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On the passage from atomic to continuum theory for thin films

by

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Abstract

We give a rigorous derivation of continuum theory from atomic models for thin films. This scheme has been proposed by Friesecke and James in [17]. The resulting continuum energy expression is obtained by integrating a stored energy density which not only depends on the deformation gradient but also on $\nu - 1$ director fields when ν is the (fixed) number of atomic film layers.

Contents

1 Introduction

The derivation of effective theories for thin elastic structures is a classical problem in elasticity theory, see, e.g., [26]. Rigorous results deriving membrane, plate or shell theories from three-dimensional elasticity have been obtained only recently (cf. [23, 24, 25, 18, 19, 20, 21]). By now there has emerged a whole hierarchy of plate theories according to different scalings of the stored energy (cf. [20]).

Another area of research concerns the passage from discrete atomic models to continuum theories. Rigorous Γ-convergence results, especially in one dimension, are proved in [8, 9, 10] for pair potentials under suitable growth assumptions on the atomic interactions. The results in [5, 6, 7] on the other hand deal with both pair potential and quantum mechanical energy models, but assume the Cauchy-Born rule to deduce continuum limits in this general framework.

The aim of the present work is to derive and discuss continuum theory for thin films, starting from a microscopic atomic model as proposed by Friesecke and James in [17]. More precisely, for $h > 0$ fixed and $k \in \mathbb{N}$ we start with reference configurations

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

(more general lattices are possible) subject to some deformation $y^{(k)} : \mathcal{L}_k \to \mathbb{R}^3$. The elastic energy of such a deformation is denoted by $E(y^{(k)})$. The natural limiting objects in the limit $k \to \infty$ (the variables of the continuum theory to be developed) are argued to be (after rescaling) given by some function $u : [0, 1] \times [0, 1] \to \mathbb{R}^3$ and vector fields $b^i : [0, 1] \times [0, 1] \to \mathbb{R}^3$, $i = 1, \dots, \nu - 1$, where the film consists of ν layers of atoms. Having defined a suitable notion of convergence, we are led to the fundamental problem:

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

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

Here, we do not want to restrict to pointwise limits, but rather calculate a variational limit of the energy allowing for some microscopic relaxation. This kind of convergence is in the spirit of Γ-convergence, cf. [14].

In section 2, we introduce the model, in particular, we discuss the admissible limiting deformations and energy functions that may be considered. We define precisely in what sense microscopic deformations are understood to converge to their macroscopic representatives.

Section 3 is the core of the theory. It shows how to pass from atomic to continuum theory in the framework set up so far. The scheme has been introduced by Friesecke and James in [17], where they suggest to follow the following strategy:

- Replace $(u, \mathbf{b})$ by their piecewise affine resp. constant approximations $(u_\varepsilon, \mathbf{b}_\varepsilon)$.

- Partition the body into mesoscopic regions where $u_\varepsilon, \mathbf{b}_\varepsilon$ are affine resp. constant and show that the energy decouples.
- Find minimizers separately on these regions.
- Patch them together.
- Obtain an integral expression in terms of ∇u and $\mathbf{b}$.

We give a rigorous version of these steps, which in part were derived formally in [17]. Note, however, that there are some major differences. In particular, the (central) notion of weak neighborhood given here is at variance with that of [17] resulting in some technical differences. These neighborhoods are not only of technical interest but also describe physically which deformation fluctuations are subject to relaxation and which will be seen in continuum theory.

Furthermore we show that the hypotheses on the decay of the energy made in [17] may be weakened. We also give a proof for the convergence of the relaxed energy on a mesoscale level under homogeneous conditions, thus showing that the continuum theory derived is indeed well-defined. This is also proved for a modified version of weak neighborhoods leading to a representation result for the limiting energy density φ. The results are extended to systems with unbounded interaction potential which are of physical interest. Finally, we discuss some extensions, in particular, to certain systems of distinguishable particles, and variants of the continuum theory.

In section 4, we examine physical energy functions and exhibit conditions under which these fit into the theory. In particular we treat pair potentials, angular forces (to incorporate materials whose binding energy depends on the bond-angles) and pair functionals (derived by the embedded atom method). We show that under reasonable hypotheses on the parameters these energies are admissible for our passage to continuum theory. To give an explicit example we also treat the case of an elementary nearest neighbor model.

It remains to study qualitative aspects of the theory derived here. This will be done in [28] in detail. The dependence of φ on a relaxation parameter introduced here will be examined. The limiting behavior of $\varphi(A, \mathbf{b})$ under very extensive or compressive strain and convexity properties will be discussed. The results for systems satisfying assumption 2.8 turn out to be different from those for nearest neighbor like interactions as in paragraph 3.6.2. In [28] we will also consider more realistic mass-spring models for which interesting phenomena will be observed when examining φ at A near $O(2, 3)$.

2 Microscopic model and macroscopic variables

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

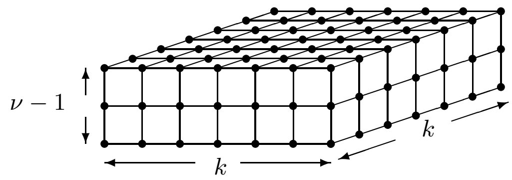
2.1 Kinematics

2.1.1 Atomistic model

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

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

where $\mathcal{L} = \mathbb{Z}^3$, $\mathcal{S}_k := [0, k] \times [0, k]$ for $k \in \mathbb{N}$ and $h := \nu - 1$ is the height of the film. (Only minor changes are necessary to treat more general Bravais-lattices $\mathcal{L}$, cf. paragraph 3.6.)



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

The deformations of this configuration will be denoted by

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

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

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

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

Assume for the moment some interpolation is chosen. As pointed out in [17], imposing regularity assumptions on the deformations y, implies existence of limiting deformations in the limit $k \to \infty$. It is argued that these limits have to be considered the natural variables of continuum theory. In detail, the assumptions on the deformations made in [17] are the following. There are constants $c_1, c_2 > 0$ such that,

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

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

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

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

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

2.1.2 Macroscopic variables

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

$$\tilde{y}^{(k)} \overset{*}{\rightharpoonup} u, \quad \nabla\tilde{y}^{(k)} \overset{*}{\rightharpoonup} \nabla u \qquad \text{in } L^\infty. \tag{1}$$

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

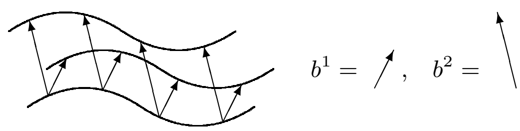
There is also a subsequence such that $(k\tilde{y}^{(k)}_{,3})$ weak*-converges in L^∞. However, this is cannot become a free variable of our continuum theory, since the limit function must be determined by the atomic positions only. We instead follow [17] and consider

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

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

$$k\left(\tilde{y}^{(k)}(\cdot,i) - \tilde{y}^{(k)}(\cdot,0)\right) \overset{*}{\rightharpoonup} b^i \qquad \text{in } L^\infty. \tag{2}$$

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



While the first condition (1) does not depend too much on the particular interpolation chosen, we can expect condition (2) to hold only for suitable interpolations (cf. below).

In our derivation – deviating from [17] – we will take the point of view that we are given u and $\mathbf{b} = (b^1,\dots,b^{\nu-1})$ and would like to assign an energy to these variables allowing for atomic relaxation. Thus reflecting the fact that we are interested in energies of macroscopic film-like configurations, we do not restrict the lattice deformations themselves, but rather impose the following conditions on u and $\mathbf{b}$.

Definition 2.1 *Let $u \in W^{1,\infty}(\mathcal{S}_1;\mathbb{R}^3)$ and $\mathbf{b} \in L^\infty(\mathcal{S}_1;(\mathbb{R}^3)^{\nu-1})$. We say that $(u,\mathbf{b})$ is admissible (for given $c_0 > 0$), i.e. $(u,\mathbf{b}) \in \mathcal{A}$, if there exists $c_1 > 0$ such that*

$$|u(x) - u(z)| \geq c_1|x-z| \quad \forall x,z \in \mathcal{S}_1 \tag{3}$$

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

$$\|b^0\|_{L^\infty}, \|b^i - b^0\|_{L^\infty} \leq c_0, \quad i = 1,\dots,\nu-1. \tag{4}$$

The first hypothesis ensures the macroscopic deformation to be 'film like'. The meaning of the second condition will become clear when we have specified our convergence scheme.

To be able to work also in un-rescaled variables, we define $U : \mathcal{S}_k \to \mathbb{R}^3$ by $\tilde{U}(x) = \frac{1}{k}U(kx) = u(x)$.

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

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

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

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

$$c_1|x - z| \le |u(x) - u(z)| \le c_2|x - z| \tag{5}$$

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

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

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

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

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

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

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

Remarks:

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

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

2.1.3 Interpolation & convergence

Weak*-convergence for bounded sequences in L^∞ is equivalent to convergence of averages (e.g. over all sub-squares of the domain). We will therefore choose our interpolation carefully such that

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

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

Note that this choice guarantees that for $Q_{\bar{x}} = \{z \in \mathcal{S}_1 : |z-\bar{x}|_\infty \le 1/2k\}$

$$\fint_{Q_{\bar{x}}} \tilde{y}(z,i)dz = \frac{1}{4} \sum_{\substack{z\in\frac{1}{k}\mathcal{L}\cap Q_{\bar{x}}\\ |z-\bar{x}|=1/\sqrt{2}k}} \tilde{y}(z,i).$$

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

$$\left| \fint_D k\Delta^i\tilde{y}(z_1,z_2)d\rho - \fint_D k\Delta^i\tilde{y}(z_1,z_2)dz_1dz_2 \right| \le C\frac{1}{kl}.$$

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

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

Definition 2.3 *Let* $u \in W^{1,\infty}(\mathcal{S}_1;\mathbb{R}^3)$, $\mathbf{b} \in L^\infty(\mathcal{S}_1;\mathbb{R}^3)$. *Choose* $c_0 > 0$, *a constant. We say that* $y^{(k)} \to (u,\mathbf{b})$ *(w.r.t.* c_0*) if*

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

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

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

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

Lemma 2.4 *Suppose* $|\tilde{y}^{(k)}(z,i) - u(z)| \le c_0/k$ *for all* $z \in \frac{1}{k}\mathbb{Z}^2 \cap \mathcal{S}_1$. *Then there exist* $w^{(k)} \in L^\infty(\mathcal{S}_1;\mathbb{R})$ *with* $\|w^{(k)}\|_{L^\infty} \le C$ *and* $w^{(k)} \to 0$ *pointwise a.e. as* $k \to \infty$ *such that*

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

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

$$|\tilde{y}(x,i) - u(x)| \le C/k \quad \forall x \in \mathcal{S}_1. \tag{6}$$

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

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

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

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

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

$$\begin{aligned}
|\tilde{y}(x,i) - u(x)| &= |\tilde{y}(x,i) - u'(x,x)| \le \max_{j \in \{0,1,2\}} |\tilde{y}(z_j,i) - u'(x,z_j)| \\
&\le \frac{c_0}{k} + \max_{j \in \{1,2,3,4\}} |u(z_j) - u'(x,z_j)|.
\end{aligned} \tag{7}$$

Choosing

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

we see by (6) and (7) and our choice of interpolating linearly between the film layers

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

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

As a consequence we obtain the following lemma.

