\big|\\ &\geqslant |a_{j_1} - a_{j_2}| - \big|f^{i_1,j_1} - f^{i_2,j_2}\big| - \big|y\big(x_1 - (z^{i_1,j_1}, 0)\big) - y\big(x_2 - (z^{i_2,j_2}, 0)\big)\big|\\ &\geqslant |a_{j_1} - a_{j_2}| - \big|f^{i_1,j_1} - f^{i_2,j_2}\big| - 2c_0 - \big|A\big((x_1)_p - z^{i_1,j_1}\big) - A\big((x_2)_p - z^{i_2,j_2}\big)\big|\end{aligned}$$

$$\begin{aligned}&\geqslant |a_{j_1} - a_{j_2}| - C'rk_0 - 2c_0 - Ck_0\\ &\geqslant 2rk_0 \quad \text{for } |a_{j_1} - a_{j_2}| \text{ sufficiently large}\\ &\geqslant |x_1 - x_2|.\end{aligned}$$

So we assume that $|a_{j_1} - a_{j_2}|$, $j_1, j_2 \in \{1, \dots, r^2\}$, 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 $|x_1 - x_2|_\infty \geqslant (r-1)(k_0+1)$. Since e is perpendicular to the graph of A' and y' lies in a $\widetilde{c_0}$-neighborhood of that graph, we find that for r not too small

$$\begin{aligned}\big|y''(x_1) - y''(x_2)\big| &= \big|(a_{j_1} - a_{j_2})e + y'(x_1) - y'(x_2)\big|\\ &\geqslant \big|(a_{j_1} - a_{j_2})e + A'(x_1 - x_2)\big| - \big|y'(x_1) - A'x_1\big| - \big|y'(x_2) - A'x_2\big|\\ &\geqslant |A'x_1 - A'x_2| - 2\widetilde{c_0}\\ &\geqslant \big|y'(x_1) - y'(x_2)\big| - 4\widetilde{c_0}\\ &\geqslant \big|f^{i_1,j_1} - f^{i_2,j_2}\big| - \big|y\big(x_1 - z^{i_2,j_1}\big) - y\big(x_2 - z^{i_2,j_2}\big)\big| - 4\widetilde{c_0}\\ &\geqslant \big|f^{i_1,j_1} - f^{i_2,j_2}\big| - 2c_0 - 2|A|k_0 - 4\widetilde{c_0}\\ &\geqslant c\big|z^{i_1,j_1} - z^{i_2,j_2}\big| - 2c_0 - 2|A|k_0 - 4\widetilde{c_0}\\ &\geqslant \frac{c}{2}\big|z^{i_1,j_1} - z^{i_2,j_2}\big|\\ &\geqslant \frac{c}{6}|x_1 - x_2|,\end{aligned}$$

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

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

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

Setting $\widetilde{\widetilde{c_0}} = \widetilde{c_0} + \max_{1 \leqslant j \leqslant r^2} |a_j e|$ we furthermore have $\|y'' - A'\| \leqslant \widetilde{\widetilde{c_0}}$. So by possibly enlarging $\widetilde{c_0}$ to $\widetilde{\widetilde{c_0}}$, we can indeed split the energy to obtain (17), and the proof is finished. □

For systems that do not satisfy Assumption 2.6, φ_∞ may be non-trivial (for an example see Proposition 4.5 in [21]). In Section 5.1 we will prove that φ_∞ is quasiconvex with respect to the first variable and convex with respect to the second.

3.2. *The limit $c_0 \to 0$*

In our definition of convergence $y^{(k)} \to (u, \mathbf{b})$, it does not make sense 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 2.3 to be less than c_0/k one could demand that

$$\|\tilde{y} - v\| \leqslant c_0/k \tag{19}$$

where v is as in (12) corresponding to $u, \mathbf{b}$ with b^0 set to zero. (Condition (2) is not needed for this definition of convergence.) This alternative set-up leads to analogous results in the passage to continuum theory, as shown in [21].

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 3.3. *Let $V_{A,\mathbf{b}}$ be as in* (12) *for constant $\nabla u = A$ and* $\mathbf{b}$. *Then*

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

In particular, the limit on the right-hand side exists (*in $\mathbb{R}$ under the usual Assumptions* 2.4 *and* 2.5, *in* $(-\infty, \infty]$ *for energies of the form* (8)).

Proof. Suppose first E is of the form (8) and there are $i \neq j \in \{0, \dots, \nu - 1\}$ such that $b^i \in b^j + A\mathbb{Z}^2$. Then, if $\|y - V_{A,\mathbf{b}}\| \leqslant r$,

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

as $r \to 0$. For the remaining cases note that $E(V_{A,\mathbf{b}})$ is bounded by Lemma 2.12 and, if $\|y - V_{A,\mathbf{b}}\| \leqslant r$,

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

Therefore,

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

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

Example. For admissible pair potentials (i.e. W satisfies the conditions of Theorem 2.10)

$$E_{\mathrm{pp}}(y) = \frac{1}{2} \sum_{i\neq j} W\big(|y_i - y_j|\big), \tag{20}$$

we get

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

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 $\mathcal{O}(kl/k^2) = \mathrm{o}(1)$. Then summing over all $z \in \mathbb{Z}^2 \times \{0, 1, \dots, \nu - 1\}$, $z \neq x$, instead of $\mathcal{L}_k \setminus \{x\}$ gives another error term of order $\mathcal{O}(l^{2-q}) = \mathrm{o}(1)$. This sum now being independent of x_p, we obtain

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

The corresponding macroscopic energy functional is given by

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

This expression can be seen as a thin-film version with directors $b^1, \dots, b^{\nu-1}$ of a formula derived in [3].

3.3. 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 the physically motivated choice $l_1(k) = \mathrm{const.}/k$ yields non-trivial results. Physically this amounts to the fact that thin film configurations are expected to be only locally energy minimizing: admitting for fracture, i.e., large interatomic distances, the film could locally (3d-) crystallize. Physically reasonable decay assumptions on atomic interactions will then lead to trivial macroscopic limits.

It is easy to see that for $l_1 \ll 1/k$ we reproduce the limit obtained in Proposition 3.3. 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 2.9) we define

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

Theorem 3.4. *Suppose E satisfies Assumptions* 2.4, 2.5, *and* 2.6. *Assume $l_1(k)$, $l_2(k)$ satisfy $kl_1(k), kl_2(k) \to \infty$. Then for all admissible u (cf.* (1)) *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 3.2, 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

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

(resp. $\leqslant -1/\delta$ for $E(u,\mathbf{b}) = -\infty$). In addition to the sets $U_i = z^i + [0,k_0+1)^2$ consider the subsets $\widehat{U}_i = z^i + [0,k_0)^2$, and construct y' similar as in the proof of Theorem 3.2 by

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

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

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

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

Considering local spatial averages, we still find $\hat{y} \in \mathcal{W}_k^{l_1,l_2}(u',\mathbf{b}')$ such that for k_0 fixed

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

(To prove this, one may choose a scale l_3 such that $1/k \ll l_3 \ll l_2$ and apply Lemmas 3.13 and 3.14 in [21] resp. Lemmas 2.2.12 and 2.213 in [22] with constants depending on k_0.)

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

$$\bigl|y''(x_1) - y''(x_2)\bigr| \geqslant C_1|x_1 - x_2| - C_3$$

with C_1, C_3 independent of k_0 and k for x_1 and x_2 that do not lie in the same $U_{i,j} \cap \widehat{U}_i$. But Lemma 2.13 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 $a_1, \ldots, a_{r^2}$. Also note that for the same reason and by translational invariance

$$\bigl|E\bigl(y'(x)\colon x \in \mathcal{L} \cap \bigl(U_i \times [0,h]\bigr)\bigr) - E(y)\bigr| \leqslant Ck_0.$$

Finally sending k to infinity gives

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

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 $E(u',\mathbf{b}')\leqslant E(u,\mathbf{b})$. Reversing the roles of $\mathbf{b}$ and $\mathbf{b}'$ respectively u and u', we obtain

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

4. Extremal strains

In this section, we examine $\varphi(A,\mathbf{b})$ for A with very large (cf. Section 4.1) or small (cf. Section 4.2) 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.

4.1. Strongly tensile deformations

Again in this paragraph we suppose that Assumption 2.6 is satisfied.

