Max-Planck-Institut
für Mathematik
in den Naturwissenschaften
Leipzig

Lattice approximation of a surface integral and convergence of a singular lattice sum

by

Anja Schlömerkemper

Preprint no.: 86 2005

Lattice approximation of a surface integral and convergence of a singular lattice sum

Anja Schlömerkemper*

October 7, 2005

Abstract

Let $\mathcal{L}$ be a lattice in $\mathbb{R}^d$, $d \geq 2$, and let $A \subset \mathbb{R}^d$ be a Lipschitz domain which satisfies some additional weak technical regularity assumption. In the first part of the paper we consider certain lattice sums over points which are close to ∂A. The main result is that these lattice sums approximate corresponding surface integrals for small lattice spacing. This is not obvious since the thickness of the domain of summation is comparable to the scale of the lattice.

In the second part of the paper we study a specific singular lattice sum in $d \geq 2$ and prove that this lattice sum converges as the lattice spacing tends to zero. This lattice sum and its convergence are of interest in lattice-to-continuum approximations in electromagnetic theories—as is the above approximation of surface integrals by lattice sums.

This work generalizes previous results [10] from $d = 3$ to $d \geq 2$ and to a more general geometric setting, which is no longer restricted to nested sets.

MSC (2000): 40A30, 31C20, 78A30, 78M35
Keywords: approximation of surface integrals, lattice-to-continuum theories, convergence of multidimensional singular series, magnetostatics

*Max-Planck-Institute for Mathematics in the Sciences, Inselstraße 22–26, D-04103 Leipzig, Germany, schloem@mis.mpg.de

1 Introduction

Lattice approximations of continuum theories have a long history and have recently regained interest, e.g., in connection with hybrid atomistic-continuum models [11] and martensitic phase transformation in shape-memory alloys [5]. One motivation is to link phenomenological models in the continuum setting to properties of materials given at a lattice scale, which is in particular of interest for the design of materials.

The motivation for the work in the first part of this paper goes back to Cauchy's work in elasticity [1]. In his molecular theory of stress, cf. also [Lo, Note B], a key step in his arguments is based on the following basic geometric fact: The volume of a (degenerate) cylinder equals the area of its base times its height. Let $\mathcal{C}_z$ be the cylinder in Figure 1 with base $\mathcal{I}$ (a 'nice' subset of $\mathbb{R}^2$) and height $n \cdot z$, where n is the normal to $\mathcal{I}$ and $z \in \mathbb{R}^3$. Then the volume of $\mathcal{C}_z$ equals the area of $\mathcal{I}$ times $n \cdot z$. In what follows we are in particular interested in cylinders of small height/thickness, i.e., small $|z|$.

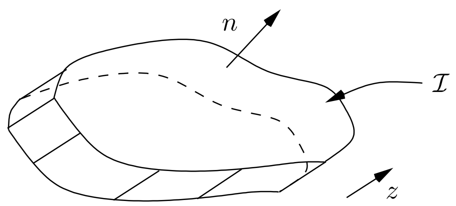

Figure 1: A (degenerate) cylinder $\mathcal{C}_z$ with base $\mathcal{I}$ and of height $n \cdot z$, where n denotes the normal to $\mathcal{I}$.

Now assume that there is a three dimensional (Bravais) lattice $\mathcal{L}$ of atoms given. Moreover assume that there acts an elastic force between any pair of atoms. Cauchy calculated the force which is exerted by all atoms on one side of a planar interface $\mathcal{I}$ on all atoms on the other side. A crucial step in his study is related to the following sum over all lattice points in a cylinder $\mathcal{C}_z$

$$\sum_{x \in \mathcal{C}_z \cap \mathcal{L}} g(x), \tag{1}$$

where g is some smooth function that reflects physical properties related to the elastic force [Lo, p. 619].

Cauchy then argued as follows: If $\mathcal{C}_z$ is large enough, the number of lattice points in $\mathcal{C}_z$ is bounded by the volume of $\mathcal{C}_z$ divided by the volume of a unit cell. For this argument he assumed that $\mathcal{I}$ is contained in a plane of lattice points and z is a lattice vector. Then, the number of lattice points in $\mathcal{C}_z$ is bounded by the area of $\mathcal{I}$ times $n \cdot z$ divided by the volume of a unit cell. To link this observation to the results of this paper, where in particular $\mathcal{I}$ does not need to be flat, we rephrase the observation as follows: Cauchy estimated the number of lattice points in $\mathcal{C}_z$ by the surface integral $\int_{\mathcal{I}} n \cdot z \, ds$ divided by the volume of a unit cell.