Lemma 2.5 *Suppose $u \in W^{1,\infty}(\mathcal{S}_1, \mathbb{R}^3)$. There exists a sequence of deformations $y^{(k)} \to (u, \mathbf{b})$ for $\mathbf{b} \in L^\infty(\mathcal{S}_1; (\mathbb{R}^3)^{\nu-1})$ if and only if (4) holds.*

Proof. Assume $y^{(k)} \to (u, \mathbf{b})$ and consider $f^{(k)}(z) = ku(z) - k\tilde{y}^{(k)}(z, 0)$. By the previous lemma, $f^{(k)}$ is bounded in L^∞, so there is a weak*-convergent subsequence $f^{(k_j)} \stackrel{*}{\rightharpoonup} b^0$, say. Now if $\chi \in L^1(\mathcal{S}_1)$ with $\|\chi\|_{L^1} = 1$, then, by lemma 2.4,

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

by dominated convergence since the $w^{(k)}$ are uniformly bounded and converge to zero pointwise. It follows that $\|b^0\|_{L^\infty} \leq c_0$.

Now considering $k_j \Delta^i \tilde{y}^{(k_j)} - f^{(k_j)} \stackrel{*}{\rightharpoonup} b^i - b^0$, $|k_j \Delta^i \tilde{y}(z) - f^{(k_j)}(z)| = |k\tilde{y}(z, i) - ku(z)| \leq c_0 + w^{(k)}(z)$, the same reasoning shows that $\|b^i - b^0\|_{L^\infty} \leq c_0$.

Conversely, suppose b^0 satisfying (4) exists. For $0 \leq i \leq \nu - 1$ set

$$\bar{b}^i(x) = \fint_{Q(x)} b^i(z) dz, \tag{8}$$

where $Q(x) = x + [-1/2k, 1/2k]^2$. (Extend b^i boundedly (constantly if b^i is constant) outside $\mathcal{S}_1$.) Now consider the function v (V in un-rescaled variables) defined by (interpolation of)

$$v(x_1, x_2, i) = \begin{cases} u(x_1, x_2) - \frac{1}{k}\bar{b}^0(x_1, x_2) & \text{for } i = 0 \\ u(x_1, x_2) + \frac{1}{k}(\bar{b}^i(x_1, x_2) - \bar{b}^0(x_1, x_2)) & \text{for } 1 \leq i \leq \nu - 1 \end{cases} \tag{9}$$

for $(x_1, x_2) \in \frac{1}{k}\mathbb{Z}^2 \cap \mathcal{S}_1$.

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

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

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

2.2 Energy

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

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

The energy of a deformation y is denoted

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

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

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

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

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

Assumption 2.6 *Suppose u is admissible. There exists a function $\psi : [0, \infty) \to \mathbb{R}$ such that*

$$|\psi| \leq M \quad \text{and} \quad \psi(r) \leq M r^{-q} \tag{10}$$

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

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

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

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

Assumption 2.7 *Let u be admissible. We assume that E is locally Lipschitz, and in any C-neighborhood of U we have*

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

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

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

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

Remarks:

(i) By assumption 2.7 we could restrict to injective y. This would result in energy errors as small as we wish.

(ii) The last requirement can be weakened to situations where E is merely translational invariant and more than one species of atoms is involved. In the latter case one has to assume some periodicity condition. Also systems of distinguishable particles as arise e.g. in nearest neighbor models can be treated. We will come back to this in paragraph 3.6.

(iii) Energy functions E satisfying 2.6 and 2.7 will be called *admissible* in the sequel. Note that the set of admissible E forms a vector space.

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

(v) In paragraph 3.5 we will see that the boundedness assumptions on ψ and $\partial E/\partial y_i$ can be weakened. Then also energies that become infinitely large as the distance between two atoms tends to zero can be considered.

In lemma 2.2 we saw how the condition $\|y - U\| \leq C$ led to a "far field minimal strain hypothesis" $|y(x)-y(z)| \geq C_1|x-z|-C_3$ (with C_1, C_3 depending on C). In fact, many interesting systems satisfy the above assumptions in a more restrictive sense (see section 4):

Assumption 2.8 *Assume that ψ and L of assumption 2.6 resp. 2.7 depend only on C_1 and C_3 where y satisfies $|y(x) - y(z)| \geq C_1|x - z| - C_3$.*

This assumption has far reaching consequences as will be detailed in [28]. For the derivation of continuum theory, we will not make use of this.

3 Passage to continuum theory

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

3.1 Results

Suppose E satisfies assumptions 2.6 and 2.7, and a relaxation parameter $c_0 > 0$ is chosen. Our main result is the following variational convergence result:

Theorem 3.1 *There exists a macroscopic stored energy function φ such that (in the spirit of Γ-convergence),*

(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*

$$E(u, \mathbf{b}) = \int_{\mathcal{S}_1} \varphi(\nabla u, b^1, \ldots, b^{\nu-1}). \tag{11}$$

In proving this theorem our strategy will be to first reduce to homogeneous conditions and study the limit for affine u and constant b^i. Assuming this in (11) leads to defining φ by solving a cell problem

$$\varphi(A, \mathbf{b}) = \liminf \frac{1}{\nu k^2} E(y^{(k)}) \quad \text{as } y^{(k)} \to (A, \mathbf{b}) \tag{12}$$

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

$$\hat{\mathcal{N}}_k^{0,1}(A, \mathbf{b}) = \left\{ y : \mathcal{L}_k \to \mathbb{R}^3 : \|y - A\| \le c_0 \text{ and } \frac{1}{(k+1)^2} \sum_{x \in \mathbb{Z}^2 \cap \mathcal{S}_k} \Delta^i y(x) = b^i \right\}. \tag{13}$$

Then we have the following representation result:

Theorem 3.2 *The macroscopic energy density* φ *of theorem 3.3 (and formula (12)) is given by*

$$\varphi(A, \mathbf{b}) = \lim_{k \to \infty} \frac{1}{\nu k^2} \inf_{y \in \hat{\mathcal{N}}_k^{0,1}(A, \mathbf{b})} E(y). \tag{14}$$

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 homogeneous version of $\mathcal{A}$, is defined by

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

consisting of *admissible* matrices A and vectors $\mathbf{b}$.

Measuring convergence of $k\Delta^i \tilde{y}^{(k)}$ in terms of negative Sobolev norms we get the following sharper version of theorem 3.1. Having introduced the notion of weak neighborhoods in the next section, we will see that this amounts to arbitrarily prescribing the scale of convergence of averages as long as the areas over which to take averages are large compared to atomic dimensions.

Theorem 3.3 *Suppose* $l = l(k)$ *is such that* $l(k) \to 0$ *and* $kl(k) \to \infty$ *as* $k \to \infty$. *Let*

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

where $\|f\|_{W^{-1,\infty}} := \sup\left\{ \int f \cdot \chi \ : \ \chi \in W_0^{1,1},\ \|\chi\|_{W_0^{1,1}} = \|\nabla \chi\|_{L^1} = 1 \right\}$. *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 3.6.2 we will sketch how to extend these results to certain finite range interaction models for distinguishable particle systems.

For many physically interesting models the requirement that the splitting function ψ be bounded (cf. (10)) is too restrictive. More generally, we should allow for energy contributions tending to infinity when atoms are getting very close.

Theorem 3.4 *Suppose the energy is of the form*

$$E(y) = \frac{1}{2} \sum_{i \neq j} W(|y_i - y_j|) + E_0(y) \tag{15}$$

where E_0 satisfies the usual assumptions (cf. paragraph 2.2, also interactions as discussed in 3.6.2 are allowed for E_0), but $W(r)$ becomes infinitely large as r tends to zero. For any $r_0 > 0$ we assume that W is Lipschitz on $[r_0, \infty)$ and there exist $M = M(r_0) \in \mathbb{R}$ and $q = q(r_0) > 3$ such that for (a.e.) $r \geq r_0$

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

for $r \geq r_0$. Then theorem 3.1 extends to energy functions of the form (15) where, as in theorem 3.2, $\varphi : \mathcal{A}_{\mathrm{hom}} \to (-\infty, \infty]$ is given by (14), continuous as a function with values in $\mathbb{R} \cup \{\infty\}$.

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

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

with $l_1(k) := c_0/k$ corresponds to a relaxation regime where the individual atoms a allowed to move in a region comparable to atomic dimensions. As is shown in [28], if assumption 2.8 holds, $l_1 = c_0/k$ is in fact the only scale which both accounts for atomistic relaxation and yields a non-trivial continuum theory. Moreover, we can not relax sending the parameter c_0 to infinity. This is due to our physically reasonable decay assumptions on the energy (cf. assumption 2.6). The main point is that finite c_0 prevents fracture from happening. Mathematically this could also be achieved by assuming growth conditions on the inter-atomic forces tending to infinity as the distance between initially close atoms becomes large. But this is physically not realistic. In our approach c_0 enters as a parameter. By its physical interpretation as an upper bound for the deviation of atoms from their macroscopic limit, however, applicability of the theory should be decidable on physical grounds.

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

3.2 Preparations

We are now going to prove these results. Note that in all that follows, k is understood to be sufficiently large, even if not explicitly stated. The constants that will appear in the energy estimates for deformations near some limiting deformation u will depend on u, but only through the constants c_1, c_2 (cf. below and assumptions 2.6 and 2.7).

3.2.1 Splitting lemmas

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

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

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

From assumption 2.6, the following lemma is easily proved by induction.

Lemma 3.5 *If $\mathcal{M}_1, \ldots, \mathcal{M}_n \subset y(\mathcal{L} \cap (\Omega \times [0,h]))$ are pairwise disjoint sets of atoms, and $\|\tilde{y} - u\| \le c/k$, then the following inequality holds:*

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

In the sequel, we will use the following statements for lattice sums the proof of which is elementary.

Lemma 3.6 *Let $d \in \mathbb{N}, q > d$. In addition, suppose $c > 0$. Then there is a constant C (depending on c) such that for $a > 0$*

$$\sum_{\substack{x \in \mathbb{Z}^{d+1}, \; 0 \le x_{d+1} \le c \\ |x| \ge a}} |x|^{-q} \le C a^{d-q}.$$

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

Lemma 3.7 *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*

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

Proof. By (remark (ii) after) lemma 2.2 there are constants C_1 and C_3 such that

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

Set $\mathcal{M} = y(\mathcal{K}), \mathcal{M}_1 = y(\mathcal{K}_2), \mathcal{M}_2 = y(\mathcal{K}_2)$. Then, by assumption 2.6,

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

Now fix $z_0 \in \mathcal{K}_2$, $y_0 = y(z_0) \in \mathcal{M}_2$. We will estimate $\sum_{x\in\mathcal{K}_1} \psi(|y(x) - y_0|)$ by splitting it into a short-range and a long-range part. Let $\delta = 2C_3/C_1$. Since the number of $x \in \mathcal{K}$ such that $|z_0 - x| \le \delta$ is bounded, we find

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

M being the global bound on ψ.

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

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

Since $q > 2$, this last expression is bounded by lemma 3.6 (with $a = 1$).