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

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

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

Proposition 4.1. *The large strain limit* $\lim_{A\to\infty}\varphi(A,\mathbf{b})$ *exists, and*

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

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

Proof. Let $y\in\widehat{\mathcal{N}}_k^{0,1}(A,\mathbf{b})$ 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 Assumption 2.4,

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

By definition of $\widehat{\mathcal{N}}_k^{0,1}$, if $c_1\leqslant s_1(A)$, then

$$\big|y(x)-y(z)\big|\geqslant c_1|x_p-z_p|-2c_0$$

which is $\geqslant \frac{c_1}{2}|x_p-z_p|$ 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

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

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 $y\in\widehat{\mathcal{N}}_k^{0,1}(A,\mathbf{b})$. By frame indifference this is the same as minimizing

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

Now the claim is an elementary consequence of Carathéodory's theorem (cf. [9] Corollary 2.9, p. 42). □

Remarks.

(i) If in Definition 2.3 we request that $\|\tilde{y}-v_{A,\mathbf{b}}\|\leqslant c_0/k$ instead of $\|\tilde{y}-A\|\leqslant c_0/k$ as in (19), the result is analogous if we replace B_{c_0} by $B_{c_0}(\mathbf{b})=\{\mathbf{y}\in(\mathbb{R}^3)^\nu\colon\ |y^i-b^i|\leqslant c_0\}$ $(b^0:=0)$. 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 2.6 be satisfied. If φ_{nn} is the continuum energy density for an interaction potential given by harmonic springs between nearest neighbors in the reference configuration (see Proposition 4.5 in [21]), then we clearly have

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

4.2. 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 $B^1,\dots,B^\nu$ from (13). We consider pair potentials with interaction function W as in (20) satisfying the conditions of Theorem 2.10. The main result of this paragraph is the following

Theorem 4.2. *Define $S_p=\sqrt{A^{\mathrm{T}}A}\in\mathbb{R}^{2\times 2}$ measuring the strain of the (constant) deformation $A\in\mathbb{R}^{3\times 2}$.*

(i) *Assume that $r^3W(r)\to\infty$ as $r\to 0$. Then*

$$\lim_{\substack{\det(S_p)\to 0\\ |S_p|\leqslant C<\infty}}\varphi(A,\mathbf{b})=\infty.$$

(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*

$$\limsup_{\substack{\det(S_p)\to 0\\ |S_p|\leqslant C<\infty}} \varphi(A,\mathbf{b}) < \infty$$

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 2.2). For $A \in \mathbb{R}^{3\times 2}$, in addition to S_p let

$$S' := \begin{pmatrix} (S_p)_{11} & (S_p)_{12} & 0 \\ (S_p)_{21} & (S_p)_{22} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad S := \begin{pmatrix} (S_p)_{11} & (S_p)_{12} \\ (S_p)_{21} & (S_p)_{22} \\ 0 & 0 \end{pmatrix}, \quad A' := \begin{pmatrix} A_{11} & A_{12} & e_1 \\ A_{21} & A_{22} & e_2 \\ A_{31} & A_{32} & e_3 \end{pmatrix},$$

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 $R \in \mathrm{SO}(3)$ 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 4.3. *Suppose $\|y - A\| \leqslant c_0$ and $x, x' \in \mathcal{L}_k$ are such that $|y(x) - y(x')| \geqslant a > 0$. Then for c such that $\frac{1-c}{c} a \geqslant 2c_0 + 2h$:*

$$\left|y(x) - y(x')\right| \geqslant c|S'x - S'x'|.$$

Proof. Clear, if $|S'x - S'x'| \leqslant a/c$. If $|S'x - S'x'| \geqslant a/c$, then

$$\begin{aligned}
\left|y(x) - y(x')\right| &\geqslant |A'x - A'x'| - \left|y(x) - Ax_p\right| - \left|Ax'_p - y(x')\right| - |Ax_p - A'x| - |A'x' - Ax'_p| \\
&= |S'x - S'x'| - \left|y(x) - Ax_p\right| - \left|Ax'_p - y(x')\right| - |Sx_p - S'x| - |S'x' - Sx'_p| \\
&\geqslant |S'x - S'x'| - 2c_0 - |x_3| - |x'_3| \\
&\geqslant c|S'x - S'x'| + (1-c)\frac{a}{c} - 2c_0 - 2h \\
&\geqslant c|S'x - S'x'|. \qquad \square
\end{aligned}$$

In the second lemma we estimate the number of atoms that are close to other atoms.

Lemma 4.4. *Suppose there are N atoms at positions $y_1, \dots, y_N$ in a bounded region $U \subset \mathbb{R}^3$. Let U_ρ, $\rho > 0$, be the ρ-neighborhood of U. Then*

$$\#\left\{(y_i, y_j)\colon i \neq j, |y_i - y_j| \leqslant \rho\right\} \geqslant N - \frac{6}{\pi\rho^3}|U_\rho|.$$

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 $\mathcal{M} \subset \{y_1, \dots, y_N\}$. Now since atoms in $\mathcal{M}$ have pairwise distances greater than ρ, we find that

$$\#\mathcal{M}\frac{4\pi}{3}\left(\frac{\rho}{2}\right)^3 \leqslant |U_\rho|.$$

It follows that

$$\#\left\{(y_i, y_j)\colon i \neq j, |y_i - y_j| \leqslant \rho\right\} \geqslant N - \#\mathcal{M} \geqslant N - \frac{6}{\pi\rho^3}|U_\rho|. \qquad \square$$

Proof of Theorem 4.2. (i) If $y \in \widehat{\mathcal{N}}_k^{0,1}(A, \mathbf{b})$, 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 4.4 we have

$$\begin{aligned}\#\big\{(y_i, y_j)\colon\ i \neq j, |y_i - y_j| \leqslant r_0\big\} &\geqslant \nu k^2 - \frac{6}{\pi r_0^3}\big(2(c_0 + r_0)\det(S_p)k^2 + \mathcal{O}(k)\big) \\ &\geqslant \frac{k^2}{2},\end{aligned}$$

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 $r_0 \leqslant a$)

$$\begin{aligned}E_{\mathrm{pp}}(y) &= \frac{1}{2}\sum_{i \neq j} W\big(|y_i - y_j|\big) \\ &\geqslant \frac{1}{2}\sum_{\substack{i\neq j\\ |y_i - y_j| \leqslant r_0}} W\big(|y_i - y_j|\big) + \frac{1}{2}\sum_{\substack{i\neq j\\ |y_i - y_j| > a}} W\big(|y_i - y_j|\big) \\ &\geqslant \frac{k^2}{4}\inf_{0\leqslant\rho\leqslant r_0} W(\rho) - \frac{Ck^2}{\det(S_p)}\end{aligned}$$

(see below). Now since $W(r) \gg r^{-3}$, we also have $\inf_{0<\rho\leqslant r} W(r) \gg r^{-3}$, and we may choose $r_0 \to 0$ as $\det(S_p) \to 0$ such that

$$\inf_{0\leqslant\rho\leqslant r_0} W(\rho) \gg \frac{1}{\det(S_p)} \gg r_0^{-3}.$$

Then indeed $E_{\mathrm{pp}}(y) \geqslant \gamma k^2$ for $\gamma = \gamma(A)$ independent of y and k with $\gamma(A) \to \infty$ as $\det(S_p) \to 0$. This proves

$$\lim_{\det(S_p)\to 0}\ \inf_{y\in\widehat{\mathcal{N}}_k^{0,1}(A,\mathbf{b})} \frac{1}{\nu k^2} E_{\mathrm{pp}}(y) = \infty.$$

It remains to show that

$$\left|\sum_{|y(x)-y(x')|\geqslant a} W\big(\big|y(x) - y(x')\big|\big)\right| \leqslant \frac{Ck^2}{\det(S_p)}.$$