In this article we consider conceptually the same problem but in a more general setting. In our case, $\mathcal{I}$ is the interface, i.e., the common boundary, of two Lipschitz domains A and B which satisfy some regularity assumptions, see Assumption $\mathcal{A}_1$ in Section 2 for details. In particular, $\mathcal{I}$ is not required to be flat as in Cauchy's work. Therefore, the interface need not be contained in a plane of lattice points and thus may intersect the interior of unit cells, which makes the problem mathematically interesting. To overcome the difficulties, we use the concept of so-called modified unit cells which was introduced in [7, 9, 10], cf. also (13) and Lemma 11 below.

Close to edges and corners of A and B and close to points of $\mathcal{I}$ where $n \cdot z$ is almost zero, Cauchy's observation about the number of points in a cylinder $\mathcal{C}_z$ is not useful anymore. However, it turns out that the volume of neighbouring regions about those points converges like $|z|^2$ and is therefore of lower order, cf. Definitions 6 and 7 and Lemmas 9 and 10.

The main result is Theorem 8. Generalizing the representation of (1) by a surface integral, we obtain an approximation of lattice sums by surface integrals for all dimensions $d \geq 2$. Analogous statements under stronger assumptions are given in [7, 9, 10] in the context of magnetic forces in continuous media. There it is in particular assumed that $d = 3$ and $\partial A \cap \partial B = \partial A$, i.e., A and B are nested sets. Estimates as in Proposition 1 were already given under stronger assumptions; the finer estimates in Theorem 8 are new.

The more general setting in this article is motivated by work on magnetic forces between two permanent magnets A and B of cuboidal or rectangular shape at distance greater or equal to zero as studied in [8]. If the distance between two magnets A and B is zero, these sets satisfy Assumption $\mathcal{A}_1$ below, but do not satisfy the assumptions of the previous result in [10, Proposition 1], even if $d = 3$ since the magnetic domains A and B are not nested.

The new geometrical setting requires a new formulation of the previous assumptions on the regularity of the domains. In particular, we need to adapt the so-called non-degeneracy condition (S), compare Definition 3 and

[10, Definition 2].

In [8], not only three-dimensional problems but also two-dimensional problems are considered; Theorem 8 is applied in the cases $d = 2$ and $d = 3$ to prove a magnetic force formula. This is the main motivation for proving Theorem 8 in two and three dimensions. However, in dimensions $d \geq 4$, Theorem 8 is for the time being only interesting from a mathematical point of view.

The first and the second part of this article are linked by their applications to the calculation of so-called short range forces, cf. [8]. See also the comment after Theorem 13.

In the second part of this article we prove the convergence of a singular lattice sum as the lattice spacing tends to zero. This continuum limit arises for instance in the context of magnetic forces, cf. [10]. In [10, Lemma 5] the convergence result is proved for $d = 3$. Here we prove the convergence also for $d = 2$ and for $d \geq 4$, see Theorem 13. The result of the former case is again of interest in [8] and is applied in the derivation of a so-called short-range part of a magnetic force formula. The case $d \geq 4$ is first of all only of mathematical interest.

The terms in the sum consist of derivatives of the fundamental solution of Laplace's equation, cf. (25). In particular, the terms are of order $|z|^{-d}$ in d dimensions. Thus the sum cannot converge absolutely. It only converges due to cancellations. In the study of sums of this type, methods from number theory, in particular form the theory of modular forms can be used, see, e.g., [12]. However, for the purpose of this article a more naive approach is sufficient: We follow the ideas from [10]. That is, we replace the sum by an integral and show that the error terms are of higher order. These estimates as well as the appropriate definition of the terms of the sum in dimensions $d = 2$ and $d \geq 4$ are new.

