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by

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Abstract

We discuss qualitative aspects of a continuum theory for thin films rigorously derived in [21]. 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 [21] is the only scale for which a limiting theory that also accounts for atomic relaxation effects is non-trivial.

Contents

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, 18, 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]. 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 [5, 6, 7]; more complicated potentials under additional assumptions as, e.g., the Cauchy-Born rule are considered in [2, 3, 4].

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 relaxations 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 $b^i : [0, 1]^2 \to \mathbb{R}^3$, $i = 1, \ldots, \nu - 1$:

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

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

In section 2, after introducing the model, we will recall the precise statements from [21]. Also we will gather 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 and study the limiting cases $c_0 \to \infty$ and $c_0 \to 0$. Moreover, we will see that the physically motivated rate of convergence for which continuum theory was derived in [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 extensive 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 $O(2, 3)$ is examined. We still find 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].

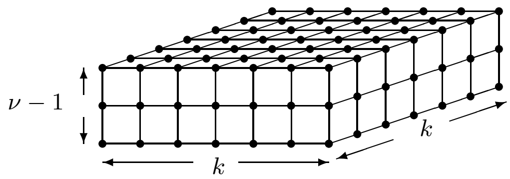
2.1 The model

Kinematics

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

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

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, $\mathcal{L} = \mathbb{Z}^3$.



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*

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

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

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

The un-rescaled version of u is denoted U, i.e. $\tilde{U} = u$. 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 $\sup_{x\in\mathcal{L}_k} |y(x) - U(x_p)| \leq c$. Then y is Lipschitz. For any (rescaled) Lipschitz interpolation $y : \mathcal{S}_k \times [0,h] \to \mathbb{R}^3$ ($\tilde{y} : \mathcal{S}_1 \times [0,h] \to \mathbb{R}^3$) there are constants $C_1, C_2, C_3 > 0$ such that,*

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

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

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*

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

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

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

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.

Energy

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

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

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

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

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

The two main 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*

$$|\psi| \leq M \qquad and \qquad \psi(r) \leq Mr^{-q} \tag{3}$$

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

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

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

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*

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

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 $|y(x) - y(z)| \geq C_1|x - z| - C_3$.*

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

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

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

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

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

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

To compute φ more directly than by the associated cell problem, set

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

where $\mathcal{L}'_k = \mathbb{Z}^2 \cap \mathcal{S}_k$.

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

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

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

Here, $\mathcal{A}_{\text{hom}} \subset \mathbb{R}^{3\cdot 2} \times (\mathbb{R}^3)^{\nu-1}$, the set of *admissible* $(A,\mathbf{b})$, is defined by

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

for matrices $A \in \mathbb{R}^{3\cdot 2}$ and vectors $b^1, \dots, b^{\nu-1}$.

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*

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

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

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

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

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

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.) $r \geq r_0$*

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

for $r \geq r_0$. Then theorem 2.7 extends to energy functions of the form (8) where, as in theorem 2.8, $\varphi : \mathcal{A}_{\text{hom}} \to (-\infty, \infty]$ 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

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

where the enumeration of elements of U_{x_i} shall be such that $x_1^i = x_i$ and if $(x_{i_1})_3 = (x_{i_2})_3$, then

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

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

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

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 $y(x_2^i), \dots, y(x_{r_a}^i)$. (The term $\mathcal{O}(k)$ is introduced to compensate for boundary effects, since U_{x_i} is not contained in $S_k \times [0, h]$ for x_i in a boundary layer of constant width.) 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 $x = (x_1, x_2, x_3) \in (\mathbb{Z}_+)^2 \times \{0, \dots, \nu - 1\}$.

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*

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

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

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

2.3 Technical results

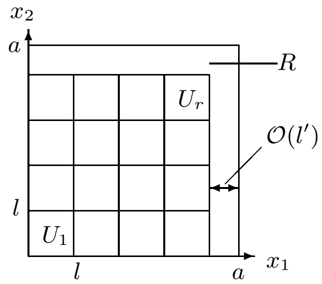
We now gather some of the technical results obtained in [21] that will be useful in the following sections.

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

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

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



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

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

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

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))

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

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

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

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*

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

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

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

and

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

(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

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

and setting

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

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 $\hat{\mathcal{N}}^{0,1}_{k,c_0}$, φ_{k,c_0}.) Our first task is to analyze this dependence of our continuum theory on the relaxation parameter c_0. It will turn out that we can not relax sending c_0 to infinity. This is due to the (physically reasonable) decay assumptions on atomic interactions. Moreover, c_0/k will prove to be the only scale which both accounts for atomistic relaxation effects and yields a non-trivial continuum theory. We start by proving the following regularity result.

Proposition 3.1 *Fix $(A, \mathbf{b}) \in \mathcal{A}_{\text{hom}}$. 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, $\varphi_{c_0}(A, \mathbf{b}) \leq \varphi_{c_0'}(A, \mathbf{b})$. Conversely, given $y \in \hat{\mathcal{N}}^{0,1}_{k,c_0}(A, \mathbf{b})$, by lemma 2.14 we find a deformation $y' \in \hat{\mathcal{N}}^{0,1}_{k,c_0'}(A, \mathbf{b})$ with $E(y') \leq E(y) + C(c_0 - c_0')^{1/5} k^2$ provided $(A, \mathbf{b})$ is admissible for c_0'. Therefore $\varphi_{c_0'}(A, \mathbf{b}) \leq \varphi_{c_0}(A, \mathbf{b}) + C(c_0 - c_0')^{1/5}$. $\square$

3.1 The limit $c_0 \to \infty$

Suppose E is an admissible pair potential with purely attractive pair interaction $W \leq 0$, $W \not\equiv 0$. 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 admissible $A, A', \mathbf{b}, \mathbf{b}'$.*

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 $2|A|$,

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

C_1, C_3 independent of $\mathbf{b}$. From assumption 2.6 and lemma 2.12 we then find a constant C such that for those $\mathbf{b}$, $E(V_{A,\mathbf{b}}) \leq Ck^2$. On the other hand, if for two vectors $\mathbf{b}_1$, $\mathbf{b}_2$

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

then $E(V_{A,\mathbf{b}_1}) = E(V_{A,\mathbf{b}_2}) + \mathcal{O}(|z|k)$. So for all $\mathbf{b}$ we obtain $\lim_{k\to\infty} \frac{1}{\nu k^2} E(V_{A,\mathbf{b}}) \leq C$, whence $\varphi_\infty(A, \cdot)$ is an upper bounded function on $\mathbb{R}^{3(\nu-1)}$ with values in $[-\infty, \infty)$. Since it is convex (by proposition 5.3 all $\varphi_{c_0}(A, \cdot)$ are convex), it must be constant.