This follows from Lemma 4.3: the left hand side can be estimated by

$$\begin{aligned}&\sum_{\substack{|y(x)-y(x')|\geqslant a\\ |S'x - S'x'|\leqslant a}} |W|\big(\big|y(x) - y(x')\big|\big) + \sum_{\substack{|y(x)-y(x')|\geqslant a\\ |S'x - S'x'| > a}} |W|\big(\big|y(x) - y(x')\big|\big) \\ &\quad\leqslant \sum_{\substack{|y(x)-y(x')|\geqslant a\\ |S'x - S'x'|\leqslant a}} Ma^{-q} + \sum_{\substack{|y(x)-y(x')|\geqslant a\\ |S'x - S'x'| > a}} M\big|y(x) - y(x')\big|^{-q} \\ &\quad\leqslant \nu(k+1)^2 Ma^{-q}\#\big\{x \in \mathbb{Z}^3\colon\ |S'x| \leqslant a\big\} + Mc^{-q}\sum_{|S'x - S'x'|\geqslant a} |S'x - S'x'|^{-q} \\ &\quad\leqslant \frac{C\nu k^2}{\det(S')} + C\nu k^2 \sum_{|S'x|\geqslant a} |S'x|^{-q} \\ &\quad\leqslant \frac{Ck^2}{\det(S')} + Ck^2 \int_{|S'x|\geqslant a} |S'x|^{-q}\,\mathrm{d}x \\ &\quad= \frac{Ck^2}{\det(S')} + Ck^2 \int_{|z|\geqslant a} |z|^{-q}\frac{\mathrm{d}z}{\det(S')} \\ &\quad= \frac{Ck^2}{\det(S_p)}.\end{aligned}$$

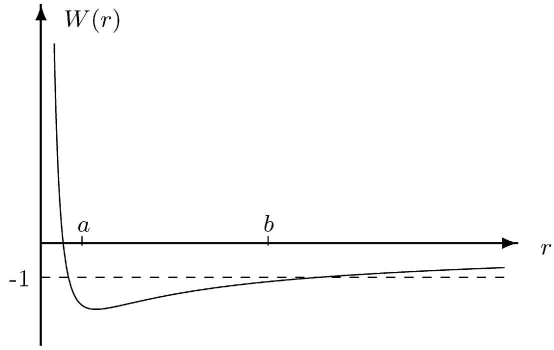

Fig. 5.

This finishes the proof of the first part of Theorem 4.2.

(ii) As before, e denotes a unit vector perpendicular to the graph of A. By convexity in $\mathbf{b}$ (cf. Proposition 5.3) 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

$$\min_{i\neq j}\left|\langle b^i - b^j, e\rangle\right| \geqslant c \quad \text{and} \quad c_0 \geqslant \sqrt{2l^2 + \left(\frac{c}{2}\right)^2} + c_3. \tag{21}$$

Consider $(k+1)^2$ points $z_{ij} = A(i, j, 0)$ at positions $A(\{0, \ldots, k\}^2)$. 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 $Q_e = \{z \in \mathbb{R}^3\colon\ \exists\lambda \in [0, c/2]\colon\ z - \lambda e \in Q\}$ 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 $|z_{ij} - z'_{ij}| \leqslant \sqrt{2l^2 + (c/2)^2}$.

Now define a deformation y by

$$y(x_1, x_2, x_3) = z'_{x_1x_2} + B^{x_3+1}.$$

By (21) and $|B^i| \leqslant c_3$, y lies in $\widehat{\mathcal{N}}_k^{0,1}(A, \mathbf{b})$. y satisfies a minimal distance hypothesis with r: $|y(x) - y(x')| \geqslant r$ 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

$$\begin{aligned}
\left|y(x) - y(x')\right| &\geqslant \left|\langle y(x) - y(x'), e\rangle\right| \\
&= \left|\langle z'_{x_1x_2} + B^{x_3+1} - z'_{x'_1x'_2} - B^{x'_3+1}, e\rangle\right| \\
&\geqslant \left|\langle B^{x_3+1} - B^{x'_3+1}, e\rangle\right| - \left|\langle z'_{x_1x_2} - z'_{x'_1x'_2}, e\rangle\right| \\
&\geqslant \left|\langle b^{x_3} - b^{x'_3}, e\rangle\right| - \frac{c}{2} \\
&\geqslant \frac{c}{2}
\end{aligned}$$

by (21) and the construction of y.

Now suppose W is admissible and as in Fig. 5, i.e. $|W(r)| \leqslant Cr^{-\alpha}$, with $\alpha < 3$, for $r \leqslant a$, and $W(r) \leqslant 0$ for $r \geqslant a$, moreover, $W(r) \leqslant -1$ for $a \leqslant r \leqslant b$, $0 < a < b$ given. Then for x fixed

$$\begin{aligned}
\sum_{x'\neq x} W\left(\left|y(x) - y(x')\right|\right) &\leqslant \sum_{|y(x)-y(x')|\leqslant a} W\left(\left|y(x) - y(x')\right|\right) + \sum_{a<|y(x)-y(x')|\leqslant b} W\left(\left|y(x) - y(x')\right|\right) \\
&\leqslant C \sum_{|y(x)-y(x')|\leqslant a} \left|y(x) - y(x')\right|^{-\alpha} + \sum_{a<|y(x)-y(x')|\leqslant b} (-1)
\end{aligned}$$

$$\begin{aligned}
&\leqslant C \sum_{x' \in \mathbb{Z}^3:\ 0<|rx'|\leqslant a} |rx'|^{-\alpha} - \#\{x':\ a < |y(x) - y(x')| \leqslant b\} \\
&= Cr^{-\alpha} \sum_{0<|x'|\leqslant a/r} |x'|^{-\alpha} - \#\{x':\ a < |y(x) - y(x')| \leqslant b\} \\
&\leqslant Cr^{-\alpha} r^{\alpha-3} - \#\{x':\ a < |y(x) - y(x')| \leqslant b\}.
\end{aligned}$$

Now since the singular values of S_p are bounded, the number of atoms that lie in $\{z:\ a < |z - y(x)| \leqslant b\}$ is bounded below by $C(b-a)/\det(S_p)$ if $b-a$ is not too small, and we find that

$$\#\{x':\ a < |y(x) - y(x')| \leqslant b\} \geqslant C \frac{(b-c_0)^2 - (a+c_0)^2}{\det(S_p)} \geqslant C \frac{b-a}{\det(S_p)}.$$

Together with the above estimate and our choice $r^3 = \tilde{c} \det(S_p)$, this shows that

$$\sum_{x' \neq x} W(|y(x) - y(x')|) \leqslant Cr^{-3} - \tilde{C} r^{-3}(b-a).$$

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)) b^0 is uniquely determined and there are B^i (cf. (13)) 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 4.2 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 (8) satisfying the conditions of Theorem 4.2(i) and $E_0 \geqslant -Ck^2$ independent of c_1.

5. 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.

5.1. Convexity properties

By frame indifference of the model, convexity of φ in A is in general not to be expected (cf. [7], p. 170, also recall Theorem 4.2(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 (9) where the c_0-relaxed energy density may be non-trivial, we show quasiconvexity resp. convexity of φ_∞ in the first resp. second component.

5.1.1. Loss of rank-one convexity

First recall the notion of rank-one convexity:

Definition 5.1. 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 $\varphi(\cdot, \mathbf{b}) : \mathcal{A}_{\mathbf{b}} := \{A \in \mathbb{R}^{3\times 2}:\ \operatorname{rank}(A) = 2\} \to \mathbb{R}$.

Proposition 5.2. *Suppose $\varphi(\cdot,\mathbf{b})$ is rank-one convex and Assumption* 2.6 *is satisfied. Then for all $A \in \mathcal{A}_{\mathbf{b}}$*

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

Here, $\lim_{A\to\infty}\varphi(A,\mathbf{b})$ *is the large strain limit discussed in Proposition* 4.1.