2 Approximation of surface integrals by lattice sums

In this section we consider the approximation of some surface integrals by certain lattice sums. Let the dimension $d \geq 2$ be fixed and let $\mathcal{L}$ be a Bravais lattice, i.e.,

$$\mathcal{L} = \Big\{ x \in \mathbb{R}^d \,:\, x = \sum_{i=1}^{d} \mu_i e_i,\ \mu_i \in \mathbb{Z} \Big\}, \tag{2}$$

where $(e_1, \dots, e_d)$ is a basis of $\mathbb{R}^d$. For simplicity we assume that the unit cell $\mathcal{U} = \{x \in \mathbb{R}^d \,:\, x = \sum_{i=1}^{d} \lambda_i e_i,\ \lambda_i \in [0,1)\}$ has unit volume. We call $\frac{1}{\ell}\mathcal{L}$, $\ell \in \mathbb{N}$, the scaled Bravais lattice, where $\frac{1}{\ell}\mathcal{L} := \{y \,:\, y = \frac{1}{\ell}x \text{ for some } x \in \mathcal{L}\}$. Similarly, we define $\frac{1}{\ell}\mathcal{U}$. Furthermore, we denote translated unit cells by $\frac{1}{\ell}\mathcal{U}(x) := x + \frac{1}{\ell}\mathcal{U}$.

A domain $A \subset \mathbb{R}^d$ is said to be *Lipschitz*, if, locally, the boundary of A is the graph of a Lipschitz continuous function and A is on one side of the boundary only. Moreover, let n denote the outer normal to ∂A and let $\mathcal{H}^k$ denote the k-dimensional Hausdorff measure. Throughout the paper, the sets A and B satisfy the following assumption.

Assumption $\mathcal{A}_1$
(i) A and B are bounded Lipschitz domains in $\mathbb{R}^d$ such that $A \cap B = \emptyset$.
(ii) A and B have some boundary in common, i.e., $\mathcal{H}^{d-1}(\partial A \cap \partial B) > 0$.
(iii) $\bar{A} \cup \bar{B}$ satisfies the outer cone property*, i.e., for each $x \in \partial(\bar{A} \cup \bar{B})$ there exists a cone, C_x^α, with opening angle $\alpha > 0$ pointed at x such that $C_x^\alpha \cap (\bar{A} \cup \bar{B}) = \{x\}$.*
(iv) ∂A, ∂B and $\partial A \cap \partial B$ satisfy the non-degeneracy condition (S), cf. Definition 3.
(v) $\partial A \cap \partial B$ satisfies the neighbourhood estimate, see Definition 4 below.

The outer cone property excludes inward pointing cusps and is for instance satisfied if $A \cup B \cup (\partial A \cap \partial B)$ is a Lipschitz domain. It is also satisfied for two domains A, B which are of polygonal shape (and of which the union might not be Lipschitz); this is of interest from an applicational point of view, cf. [8].

Note that Assumption $\mathcal{A}_1$ includes the case of A and B being nested sets, which is supposed in [10] for $d = 3$.

Assumptions $\mathcal{A}_1$ (iv) and $\mathcal{A}_1$ (v) are restrictions on the shape of ∂A, ∂B and $\partial A \cap \partial B$, respectively. They are for instance satisfied if A and B are polyhedra which are Lipschitz domains. Before giving the precise definition of these conditions and commenting on the notions further, we state a first result. To this end we fix a vector $z \in \frac{1}{\ell}\mathcal{L} \setminus \{0\}$ and set, cf. Figure 2,

$$A_z := \{x \in \bar{A} \ : \ x + z \in B\} \equiv \bar{A} \cap (B - z). \tag{3}$$

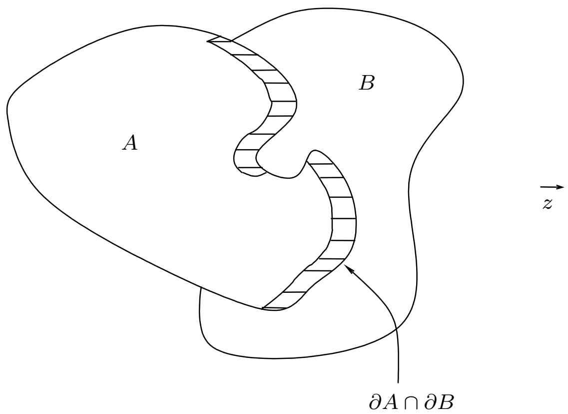

Figure 2: A slice of A and B indicating A_z.