For the remaining part it suffices to show that

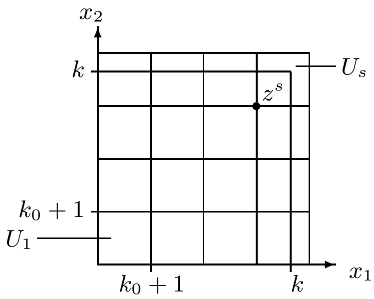
$$\varphi_\infty(A', \mathbf{b}) \leq \varphi_\infty(A, \mathbf{b}).$$

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 $y \in \hat{\mathcal{N}}^{0,1}_{k_0,c_0}(A, \mathbf{b})$ with

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

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 $U_1, \ldots, U_s$ be translates of $[0, k_0 + 1)^2$.



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

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

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

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

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

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

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

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

such that

$$\left| \frac{1}{\nu k^2} E(y') - \frac{1}{\nu k^2} E(\hat{y}) \right| \le C(\tilde{c_0}) \left(\frac{k_0^2}{k}\right)^{1/5}. \tag{16}$$

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

$$\left| \frac{1}{\nu k^2} E(y'(x) : x \in \mathcal{L}_k) - \frac{1}{\nu k_0^2} E(y(x) : x \in \mathcal{L}_{k_0}) \right| \le C \left(\frac{1}{k_0} + \frac{k_0}{k} \right). \tag{17}$$

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

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

Letting first $k \to \infty$, then $\tilde{c_0} \to \infty$, we deduce from proposition 3.1

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

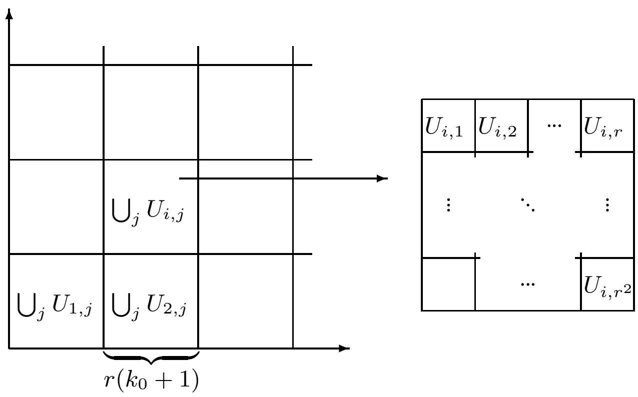
Since δ was arbitrary we finally get sending $c_0 \to \infty$

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

It remains to justify the application of lemma 2.13. The problem is that $\tilde{c_0}$ 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 $\|y'' - A\| \le \tilde{c_0}$ depends only on k_0 and y'' consists of translates of $y(\mathcal{L}_{k_0})$, but in addition satisfies a far-field minimal strain hypothesis with constants C_1, C_3 independent of k_0, i.e.

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

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



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

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

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

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 $y \in \hat{\mathcal{N}}^{0,1}_{k_0, c_0}(A, \mathbf{b})$.

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

$$|y''(x_1) - y''(x_2)| \ \ge \ |a_{j_1} - a_{j_2}| - |y'(x_1) - y'(x_2)|$$

$$
\begin{aligned}
&\geq |a_{j_1} - a_{j_2}| - |f^{i_1,j_1} - f^{i_2,j_2}| - |y(x_1 - z^{i_1,j_1}) - y(x_2 - z^{i_2,j_2})| \\
&\geq |a_{j_1} - a_{j_2}| - |f^{i_1,j_1} - f^{i_2,j_2}| - 2c_0 \\
&\quad -|A(x_1 - z^{i_1,j_1}) - A(x_2 - z^{i_2,j_2})| \\
&\geq |a_{j_1} - a_{j_2}| - C'rk_0 - 2c_0 - Ck_0 \\
&\geq 2rk_0 \qquad \text{for } |a_{j_1} - a_{j_2}| \text{ sufficiently large} \\
&\geq |x_1 - x_2|.
\end{aligned}
$$

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

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

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

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

$$
\frac{c}{2}|z^{i_1,j_1} - z^{i_2,j_2}| \geq \frac{crk_0}{4} \geq 2c_0 + 2|A|k_0 + 4\tilde{c_0},
$$

if we choose r sufficiently big.

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

For systems that do not satisfy assumption 2.6, φ_∞ may be nontrivial (for an example see proposition 4.5 in [21]). In paragraph 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

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

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*

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

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

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

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

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

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

Therefore,

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

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)

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

we get

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

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

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

By theorems 2.7 resp. 2.9, the macroscopic energy is given by

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

This expression can be seen as a thin-film version with directors $b^1,\dots,b^{\nu-1}$ of a formula derived in [4].

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 $l_1(k) = \text{const.}/k$ yields non-trivial results.

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 $\mathbf{b} \in (\mathbb{R}^3)^{(\nu-1)}$ will be admissible.) In analogy to $\mathcal{W}_k^l$ (cf. theorem 2.9) we define

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

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. The proof follows along the lines of the proof of theorem 3.2. We indicate the necessary modifications.