Proof. First note that φ is in fact bounded on each $\mathcal{A}_{\mathbf{b}}(c_1) := \{A \in \mathbb{R}^{3\times 2}\colon s_1(A) \geqslant c_1\}$, $c_1 > 0$, by Lemma 2.12 and Assumption 2.6. 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 $\lambda_1,\lambda_2 \geqslant 1$. Note that

$$\inf_{x\neq 0}\frac{\langle A\Lambda x, A\Lambda x\rangle}{\langle x,x\rangle} = \inf_{x\neq 0}\frac{\langle Ax,Ax\rangle}{\langle \Lambda^{-1}x,\Lambda^{-1}x\rangle} \geqslant \min\{\lambda_1^2,\lambda_2^2\}\inf_{x\neq 0}\frac{\langle Ax,Ax\rangle}{\langle x,x\rangle}.$$

From Proposition 4.1 we infer that for λ_1,λ_2 sufficiently large $f(\lambda_1,\lambda_2) \geqslant \overline{E}^{**}(\mathbf{b}) - \delta$. Fix such λ_1,λ_2. By convexity of $\lambda \mapsto f(\lambda_1,\lambda)$ on $[1,\infty)$ we deduce that $f(\lambda_1,1) \geqslant \overline{E}^{**}(\mathbf{b}) - \delta$. Now convexity of $\lambda \mapsto f(\lambda,1)$ implies that $f(1,1) \geqslant \overline{E}^{**}(\mathbf{b}) - \delta$. □

5.1.2. Convexity in **b**

Discussing convexity in **b**, have to we insist on $y^{(k)} \to (u,\mathbf{b})$ being defined as usual, i.e. not as proposed in (19) 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 **b**. So by lower semicontinuity of Γ-limits we obtain:

Proposition 5.3. *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 $y_{ij}^{(k)} \in \widehat{\mathcal{N}}_{k,Q_{ij}}^{0,1/2}(A,\mathbf{b}_j)$ satisfying

$$\frac{1}{\nu(k/2)^2}E\big(y_{ij}^{(k)}\big) \leqslant \varphi(A,\mathbf{b}_j) + \mathrm{o}(1), \quad i,j = 1,2,$$

by Theorem 2.8 and frame indifference. Defining $y^{(k)}$ by

$$y^{(k)}(x) = y_{ij}^{(k)}(x) \quad \text{for } x \in \mathcal{L} \cap \big(kQ_{ij}\times[0,h]\big),$$

it is easily seen that $y \in \widehat{\mathcal{N}}^{0,1}(A,\mathbf{b})$ and

$$\varphi\left(A,\frac{\mathbf{b}_1+\mathbf{b}_2}{2}\right) \leqslant \liminf_{k\to\infty} E\big(y^{(k)}(x)\colon x \in \mathcal{L}_k\big) \leqslant \frac{1}{2}\big(\varphi(A,\mathbf{b}_1) + \varphi(A,\mathbf{b}_2)\big), \qquad \square$$

which concludes the proof.

Remark. Defining convergence as in (19), it is not clear (and for c_0 small enough false) that y constructed in the previous proof satisfies $\|y - v_{A,\mathbf{b}}\| \leqslant c_0$. Consider the example from Paragraph 3.2. For $\nu = 2$ and $A = \mathrm{Id}$

$$\varphi_0(A,\mathbf{b}) = \frac{1}{2\nu}\sum_{i,j=0}^{1}\sum_{\substack{z\in\mathbb{Z}^2\\(z,j)\neq(0,0,i)}} W\big(\big|Az + b^j - b^i\big|\big)$$
$$= \frac{1}{2}\bigg(\sum_{z\in\mathbb{Z}^2\setminus\{0\}} W\big(|Az|\big) + \sum_{z\in\mathbb{Z}^2} W\big(\big|Az + b^1\big|\big)\bigg).$$

Now if $W:[0,\infty)\to\mathbb{R}$ satisfies $W(0)>0$ and $W(r)=0$ for $r\geqslant 1$, then $\varphi_0(\mathrm{Id}_{2,3},0)>0$, while

$$\varphi_0\big(\mathrm{Id}_{2,3},(0,0,\pm 1)\big)=0.$$

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.

5.1.3. Quasiconvexity of φ_∞

For energy functions that do not satisfy Assumption 2.6 the limit $c_0\to\infty$ can be non-trivial. In the following proposition we examine this limit for convexity properties. As in Theorem 3.2 we define $\varphi_\infty=\lim_{c_0\to\infty}\varphi_{c_0}$. If Assumption 2.6 holds, the following is trivial by Theorem 3.2. We therefore treat only finite range energies given by (9). For such energies, φ_∞ is defined on all of $\mathbb{R}^{3\times 2}\times\mathbb{R}^{3(\nu-1)}$, cf. [21].

Recall the definition of quasiconvexity (cf., e.g., [1], p. 350):

Definition 5.4. A continuous function $f:\mathbb{R}^{m\times n}\to\mathbb{R}$ is said to be quasiconvex if

$$\fint_\Omega f(F+\nabla\zeta)\,\mathrm{d}x\geqslant f(F)$$

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 5.5. *Suppose that E is of the form* (9). *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 3.2. We indicate the modifications.

Sketch of the Proof. Convexity in $\mathbf{b}$ is clear since by Proposition 5.3 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

$$\varphi_\infty(A,\mathbf{b})\leqslant\int_{\mathcal{S}_1}\varphi_\infty(A+\nabla f,\mathbf{b})\,\mathrm{d}x.$$

Let $\delta>0$ and c_0 be given. By Theorem 2.7, for arbitrarily large k_0 we find a deformation $y:\mathcal{L}_{k_0}\to\mathbb{R}^3$ with $\|\tilde{y}-u\|\leqslant c_0/k_0$ and $|\fint_{[0,1]^2}(k_0\Delta^i\tilde{y}-b^i)\,\mathrm{d}\rho|$ as small as we wish such that

$$\frac{1}{\nu k_0^2}E(y)\leqslant\int_{\mathcal{S}_1}\varphi_{c_0}(\nabla u,\mathbf{b})+\frac{\delta}{3}.$$

Using Lemma 2.14, we may even assume that $\fint_{[0,1]^2}(k_0\Delta^i\tilde{y}-b^i)\,\mathrm{d}\rho=0$.

Proceeding as in Theorem 3.2 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

$$\sup_{x\in\mathcal{L}_k}\big|y'(x)-Ax_p\big|=\sup_{x\in\mathcal{L}_{k_0}}\big|y(x)-Ax_p\big|.$$

The crucial point to observe is that since $y\in\widehat{\mathcal{N}}^{0,1}_{k_0,c_0}(u,\mathbf{b})$ and u satisfies the same boundary conditions as A, in contrast to Theorem 3.2 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 $y'\in\widehat{\mathcal{N}}^{0,1}_{k,\tilde{c}_0}(A,\mathbf{b})$ ($\tilde{c}_0$ depending on f,k_0) with

$$\frac{1}{\nu k^2}E(y')\leqslant\frac{1}{\nu k_0^2}E(y)+\frac{\delta}{3}$$

if k_0 and k are large enough. Taking the limit $k \to \infty$, it follows that

$$\varphi_\infty(A, \mathbf{b}) \leqslant \varphi_{\tilde{c}_0}(A, \mathbf{b}) \leqslant \int_{\mathcal{S}_1} \varphi_{c_0}(\nabla u, \mathbf{b}) + \delta.$$

Now sending $c_0 \to \infty$ the claim follows from monotone convergence and the arbitrariness of δ. □

5.2. 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,

$$\varphi\big(A, b^1, \dots, b^{\nu-1}\big) = \varphi\big(RA, Rb^1, \dots, Rb^{\nu-1}\big) \tag{22}$$

for all $R \in \mathrm{SO}(3)$. So to evaluate $\varphi(A, \mathbf{b})$, we may only look at matrices

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{12} & a_{22} \\ 0 & 0 \end{pmatrix} \tag{23}$$

whose last row is 0 and whose top part is symmetric. Moreover, for systems of indistinguishable particles we have

Proposition 5.6. φ *satisfies the following symmetry properties*:

(i) *If* σ *is a permutation of* $\{1, \dots, \nu - 1\}$, *then*

$$\varphi\big(A, b^1, \dots, b^{\nu-1}\big) = \varphi\big(A, b^{\sigma(1)}, \dots, b^{\sigma(\nu-1)}\big).$$

(ii) *For* $1 \leqslant j \leqslant \nu - 1$

$$\varphi\big(A, b^1, \dots, b^{\nu-1}\big) = \varphi\big(A, b^1 - b^j, \dots, b^{j-1} - b^j, -b^j, b^{j+1} - b^j, \dots, b^{\nu-1} - b^j\big).$$

(iii) *If* $\nu \leqslant 2$, *then for all* $R \in \mathrm{O}(3)$

$$\varphi\big(A, b^1, \dots, b^{\nu-1}\big) = \varphi\big(RA, Rb^1, \dots, Rb^{\nu-1}\big).$$

(iv) *If* $R = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$, *then*

$$\varphi\big(A, b^1, \dots, b^{\nu-1}\big) = \varphi\big(AR, b^1, \dots, b^{\nu-1}\big).$$

(v) *If* $P = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, *then*

$$\varphi\big(A, b^1, \dots, b^{\nu-1}\big) = \varphi\big(AP, b^1, \dots, b^{\nu-1}\big).$$

Proof. Without loss of generality we may switch to the reference configuration

$$\mathcal{L} \cap \big(\big[-k/2, k/2\big]^2 \times [0, h]\big).$$

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 0th and the jth layer gives (ii). Finally, (iii) is trivial for $\nu = 1$, and for $\nu = 2$ it follows from (22) since by (ii) and (iv)

$$\varphi\big(A, b^1\big) = \varphi\big(AR^2, b^1\big) = \varphi\big(AR^2, -b^1\big) = \varphi\big(-A, -b^1\big). \qquad \square$$

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 $\nu \leqslant 1$, then (i) and (ii) are trivial. For $\nu = 2$, (ii) states that

$$\varphi\big(A, b^1\big) = \varphi\big(A, -b^1\big).$$

(iii) The above statements only hold for systems of indistinguishable atoms. For situations as in (9) we cannot permute the b^i or rotate the lattice.