It follows that

$$|E(\mathcal{M}) - E(\mathcal{M}_1)| \le E(\mathcal{M}_2) + \sum_{z\in\mathcal{K}_2} C.$$

But, by lemma 3.5,

$$\left|E(\mathcal{M}_2) - \sum_{v\in\mathcal{M}_2} E(\{v\})\right| \le \frac{1}{2} \sum_{\substack{x,z\in\mathcal{K}_2\\ x\neq z}} \psi(|y(x) - y(z)|).$$

Just as before this sum can be bounded by $\sum_{z\in\mathcal{K}_2} C$. Hence,

$$|E(\mathcal{M}) - E(\mathcal{M}_1)| \le C\#\mathcal{K}_2 + \sum_{v\in\mathcal{M}_2} E(\{v\}).$$

Observing that by frame indifference of the energy the term $E(\{v\})$ is a constant, finishes the proof. □

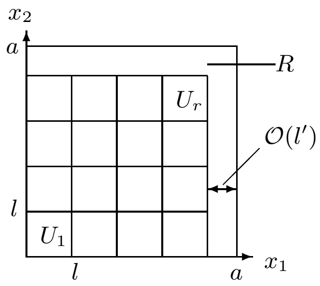
As an immediate consequence we get

Corollary 3.8 *Let y, y' be two deformations satisfying the hypotheses of lemma 3.7, and $\mathcal{K} \subset \mathcal{L} \cap (k\Omega \times [0, h])$. Then there is a constant C such that*

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

Proof. Apply lemma 3.7 with $\mathcal{K}_2 = \{x \in \mathcal{K} : y(x) \neq y'(x)\}$ to y and y'. □

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



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

Lemma 3.9 *Suppose $y : kQ \times [0,h]$ satisfies $|\tilde{y} - u| \le c/k$ for some admissible u. Then*

$$E(y(x) : x \in \mathcal{L} \cap (kQ \times [0,h])) = \sum_{i=1}^{r} E(\mathcal{M}_i) + \mathcal{O}(ka^2/l) + \mathcal{O}(k^2 a l').$$

Proof. By lemma 3.7 we get

$$\left| E(y(x) : x \in \mathcal{L} \cap (kQ \times [0,h])) - E(y(x) : x \in \bigcup_{i=1}^{r} \mathcal{K}_i) \right| = \mathcal{O}(k^2 a l'). \qquad (16)$$

Lemma 3.5 implies that

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

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

1. short range term: Since $|\psi| \le M$, we have

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

For fixed $x \in \mathcal{K}_i$, the number of $z \in \mathcal{L}$ with $|x - z| \le \delta$ is bounded. On the other hand, in order to have at least one $z \in \mathcal{K}_j$ with $|x - z| \le \delta$ and $i \ne j$, we must have $\operatorname{dist}(x_p, \partial kU_i) \le \delta$. For fixed i, the number of these x is bounded by Ckl, C constant. (The perimeter of kU_i is $4kl$.) This yields, since $r = \mathcal{O}((ka)^2/(kl)^2)$,

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

2. long range term: As in the proof of lemma 3.7, $|x-z|>\delta$ implies $|y(x)-y(z)|>\frac{C_1}{2}|x-z|$, and thus

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

C some constant. Now for fixed $x\in\mathcal{K}_i$ with $\operatorname{dist}(x_p,\partial(kU_i))=: d(x)=d$ we have by lemma 3.6 (i fixed)

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

So we obtain for i fixed:

$$\frac{1}{2}\sum_{j\neq i}\sum_{\substack{x\in\mathcal{K}_i\\ z\in\mathcal{K}_j\\ |x-z|>\delta}}\psi(|y(x)-y(z)|)\le C\sum_{x\in\mathcal{K}_i}\max\{\delta,d(x)\}^{2-q}. \tag{17}$$

The number of x with $d(x)\le\delta$ is bounded by Ckl. So summing over these x will give a term of order $C\delta^{2-q}kl=Ckl$ in (17). Now let x be such that $d(x)>\delta$. There exists a unique $m\in\mathbb{N}_0$ such that $d\in(\delta+m,\delta+m+1]$. The number of the x corresponding to the same m is bounded by $C\nu(kl-2(\delta+m))\le Ckl$. So ($i$ fixed)

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

by lemma 3.6 with $c=0$. Hence this part of the sum is also bounded by Ckl.

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

$$Crkl\le C\left(\frac{ka}{kl}\right)^2kl=Cka^2/l.$$

This is the same bound as for the short range term. We have thus shown that the remaining error term is indeed $\mathcal{O}(ka^2/l)$. Together with (16) this yields the desired estimate. $\square$

3.2.2 Weak neighborhoods

It is illuminating to describe deformations that we will take into account for atomic energy relaxation more directly by weak neighborhoods about the limit points u and $\mathbf{b}$ in terms of the atomic positions. While the distance from u is measured by the maximum norm, the convergence of the relative displacements of the film layers is in the weak*-sense in L^∞. By boundedness of $k\Delta^i\tilde{y}$ this is equivalent to convergence of averages

$$\fint_D k\Delta^i\tilde{y} \to \fint_D b^i$$

for all squares $D = a_1 + [0, a_2]^2 \subset \mathcal{S}_1$ (cf. [13]).

We now consider mesoscopic local averages. For this we define $\rho = \rho(k)$ to be the measure $\sum_{x\in\mathbb{Z}^2} \delta_{x/k}$ where $\delta_{x/k}$ is the Dirac measure at x/k. Let $Q \subset \mathcal{S}_1$ be a sub-square of side-length l_4, and recall the definition of $\bar{\mathbf{b}}$ from (8). For admissible u, $\mathbf{b}$ define:

Definition 3.10 *A deformation* $y : \mathcal{L} \cap (kQ \times [0,h]) \to \mathbb{R}^3$ *(resp. its interpolation) belongs to the weak neighborhood*

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

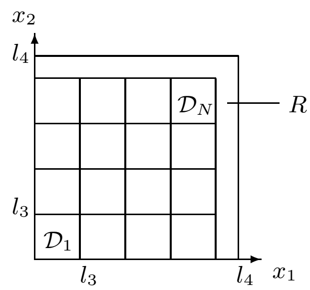
$$\|\tilde{y} - u\| \le l_1 \text{ and } \left|\fint_{\mathcal{D}} k\Delta^i\tilde{y} - \bar{b}^i d\rho\right| \le l_2 \tag{18}$$

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

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

$$\|\tilde{y} - u\| \le l_1 \text{ and } \left|\fint_{\mathcal{D}_j} k\Delta^i\tilde{y} - \bar{b}^i d\rho\right| \le l_2 \tag{19}$$

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



In case $l_3 = l_4$ *we require that (18) resp. (19) holds with* $\mathcal{D} = Q$ *resp.* $\mathcal{D}_1 = Q$.

Remark: Clearly, $\mathcal{N}^{l_1,l_2,l_3}_{k,Q}(u,\mathbf{b}) \subset \hat{\mathcal{N}}^{l_1,l_2,l_3}_{k,Q}(u,\mathbf{b})$, and V as defined in (9) lies in $\mathcal{N}^{l_1,l_2,l_3}_{k,Q}(u,\mathbf{b})$ for admissible $(u,\mathbf{b})$ and $l_1 = c_0/k$. Since we will mainly deal with the choice $l_1 = c_0/k$, we will drop l_1 from our notation.

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

$$\|b^0\|_\infty, \|b^i - b^0\|_\infty \leq c_3 \tag{20}$$

for all $i \in \{1, \ldots, \nu - 1\}$ and some constant $0 < c_3 < c_0$. So $v : \Omega \to \mathbb{R}^3$ as defined in (9) satisfies $\|v - u\| \leq c_3$.

Lemma 3.11 *Suppose $\|y - U\| \leq c_0 + \delta$, $0 \leq \delta \leq c$. Then there exists y' with $\|y' - U\| \leq c_0$ such that*

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

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

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

where $C = L\nu \frac{c_0 + c_3}{c_0 - c_3}$, L as in assumption 2.7.

Proof. Let v be as in (9) and define y' such that

$$\tilde{y}' := \lambda \tilde{y} + (1 - \lambda) v, \quad \lambda = \frac{c_0 - c_3}{c_0 - c_3 + \delta}. \tag{21}$$

Then indeed by (20),

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

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

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

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

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

By (remark (iv) after) assumption 2.7 the claim follows. □

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

Lemma 3.12 *Let $\mathcal{D}_j$ be as in definition 3.10. Suppose $|\fint_{\mathcal{D}_j} (k\Delta^i \tilde{y} - \bar{b}^i) d\rho| \leq \delta \leq 1$, $j = 1, \ldots, N$, and $\|y - U\| \leq c_0 + \varepsilon$, $\varepsilon \leq 1$. Then there exists y' with $\|y' - U\| \leq c_0$,*

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

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

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

Set

$$B^i = \bar{b}^{i-1} - \bar{b}^0 \quad \text{for } i = 2,\dots,\nu, \qquad B^1 = -\bar{b}^0, \tag{22}$$

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

$$Y^i(x_p) = k(\tilde{y}(x_p, i-1) - u(x_p)), \quad \overline{Y^i} = \fint_{\mathcal{D}_j} Y^i d\rho \tag{23}$$

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

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

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

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

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

$$\left|\overline{Y^i} - B^i\right| \le C\sqrt{\varepsilon' + \delta} \qquad \text{for } i = 1,\dots,\nu. \tag{24}$$

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

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

The second and third component can be estimated by noting that

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

for $m = 2, 3$, hence also

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

Together with (24) this proves that

$$\sum_{z\in\frac{1}{k}\mathbb{Z}^2\cap\mathcal{D}_j} \left|Y^i(z) - B^i\right| \leq C(kl_3)^2(\sqrt[4]{\varepsilon'} + \sqrt[4]{\delta}). \tag{25}$$

Now define a new configuration y'' by replacing Y^i by B^i for those i with $|B^i| \geq c_0 - \varepsilon'$, i.e. Y''^i defined analogously to Y^i equals to B^i for these i and equals Y^i for the other i. By (remark (iv) after) assumption 2.7,

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

Finally, exactly as in the proof of lemma 3.11, we choose $\tilde{y}'$ as a convex combination of $\tilde{y}''$ and v with $c_3 = c_0 - \varepsilon'$. Noting that

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

finishes the proof. □

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

Lemma 3.13 *Suppose u and* $\mathbf{b}$ *are admissible, and scales* $0 \leq l_2, l_2' \leq 1$, $1/k \leq l_3, l_3' \leq 1$ *are given with* $l_2' \gg l_3/l_3'$. *Then*

$$\begin{aligned}
\inf_{y\in\hat{\mathcal{N}}^{0,l_3}_{k,Q}(u,\mathbf{b})} E(y) &\leq \inf_{y\in\hat{\mathcal{N}}^{l_2,l_3}_{k,Q}(u,\mathbf{b})} E(y) + O(k^2 l_4^2 l_2^{1/5}), \\
\inf_{y\in\mathcal{N}^{l_2',l_3'}_{k,Q}(u,\mathbf{b})} E(y) &\leq \inf_{y\in\hat{\mathcal{N}}^{0,l_3}_{k,Q}(u,\mathbf{b})} E(y).
\end{aligned}$$

Furthermore, if there is $c_3 < c_0$ *such that (20) holds, then the error term* $\mathcal{O}(k^2 l_4^2 l_2^{1/5})$ *may be replaced by* $\mathcal{O}(k^2 l_4^2 l_2)$.