Let $E(u,\mathbf{b}) = \liminf_{k\to\infty} \frac{1}{\nu k^2} \inf_{y\in\mathcal{W}_k^{l_1,l_2}(u,\mathbf{b})} E(y)$. Choosing a suitable large k_0, we find $y \in \mathcal{W}_k^{l_1,l_2}(u,\mathbf{b})$ with

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

(resp. $\leq -1/\delta$ for $E(u,\mathbf{b}) = -\infty$). Construct y' as in the proof of theorem 3.2 with A' replaced by u'. Considering local spatial averages we still find $\hat{y} \in \mathcal{W}_k^{l_1,l_2}(u',\mathbf{b}_i)$ such that

$$\left| \frac{1}{\nu k^2} E(y') - \frac{1}{\nu k^2} E(\hat{y}) \right| \leq g(k,k_0)$$

with $\lim_{k\to\infty} g(k,k_0) = 0$. (To prove this, one may use the estimates for $\mathcal{W}_k^{l_1,l_2}$ obtained in [21], lemma 3.14.) Letting k tend to infinity gives

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

For the construction of y'' we can only guarantee that

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

for x_1 and x_2 that do not lie in the same $U_{i,j}$. 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 $a_1, \ldots, a_{r^2}$.

Now first setting $u' = u$ 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, for $\mathbf{b}$ fixed and general u, u' we obtain

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

Independence of $\mathbf{b}$ is seen as in the proof of theorem 3.2. Note that if in the above construction y' is patched together from translates of two deformations y_1 and y_2 in a checker-board pattern where $y_i \in \mathcal{W}_k^{l_1,l_2}(u, \mathbf{b}_i)$ with $\mathbf{b} = \frac{1}{2}(\mathbf{b}_1 + \mathbf{b}_2)$, then the argument shows that for $u = u'$

$$E\left(u, \frac{\mathbf{b}_1 + \mathbf{b}_2}{2}\right) \leq \frac{1}{2}(E(u, \mathbf{b}_1) + E(u, \mathbf{b}_2)).$$

As in the proof of theorem 3.2 we see that $\mathbf{b} \mapsto E(u, \mathbf{b})$ is bounded from above. Hence it must be constant. □

4 Extremal strains

In this section, we examine $\varphi(A, \mathbf{b})$ for A with very large (cf. paragraph 4.1) or small (cf. paragraph 4.2) singular values. Physically, the limit $A \to \infty$ is of limited relevance since 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 extensive deformations

Again in this paragraph we suppose that ψ satisfies assumption 2.6.

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

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

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

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

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

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

Proof. Let $y\in\hat{\mathcal{N}}_k^{0,1}(A,\mathbf{b})$ and $\mathbf{y}_{x_p}=(y(x_p,0),\dots,y(x_p,\nu-1))$, $\Delta\mathbf{y}_{x_p}=(y(x_p,1)-y(x_p,0),\dots,y(x_p,\nu-1)-y(x_p,0))$. By assumption 2.4,

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

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

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

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

so

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

as $c_1\to\infty$.

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

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

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

Remarks:

(i) If in definition 2.3 we request that $\|\tilde{y}-v_{A,\mathbf{b}}\|\le c_0/k$ instead of $\|\tilde{y}-A\|\le c_0/k$ as in (19), the result is analogous if we replace B_{c_0} by $B_{c_0}(\mathbf{b})=\{\mathbf{y}\in(\mathbb{R}^3)^\nu : |y^i-b^i|\le c_0\}$ ($b^0:=0$). Then, while holding c_0 fixed, we may send $(A, \mathbf{b}) \to \infty$ in the following sense. Let $A \to \infty$ as above. If e is a unit normal to graph(A), suppose that $|\langle b^i - b^j, e\rangle| \to \infty$ for $i \neq j \in \{0, \ldots, \nu - 1\}$. 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 $B^1, \ldots, B^\nu$ 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 *(i) Assume that $r^3 W(r) \to \infty$ as $r \to 0$. Then*

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

(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

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

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 $A \in \mathbb{R}^{3\cdot 2}$, let $S_p = \sqrt{A^T A} \in \mathbb{R}^{2\times 2}$,

$$S' = \begin{pmatrix} (S_p)_{11} & (S_p)_{12} & 0 \\ (S_p)_{21} & (S_p)_{22} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \qquad S = \begin{pmatrix} (S_p)_{11} & (S_p)_{12} \\ (S_p)_{21} & (S_p)_{22} \\ 0 & 0 \end{pmatrix}.$$

Define $A' \in \mathbb{R}^{3\cdot 3}$ by $A' = A \otimes e$, where e is the unit vector perpendicular to graph(A) such that $\det(A') > 0$. By the singular value decomposition there is an orthogonal matrix $R \in SO(3)$ such that

$$A = RS, \qquad A' = RS'.$$

We will investigate the limit $\det(S_p) \to 0$ while the singular values of A, i.e. the eigenvalues of S_p, remain bounded, which we will assume for the rest of this paragraph.

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

$$|y(x) - y(x')| \ge c|S'x - S'x'|.$$

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

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

□

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

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

$$\#\{(y_i, y_j) : i \ne j, |y_i - y_j| \le \rho\} \ge N - \frac{6}{\pi \rho^3}|U_\rho|.$$

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

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

It follows that

$$\#\{(y_i, y_j) : i \ne j, |y_i - y_j| \le \rho\} \ge N - \#\mathcal{M} \ge N - \frac{6}{\pi \rho^3}|U_\rho|.$$

□

Proof of theorem 4.2. (i) If $y \in \hat{\mathcal{N}}_k^{0,1}(A, \mathbf{b})$, then all the atoms lie in the c_0-neighborhood of $A([0,k]^2)$. The volume of the r_0-neighborhood of this set is $2(c_0 + r_0)\det(S_p)k^2 + \mathcal{O}(k)$. By lemma 4.4 we have

$$\begin{aligned}
\#\{(y_i, y_j) : i \ne j, |y_i - y_j| \le r_0\} \ &\ge\ \nu k^2 - \frac{6}{\pi r_0^3}(2(c_0 + r_0)\det(S_p)k^2 + \mathcal{O}(k)) \\
&\ge\ k^2/2,
\end{aligned}$$

provided $r_0^3 \gg \det(S_p)$, and therefore (fix $a > 0$ such that W is positive on $(0, a]$ and suppose that $r_0 \leq a$)