We also consider a function $f : \mathbb{R}^d \to \mathbb{R}$ which is assumed to be Lipschitz continuous on A_z. Note that $f(x)$ is in particular defined for each $x \in \frac{1}{\ell}\mathcal{L}$. For later reference we set

Assumption $\mathcal{A}_2$ *The function $f : \mathbb{R}^d \to \mathbb{R}$ is Lipschitz continuous on A_z.*

Finally, we set $(\cdot)_+ = \max\{0, \cdot\}$ and are now in a position to state

Proposition 1 *Let A, B and f satisfy Assumptions $\mathcal{A}_1$ and $\mathcal{A}_2$, respectively. Fix $0 < \delta \ll 1$ and $z \in \frac{1}{\ell}\mathcal{L} \setminus \{0\}$ such that $|z| \leq \delta$. Then there exists an $\ell_0 \in \mathbb{N}$ such that for all $\ell \geq \ell_0$*

$$\Big| \frac{1}{\ell^d} \sum_{x \in A_z \cap \frac{1}{\ell}\mathcal{L}} f(x) - \int_{\partial A \cap \partial B} f(\xi)(n(\xi) \cdot z)_+ \, d\mathcal{H}^{d-1}(\xi) \Big| \leq C|z|^{4/3}. \tag{4}$$

The constant C only depends on the dimension d, $\sup|f|$, *the Lipschitz constant of f and on A and B.*

We give the proof of Proposition 1 below. It is an easy consequence of the following theorem, Theorem 8, which asserts a sharper error estimate that involves also the lattice parameter ℓ. In order to state the theorem, we need to introduce further notions, which are used in the proof of the theorem. First we give the precise definition of the non-degeneracy condition (S). For brevity and notational reasons, we write out the definition only for $\partial A \cap \partial B$. The definitions for ∂A and ∂B satisfying the non-degeneracy condition (S) go analogously.

Definition 2 *We say that $\partial A \cap \partial B$ is* piecewise $C^{1,1}$ *if there exist finitely many pairwise disjoint sets $U_i \subset \partial A \cap \partial B$ which are relatively open in $\partial A \cap \partial B$ and have the following properties:*
(i) U_i is a connected, orientable $C^{1,1}$ submanifold of $\mathbb{R}^d$ and the normal n to ∂A restricted to U_i is Lipschitz continuous up to the boundary,
(ii) $(\partial A \cap \partial B) \subset \bigcup_i \bar{U}_i$ and
(iii) the relative boundary ∂U_i is a finite union of connected $C^{1,1}$ submanifolds of $\mathbb{R}^d$. If $d = 2$, ∂U_i is required to be a union of finitely many points in $\mathbb{R}^d$.

In $d = 3$, condition (iii) in Definition 2 can be replaced with: ∂U_i is a finite union of rectifiable curves, cf. [10, Definition 1].

Definition 3 *We say that $\partial A \cap \partial B$ satisfies the* non-degeneracy condition (S) *if it is piecewise $C^{1,1}$ and if for all $z \in \mathbb{R}^d \setminus \{0\}$ the relative boundary of the set*

$$(\partial A \cap \partial B)^+ = \Big\{ x \in (\partial A \cap \partial B) \cap \big(\bigcup_i U_i \big) \ : \ n(x) \cdot z > 0 \Big\} \tag{5}$$

is a finite union of connected $C^{1,1}$ submanifolds of $\mathbb{R}^d$ of which the number and the total $\mathcal{H}^{d-2}$ measure are bounded independently of z. If $d = 2$, we simply assume that the boundary of the set in (5) *is a finite union of points of which the number is uniformly bounded in z.*

The non-degeneracy condition (S) was introduced in [9, Definition 3.4], cf. also [10, Definition 2], for the case $d = 3$. It controls the number of isolated boundary points which have the same tangent. That is, this condition excludes 'rough' boundaries which have an infinite number of indentations and protrusions. However, it is for instance satisfied for polyhedra which are Lipschitz. For further examples and a discussion of this notion for $d = 3$ see [10, p. 236]. We make use of the non-degeneracy condition (S) in the proof of Lemma 9.