Proof. Let $y \in \hat{\mathcal{N}}^{l_2,l_3}_{k,Q}(u,\mathbf{b})$ be arbitrary. Write Q as a disjoint union of N translates of $[0, l_3)^2$, $\mathcal{D}_1, \ldots, \mathcal{D}_N$, and a rest R whose area is of order $\mathcal{O}(l_3 \cdot l_4)$ as in definition 3.10 (ii). Set $m_j^i = \fint_{\mathcal{D}_j} k\Delta^i \tilde{y} - \bar{b}^i d\rho$ and define $y_0 : kQ \times [0,h] \to \mathbb{R}^3$ by (interpolation of)

$$\tilde{y}_0(x_p, i) = \begin{cases} \tilde{y}(x_p, 0) & \text{for } i = 0,\ x_p \in \frac{1}{k}\mathcal{L} \cap \mathcal{D}_j \\ \tilde{y}(x_p, i) - \frac{1}{k} m_j^i & \text{for } 1 \leq i \leq \nu - 1,\ x_p \in \frac{1}{k}\mathcal{L} \cap \mathcal{D}_j \\ \tilde{y}_0(x_p, i) & \text{for } 0 \leq i \leq \nu - 1,\ x_p \in \frac{1}{k}\mathcal{L} \cap R. \end{cases} \tag{26}$$

Then we have

$$\|y_0 - y\| \leq \max_{\substack{1 \leq i \leq \nu - 1 \\ 1 \leq j \leq N}} |m_j^i| \leq l_2 \tag{27}$$

since $y \in \hat{\mathcal{N}}_{k,Q}^{l_2,l_3}(u, \mathbf{b})$. In particular, $\|y_0 - U\| \leq c_0 + l_2$, so invoking lemma 3.12 (resp. 3.11), we find y' satisfying $\|y' - U\| \leq c_0$,

$$\left| \fint_{\mathcal{D}_j} k\Delta^i \tilde{y}' - \bar{b}^i d\rho \right| \;\leq\; \left| \fint_{\mathcal{D}_j} k\Delta^i \tilde{y}_0 - \bar{b}^i d\rho \right| \;=\; \left| \fint_{\mathcal{D}_j} \left(k\Delta^i \tilde{y} - m^i \right) - \bar{b}^i d\rho \right| \;=\; 0$$

by construction of y_0, i.e. $y' \in \hat{\mathcal{N}}_{k,Q}^{0,l_3}(u, \mathbf{b})$, and

$$|E(y') - E(y_0)| \leq C l_2^{1/5} (kl_4)^2 \qquad (\text{resp. } \leq C l_2 (kl_4)^2).$$

Now by (27) and the Lipschitz assumption 2.7 on E we also have

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

whence

$$\inf_{y \in \hat{\mathcal{N}}_{k,Q}^{0,l_3}(u,\mathbf{b})} E(y) \leq E(y') \leq E(y) + \mathcal{O}(k^2 l_4^2 l_2^{1/5}) \quad (\text{resp. } \leq E(y) + \mathcal{O}(k^2 l_4^2 l_2)).$$

Since $y \in \hat{\mathcal{N}}_{k,Q}^{l_2,l_3}(u, \mathbf{b})$ was arbitrary, the first inequality is proven.

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

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

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

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

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

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

i.e. $y \in \mathcal{N}_{k,Q}^{l_2',l_3'}(u,\mathbf{b})$. It follows that $\hat{\mathcal{N}}_{k,Q}^{0,l_3}(u,\mathbf{b}) \subset \mathcal{N}_{k,Q}^{l_2',l_3'}(u,\mathbf{b})$. □

The connection between $\mathcal{W}_k^l(u,\mathbf{b})$ (see theorem 3.3) and the neighborhoods defined in definition 3.10 is described by the following lemma.

Lemma 3.14 *Let $u, \mathbf{b}$ be admissible. Assume $1/k \leq l_3 \ll l$, and $1/k \leq l' \ll l_2' l_3'$. Then*

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

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

$$\begin{aligned}
&\int_{\mathcal{S}_1} f \cdot (k\Delta^i \tilde{y} - b^i) \\
&= \frac{1}{k^2}\int_{\mathcal{S}_1} f \cdot (k\Delta^i\tilde{y} - \bar{b}^i)d\rho + \mathcal{O}(1/k) \\
&= \frac{1}{k^2}\sum_j \int_{\mathcal{D}_j} f \cdot (k\Delta^i\tilde{y} - \bar{b}^i)d\rho + \mathcal{O}(1/k + l_3) \\
&= \frac{1}{k^2}\sum_j \int_{\mathcal{D}_j} \Big(f(x_j) + \nabla f(x_j)(x - x_j) + o(l_3)\Big) \cdot (k\Delta^i\tilde{y} - \bar{b}^i)d\rho + \mathcal{O}(l_3) \\
&\leq \frac{1}{k^2}\sum_j \int_{\mathcal{D}_j} |\nabla f(x_j)||x - x_j| \cdot |(k\Delta^i\tilde{y} - \bar{b}^i)|d\rho + \mathcal{O}(l_3) \\
&\leq \frac{1}{k^2}\sum_j \int_{\mathcal{D}_j} C|\nabla f(x_j)|\sqrt{2}l_3 + \mathcal{O}(l_3) \\
&\leq C(1 + \|\nabla f\|_{L^1})l_3 \ \leq \ Cl_3 \ \ll \ l,
\end{aligned}$$

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

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

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

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

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

In particular, sending $a \to 0$,

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

This implies

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

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

3.3 Proof of theorem 3.2

In this paragraph we will prove theorem 3.2, the representation formula for φ. Setting

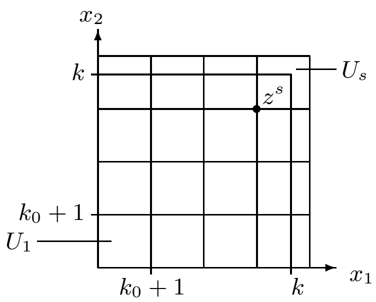
$$\varphi_k(A, \mathbf{b}) = \frac{1}{\nu k^2} \inf_{y \in \hat{\mathcal{N}}_k(A,\mathbf{b})} E(y), \tag{28}$$

we need to show that φ_k converges uniformly on compact subsets of $\mathcal{A}_{\text{hom}}$ to some continuous function φ.

In the first part of this paragraph we will show that φ exists as a pointwise limit (cf. proposition 3.16), while the in second we will investigate the continuity properties of the functions φ_k (cf. corollary 3.20) leading to the final result.

Existence

We start with a preparatory lemma. Throughout this paragraph $A \in \mathbb{R}^{3\cdot 2}$ is some admissible matrix and $\mathbf{b} \in (\mathbb{R}^3)^{\nu-1}$ some admissible vector. Let $y \in \hat{\mathcal{N}}_{k_0}(A, \mathbf{b})$ for $k \geq k_0$ and cover $\mathcal{S}_k$ by translates of $[0, k_0+1)^2$, denoted $U_1, \ldots, U_s$ as in the following picture:



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

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

for $x \in \mathcal{L} \cap ((U_j \cap S) \times [0, h]),\ 1 \leq j \leq s$.

For y' constructed this way it is easy to see that

$$\|y' - A\| \leq c_0 \quad \text{and} \quad \frac{1}{(k+1)^2} \sum_{x \in \mathbb{Z}^2 \cap \mathcal{S}_k} \Delta^i y'(x) = b^i + \mathcal{O}\left(\frac{k_0}{k}\right). \tag{29}$$

From lemma 3.9 and (29) we derive the main ingredient into the proof of the next proposition:

Lemma 3.15 *Suppose $k_0 \in \mathbb{N}$. Then there is a constant C (independent of k_0) such that for $k > k_0$ sufficiently large for every $y \in \hat{\mathcal{N}}_{k_0}(A, \mathbf{b})$ there is a $\hat{y} \in \hat{\mathcal{N}}_k(A, \mathbf{b})$ with*

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

Proof. For $y \in \hat{\mathcal{N}}_{k_0}(A, \mathbf{b})$ we define y' as above. From (29) we deduce

$$\|y' - A\| \le c_0 \quad \text{and} \quad \left| \fint_{\mathcal{S}_1} k\Delta^i \tilde{y}' d\rho_k - b^i \right| = \mathcal{O}\left(\frac{k_0}{k}\right). \tag{30}$$

So by lemma 3.13 (and $\hat{\mathcal{N}}_k^{0,l_3} \subset \hat{\mathcal{N}}_k^{l_2,l_3}$) there exists $\hat{y} \in \hat{\mathcal{N}}_k(A, \mathbf{b})$ with

$$\left| \frac{1}{k^2} E(\hat{y}) - \frac{1}{k^2} E(y') \right| \le C \left(\frac{k_0}{k}\right)^{1/5}. \tag{31}$$

We estimate the energy of y'. Using lemma 3.9 for translates of $[0, \frac{k_0+1}{k})^2$ and denoting the set of indices i for which $U_i \subset \mathcal{S}_k$ by $\mathcal{I}$, we see that

$$E(y'(x) : x \in \mathcal{L}_k) = \sum_{i \in \mathcal{I}}^{r} E(y'(x) : x \in \mathcal{L} \cap (U_i \times [0, h])) + \mathcal{O}(k^2/k_0 + kk_0).$$

By the periodic construction of y' we get

$$E(y'(x) : x \in \mathcal{L}_k) = \#\mathcal{I} \cdot E(y(x) : x \in \mathcal{L}_{k_0}) + \mathcal{O}(k^2/k_0) + \mathcal{O}(k_0 k). \tag{32}$$

Since $\#\mathcal{I} = \lfloor k/k_0 \rfloor^2 = (k/k_0)^2(1 + \mathcal{O}(k_0/k))$, we obtain from (32), noting that $E(y(x) : x \in \mathcal{L}_{k_0}) = \mathcal{O}(k_0^2)$ by lemma 3.7,

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

This finishes the proof by (31). □

Recall the definition of φ_k from (28).

Proposition 3.16 *The limit*

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

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

Proof. By lemma 3.7 (cf. the remark above that lemma) we have for $y \in \hat{\mathcal{N}}_k(A, \mathbf{b})$

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

so $(\varphi_k(A, \mathbf{b}))_k$ is a bounded sequence. We may therefore define φ by

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

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

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

where C is the constant from lemma 3.15. Then there is $\hat{y} \in \hat{\mathcal{N}}_k(A, \mathbf{b})$ such that

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

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

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

Continuity

Here we investigate the remaining parts of theorem 3.2, namely if $\varphi_k \to \varphi$ uniformly on compact subsets of $\mathcal{A}_{\text{hom}}$ and if $(A, \mathbf{b}) \mapsto \varphi(A, \mathbf{b})$ is continuous. We start by investigating the continuity properties of φ_k, first with respect to the variables b^i.