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

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

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

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

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

It remains to show that

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

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

$$\begin{aligned} &\sum_{\substack{|y(x)-y(x')|\geq a \\ |S'x-S'x'|\leq a}} |W|(|y(x) - y(x')|) + \sum_{\substack{|y(x)-y(x')|\geq a \\ |S'x-S'x'|>a}} |W|(|y(x) - y(x')|) \\ &\leq \sum_{\substack{|y(x)-y(x')|\geq a \\ |S'x-S'x'|\leq a}} Ma^{-q} + \sum_{\substack{|y(x)-y(x')|\geq a \\ |S'x-S'x'|>a}} M|y(x) - y(x')|^{-q} \\ &\leq \nu(k+1)^2 Ma^{-q} \#\{x \in \mathbb{Z}^3 : |S'x| \leq a\} + Mc^{-q} \sum_{|S'x-S'x'|\geq a} |S'x - S'x'|^{-q} \\ &\leq \frac{C\nu k^2}{\det(S')} + C\nu k^2 \sum_{|S'x|\geq a} |S'x|^{-q} \\ &\leq \frac{Ck^2}{\det(S')} + Ck^2 \int_{|S'x|\geq a} |S'x|^{-q} dx \\ &= \frac{Ck^2}{\det(S')} + Ck^2 \int_{|z|\geq a} |z|^{-q} \frac{dz}{\det(S')} \\ &= \frac{Ck^2}{\det(S_p)}. \end{aligned}$$

This finishes the proof of the first part of theorem 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 $c > 0$ and l small such that

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

Consider $(k+1)^2$ points $z_{ij} = A(i, j, 0)$ at positions $A(\{0, \dots, k\}^2)$. Since the singular values of S_p are bounded, for each of these points there is another one closer than d to it for d sufficiently large. Now partition the graph of A by disjoint translates of a square of side-length l, such that every such point is covered. The number those points in such a square Q is bounded by $C/\det(S_p)$.

On the other hand, if $A = RS$, each set $Q_e = \{z \in \mathbb{R}^3 : \exists\lambda \in [0, c/2] : z - \lambda e \in Q\}$ contains at least Cr^{-3} points of the lattice $rR\mathbb{Z}^3$, if r is small. Choosing r such that $r^3 = \tilde{c}\det(S_p)$, $\tilde{c}$ sufficiently small, we can move the original points z_{ij} within the sets Q_e onto distinct lattice points z'_{ij} of $rR\mathbb{Z}^3$ such that $|z_{ij} - z'_{ij}| \leq \sqrt{2l^2 + (c/2)^2}$.

Now define a deformation y by

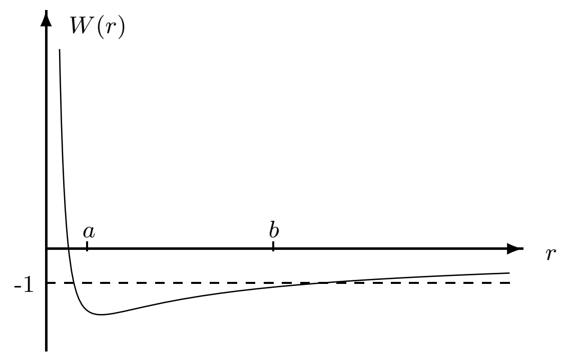
$$y(x_1, x_2, x_3) = z'_{x_1 x_2} + B^{x_3+1}.$$

By (21) and $|B^i| \leq c_3$, y lies in $\hat{\mathcal{N}}_k^{0,1}(A, \mathbf{b})$. y satisfies a minimal distance hypothesis with r: $|y(x) - y(x')| \geq r$ for $x \neq x'$. If $x_3 = x'_3$ this follows from the definition of y. If $x_3 \neq x'_3$ this follows from

$$\begin{aligned}
|y(x) - y(x')| &\geq |\langle y(x) - y(x'), e\rangle| \\
&= |\langle z'_{x_1 x_2} + B^{x_3+1} - z'_{x'_1 x'_2} - B^{x'_3+1}, e\rangle| \\
&\geq |\langle B^{x_3+1} - B^{x'_3+1}, e\rangle| - |\langle z'_{x_1 x_2} - z'_{x'_1 x'_2}, e\rangle| \\
&\geq |\langle b^{x_3} - b^{x'_3}, e\rangle| - c/2 \\
&\geq c/2
\end{aligned}$$

by (21) and construction of y.

Now suppose W is admissible and as in the picture below,



i.e. $|W(r)| \le Cr^{-\alpha}$, with $\alpha < 3$, for $r \le a$, and $W(r) \le 0$ for $r \ge a$, moreover $W(r) \le -1$ for $a \le r \le b$, $0 < a < b$ given. Then for x fixed

$$\begin{aligned}
&\sum_{x' \neq x} W(|y(x) - y(x')|) \\
\le\ & \sum_{|y(x)-y(x')| \le a} W(|y(x) - y(x')|) + \sum_{a < |y(x)-y(x')| \le b} W(|y(x) - y(x')|) \\
\le\ & C \sum_{|y(x)-y(x')| \le a} |y(x) - y(x')|^{-\alpha} + \sum_{a < |y(x)-y(x')| \le b} (-1) \\
\le\ & C \sum_{x' \in \mathbb{Z}^3 \,:\, 0 < |rx'| \le a} |rx'|^{-\alpha} - \#\{x' : a < |y(x) - y(x')| \le b\} \\
=\ & Cr^{-\alpha} \sum_{0 < |x'| \le a/r} |x'|^{-\alpha} - \#\{x' : a < |y(x) - y(x')| \le b\} \\
\le\ & Cr^{-\alpha} r^{\alpha - 3} - \#\{x' : a < |y(x) - y(x')| \le b\}
\end{aligned}$$

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

$$\#\{x' : a < |y(x) - y(x')| \le b\} \ge C \frac{b-a}{\det(S_p)}.$$

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

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

So if $b - a$ is chosen sufficiently large, this energy is negative. Now sum over all x to deduce that also the overall energy is negative. □

Remarks:

(i) It is not hard to see that if (cf. (2)) 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 is 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 $E_0 \ge -Ck^2$ independent of c_1 or assumption 2.4 is satisfied with ψ not depending on c_1. The latter follows from applying theorem 4.2 (i) to the right hand side of

$$E(y) \ge \frac{1}{2} \sum_{i \neq j} (W(|y_i - y_j|) - \psi(|y_i - y_j|)) - Ck^2.$$

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

In this paragraph, we explore if φ satisfies certain convexity properties. By frame indifference of the model, convexity of φ is in general not to be expected (cf. [8], p. 170, and 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.