Suppose now our reference configuration is a natural state. By the results in Section 6 and Proposition 5.3 we cannot expect that there is a unique quadratic form approximating φ for small strains. (An example of a macroscopic energy density φ which is zero on contractions is given in Proposition 4.5 of [21].) However (as e.g. in Proposition 4.5 of [21]), for purely tensile deformations, i.e. $s_1(A) \geqslant 1$, $|b^i - b^j| \geqslant 1$ for $i \neq j$, there can be a symmetric quadratic form Q such that for A (of the form (23)) 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

$$E(A, \mathbf{b}) \approx Q\big(A - \mathrm{Id}_{2,3}, b^1 - e_3, b^2 - b^1 - e_3, \ldots, b^{\nu-1} - b^{\nu-2} - e_3\big).$$

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 5.7. *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 the Proof. First note that by symmetry of Q

$$q_{ij} = q_{ji}. \tag{24}$$

Define

$$S = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad \widetilde{P} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad \widetilde{R} = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

From (iii) and (ii) of Proposition 5.6 we get that $\varphi(A, b) = \varphi(SA, Sb) = \varphi(SA, -Sb)$ which implies

$$q_{4j} = q_{5j} = 0 \quad \text{for } j = 1, 2, 3, 6. \tag{25}$$

Next from (iii) and (v) of Proposition 5.6 we deduce $\varphi(A, b) = \varphi(\widetilde{P}AP, \widetilde{P}b)$ and hence

$$q_{11} = q_{22}, \quad q_{44} = q_{55}, \quad q_{13} = q_{23}, \quad q_{16} = q_{26}. \tag{26}$$

Finally by (22) and (iv) of Proposition 5.6 we have $\varphi(A, b) = \varphi(\widetilde{R}AR, \widetilde{R}b)$ which leads to

$$q_{13} = -q_{23}, \qquad q_{45} = q_{36} = 0. \tag{27}$$

Summarizing (24)–(27) 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 cannot 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 Section 6.2). 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 2.11 are satisfied, and all the assertions of Proposition 5.6 apply.

6. Small strains

In this section, we study the response of our continuum theory to deformations that are locally close to rigid motions. For a simple mass-spring model with nearest neighbor interaction discussed in [21], we could give an explicit formula for φ which turned out to give zero energy response under contractive boundary conditions due to microscopic 'crumpling'. This model, however, lacks some physically desirable features, in particular it has no shear resistance. We will 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 $\operatorname{dist}(A, \mathrm{O}(2,3))$ 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.

6.1. 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

$$E(y) = \sum_{i=1}^{L} W_1\big(|y_i - y_{i-1}|\big) + \sum_{i=1}^{L-1} W_2(\phi_i),$$

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

$$W_1(r) \geqslant \begin{cases} \alpha_1 (r-1)^2 & \text{for } |r-1| \leqslant \rho, \\ \alpha_2 & \text{for } |r-1| \geqslant \rho, \end{cases} \qquad W_2(\phi) \geqslant \begin{cases} \alpha_1 \phi^2 & \text{for } |\phi| \leqslant \rho, \\ \alpha_2 & \text{for } \rho \leqslant |\phi| \leqslant \pi. \end{cases}$$

For given $a > 0$, we would like to examine

$$\varphi(a) := \lim_{L\to\infty} \frac{1}{L} \inf_{\mathcal{N}_L(a)} E(y), \quad \mathcal{N}_L(a) = \big\{y\colon \big|y_i - (ia, 0, 0)\big| \leqslant c_0\big\}. \tag{28}$$

($\mathcal{N}_L(a)$ is a one-dimensional version of $\widehat{\mathcal{N}}_k^{0,1}$.) 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 6.1. *For each $a > 0$ the limit in* (28) *exists.*

Proof. This is just an easy one-dimensional special case of Theorem 2.8. 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 $|E(y)/L| \leqslant 2C$, 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

$$\frac{1}{L_0}\inf_{y\in\mathcal{N}_{L_0}(a)} E(y) \leqslant \varphi(a)+\varepsilon \quad\text{and}\quad \frac{1}{L}\inf_{y\in\mathcal{N}_L(a)} E(y) \geqslant \varphi(a)-\varepsilon\ \forall L\geqslant L_0.$$

Then choose $y^0 \in \mathcal{N}_{L_0}(a)$ such that

$$\frac{1}{L_0}E\big(y^0\big) \leqslant \varphi(a)+2\varepsilon.$$

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 $L \geqslant L_0$ 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 $(0\leqslant r < L_0)$

$$y_{kL_0+r} = (kL_0 a, 0, 0) + y_r^0.$$

Clearly, y is in $\mathcal{N}_L(a)$, and, by translational invariance,

$$E(y_0,\dots,y_L) \leqslant \lfloor L/L_0\rfloor E\big(y_0^0,\dots,y_{L_0}^0\big) + 2CL_0 + 2C\lfloor L/L_0\rfloor.$$

So dividing by L and choosing L_0 large enough, this shows that for L sufficiently large indeed

$$\varphi(a)-\varepsilon \leqslant \frac{1}{L}E(y_0,\dots,y_L) \leqslant \varphi(a)+3\varepsilon. \qquad \square$$

The main result for our one-dimensional model problem is the following

Proposition 6.2. *There exist $\delta, c > 0$ such that for all $1-\delta \leqslant a \leqslant 1+\delta$*

$$\varphi(a) \geqslant c(1-a)^2.$$

If in addition there exists $\alpha_3 \geqslant \alpha_1$ such that $W_1(r) \leqslant \alpha_3(r-1)^2$ if $|r-1|\leqslant\delta$, and $W_2(0)=0$, then there are $C, c > 0$ such that

$$c(a-1)^2 \leqslant \varphi(a) \leqslant C(a-1)^2.$$

So the energy scales quadratically with the distance of a to 1. However, we will see that even for quadratic energy wells φ will not be C^2 at $a=1$.