Lemma 3.17 *Let* $(A, \mathbf{b}), (A, \mathbf{b}') \in \mathcal{A}_{\text{hom}}$. *Then*

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

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

Proof. For $y \in \hat{\mathcal{N}}_k(A, \mathbf{b})$, $\left| \fint_{\mathcal{S}_1} k \Delta^i \tilde{y} d\rho - b'^i \right| \leq \left| \fint_{\mathcal{S}_1} k \Delta^i \tilde{y} d\rho - b^i \right| + |b^i - b'^i| = |b^i - b'^i|$. So $y \in \hat{\mathcal{N}}^{l_2,1}_{k,\mathcal{S}_1}(A, \mathbf{b}')$ for $l_2 = \max_i |b^i - b'^i|$ fixed. By lemma 3.13,

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

so, since y was arbitrary, we get

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

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

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

Lemma 3.18 *Let* $(A, \mathbf{b}), (A', \mathbf{b}) \in \mathcal{A}_{\text{hom}}$. *Then there exist constants $c, C > 0$ such that*

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

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

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

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

Then $\|y' - y\| \le |A - A'|\sqrt{2k^2 + h^2} \le C|A - A'|k$, so by assumption 2.7

$$|E(y') - E(y)| \le Ck^2|A - A'|k. \tag{33}$$

On the other hand, we clearly have $y' \in \hat{\mathcal{N}}_k(A', \mathbf{b})$. Together with (33) it follows that $\varphi_k(A', \mathbf{b}) \le \frac{1}{\nu k^2} E(y) + C|A - A'|k$. Since y was arbitrary we get

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

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

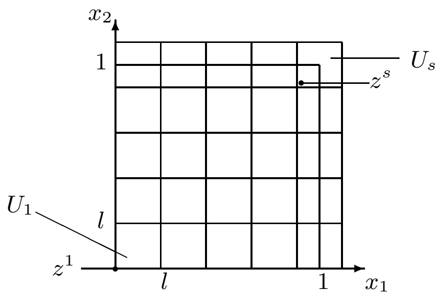
This lemma proves continuity of the φ_k with respect to A. The condition that $|A - A'| \le c/k$ can easily be dropped considering intermediate points between A and A'. However, the Lipschitz constant Ck obtained this way blows up as $k \to \infty$. In order to prove the main continuity result, we therefore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

Lemma 3.19 *Let* $(A, \mathbf{b}), (A', \mathbf{b}) \in \mathcal{A}_{\text{hom}}$. *Suppose* $1/k \le l = l(k) \le 1$. *Then there are constants* $c, C > 0$ *such that*

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

for $|A - A'| \le c/kl$.

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



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

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

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

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

so assumption 2.7 shows that

$$|E(y') - E(y)| \le Ck^2 kl|A - A'|. \tag{34}$$

Now let $\mathcal{I}$ denote the set of those indices i for which $U_i \subset \mathcal{S}_1$. Applying lemma 3.9 to y' first, then using frame indifference, and finally applying lemma 3.9 to $y''(x) = y(x) - Ax_p + A'x_p$ gives

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

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

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

by (34). Since y was arbitrary we get

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

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

As a consequence of lemmas 3.17, 3.18 and 3.19 we get:

Proposition 3.20 *The set $\{\varphi_k\}$ is equicontinuous.*

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

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

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

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

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

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

This shows equicontinuity of $\{\varphi_k(\cdot, \mathbf{b}) : k \in \mathbb{N}\}$, since the remaining finitely many $\varphi_1(\cdot, \mathbf{b}), \ldots, \varphi_{k_0}(\cdot, \mathbf{b})$ are continuous by lemma 3.18. By lemma 3.17 the family $\{\varphi_k(A, \cdot) : A \text{ admissible with } s_1(A), s_2(A) \in [c_1, c_2], k \in \mathbb{N}\}$ is also equicontinuous for all $c_2 \geq c_1 > 0$. The claim follows. □

From propositions 3.16 and 3.20 we can now easily finish the proof of theorem 3.2.

Proof of theorem 3.2. By proposition 3.16 $\varphi_k(A, \mathbf{b}) \to \varphi(A, \mathbf{b})$ pointwise and by proposition 3.20 $\{\varphi_k\}$ is equicontinuous. This implies that $\varphi_k(A, \mathbf{b}) \to \varphi(A, \mathbf{b})$ uniformly on compact subsets of $\mathcal{A}_{\text{hom}}$, in particular that φ is continuous, since by Arzela-Ascoli every subsequence has a further subsequence that converges. By the pointwise convergence its limit must be φ. □

3.4 Proof of theorems 3.1 and 3.3

First note that theorem 3.1 is an immediate consequence of theorem 3.3. So we only have to prove the latter result.

Fix admissible $u \in W^{1,\infty}(\mathcal{S}_1), \mathbf{b} \in L^\infty(\mathcal{S}_1)$ and constants $c_1, c_2 > 0$ as in (5). We will show that, for $l_3 \to 0$, $kl_3 \to \infty$,

$$\lim_{k\to\infty} \frac{1}{\nu k^2} \inf_{\hat{\mathcal{N}}_k^{0,l_3}(u,\mathbf{b})} E(y) = E(u,\mathbf{b}). \tag{35}$$

This will be sufficient since from lemmas 3.13 and 3.14 we obtain the following corollary which precisely describes our relaxation procedure in terms of weak neighborhoods.

Corollary 3.21 *Suppose (35) holds. Then in fact*

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

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

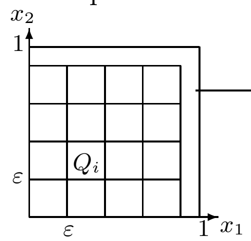
If $Q \subset \mathcal{S}_1$ is some square in $\mathcal{S}_1$ of side-length $l = l(k)$ we write $\hat{\mathcal{N}}_Q(u,\mathbf{b}) := \hat{\mathcal{N}}_{k,Q}^{0,l}(u,\mathbf{b})$.

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

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

Furthermore, there exists $\bar{c}_2$ only depending on c_2 such that $\sup_{x\in\mathcal{S}_1} |\nabla\bar{u}(x)| \le \bar{c}_2$ (cf. [16]).

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



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

$$\|\bar{u} - u_\varepsilon\|_\infty < \varepsilon g(\varepsilon) \tag{36}$$

where u_ε is affine on each of the squares Q_i. (If $\bar{u} \in C^{1,\alpha}$, one can e.g. choose $g(\varepsilon) = C\varepsilon^\alpha$.) We fix such a function g satisfying (36) from now on.

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

$$k\varepsilon' g(\varepsilon')^\gamma \equiv c_0. \tag{37}$$

Note that (36) and (37) imply that

$$\|\bar{u} - u_\varepsilon\|_\infty \ll c_0/k \quad \text{if } \varepsilon \le \varepsilon' \tag{38}$$

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

Lemma 3.22 *Let $Q \subset \mathcal{S}_1$ be one of the squares $Q_1, \ldots, Q_{m_\varepsilon}$ (on which ∇u_ε is constant). Suppose $c_1 - \delta \le s_1(\nabla u_\varepsilon) \le s_2(\nabla u_\varepsilon) \le c_2 + \delta$ on Q, and let $\mathbf{b}$ be a constant admissible vector in $\mathbb{R}^{3(\nu-1)}$. Then, if $\varepsilon \le \varepsilon'$,*

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

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

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

and define y' by

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

for $x_p \in \frac{1}{k}\mathbb{Z}^2 \cap Q$ and interpolation (v_ε defined analogously to (9) with respect to u_ε and $\mathbf{b}$.). Then by (38) for $\varepsilon \le \varepsilon'$,

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

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

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

Furthermore, by corollary 3.8,

$$|E(y) - E(y')| \le Cr_Q. \tag{39}$$

Invoking lemma 3.13 (with c_0 replaced by $c_0 + 2\delta$ and c_3 by c_0) we find a deformation y'' on Q with

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

satisfying

$$E(y'') \le E(y') + \frac{1}{\delta}\frac{Cr_Q}{|kQ|}|kQ|. \tag{40}$$

(Note that the constant found in the proof of lemma 3.13 by applying lemma 3.11 is – in the terminology of this lemma – $Cl_2/(c_0 - c_3)$. Here, this equals $Cr_Q/|kQ|\delta$.) Finally, by lemma 3.12, there is yet another deformation y''' with

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

and

$$|E(y''') - E(y'')| \leq C\delta^{1/5}|kQ|. \tag{41}$$

Since $y''' \in \hat{\mathcal{N}}_Q(u_\varepsilon, \mathbf{b})$ and $y \in \hat{\mathcal{N}}_Q(u, \mathbf{b})$ was arbitrary, we deduce from (39), (40) and (41)

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

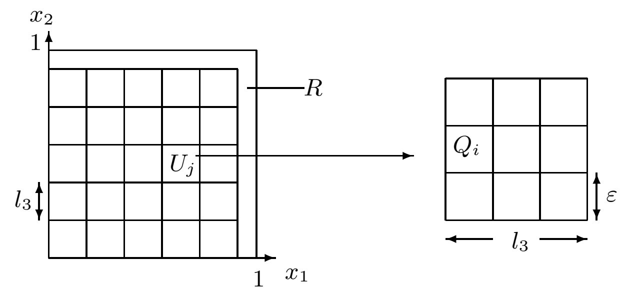
Interchanging the roles of u and u_ε (but defining r_Q as before and only replacing v_ε by v in the definition of y') gives an analogous inequality.

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

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

□

Now consider a partition of $\mathcal{S}_1$ with squares $\mathcal{D}_j$ of side-length l_3 and R, $|R| \leq 2l_3$ (see the next picture). Since $kl_3 \to \infty$ and $k\varepsilon' \to \infty$ (cf. (37)), we may choose $\varepsilon = \varepsilon(k) \leq \varepsilon' \to 0$ with $k\varepsilon \to \infty$ as $k \to \infty$ such that eventually $l_3/\varepsilon \in \mathbb{N}$. This also induces a partition of $\mathcal{S}_1$ into squares Q_i of side-length ε and R as in the picture below.



Proof of Theorem 3.3. Define G to be the union of those $\mathcal{D}_j$ where $c_1 - \delta < s_1(\nabla\bar{u}) \leq s_2(\nabla\bar{u}) < c_2 + \delta$. Since $\nabla\bar{u}$ is continuous, for k large enough, $G \supset \{x : c_1 \leq s_1(\nabla\bar{u}(x)) \leq s_2(\nabla\bar{u}(x)) \leq c_2\} \setminus R \supset \mathcal{S}_1 \setminus (B \cup R)$, whence $|G| \geq 1 - |B| \geq 1 - \sigma - 2l_3$.