Loss of rank-one convexity

In this paragraph we again suppose assumption 2.6 holds. Recall the notion of rank-one convexity:

Definition 5.1 *Suppose $f : \Omega \to \mathbb{R}$, where $\Omega \subset \mathbb{R}^{m \cdot n}$ 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 $\varphi(\cdot, \mathbf{b}) : \mathcal{A}_{\mathbf{b}} := \{A \in \mathbb{R}^{3 \cdot 2} : \operatorname{rank}(A) = 2\} \to \mathbb{R}$.

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

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

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

Proof. First note that φ is in fact bounded on each $\mathcal{A}_{\mathbf{b}}(c_1) := \{A \in \mathbb{R}^{3 \cdot 2} : s_1(A) \geq c_1\}$, $c_1 > 0$, by lemma 2.12 and assumption 2.6. Let $\delta > 0$. Set

$$f(\lambda_1, \lambda_2) := \varphi(A \cdot \Lambda, \mathbf{b}), \quad \Lambda = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}, \lambda_1, \lambda_2 \geq 1.$$

Note that

$$\begin{aligned} \inf_{|x|=1} |A\Lambda x|^2 &= \inf_{x \neq 0} \frac{\langle A\Lambda x, A\Lambda x\rangle}{\langle x, x\rangle} = \inf_{x\neq 0} \frac{\langle Ax, Ax\rangle}{\langle \Lambda^{-1}x, \Lambda^{-1}x\rangle} \\ &\geq \min\{\lambda_1^2, \lambda_2^2\} \inf_{x \neq 0} \frac{\langle Ax, Ax\rangle}{\langle x, x\rangle} = \min\{\lambda_1^2, \lambda_2^2\} \inf_{|x|=1} |Ax|^2. \end{aligned}$$

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

$$f(\lambda_1, 1) \geq \bar{E}^{**}(\mathbf{b}) - \delta.$$

Now convexity of $\lambda \mapsto f(\lambda, 1)$ implies that

$$f(1, 1) \geq \bar{E}^{**}(\mathbf{b}) - \delta.$$

□

Convexity in b

Discussing convexity in $\mathbf{b}$ we now 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 $\mathbf{b}$. 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 straight forward:

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 $Q_{11}, Q_{12}, Q_{21}, Q_{22}$ choose $y_{ij}^{(k)} \in \hat{\mathcal{N}}_{k,Q_{ij}}^{0,1/2}(A, \mathbf{b}_j)$ satisfying

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

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

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

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

$$\liminf_{k \to \infty} E(y^{(k)}(x) : x \in \mathcal{L}_k) \leq \frac{1}{2}(\varphi(A, \mathbf{b}_1) + \varphi(A, \mathbf{b}_2)).$$

□

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 $\|y - v_{A,\mathbf{b}}\| \leq c_0$. Consider the example from paragraph 3.2. For $\nu = 2$ and $A = \mathrm{Id}$

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

Now if $W : [0, \infty) \to \mathbb{R}$ satisfies $W(0) > 0$ and $W(r) = 0$ for $r \geq 1$, then $\varphi_0(\mathrm{Id}_{2,3}, 0) > 0$, while $\varphi_0(\mathrm{Id}_{2,3}, (0, 0, \pm 1)) = 0$. Hence, φ_0 is not convex in $\mathbf{b}$. Since $\varphi_0 = \lim_{c_0 \to 0} \varphi_{c_0}$, convexity also fails for values of c_0 bigger than 0.

Quasiconvexity of φ_∞

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

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

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

$$\fint_\Omega f(F + \nabla\zeta)dx \geq f(F)$$

for every bounded open subset $\Omega \subset \mathbb{R}^n$, $\zeta \in C_c^\infty(\Omega)$, and all $F \in \mathbb{R}^{m\cdot n}$.

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 limit $c_0 \to \infty$ corresponds to the unconstrained limit $y \overset{*}{\rightharpoonup} u$ in $W^{1,\infty}$, i.e. the full (lower semicontinuous) Γ-limit of E.

The proof is very similar to the proof of proposition 3.2. We indicate the modifications.

Sketch of 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

$$\varphi_\infty(A, \mathbf{b}) \leq \int_{\mathcal{S}_1} \varphi_\infty(A + \nabla f, \mathbf{b})dx.$$

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 $\|\tilde{y} - u\| \leq c_0/k_0$ and $|\fint_{[0,1]^2}(k_0\Delta^i\tilde{y} - b^i)d\rho|$ as small as we wish such that

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

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

Proceeding as in theorem 3.2 we construct a deformation $y' : \mathcal{L}_k \to \mathbb{R}^3$ for $k \gg k_0$ by patching together appropriately translated copies of y, so that

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

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

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

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

$$\varphi_\infty(A, \mathbf{b}) \leq \varphi_{\tilde{c_0}}(A, \mathbf{b}) \leq \frac{1}{\nu k^2} E(y') \leq \int_{\mathcal{S}_1} \varphi_{c_0}(\nabla u, \mathbf{b}) + \delta.$$

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,

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

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

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

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 $\{1, \ldots, \nu - 1\}$, then

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

(ii) For $1 \leq j \leq \nu - 1$

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

(iii) If $\nu \leq 2$, then for all $R \in O(3)$

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

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

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

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

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

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

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

Then $(x_p, x_3) \mapsto (Px_p, x_3)$ and $(x_p, x_3) \mapsto (Rx_p, x_3)$ are lattice restoring, so (iv) and (v) follow. Also (i) is clear, since this only amounts to a renumbering of the film layers, the 0-layer held fixed. Interchanging the 0^{th} and the j^{th} layer gives (ii). Finally, (iii) is trivial for $\nu = 1$, and for $\nu = 2$ it follows from (22) since by (ii) and (iv)

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

□

Remarks:

(i) Note that the reflection P and R, rotation about 90°, span the set of symmetry operations of $[-1/2, 1/2]^2$.