Before we come to the rather technical proof of the lower bound in Proposition 6.2, note that it is easy to get upper bounds for $\varphi(a)$:

Lemma 6.3. *Suppose there exists $\alpha_3 \geqslant \alpha_1$ such that $W_1(r) \leqslant \alpha_3(r-1)^2$ if $|r-1|\leqslant\rho$, and $W_2(0)=0$. Then for $|a-1|\leqslant\rho$*

$$\varphi(a) \leqslant \alpha_3(a-1)^2.$$

Proof. Just insert the Cauchy–Born state $y_k = (ka, 0, 0)$ and let $L\to\infty$. $\square$

We will now prove lower bounds for φ. Suppose first $1\leqslant a\leqslant 2$. Noting that imposing the additional constraint that $y_0 = 0$ and $y_L = La$ only leads to negligible energy errors (of order $\mathcal{O}(1/L)$) we define E_L by

$$E_L(a) = \inf\big\{E(y)\colon\ \big|y_i - (ia,0,0)\big| \leqslant c_0 \text{ and } y_0 = 0,\ y_L = (La,0,0)\big\}.$$

But if $|y_i - (ia,0,0)| \leqslant c_0$, then $|y_{i+1}-y_i| \leqslant a + 2c_0 \leqslant 2(c_0+1)$, so we have

$$E_L(a) \geqslant \inf\left\{\sum_{i=1}^{L} f(z_i)\colon\ z_1,\dots,z_L\in\mathbb{R}^3 \text{ and } z_1+\dots+z_L = (La,0,0)\right\},$$

where $f:\mathbb{R}^3\to\mathbb{R}\cup\{\infty\}$ is given by

$$f(z) = \begin{cases} W_1(|z|) & \text{for } |z|\leqslant 2c_0+2,\\ \infty & \text{for } |z| > 2c_0+2.\end{cases}$$

Now clearly there exists $\alpha_4 > 0$ such that

$$f^{**}(z) \geqslant \begin{cases} 0 & \text{for } |z| \leqslant 1, \\ \alpha_4(|z|-1)^2 & \text{for } 1 < |z| \leqslant 2c_0 + 2, \\ \infty & \text{for } |z| > 2c_0 + 2. \end{cases}$$

It follows that

$$\varphi(a) = \lim_{L\to\infty} \frac{1}{L} E_L(a) \geqslant \lim_{L\to\infty} f^{**}(a,0,0) \geqslant \alpha_4(a-1)^2. \tag{29}$$

This establishes the desired lower bound for tensile deformations $a \geqslant 1$.

Suppose now $a < 1$. Since the inter-atomic distances $|y_i - y_{i-1}|$ remain bounded, by rescaling E we may assume that

$$W_1(r) \geqslant (r-1)^2, \qquad W_2(\phi) \geqslant \phi^2.$$

Lemma 6.4. *If y is any deformation with $E(y) \leqslant L^{-3}$, then*

$$|y_L - y_0|^2 \geqslant L^2\big(1 - 3L^{-2}\big). \tag{30}$$

Proof. Suppose $E(y) \leqslant \delta$. Then

$$\sum_{i=1}^{L} \big(|y_i - y_{i-1}| - 1\big)^2 \leqslant \delta, \qquad \sum_{i=1}^{L-1} \phi_i^2 \leqslant \delta$$

and hence by Cauchy–Schwarz

$$\sum_{i=1}^{L} \big||y_i - y_{i-1}| - 1\big| \leqslant \sqrt{L}\sqrt{\delta}, \qquad \sum_{i=1}^{L-1} |\phi_i| \leqslant \sqrt{L-1}\sqrt{\delta}.$$

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 $\delta L \leqslant 1$

$$\begin{aligned} |y_L - y_0|^2 &= \left| \sum_{i=1}^{L} y_i - y_{i-1} \right|^2 \\ &= \sum_{\substack{1\leqslant i\leqslant L \\ 1\leqslant j\leqslant L}} \langle y_i - y_{i-1}, y_j - y_{j-1} \rangle \\ &\geqslant \sum_{\substack{1\leqslant i\leqslant L \\ 1\leqslant j\leqslant L}} |y_i - y_{i-1}||y_j - y_{j-1}| \cos\big(\sqrt{L\delta}\big) \\ &= \Big(\sum_{1\leqslant i\leqslant L} |y_i - y_{i-1}| \Big)^2 \cos\big(\sqrt{L\delta}\big) \\ &\geqslant \big(L - \sqrt{L\delta}\big)^2 (1 - L\delta). \end{aligned}$$

Now choosing $\delta = \delta(L) = L^{-3}$, the claim follows. □

If y satisfies $|y_i - (ia, 0, 0)| \leqslant c_0$ for $i = 0, \ldots, L$, then $La - 2c_0 \leqslant (y_L)_1 - (y_0)_1 \leqslant La + 2c_0$. So, for $|a - a'| \leqslant 2c_0/L$, we define E_L depending on two parameters a, a' by

$$\mathcal{N}_L(a, a') := \big\{ y \in \mathcal{N}_L(a) \colon\ (y_L)_1 - (y_0)_1 = La' \big\}$$

and

$$E_L(a, a') = \inf_{\mathcal{N}_L(a,a')} E(y).$$

Also, let $m = \lceil \sqrt{3 + 4c_0^2} + 1 \rceil$ and define $a_0, a_1, \ldots$ and $L_0, L_1, \ldots$ by

$$1 - a_n = 4^{-1-n} \quad \text{and} \quad L_n = \frac{4m}{\sqrt{1 - a_n}} = 2^{3+n} m.$$

Lemma 6.5. *There exists $c > 0$ such that for all $k \in \mathbb{N}$,*

$$\frac{1}{kL_n} E_{kL_n}(a, a') \geqslant c(1 - a')^2 \quad \forall a' \in \left[\frac{3}{4}, a_n\right], \ |a - a'| \leqslant \frac{2c_0}{kL_n}.$$

Proof. The lemma is proven by induction on n. The case $n = 0$ follows directly from the following claim which will be proven later.

Claim. *There exists $C > 0$ such that, for all $k \in \mathbb{N}$,*

$$\frac{1}{kL_0} E_{kL_0}(a, a') \geqslant C \quad \forall a' \in \left[\frac{1}{2}, a_0\right], \ |a - a'| \leqslant \frac{2c_0}{kL_0}.$$

Suppose the lemma is proven for n and choose $c = \min\{(4m)^{-4}, C\}$.

$$L_n = \frac{4m}{\sqrt{1 - a_n}} = \frac{m}{\sqrt{1 - a_{n+2}}} \geqslant \frac{m}{\sqrt{1 - a'}}$$

for $a' \leqslant a_{n+2}$ implies

$$L_n^2(1 - a') > 3 + (2c_0)^2,$$

and thus

$$(L_n a')^2 + (2c_0)^2 < L_n^2\big(1 - 3L_n^{-2}\big).$$

But if $y \in \mathcal{N}_{L_n}(a, a')$, then $|y_{L_n} - y_0|^2 \leqslant (L_n a')^2 + (2c_0)^2$, so (30) cannot hold. It follows from Lemma 6.4 that

$$\frac{1}{L_n} E(y) \geqslant L_n^{-4} \quad \forall y \in \mathcal{N}_{L_n}(a, a'), \ 0 < a' \leqslant a_{n+2}. \tag{31}$$

Now let $3/4 \leqslant a' \leqslant a_{n+1}$, $|a - a'| \leqslant 2c_0/(kL_{n+1})$. 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

$$E_{kL_{n+1}}(a, a') \geqslant \sum_{i=1}^{2k} E_{L_n}(a, x_i),$$

where $x_1 + \cdots + x_{2k} = 2ka'$ and $x_i > 1/2$, because

$$L_n x_i \geqslant L_n a - 2c_0 \geqslant L_n a' - L_n \frac{2c_0}{kL_{n+1}} - 2c_0 \geqslant \frac{3L_n}{4} - 3c_0 > \frac{L_n}{2}.$$

So if $f : \mathbb{R} \to \mathbb{R} \cup \{\infty\}$ is defined by

$$f(x) = \begin{cases} \infty & \text{for } x \leqslant 1/2, \\ c(1 - x)^2 & \text{for } 1/2 < x \leqslant a_n, \\ L_n^{-4} & \text{for } a_n < x \leqslant a_{n+2}, \\ 0 & \text{for } a_{n+2} < x, \end{cases}$$

we have by (31), the above claim (note that $C \geqslant c(1/2)^2$) and induction hypothesis,

$$\frac{1}{kL_{n+1}} E_{kL_{n+1}}(a, a') \geqslant \frac{1}{2k} \sum_{i=1}^{2k} \frac{1}{L_n} E_{L_n}(a, x_i) \geqslant \frac{1}{2k} \sum_{i=1}^{2k} f(x_i) \geqslant f^{**}(a').$$

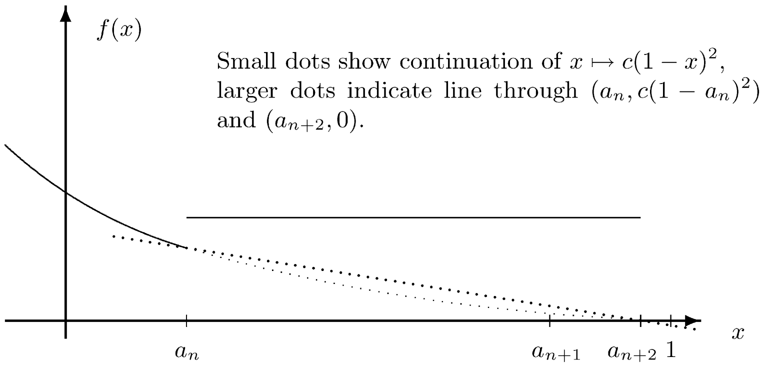

Fig. 6.