Let $\mathcal{M}_j = y(\mathcal{L} \cap (k\mathcal{D}_j \times [0, h]))$. It follows from lemmas 3.9 and 3.7 that

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

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

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

Now, using lemma 3.9 again,

$$\left|\inf_{y\in\hat{\mathcal{N}}_{\mathcal{D}_j}(u,\mathbf{b})}E(y)-\min\sum_{Q_i\subset\mathcal{D}_j}\inf_{y\in\hat{\mathcal{N}}_{Q_i}(u,\mathbf{b}_{j,i})}E(y)\right|\le C\frac{kl_3^2}{\varepsilon}\tag{42}$$

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

Since $\nabla u_\varepsilon\to\nabla\bar{u}$ uniformly, we may choose matrices A_j such that $\sup_j|A_j-\nabla u_\varepsilon|=o(1)$ on $\mathcal{D}_j$. We now want to replace u by A_j in the right hand side of (42). First replacing u by u_ε on Q_i leads to an error bounded by $C(\delta^{1/5}|Q_i|+|B\cap Q_i|/\delta^3)k^2$ by lemma 3.22. Now replacing ∇u_ε by A_j leads to an additional error of order $o(|kQ_i|)$ because for matrices A,

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

where $m=\lfloor k\varepsilon\rfloor$ or $\lfloor k\varepsilon\rfloor-1$ (use translational invariance) and $(\varphi_k)_k$ is equicontinuous by proposition 3.20. It follows that

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

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

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

Summarizing (using theorem 3.2 to choose $n=\lfloor kl_3\rfloor$ uniquely), we obtain

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

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

approximate **b** by continuos functions in measure.) So we deduce from lemma 3.23 and theorem 3.2

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

Since $\mathcal{S}_1 \setminus \Omega \subset B$, $B \leq \sigma$, and φ is bounded on compact subsets of admissible matrices, we finally deduce that

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

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

Remark: Assuming regularity for ∇u, **b**, e.g. requiring them to lie in some Hölder class, the above proof gives explicit error estimates.

Lemma 3.23 *Let $\Omega \subset \mathbb{R}^n$ be of finite measure, $v_k : \Omega \to K$, $k = 1, 2, \ldots$, measurable, K some compact subset of $\mathbb{R}^m$, and $f_k : K \to \mathbb{R}$ such that $f_k \circ v_k$ is integrable. Furthermore suppose that $\Omega_k \subset \Omega$ is measurable with $|\Omega \setminus \Omega_k| \to 0$ as $k \to \infty$. If $f_k \to f$, uniformly on K, $f : K \to \mathbb{R}$ continuous, and $v_k \to v$ in measure, then*

$$\lim_{k\to\infty} \int_{\Omega_k} f_k(v_k) = \int_\Omega f(v).$$

The proof of this lemma is a straight forward $\varepsilon/4$-argument.

3.5 Extension to infinite pair-interaction

We will now prove theorem 3.4. For this paragraph we assume that proposition 4.1 is already proven.

Suppose E is given as in (15). For given δ we choose

$$E_\delta(y) = \frac{1}{2} \sum_{i \neq j} W_\delta(|y_i - y_j|) + E_0(y) \tag{43}$$

where $W_\delta \leq W$ satisfies the hypotheses of proposition 4.1, and

$$W_\delta(r) = W(r) \text{ for } r \geq \delta, \quad W_\delta(r) \geq \min_{0<s\leq\delta} W(s) \text{ for } r \leq \delta. \tag{44}$$

Proposition 4.1 implies that E_δ is an admissible energy function. If δ is small enough, we may assume that $W(r) > 0$ for $r \leq \delta$. Note also that there exists $C = C(\delta, c)$ such that for all $z \in \mathcal{L}_k$ and y with $\|\tilde{y} - u\| \leq c/k$ (u admissible)

$$\sum_{\substack{x \in \mathcal{L}_k \\ x \neq z}} |W_\delta(|y(x) - y(z)|)| \leq C \tag{45}$$

This follows from lemma 3.7 (with $\mathcal{K}_2 = \{z\}$) applied to the (admissible) pair potential given by $|W_\delta|$.

Definition 3.24 *Let $\delta > 0$.*

(i) We call (y_i, y_j), $i \neq j$, a δ-critical bond if $|y_i - y_j| < \delta$.

(ii) We say that y satisfies a minimal distance hypothesis with δ if

$$|y_i - y_j| \geq \delta \text{ for all } i \neq j.$$

Lemma 3.25 *Suppose y is a deformation with $\|\tilde{y} - u\| \leq c/k$, u admissible*

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

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

Proof. (i) Suppose $y_i = y(x_i) \in B$. Choose $\delta = 2C_3/C_1$ as in the proof of lemma 3.7. Then for $|x - z| \geq \delta$ we have $\frac{C_1}{2}|x - z| \leq |y(x) - y(z)|$ and thus

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

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

(ii) Just note that, by lemma 2.2 (ii), $|x - z| \leq (|y(x) - y(z)| + C_3)/C_1$. $\square$

We will prove theorem 3.4 by reducing to the case of admissible energy functions already treated. The main point is to show that we may impose an additional minimal distance hypothesis on the deformations. To this end for given y, we have to find a new configuration y' satisfying this hypothesis whose energy does not exceed $E(y)$ too much. The main difficulty comes again from the condition on local spatial averages.

Let $(A, \mathbf{b}) \in \mathcal{A}_{\text{hom}}$. As in the proof of lemma 3.12 we choose

$$b^0 \in \underset{b^0}{\operatorname{argmin}} \max \left\{ \max_{1 \leq i \leq \nu - 1} |b^i - b^0|, |b^0| \right\} \tag{46}$$

and set

$$B^i = b^{i-1} - b^0, \ i = 2, \ldots, \nu, \quad B^1 = -b^0. \tag{47}$$

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

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

$$0 < \delta_1 < \delta_1' < \frac{\delta_2}{6n(2\delta_2)}, \quad 3\delta_2 < \delta_2' \leq \min\{1, c_1\} \tag{48}$$

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

Step 1. We first derive an intermediate deformation from y successively moving the atoms around. At each intermediate step we are dealing with deformations $\hat{y}$ such that $\|\hat{y} - A\| \leq c_0$, so lemma 3.25 is applicable.

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

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

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

$$y(x) + re \in B_{c_0}(Ax_p) \quad \text{ and } \quad y(x') - re \in B_{c_0}(Ax'_p)$$

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

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

such that

$$|Y(x) - Y(x')|, |Y(x) - y(z)|, |Y(x') - y(z)| \ge \delta'_1$$

for all $z \in \mathcal{L}_k$, $z \neq x, x'$.
Proof of the claim: Let B, B' be balls of radius $2\delta_2$ centered at $y(x)$ resp. $y(x')$. Clearly, $\text{dist}(z, \bar{z}) \ge \delta_2 > \delta_1$ if $z \in L$ and $\bar{z} \notin B$ (resp. if $z \in L'$ and $\bar{z} \notin B'$). By the preceding lemma there are at most $n(2\delta_2)$ atoms in these balls. Consider balls B_l, resp. $B'_{l'}$ with radius δ'_1 around the atoms in the balls B, resp. B'. Since by assumption $\delta'_1 < \delta_2/6n(2\delta_2)$ we get ($\mathcal{H}^1$ denoting one-dimensional Hausdorff measure)

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

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

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

Noting that $|z - z'| \le \delta'_1 \Rightarrow |y(x) + y(x') - 2z| \le \delta'_1$ we also get that

$$\mathcal{H}^1(\{z \in L : |z - z'| \le \delta'_1\}) \le \delta'_1,$$

so we have shown that

$$\mathcal{H}^1(\{z \in L \setminus \bigcup_l B_l : z' \notin \bigcup_{l'} B'_{l'}, |z - z'| \ge \delta'_1\}) \ge \delta_2/3 - \delta'_1 > 0.$$

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

We now update the deformation by replacing $y(x)$ by $Y(x)$ and $y(x')$ by $Y(x')$. If each atom has been considered this way we arrive at a new configuration again denoted y. We repeat the process until there are no more δ_1-critical bonds that can be removed this way. (There may still be δ_1-critical bonds left.)
Step 2. If there are no more δ_1-critical bonds, we are done. If there still are, using the new configuration constructed in step 1 (again called y), we now

construct y'. Suppose $y(x)$ takes part in a δ_1-critical bond. Then it is not possible to find another atom in the same film layer and the unit vector e as described above. But then, for all $x' \in \mathcal{L} \cap (kQ \times [0,h])$ with $x_3 = x_3'$,

$$|y(x') - Ax_p' - [y(x) - Ax_p]| \leq \delta_2, \tag{49}$$

for otherwise we could define

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

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

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

we had

$$|Ax_p' - Ax_p''| \leq 2\delta_2 + \delta_1 < c_1$$

in contradiction to (48).)

Now suppose $(y(x), y(x'))$ is critical where $x' = (x_p', i')$, $i' \neq i$. Then again as in (49) for all $z_p, z_p' \in \mathbb{Z}^2 \cap kQ$,

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

In particular for $z_p' - z_p = x_p' - x_p$

$$\left| y(z_p', i') - Az_p' - [y(x') - Ax_p'] - \Big(y(z_p, i) - Az_p - [y(x) - Ax_p] \Big) \right| \leq 2\delta_2,$$

so

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

Since $|x_p - x_p'| \leq C$ (cf. lemma 3.25 (ii)), we find (up to a constant boundary layer) at least one $3\delta_2$-critical bond per atom of the i-th layer. If this case occurs, i.e. we have more than $(kl_3)^2 - Ckl_3$ $3\delta_2$-critical bonds, we reorder all the atoms in $kQ \times [0,h]$, first by placing atom x at position $V(x)$ (V such that $\tilde{V} = v$, cf. (9)). Now suppose δ_2' is small enough. Then, since $|B^i| < c_0 - \theta$ or $|B^j| < c_0 - \theta$ if $|B^i - B^j - Az| \leq \theta$ for $i \neq j$ and some $z \in \mathbb{Z}^2$, we can eliminate all $3\delta_2$-critical bonds as in step 1, arriving at a new deformation y such that no atom in $y(kQ \times [0,h])$ takes part in a δ_2'-critical bond.