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

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

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

Suppose now our reference configuration is a natural state. By the results in section 6 and proposition 5.3 we can not 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 extensive deformations, i.e. $s_1(A) \geq 1$, $|b^i - b^j| \geq 1$ for $i \neq j$, there can be a symmetric quadratic form Q such that for A (of the form (23)) and b^i with

$$A \approx Id_{2,3} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{pmatrix}, \qquad b^i - b^{i-1} \approx e_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

the energy can be written as

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

Then Q is a symmetric form on $\mathbb{R}^3 \times (\mathbb{R}^3)^{\nu-1} = \mathbb{R}^{3\nu}$ leading to $(9\nu^2 + 3\nu)/2$ elastic constants.

In the following we examine the cases $\nu = 1$ and $\nu = 2$ to show how symmetry reduces this number. We only treat the case $\nu = 2$ and comment on the much easier case $\nu = 1$ thereafter. Here, $(9\nu^2 + 3\nu)/2 = 21$.

Set $b := b^1$ and let Q be given by

$$Q(\epsilon, \epsilon) = q_{ij}\epsilon_i\epsilon_j,$$

where $1+\epsilon_1 = a_{11}$, $1+\epsilon_2 = a_{22}$, $\epsilon_3 = a_{12}$, $\epsilon_4 = b_1$, $\epsilon_5 = b_2$ and $1+\epsilon_6 = b_3$.

Proposition 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 Proof. First note that by symmetry of Q

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

Define

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

From (iii) and (ii) of proposition 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 from (iii) and (v) of proposition 5.6 we deduce $\varphi(A, b) = \varphi(\tilde{P}AP, \tilde{P}b)$ and hence

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

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

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

Summarizing (24) – (27) yields the result. □

If $\nu = 1$, $(9\nu^2 + 3\nu)/2 = 6$, a similar reasoning shows that

$$Q = \begin{pmatrix} q_{11} & q_{12} & q_{13} \\ q_{21} & q_{22} & q_{23} \\ q_{31} & q_{32} & q_{33} \end{pmatrix} = \begin{pmatrix} q_{11} & q_{12} & 0 \\ q_{12} & q_{11} & 0 \\ 0 & 0 & q_{22} \end{pmatrix}.$$

In particular, there remain three elastic constants.

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 extensive strains. Again, the crucial parameter is c_0. Still, the relevant scaling of energy with respect to $\operatorname{dist}(A, O(2,3))$ turns out to be quadratic. At first we study a one-dimensional atomic chain in detail, which might be of independent interest modeling a polymer chain in a confined region. Using these results we also obtain estimates for thin films.

6.1 Energy scaling of an atomic chain

Consider $L+1$ atoms at $y_0, \ldots, y_L \in \mathbb{R}^3$ whose energy is given by

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

where $\phi_i \in (-\pi, \pi]$ denotes the angle between $y_{i+1} - y_i$ and $y_i - y_{i-1}$. Assume that W_1 is locally bounded, W_2 bounded and symmetric, $W_1(1) = 0 = W_2(0)$, and there are $\alpha_1, \alpha_2 > 0$ and $\rho > 0$ such that

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

For given $a > 0$, we want to examine

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

($\mathcal{N}_L(a)$ is a one-dimensional version of $\hat{\mathcal{N}}_k^{0,1}$.) In particular, we are interested in the energy scaling for deformations near the zero-energy state $y_k = (k, 0, 0)$, i.e. $a \approx 1$.

Lemma 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 sake of completeness. First note that since W_1 restricted to $[0, 2c_0 + a]$ and W_2 are bounded, say by $C > 0$, we have $|E(y)/L| \leq 2C$, so

$$\varphi(a) := \liminf_{L\to\infty} \frac{1}{L} \inf_{y\in\mathcal{N}_L(a)} E$$

exists in $\mathbb{R}$. For $\varepsilon > 0$ choose L_0 such that

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

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

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

We may assume that $y_0^0 = (0,0,0)$ and $y_{L_0}^0 = (L_0 a, 0, 0)$ if L_0 is large enough. For $L \geq L_0$ we can break the atomic chain into pieces of length L_0 plus a remaining part of length smaller than L_0 and define y by $(0 \leq r < L_0)$

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

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

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

So

$$\frac{1}{L} E(y_0, \ldots, y_L) \leq \frac{1}{L_0} E(y_0^0, \ldots, y_{L_0}^0) + \frac{2CL_0}{L} + \frac{2C}{L_0}.$$

Choosing L_0 large enough, this shows that for L sufficiently large indeed

$$\varphi(a) - \varepsilon \leq \frac{1}{L} E(y_0, \ldots, y_L) \leq \varphi(a) + 3\varepsilon.$$

□

It is easy to get upper bounds for $\varphi(a)$:

Lemma 6.2 *Suppose that in addition there exists $\alpha_3 \geq \alpha_1$ such that $W_1(r) \leq \alpha_3(r-1)^2$ if $|r-1| \leq \rho$, and $W_2(0) = 0$. Then for $|a-1| \leq \rho$*