Now, since

$$L_n^{-4} = (4m)^{-4}(1-a_n)^2 \geqslant c(1-a_n)^2, \quad 1-a_n = 16(1-a_{n+2}) \quad \text{and} \quad -2c(1-a_n) < -\frac{16}{15}c(1-a_n),$$

f^{**} is given by

$$f^{**}(x) = \begin{cases} \infty & \text{for } x \leqslant 1/2, \\ c(1-x)^2 & \text{for } 1/2 < x \leqslant a_n, \\ \frac{c(1-a_n)}{15}(16(1-x)-(1-a_n)) & \text{for } a_n < x \leqslant a_{n+2}, \\ 0 & \text{for } a_{n+2} < x \end{cases}$$

(see Fig. 6). So for $a' \leqslant a_n$ we are done. But also for $a' \in [a_n, a_{n+1}]$

$$f^{**}(a') = \frac{c(1-a_n)}{15}\big(16(1-a') - (1-a_n)\big) \geqslant c(1-a')^2.$$

(Set $1-a' = \lambda(1-a_n)$, then this is equivalent to $\frac{1}{15}(16\lambda - 1) \geqslant \lambda^2$ 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

$$\frac{1}{L_0}E(y_0, \ldots, y_{L_0}) \geqslant \frac{\delta(L_0)}{L_0} = L_0^{-4} \quad \text{for } 0 \leqslant a' \leqslant a_1.$$

For $1/2 \leqslant a' \leqslant a_0$ gain considering the first components of the atomic sites $y_0, y_{L_0}, \ldots, y_{kL_0}$, $x_1 + \ldots + x_k = ka'$, $x_i > 0$, we deduce

$$\frac{1}{kL_0}E_{kL_0}(a, a') \geqslant \frac{1}{k}\sum_{i=1}^{k}\frac{1}{L_0}E_{L_0}(a, x_i) \geqslant \frac{1}{k}\sum_{i=1}^{k} f(x_i) \geqslant f^{**}(a') \geqslant C > 0,$$

where now $f : \mathbb{R} \to \mathbb{R} \cup \{\infty\}$ is defined by

$$f(x) = \begin{cases} \infty & \text{for } x \leqslant 0, \\ L_0^{-4} & \text{for } 0 < x \leqslant a_1, \\ 0 & \text{for } a_1 < x. \end{cases} \qquad \Box$$

After these preparations the proof of Proposition 6.2 is straightforward:

Proof of Proposition 6.2. The upper bound is immediate from Lemma 6.3. The lower bound for $a \geqslant 1$ was established in (29). The additional constraint in $\mathcal{N}(a, a')$ is negligible, so the lower bound for $a < 1$ follows by choosing n such that $a = a' \leqslant a_n$ and letting $k \to \infty$ in Lemma 6.5 noting that, by Lemma 6.1, it suffices to consider a subsequence in (28). $\Box$

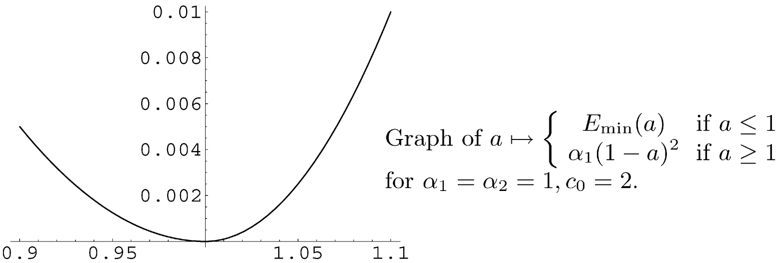

Fig. 7.

The following examples show that even for quadratic energy wells

$$W_1(r) = \alpha_1(r-1)^2 \quad \text{resp.} \quad W_2(\phi) = \alpha_2\phi^2, \tag{32}$$

φ will not be C^2 at $a = 1$.

Examples. 1. Let W_1, W_2 be as in (32). If $a \geqslant 1$, then, as in the derivation of (29), we see that the Cauchy–Born state $y_k = (ka, 0, 0)$ is asymptotically optimal, leading to

$$\varphi(a) = \alpha_1(a-1)^2.$$

For $0 < a < 1$ consider the spiral deformation $y_k = (ka, c_0\cos(k\psi), c_0\sin(k\psi))$, $k = 1, \ldots, L$ with $|\psi| \ll 1$. 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

$$E_{\min} = \frac{\alpha_1\alpha_2}{\alpha_2 + \alpha_1 c_0^2/4}(1-a)^2 + \mathcal{O}\big((1-a)^3\big)$$

(see Fig. 7). 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 $a \geqslant 1$ 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 pure bending energies for $a < 1$ that occur only at lower energy scales.

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):

$$\gamma \mapsto \big(R\sin(\gamma), 0, R\big(1-\cos(\gamma)\big) - d\big)$$

for $0 \leqslant \gamma \leqslant \gamma_{\max}$, $\gamma_{\max}$ given by $R(1-\cos(\gamma_{\max})) = d$. We place atoms on this curve starting at $\gamma = 0$ with distances 1 between neighboring atoms:

$$y_k = \big(R\sin(k\Phi/L), 0, R\big(1-\cos(k\Phi/L)\big) - d\big), \quad k = 0, \ldots, L, \tag{33}$$

where $2R\sin(\Phi/2L) = 1$ and $\Phi \leqslant \gamma_{\max}$, $\Phi + \Phi/L > \gamma_{\max}$. 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 $(1-a)$)

$$\Phi \approx \gamma_{\max} \approx \sqrt{6}(1-a)^{1/2}, \quad R \approx 3d(1-a)^{-1}, \quad L \approx \frac{\sqrt{2}d}{\sqrt{3}}(1-a)^{-1/2}.$$

The mean energy of y is thus

$$\frac{1}{L}E(y) = \alpha_2\left(\frac{\Phi}{L}\right)^2 = \frac{9\alpha_2}{d^2}(1-a)^2 + \mathcal{O}\big((1-a)^3\big).$$

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 $\approx (9\alpha_2/d^2)(1-a)^2$. Finally, set $y' = \bar{a}y \in \mathcal{N}_L(a\bar{a})$ for $\bar{a} \leqslant 1$ near 1 and, for given $x \leqslant 1$ near 1 minimize $E(y')$ subject to $a\bar{a} = x$. It follows that

$$\varphi(x) \leqslant \frac{9\alpha_1\alpha_2}{d^2\alpha_1 + 9\alpha_2}(1-x)^2 + \mathcal{O}\big((1-x)^3\big).$$

Again, this is preferable to the Cauchy–Born energy $\alpha_1(1-x)^2$.

Remark. In terms of scaling with c_0 the lower and upper bound for $\varphi(a)$ derived in the preceding examples respectively in Proposition 6.2 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 6.5). In fact, the lower bound can be improved as we shall now detail.