Lemma 3.26 *Suppose $|B^i| = |B^j| = c_0$ and $B^i - B^j \in A\mathbb{Z}^2$ only for $i = j$. (So θ as above can be chosen.) There are $0 < \delta_1, \delta_1', \delta_2, \delta_2'$ (only depending on W, E_0, and θ) such that (48) holds and (cf. (43)) for all $y \in \hat{\mathcal{N}}_Q^{l_2,l_3}(A, \mathbf{b})$*

$$E_{\delta_1}(y') \leq E_{\delta_1}(y)$$

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

Proof. We prove that each step of the above construction lowers energy. Assume δ_2' is so small that $W(r) \ge 0$ on $(0, \delta_2']$ and thus also $W_\delta \ge 0$ on $(0, \delta_2']$ for $\delta \le \delta_2'$ (cf. (44)). Suppose $\hat{y}$, $\hat{y}'$ are intermediate configurations in step 1 above and $\hat{y}'$ arises from $\hat{y}$ by moving the atoms x and x'. By corollary 3.8 changing the position of two atoms yields an energy error in E_0 bounded by some constant C. For given (small) δ_1', δ_2 choose δ_1 so small that

$$W_{\delta_1}(r) > C + 5 \sup_{\|\tilde{y}-u\| \le c_0/k} \sup_z \sum_{z' \neq z} |W_{\delta_1'}(|y(z') - y(z)|)|$$

for all $r \le \delta_1$ (which is possible by (45) and (44)). Now, $y(x)$ having a critical bond of length $r < \delta_1$,

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

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

$$W_{\delta_1}(r) > 2C + \sup_{\|\tilde{y}-u\| \le c_0/k} \sup_x 2\nu \sum_{x' \neq x} |W_{\delta_2'}(|y(x') - y(x)|)|$$

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

$$\begin{aligned}
&E_{\delta_1}(y) - E_{\delta_1}(y') \\
&= \frac{1}{2} \sum_{x' \neq x} W_{\delta_1}(|y(x') - y(x)|) - \frac{1}{2} \sum_{x' \neq x} W_{\delta_1}(|y'(x') - y'(x)|) \\
&\quad + E_0(y) - E_0(y') \\
&\ge \frac{1}{2} \sum_{\substack{x' \neq x \\ |y(x)-y(x')| \le 3\delta_2}} W_{\delta_1}(|y(x) - y(x')|) + \frac{1}{2} \sum_{\substack{x' \neq x \\ |y(x)-y(x')| > \delta_2'}} W_{\delta_2'}(|y(x') - y(x)|) \\
&\quad - \frac{1}{2} \sum_{x' \neq x} W_{\delta_2'}(|y'(x') - y'(x)|) + E_0(y) - E_0(y')
\end{aligned}$$

$$\geq \frac{(\lceil kl_3\rceil+1)^2}{2}\left(2C+2\nu \sup_{\|\tilde{y}-u\|\leq c_0/k}\sup_x \sum_{x'\neq x}|W_{\delta_2'}(|y(x')-y(x)|)|\right)$$
$$-\frac{1}{2}\nu\lceil kl_3\rceil^2 \sup_x \sum_{x'\neq x}|W_{\delta_2'}(|y(x')-y(x)|)|$$
$$-\frac{1}{2}\nu\lceil kl_3\rceil^2 \sup_x \sum_{x'\neq x}|W_{\delta_2'}(|y'(x')-y'(x)|)|-C(kl_3)^2$$
$$\geq 0.$$

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

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

Lemma 3.27 *For all $y\in\hat{\mathcal{N}}_{k,c_0-\delta_2}^{l_2,l_3}(u,\mathbf{b})$ there exists $y'\in\hat{\mathcal{N}}_{k,c_0}^{l_2,l_3}(u,\mathbf{b})$ with $E(y')\leq E_{\delta_1}(y)$ if δ_1 is sufficiently small.*

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

We first analyze φ. The first part of theorem 3.4 is contained in the following proposition.

Proposition 3.28 *Suppose A and $\mathbf{b}$ are admissible. Then the limit*

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

exists in $(-\infty,\infty]$, φ is continuous on $\mathcal{A}_{\mathrm{hom}}$ (as a function with values in $\mathbb{R}\cup\{\infty\}$), and $\varphi(A,\mathbf{b})=\infty$ iff there are $z\in\mathbb{Z}^2$, $i\neq j\in\{1,\ldots,\nu\}$ such that $B^i-B^j=Az$ and $|B^i|=|B^j|=c_0$. (B^i as in (47), (46).)

Furthermore, φ_δ denoting the limiting energy density corresponding to E_δ (cf. (43)), $\varphi_\delta\nearrow\varphi$ pointwise on $\mathcal{A}_{\mathrm{hom}}$ as $\delta\searrow 0$.

Proof. Suppose first that $B^i-B^j\notin A\mathbb{Z}^2$ if $|B^i|=|B^j|=c_0$, $i\neq j$. By lemma 3.26

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

for δ_1 sufficiently small. But $E_{\delta_1}\leq E$, so the reverse inequality it true, too. We may therefore replace E by E_{δ_1} and infer from theorem 3.2 that $\varphi(A,\mathbf{b})$ exists in $\mathbb{R}$, and φ is continuous at these $A,\mathbf{b}$.

For $0<\theta\leq 1$ given, suppose now there are $z\in\mathbb{Z}^2$ and $i\neq j$ such that $|B^i|,|B^j|\geq c_0-\theta$, $|B^i-B^j-Az|\leq\theta$. We define Y^i and $\overline{Y^i}$ as in the proof of lemma 3.12. There it was shown that for $|B^{i_0}| \geq c_0 - \theta$ we have (cf. (24) and (25) with $\varepsilon' = \theta$ and $\delta = 0$)

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

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

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

Now if $i \neq j$, then this shows that the number of $4C\sqrt[4]{\theta}$-critical bonds is at least $k^2/2$. This holds for all $y \in \hat{\mathcal{N}}_k^{0,1}(A, \mathbf{b})$, so by (28)

$$\varphi_k(A, \mathbf{b}) \geq \frac{1}{2\nu} \inf_{0 < s \leq 4C\sqrt[4]{\theta}} W(s) - C,$$

and thus

$$\varphi(A, \mathbf{b}) \geq \frac{1}{2\nu} \inf_{0 < s \leq 4C\sqrt[4]{\theta}} W(s) - C \to \infty \text{ as } \theta \to 0.$$

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

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

□

Define

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

Proof of theorem 3.4. By proposition 3.28 it remains to prove upper and lower bounds for general admissible $(u, \mathbf{b})$. This is done in four steps:

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

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

for all $\delta_1 > 0$. Now, by proposition 3.28, $\varphi_{\delta_1} \nearrow \varphi$ pointwise as $\delta_1 \to 0$, so

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

by monotone convergence.

2. First suppose that $|B^i(x)| \leq c_0 - \theta$ a.e. for some $\theta > 0$. Then by lemma 3.27 for appropriately chosen δ_1, δ_2 small

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

Now by theorems 3.2 and 3.3 (see also corollary 3.21), denoting the macroscopic energy density corresponding to E_δ by φ^δ,

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

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

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

Now this holds for all δ_2, therefore

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

by dominated convergence, provided $\varphi_{c_0-\delta} \to \varphi_{c_0}$ boundedly on $\{|B^i| \leq c_0 - \theta\}$ as $\delta \to 0$. To see this, note first that on this set we may replace φ by φ^{δ_0} for $\delta_0 > 0$ small enough only depending on θ (see the proof of proposition 3.28). Now an easy consequence of lemma 3.12 is that $|\varphi^{\delta_0}_{k,c_0-\delta} - \varphi^{\delta_0}_{k,c_0}| \leq C\delta^{1/5}$. It remains to note that $y^{(k)} \in \hat{\mathcal{N}}^{l_2,l_3}_{k,c_0}(u,\mathbf{b})$ for all k implies $y^{(k)} \to (u, \mathbf{b})$.

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

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

By continuity and boundedness of φ,

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

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

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

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

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

□

3.6 Extensions & variants

We discuss some extensions of the theory and possible changes of our set-up.

3.6.1 Basic extensions

More general Bravais lattices and domains

More generally, we could deal with Bravais-lattices

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

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

Covering $\mathcal{S}$ with mesoscopic squares up to a negligible error at the boundary, it is not hard to see that the convergence scheme in fact applies to bounded Lipschitz domain $\mathcal{S} \subset \mathbb{R}^2$ (where φ is given as in theorem 3.2).

Alternative definition of convergence

In our definition of convergence $y^{(k)} \to (u, \mathbf{b})$, it is not possible to consider the limiting case of very restricted relaxation, i.e. $c_0 \to 0$, unless all b^i are zero. Instead of asking $\|\tilde{y} - u\|$ in definition 2.3 to be less than c_0/k one could demand that

$$\|\tilde{y} - v\| \leq c_0/k \tag{50}$$

where v is as in (9) corresponding to $u, \mathbf{b}$ with b^0 set to zero. (Condition (4) is not needed for this definition of convergence.) The results are analogous.

Different types of atoms

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

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

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

3.6.2 Distinguishable particle systems

Similarly, the convergence scheme also applies to certain systems with distinguishable particles. In this paragraph we will state a general result for systems with finite range interaction. The basic assumption is that only atoms that are close in the reference configuration are supposed to interact. This violates assumption 2.7 since the energy is not a function of atomic positions in the deformed configuration any more. It rather also depends on the reference configuration, i.e. the atoms are distinguishable. It will be clear, however, that the convergence scheme of section 3 still applies.

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

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

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

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

$$E_{\text{fr}}(y) = \sum_{x_i \in \mathcal{L} \cap (S_k^a \times [0,h])} f_{x_i}(y(x_2^i) - y(x_1^i), \ldots, y(x_{r_a}^i) - y(x_1^i)) + \mathcal{O}(k) \qquad (51)$$

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

$$f_{(x_1+p_1, x_2, x_3)} = f_x = f_{(x_1, x_2+p_2, x_3)} \qquad (52)$$

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

Proposition 3.29 *Suppose E_{fr} is defined as in (51) and (52) holds. Assume that the f_{x_i} are locally Lipschitz. Then the limit φ_{fr} of theorem 3.2 exists and we have*

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

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

(Adopting the notion of δ-criticality suitably (cf. definition 3.24), also unbounded pair-interaction parts can be treated analogously to theorem 3.4.)

Sketch of Proof. First note that by (52) there are only finitely many different functions f_x. Due to lemma 2.2, a bound on the distance of two atoms in the reference configuration implies a bound on their distance in the deformed state. So by a cut-off argument we may suppose that the functions f_{x_i} are uniformly bounded and have common local Lipschitz constants. It is then clear that the decay-assumptions on E are sufficient. By the periodicity assumption (52) the passage scheme of section 3 is applicable once we have shown that E satisfies the Lipschitz property of assumption 2.7. But each atom occurs in at most r_a summands of (51). The claim is proven. □

Remark: Dealing only with energies whose range is bounded in the reference configuration, there is no need for a minimal strain hypothesis on u, i.e. for these interactions we might set $c_1 = 0$ in (3).

4 Examples/applications

In this section we will investigate some examples of atomic interactions and explore under what circumstances these models fit into the theory developed in the last section. The first three models will satisfy assumptions 2.6 and 2.7 even in the more restrictive sense of assumption 2.8. For the last one this will be obviously false. Throughout this discussion we will assume that $u \in W^{1,\infty}(\mathcal{S}_1;\mathbb{R}^3)$, $b^i \in L^\infty(S_1;\mathbb{R}^3)$ are admissible.

4.1 Pair potentials

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

$$E_{\rm pp}(y) = \frac{1}{2}\sum_{i\neq j} W(|y_i - y_j|), \tag{53}$$

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

Proposition 4.1 *Suppose $E_{\rm pp}$ is defined as in (53). Assume that $W : [0,\infty) \to \mathbb{R}$ is Lipschitz. If there exist $M > 0$ and $q > 3$ such that for a.e. $r \geq 0$*

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

then $E_{\rm pp}$ is admissible.