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

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

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

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

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

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

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

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

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

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

It follows that

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

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

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

If y is any deformation with $E(y) \leq \delta$, then

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

and hence by Cauchy-Schwarz

$$\sum_{i=1}^{L} ||y_i - y_{i-1}| - 1| \leq \sqrt{L}\sqrt{\delta}, \quad \sum_{i=1}^{L-1} |\phi_i| \leq \sqrt{L-1}\sqrt{\delta}.$$

Noting that the absolute value of the angle between $y_i - y_{i-1}$ and $y_j - y_{j-1}$ is bounded by $\sum_{k=1}^{L-1} |\phi_k|$ we find that for $\delta L \leq 1$

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

in particular, choosing $\delta = \delta(L) = L^{-3}$, we obtain

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

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

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

and

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

Also, let $m = \left\lceil \sqrt{3+4c_0^2}+1 \right\rceil$ and define $a_1, a_2, \ldots$ and $L_1, L_2, \ldots$ by

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

Lemma 6.3 *There exists $c > 0$ such that for all $k \in \mathbb{N}$,*

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

Proof. The lemma is proved by induction on n. The case $n = 0$ follows directly from the following

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

$$\frac{1}{kL_0} E_{kL_0}(a,a') \geq C \quad \forall\, a' \in [1/2, a_0],\ |a-a'| \leq \frac{2c_0}{kL_0}.$$

Suppose it is proven for n and choose $c = \min\{(4m)^{-4}, C\}$. For $a' \leq a_{n+2}$

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

implies

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

and thus

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

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

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

Now let $3/4 \leq a' \leq a_{n+1}$, $|a-a'| \leq \frac{2c_0}{kL_{n+1}}$. Considering the first components of the atoms $y_0, y_{L_n}, \ldots, y_{2kL_n}$ (note that $L_{n+1}/L_n = 2$) we deduce

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

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

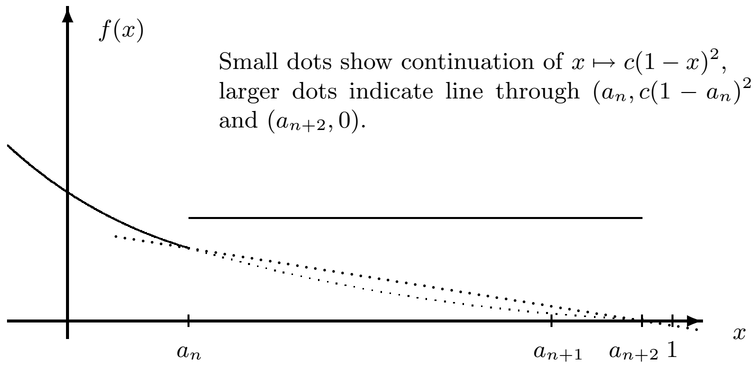
$$L_n x_i \geq L_n a - 2c_0 \geq L_n a' - L_n \frac{2c_0}{kL_{n+1}} - 2c_0 \geq 3L_n/4 - 3c_0 > L_n/2.$$

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

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

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

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



Now, since $L_n^{-4} = (4m)^{-4}(1-a_n)^2 \geq c(1-a_n)^2$ and $1-a_n = 16(1-a_{n+2})$, f^{**} is given by

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

So for $a' \leq a_n$ we are done. But also for $a' \in [a_n, a_{n+1}]$

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

(Set $1-a' = \lambda(1-a_n)$, then this is equivalent to $\frac{1}{15}(16\lambda - 1) \geq \lambda^2$ which in turn is equivalent to $\lambda \in [1/15, 1]$. This is guaranteed by $a \in [a_n, a_{n+1}]$.)

The claim at the beginning of the proof can now be shown by analogous arguments: $y \in \mathcal{N}_{L_0}(a,a')$ implies

$$\frac{1}{L_0}E(y_0,\ldots,y_{L_0}) \geq \frac{\delta(L_0)}{L_0} = L_0^{-4} \quad \forall y \in \mathcal{N}_{L_0}(a,a'),\ 0 < a' \leq a_1.$$

Again 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

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

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

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

□

We can now state the main result of our one-dimensional model problem:

Proposition 6.4 *There exist $\delta, c > 0$ such that for all $1-\delta \le a \le 1+\delta$*

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

If in addition W_1 and W_2 are bounded from above as in lemma 6.2, then there are $C, c > 0$ such that

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

Proof. The upper bound is immediate from lemma 6.2. The lower bound for $a \ge 1$ 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 $a = a' \le a_n$ and letting $k \to \infty$ in lemma 6.3 noting that, by lemma 6.1, it suffices to consider a subsequence in (28). □

So the energy scales quadratically with the distance of a to 1. The following example shows 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 $a \ge 1$, then, as in the derivation of (29), we see that the Cauchy-Born state $y_k = (ka, 0, 0)$ is asymptotically optimal, leading to

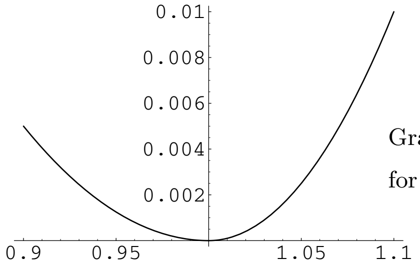
$$\varphi(a) = \alpha_1(a-1)^2.$$

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

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

This is by a c_0-dependent factor smaller than the Cauchy-Born minimizer $y_k = (ka, 0, 0)$ which has mean energy $\alpha_1(1-a)^2$.

Also this shows that the minimal energy is not twice differentiable in a at $a = 1$ since for $a \ge 1$ 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.



Graph of $a \mapsto \begin{cases} E_{\min}(a) & \text{if } a \le 1 \\ \alpha_1(1-a)^2 & \text{if } a \ge 1 \end{cases}$ for $\alpha_1 = \alpha_2 = 1, c_0 = 2$.