Fix c_0 and let $k \in \mathbb{N}$. Suppose $y \in \mathcal{N}_{kL,kc_0}(a)$ and consider the corresponding k-step chain $Y = (Y_0, \dots, Y_L)$ defined by $Y_j = y_{kj}$. For the corresponding angles we obtain

$$|\Phi_j| \leqslant \sum_{i=k(j-1)+1}^{k(j+1)-1} |\phi_i|.$$

To estimate $|Y_j - Y_{j-1}|$, let $\bar{\Phi}_j = \sum_{i=k(j-1)+1}^{kj-1} |\phi_i|$. Then, if $\bar{\Phi} \leqslant 1$, similar as on page 68, we obtain

$$|Y_j - Y_{j-1}| = \left| \sum_{i=k(j-1)+1}^{kj} (y_i - y_{i-1}) \right| \geqslant \sum_{i=k(j-1)+1}^{kj} |y_i - y_{i-1}|\big(1 - \bar{\Phi}_j^2\big).$$

On the other hand, clearly $|Y_j - Y_{j-1}| \leqslant \sum_{i=k(j-1)+1}^{kj} |y_i - y_{i-1}|$, so setting $\gamma k := \sum_{i=k(j-1)+1}^{kj} |y_i - y_{i-1}|$,

$$\begin{aligned}
\big(|Y_j - Y_{j-1}| - k\big)^2 &\leqslant \max\big\{(\gamma k - k)^2, \big(\gamma k - k - \gamma k \bar{\Phi}_j^2\big)^2\big\} \\
&\leqslant 2(\gamma k - k)^2 + 2\big(\gamma k \bar{\Phi}_j^2\big)^2 \\
&\leqslant 10(\gamma k - k)^2 + 2(2k\bar{\Phi}_j)^2.
\end{aligned}$$

(If $\gamma \leqslant 2$, this is clear. If $\gamma \geqslant 2$, it follows from $10(\gamma-1)^2 \geqslant 2(\gamma-1)^2 + 2\gamma^2$ and $\bar{\Phi}_j^2 \leqslant 1$. If $\bar{\Phi}_j \geqslant 1$, we get such an estimate even easier:

$$\big(|Y_j - Y_{j-1}| - k\big)^2 \leqslant 2\big((2c_0 + a)k\big)^2 + 2k^2 \leqslant Ck^2\bar{\Phi}_j^2.$$

Now let $y' := Y/k$. Then clearly $y' \in \mathcal{N}_{L,c_0}(a)$. Without loss of generality we may assume there exists α_3 as in Lemma 6.3. By Cauchy–Schwarz,

$$\begin{aligned}
E_L(y') &\leqslant \alpha_3 \sum_{j=1}^{L} \big(|y'_j - y'_{j-1}| - 1\big)^2 + \alpha_3 \sum_{j=1}^{L-1} \Phi_j^2 \\
&= \frac{\alpha_3}{k^2} \sum_{j=1}^{L} \big(|Y_j - Y_{j-1}| - k\big)^2 + \alpha_3 \sum_{j=1}^{L-1} \Phi_j^2 \\
&\leqslant \alpha_3 \sum_{j=1}^{L} \big(10(\gamma-1)^2 + C\bar{\Phi}_j^2\big) + \alpha_3 \sum_{j=1}^{L-1} \Phi_j^2 \\
&\leqslant \alpha_3 \sum_{j=1}^{L} \left(\frac{10}{k^2} k \sum_{i=k(j-1)+1}^{kj} \big(|y_i - y_{i-1}| - 1\big)^2 \right) + \alpha_3 \sum_{j=1}^{L-1} \left(Ck \sum_{i=k(j-1)+1}^{k(j+1)-1} |\phi_i|^2 \right) \\
&\leqslant C \left(\frac{1}{k} \sum_{i=1}^{Lk} \big(|y_i - y_{i-1}| - 1\big)^2 + k \sum_{i=1}^{Lk} |\phi_i|^2 \right).
\end{aligned}$$

It follows that

$$\frac{1}{L}E_L(y') \leqslant \frac{Ck^2}{Lk}E_{Lk}(y)$$

and since $y \in \mathcal{N}_{kL,kc_0}(a)$ was arbitrary, letting $L \to \infty$ in fact

$$\varphi_{kc_0}(a) \geqslant c(c_0)k^{-2}\varphi_{c_0}(a).$$

This proves that also the lower bound scales like c_0^{-2}. □

6.1.1. 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

$$H(a) = \begin{cases} \alpha_1(1-a)^2 & \text{for } a \leqslant 1, \\ \alpha_2(1-a)^2 & \text{for } a \geqslant 1, \end{cases}$$

where $0 < \alpha_1 < \alpha_2$. The corresponding Boltzmann distribution of statistical mechanics is

$$d\mathbb{P}_\beta(a) = \frac{1}{Z_\beta}\mathrm{e}^{-\beta H(a)}\,\mathrm{d}a,$$

$\beta = 1/kT > 0$, 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:

$$\int a\,\mathrm{d}\mathbb{P}_\beta(a) = 1 - \frac{1}{\sqrt{\pi\beta}}\left(\sqrt{\frac{1}{\alpha_1}} - \sqrt{\frac{1}{\alpha_2}}\right).$$

Since $\alpha_2 > \alpha_1$, this is strictly less than 1 and increasing in β, reflecting thermal contraction as expected for polymers (cf. [23]).

6.2. Energy scaling near O(2,3)

Taking into account only next neighbor interactions leads to zero energy response to compressions, as noted earlier (see Proposition 4.5 of [21]). 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

$$W_1(r) \geqslant \alpha(r-1)^2, \quad W_1'(r) \geqslant \alpha\big(r-\sqrt{2}\big)^2, \quad W_2(\phi) \geqslant \alpha\phi^2$$

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

$$E_{\mathrm{an}}(y) = \frac{1}{2}\sum_{|x_i - x_j| = 1} W_1\big(|y_i - y_j|\big) + \frac{\delta}{2}\sum_{|x_i - x_j| = 2} \chi_{[0,r_0)}\big(|y_i - y_j|\big) + \frac{1}{2}\sum |y_i - y_k||y_j - y_k| W_2\left(|\theta_{ikj}| - \frac{\pi}{2}\right) \tag{34}$$

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

$$E_{\mathrm{nnn}}(y) = \frac{1}{2}\sum_{|x_i - x_j| = 1} W_1\big(|y_i - y_j|\big) + \frac{1}{2}\sum_{|x_i - x_j| = \sqrt{2}} W_1'\big(|y_i - y_j|\big) + \frac{\delta}{2}\sum_{|x_i - x_j| = 2} \chi_{[0,r_0)}\big(|y_i - y_j|\big). \tag{35}$$

Proposition 6.6. *Both E_{an} and E_{nnn} are admissible energy functions leading to continuum stored energy functions φ_{an} resp. φ_{nnn}. For $\nu \geqslant 2$ there exist $\delta, c > 0$ such that for* $\operatorname{dist}(A, O(2,3)) \leqslant \delta$,

$$\varphi_{\mathrm{an}}(A, \mathbf{b}), \varphi_{\mathrm{nnn}}(A, \mathbf{b}) \geqslant c\operatorname{dist}^2\big(A, O(2,3)\big).$$

Clearly, E_{an} and E_{nnn} are admissible energy functions (see Proposition 2.11). It remains to prove the lower bound on φ in terms of $\operatorname{dist}^2(A, O(2,3))$. To give a detailed proof is cumbersome, we mention the main ideas.

Sketch of the Proof. The film contains various atomic chains. For $\nu \geqslant 2$, 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. Similarly 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 6.2 gives the result. □

Remarks.

(i) Proposition 6.6 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 $\nu \geqslant 2$ this result implies that $\bar\varphi$ (defined on $\mathbb{R}^{3\times 2}$, cf. the remark below Proposition 2.11) is not rank-one convex. This is because φ vanishes on $O(2,3)$, but not on its rank-one convex hull $\{A \in \mathbb{R}^{3\times 2}\colon s_2(A) \leqslant 1\}$ (see [11], page 50, Corollary 2.3.2).

In the rest of this Section 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 (33) for the atomic chain. Let R, L and Φ be the same as in (33). Set $R(x_3) = R + \frac{\nu-1}{2} - x_3$. We define a film deformation patching together appropriately cylindrical configurations

$$y(x_1, x_2, x_3) = \big(R(x_3)\sin(x_1\Phi/L), x_2, R(x_3)\big(1 - \cos(x_1\Phi/L)\big) - d\big),$$

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 (33), for $A = (ae_1, e_2)$, $a \leqslant 1$ near 1,

$$\bar\varphi(A) \leqslant \frac{\text{const.}}{c_0^2}(1 - a)^2,$$

provided there exists $\beta > 0$ such that, in a neighborhood of 1 resp. $\sqrt{2}$ resp. 0,

$$W_1(r) \leqslant \beta(r - 1)^2, \quad W_1'(r) \leqslant \beta\big(r - \sqrt{2}\big)^2, \quad W_2(\phi) \leqslant \beta\phi^2.$$

For $a \geqslant 1$, however, it is not hard to prove that $\bar\varphi(A) \geqslant \alpha_1(1 - a)^2$. (This can be seen considering the one dimensional atomic chains $i \mapsto y(i, x_2, x_3)$.) □

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