Proof. We need only check that $E_{\rm pp}$ satisfies assumptions 2.6 and 2.7. Clearly, $E_{\rm pp}$ only depends on atomic positions, is frame indifferent, and satisfies assumption 2.6 with $\psi(r) = |W(r)|$. Furthermore, W Lipschitz (with Lipschitz constant M', say) implies that E is Lipschitz and we have for each l whenever $y_m \neq y_l$ for all $m \neq l$ and $W'(|y_l - y_j|)$ exists, i.e. almost everywhere,

$$\begin{aligned} \left|\frac{\partial E}{\partial y_l}(y)\right| &= \left|\frac{1}{2}\sum_{i\neq j} W'(|y_i - y_j|)\cdot\frac{y_i - y_j}{|y_i - y_j|}\cdot(\delta_{il} - \delta_{jl})\right| \\ &\leq \sum_{j\neq l} \left|W'(|y_l - y_j|)\right|. \end{aligned} \tag{54}$$

We have to find a bound on this quantity assuming $\|\tilde{y} - u\| \leq C/k$. But then, as in lemma 2.2, y satisfies $|y(x) - y(z)| \geq C_1|x - z| - C_3$ and we can apply the technique of splitting the sum into long-range and short-range terms as in the proof of lemma 3.7. From $|W'(r)| \leq M'$ and $|W'(r)| \leq Mr^{-q+1}$, $q > 3$, we then deduce that the right hand side of (54) is bounded (independently of k and l). $\square$

As an example consider the Morse potential with interaction function

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

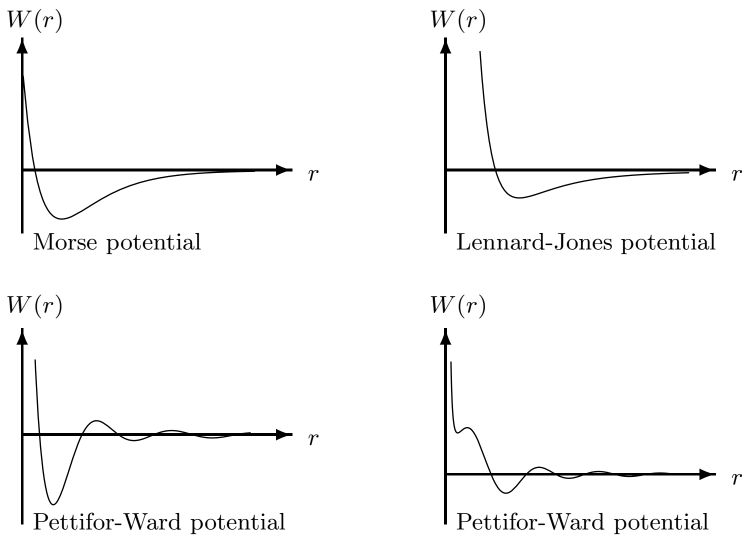
for positive parameters W_0, a and r_0 (cf. [27]). By theorem 3.4 we also see that our convergence scheme applies to, e.g., the Lennard-Jones potential given by

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

$W_0 > 0$ and σ constants (cf. [27]), and the Pettifor-Ward pair potentials (cf. [30]) given by

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

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



4.2 Pair functionals

More generally, in this paragraph we will discuss pair functionals as examples of the embedded atom method. These models have the advantage of also covering some environmental dependence of the bond strength between the nuclei at positions $\{y_i\}$ (cf. [27]). We let

$$E_{\mathrm{pf}}(y) = \frac{1}{2} \sum_{i \neq j} W(|y_i - y_j|) + \sum_i F(\rho_i), \tag{55}$$

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

$$\rho_i = \sum_{j \neq i} f(|y_i - y_j|), \tag{56}$$

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

The interpretation of such an energy function is the following (cf. [27]). As always $\{y_i\}$ denotes the positions of the nuclei of some material. These nuclei are supposed to be embedded in some electron gas consisting of the valence electrons of the atoms of that material. Now suppose that the total energy associated with y can be split into two parts: one that describes the interaction of the various nuclei, leading to the first summand in (55), and the sum of the energy it costs to embed a single nucleus into an electron gas of some density ρ. Denoting this energy

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

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

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

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

We aim at exhibiting conditions on W, F and f such that E_{pf} satisfies assumptions 2.6 and 2.7. First note that since

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

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

Lemma 4.2 *Suppose E_{pf} is defined as in (55) and W is as in proposition 4.1 (resp. theorem 3.4). Assume $F : [0, \infty) \to (-\infty, 0]$ is convex and Lipschitz, $f : [0, \infty) \to [0, \infty)$ is Lipschitz and for a.e. $r \geq 0$*

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

Then E_{pf} is admissible (resp. theorem 3.4 applies).

Note that, as is plausible, by the decay hypothesis and assumptions on F, necessarily $f(r) \to 0$ as $r \to \infty$ (if F is not trivial). In the following proposition we will see that F need not be Lipschitz. While the decay assumption on f' is in the spirit of the previous result, $|F \circ f(r)| \leq M r^{-q}$ poses quite severe decay conditions on f, if we take e.g. $F(a) \sim \sqrt{a}$. This will be remedied in proposition 4.3.

Proof. First note $F \leq 0$ convex implies that $-F$ is subadditive. By propoition 4.1 it remains to verify assumptions 2.6 and 2.7 for the embedding term $E_{\text{emb}}(y) = \sum_i F(\rho_i)$. So let $\mathcal{M}$ and $\mathcal{N}$ be disjoint sets of atoms. Setting

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

we find

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

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

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

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

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

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

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

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

For the remaining part we again only need to consider the embedding term of the energy. (The first one is dealt with as in the proof of proposition 4.1.) F is Lipschitz, say $\|F'\|_\infty \le M'$. So almost everywhere

$$
\begin{aligned}
&\left| \frac{\partial}{\partial y_l} \sum_i F\left(\sum_{j\neq i} f(|y_i - y_j|) \right) \right| \\
&= \left| \sum_i \left(F'\left(\sum_{j\neq i} f(|y_i - y_j|) \right) \cdot \sum_{j\neq i} f'(|y_i - y_j|) \cdot \frac{y_i - y_j}{|y_i - y_j|} \cdot (\delta_{il} - \delta_{jl}) \right) \right| \\
&\le \ M' \left| \sum_{i\neq j} f'(|y_i - y_j|) \cdot \frac{y_i - y_j}{|y_i - y_j|} \cdot (\delta_{il} - \delta_{jl}) \right| \\
&\le \ 2M' \sum_{j\neq l} \left| f'(|y_l - y_j|) \right|. \qquad (57)
\end{aligned}
$$

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

Proposition 4.3 *Suppose W is as in proposition 4.1 (resp. theorem 3.4). Assume now $F : [0,\infty) \to (-\infty, 0]$ is convex, $f : [0,\infty) \to (0,\infty)$ is Lipschitz, and, for a.e. $r \geq 0$,*

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

Then theorems 3.1, 3.2, and 3.3 (resp. 3.4) apply to E_{pf} as given in (55).

Remark: Before we prove this proposition we would like to comment on the plausability of the various assumption made. F is non-positive since placing a positively charged particle into an electron cloud yields energy. The non-negativity of f is clear, since f is supposed to be a density. Strict posivity is plausible, since perfect screening is not to be expected. The convexity condition on F can be understood as reflecting the fact that due to screening adding more electrons (i.e. raising the electron density) results in smaller and smaller effects. This seems to match experimental data (cf. [27], p. 171). A qualitatively reasonable scaling would be given by $F(a) \sim -\sqrt{a}$ as e.g. in the Finnis-Sinclair model where $F(a) \propto -\sqrt{a}$ (cf. [27]). The remaining are decay assumptions on f as those for W.

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

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

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

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

theorems 3.1, 3.2, and 3.3 also apply to E. $\square$

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

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

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

4.3 Angular forces

In this paragraph we consider energy functions that may also depend on the angles between atomic bonds. For a physical motivation of such models we refer to [27]. Mathematically, this leads to consideration of potentials depending on triplets of atomic positions:

$$E_{\rm af}(y) = \frac{1}{2}\sum_{i\neq j} W(|y_i - y_j|) + \frac{1}{6}\sum_{\substack{i,j,k\\ i\neq j\neq k\neq i}} \hat{W}(y_i, y_j, y_k), \tag{58}$$

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

$$\begin{aligned} \hat{W}(y_i, y_j, y_k) \;=\; & h(|y_i - y_j|, |y_j - y_k|, \theta_{ijk}) + h(|y_j - y_k|, |y_k - y_i|, \theta_{jki}) \\ & + h(|y_k - y_i|, |y_i - y_j|, \theta_{kij}), \end{aligned} \tag{59}$$

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

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

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

Again we are seeking for conditions on W and $\hat{W}$ (resp. h) such that $E_{\rm af}$ satisfies assumptions 2.6 and 2.7. As before it is easy to see that $E_{\rm af}(y)$ depending only on interatomic distances and angles is determind by atomic positions and is frame indifferent.

Proposition 4.4 *Suppose $E_{\rm af}$ is defined as in (58). Assume that W is as in proposition 4.1 (resp. theorem 3.4) and h is Lipschitz. Furthermore, there are bounded functions $\chi_1, \chi_2, \alpha_1, \alpha_2 : [0,\infty) \to [0,\infty)$ with*

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

such that

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

and (a.e.)

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

and

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

Then $E_{\rm af}$ is admissible (resp. theorem 3.4 applicable).

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

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

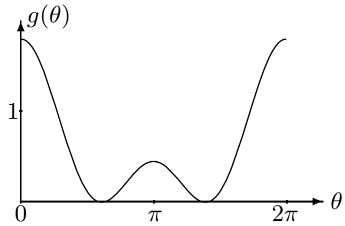
Example: If h splits into

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

as e.g. for Stillinger-Weber-type energies (cf. [27]). Then h satisfies the conditions of proposition 4.4 if f_μ, f'_μ are bounded, $|f_\mu| \le M r^{-q}$, $|f'_\mu| \le M r^{-q+1}$ for $\mu = 1, 2$, $f_1(r_1) f_2(r_2) \le \min\{r_1, r_2\}$ and g and g' are bounded. This is satisfied e.g. for the angular term

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

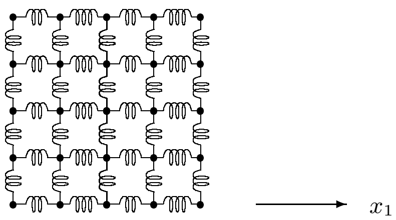
discussed in [27].



4.4 A simple example

Even for fairly elementary microscopic energies as e.g. given by pair potentials, not much is known about their ground state deformations. (Some one-dimensional results in this direction can be found in [5], a recent two-dimensional result for certain pair potentials is proved in [31].) We conclude this section calculating φ explicitly for a simple nearest neighbor model. Although it lacks some physical requirements (e.g. shear resistance), it captures some realistic features as e.g. quadratic energy growth near the reference configuration (a natural state) for pure extensions. The model consisting of two different types of bonds, the energy minimizer will not be a simple crystal. A pointwise limit would overestimate the energy.

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



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

$$E_{\rm nn}(y) = \frac{1}{2} \sum_{|x_i - x_j| = 1} d_{ij} (|y_i - y_j| - 1)^2, \qquad (60)$$

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

Proposition 4.5 *$E_{\rm nn}$ is admissible in the sense of proposition 3.29. In particular, the limit $\varphi_{\rm nn}$ of theorem 3.2 exists for $E_{\rm nn}$ and*

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

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

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

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

This is clearly a special case of (51) with $a = 1$ and periodicity $p_1 = 2, p_2 = 1$. So we only have to prove the representation formula for $\varphi_{\rm nn}$.

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

$$i \mapsto y(x_1 + i, x_2, x_3), \quad \text{resp.} \quad i \mapsto y(x_1, x_2 + i, x_3)$$

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

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

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

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