2. To extend this observation to thin films, we also study the following two dimensional deformation (E as in the preceding example). Consider a piece of a circle in the x_1-x_3-plane with radius R (large):

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

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

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

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

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

Now patching together appropriately translated and reflected copies of this configuration leads to y in $\mathcal{N}_L(a)$ with arbitrarily large L and mean energy $\approx \frac{9\alpha_2}{d^2}(1-a)^2$. Finally, set $y' = \bar{a}y \in \mathcal{N}_L(a\bar{a})$ for $\bar{a} \le 1$ near 1 and, for given $x \le 1$ near 1 minimize $E(y')$ subject to $a\bar{a} = x$. It follows that

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

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

Remark: In terms of scaling with c_0 the lower and upper bound for $\varphi(a)$ derived in the preceding examples respectively in proposition 6.4 do not match: the factors of $(1-a)^2$ scale like c_0^{-2} respectively $c \sim m^{-4} \sim c_0^{-4}$ (cf. lemma 6.3). In fact, the lower bound can be improved as we shall now detail.

Fix c_0 and let $k \in \mathbb{N}$. Suppose $y \in \mathcal{N}_{kL,kc_0}(a)$ 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

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

To estimate $|Y_j - Y_{j-1}|$, let $\bar{\Phi}_j = \sum_{i=k(j-1)+1}^{kj-1} |\phi_i|$. Then, if $\bar{\Phi} \le 1$, similar as on page 31, we obtain

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

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

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

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

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

Now let $y' := Y/k$. Then clearly $y' \in \mathcal{N}_{L,c_0}(a)$. Without loss of generality we may assume there exists α_3 as in lemma 6.2. By Cauchy-Schwarz,

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

It follows that

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

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

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

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

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

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

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

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

$\beta = 1/kT > 0$, where k is Boltzmann's constant and T temperature. For large β, i.e. sufficiently small temperature, we may take this as an approximation for all a.

It is elementary to see that the partition function Z_β is given by

$$Z_\beta = \frac{1}{2}\sqrt{\frac{\pi}{\beta}}\left(\sqrt{\frac{1}{\alpha_1}} + \sqrt{\frac{1}{\alpha_2}}\right).$$

The mean of this distribution, i.e. the preferred elongation of the atomic chain, can also be calculated explicitly:

$$\int a d\mathbb{P}_\beta(a) = 1 - \frac{2}{\sqrt{\pi\beta}}\left(\sqrt{\frac{1}{\alpha_1}} - \sqrt{\frac{1}{\alpha_2}}\right).$$

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

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

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 $E_{\rm an}$ by

$$\begin{aligned} E_{\rm an}(y) \;=\; & \frac{1}{2}\sum_{|x_i-x_j|=1} W_1(|y_i-y_j|) + \frac{\delta}{2}\sum_{|x_i-x_j|=2} \chi_{[0,r_0)}(|y_i-y_j|) \\ & + \frac{1}{2}\sum |y_i-y_k||y_j-y_k| W_2(\theta_{ikj}) \end{aligned} \qquad (34)$$

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

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

Proposition 6.5 *Both $E_{\rm an}$ and $E_{\rm nnn}$ are admissible energy functions leading to continuum limits $\varphi_{\rm an}$ resp. $\varphi_{\rm nnn}$. For $\nu \geq 2$ there exist $\delta, c > 0$ such that for dist$(A, O(2,3)) \leq \delta$,*

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

Clearly, $E_{\rm an}$ and $E_{\rm nnn}$ are admissible energy functions (see proposition 2.11). It remains to prove the lower bound on φ in terms of $\mathrm{dist}^2(A, O(2,3))$. To give a detailed proof is cumbersome, we mention the main ideas.
Sketch of proof. The film contains various atomic chains. For $\nu \geq 2$, the film energy can be bounded from below, e.g., by the energies of the chains $y(j, x_2, x_3)$, $j = 0, \dots, k$, where these chain energies also contain angular terms as in the previous paragraph due to the angular resp. next nearest neighbor part in E. Similar this holds for the diagonal chains. Since the deviation of A from $O(2,3)$ for A in the vicinity of $O(2,3)$ can be estimated by the deviation of $|A(1,0)|$ and $|A(0,1)|$ from 1 and the deviation of $|A(1,1)|$ and $|A(1,-1)|$ from $\sqrt{2}$, applying proposition 6.4 gives the result. □

Remarks:

(i) Proposition 6.5 is false for $\nu = 1$, i.e. films consisting of only one single layer. (This can be seen by considering folded configurations.)

(ii) Define $\bar{\varphi}(A) := \inf_{\mathbf{b}} \varphi(A, \mathbf{b})$. For $\nu \geq 2$ this result implies that $\bar{\varphi}$ (defined on $\mathbb{R}^{3\cdot 2}$, 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 $\{A \in \mathbb{R}^{3\cdot 2} : s_2(A) \leq 1\}$ (see [11], page 50, corollary 2.3.2).

In the rest of this paragraph we will see that $\bar{\varphi}$ is not twice differentiable at $A = \mathrm{Id}$. For 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

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

for $x \in \{0, \dots, L\} \times \{0, \dots, k\} \times \{0, \dots, \nu-1\}$. The nearest neighbor, next nearest neighbor lengths and bond angles are approximately

$$\frac{1}{R}\left(\frac{\nu-1}{2} - x_3\right), \quad \sqrt{2} + \frac{1}{\sqrt{2}R}\left(\frac{\nu-1}{2} - x_3\right) + \frac{1}{\sqrt{2}}\frac{\Phi}{L}, \quad \frac{\Phi}{2L},$$

respectively. Since $\Phi/L \approx R^{-1} \approx 3(1-a)/d$, this implies that, similar as in (33), for $A = (ae_1, e_2)$, $a \le 1$ near 1,

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

provided there exists $\beta > 0$ such that, in a neighborhood of 1 resp. $\sqrt{2}$ resp. 0, $W_1(r) \le \beta(r-1)^2$, $W_1'(r) \le \beta(r-\sqrt{2})^2$, $W_2(\phi) \le \beta\phi^2$. For $a \ge 1$, however, it is not hard to prove that $\bar{\varphi}(A) \ge \alpha_1(1-a)^2$. (This can be seen considering the one dimensional atomic chains $i \mapsto y(i, x_2, x_3)$.) □

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