Here and in the following, let $z \in \mathcal{L} \setminus \{0\} \cap B_\delta$ for some fixed $0 < \delta \ll 1$. We split the set A_z into a bad set $\mathcal{B} \cap A_z$, which essentially gives rise to the right hand side of (4) and a good set $\mathcal{G}$, which contributes to the surface integral in (4) (cf. Figure 3). To define these sets, we introduce

$$\Gamma := \partial((\partial A \cap \partial B)^+) \cup \bigcup_i \partial U_i \tag{6}$$

with $(\partial A \cap \partial B)^+$ as in Definition 3. Note that Γ is a union of finitely many connected $C^{1,1}$ submanifolds. These submanifolds are denoted by Γ_i, $i = 1, \dots, k$. Then $\Gamma = \bigcup_{i=1}^k \Gamma_i$. Before we define the good and bad sets, we give the precise definition of the neighbourhood estimate.

Definition 4 *Let $\partial A \cap \partial B$ satisfy the non-degeneracy condition (S), let Γ and Γ_i be as above and let $r > 0$. The* r-neighbourhood *of Γ_i is*

$$\Gamma_i(r) = \big\{x \in \mathbb{R}^d \,:\, \operatorname{dist}(x, \Gamma_i) \leq r\big\}. \tag{7}$$

Its d dimensional Lebesgue measure is denoted by $|\Gamma_i(r)|$. We say that $\partial A \cap \partial B$ satisfies the neighbourhood estimate *if there exist constants $c > 0$ and $r_0 > 0$ such that for any Γ_i*

$$|\Gamma_i(r)| \leq cr^2 \tag{8}$$

for all $r < r_0$.

Remark 5 (i) If $d = 2$, (8) always holds, trivially.
(ii) If $d = 3$, we proceed as in [10, p. 238] in order to show: If Γ is a finite union of rectifiable curves Γ_i, (8) holds for small enough r. Indeed, let L_i denote the length of Γ_i. Then we can cover Γ_i by $\lfloor \frac{L_i}{4r} \rfloor + 2$ balls of dimension 3 and radius $2r$, where $\lfloor a \rfloor$ is the integer part of a. Then $|\Gamma_i(r)| \leq cr^3(\lfloor \frac{L_i}{4r} \rfloor + 2)$. If $r \leq \frac{3}{2} L_i$, we obtain $|\Gamma_i(r)| \leq cr^3 \frac{L_i}{r} \leq cr^2$.
(iii) In $d > 3$ dimensions, the situation is more subtle. However, under certain assumptions on the regularity of Γ, we can estimate $\Gamma_i(r)$ by the volume of tubes. Consider $\mathbb{R}^d$ as a Riemannian manifold with Euclidean metric and let P be a smooth submanifold. Then a tube $T(P, r)$ of radius $r \geq 0$ about P is the set

$$T(P, r) = \{x \in \mathbb{R}^d \,:\, \exists \text{ a geodesic } \xi \text{ of length } L(\xi) \leq r \text{ from } x \text{ meeting } P \text{ orthogonally}\},$$

cf. [4, Section 3.1] for details. The volume of such a tube is a polynomial in r by Weyl's formula, see, e.g., [4, Eqn. (1.1)]. The smallest power in the polynomial is $d-q$ where q denotes the dimension of the submanifold P. Hence, if $q=d-2$, we have $|T(P,r)| \leq cr^2$ for small r.

We apply this estimate to our setting in order to give an example for (8) in $d>3$: Let us assume for a moment that Γ_i is not only $C^{1,1}$ but smooth and that the relative boundary $\partial\Gamma_i$ is a finite union of smooth $d-3$ dimensional submanifolds of $\mathbb{R}^d$. Let V be the sum of the volumes of the r tubes about these submanifolds. By Weyl's tube formula, V is of the order of r^3 for small r, so, in particular, $V \leq cr^2$ for small r.

The volume of $\Gamma_i(r)$ is bounded by the volume of the tube $T(\Gamma_i,r)$ plus V. If Γ_i is a smooth $d-2$ dimensional submanifold in $\mathbb{R}^d$, we have $|T(\Gamma_i,r)| \leq cr^2$ by Weyl's tube formula. Hence we have (8) for small r.

Now we give the definitions of the so-called good and bad sets of A_z, cf. Figure 3. The bad set $\mathcal{B}$ consists of two parts. The first part, called $\mathcal{B}_I$ contains points close to Γ, i.e., it contains the lattice points which are close to edges and corners of A and B which belong to $\partial A \cap \partial B$. The remaining part $\mathcal{B}_{II}$ contains the points which are close to those boundary points at which z is nearly tangential. We always assume $z \in \mathcal{L} \setminus \{0\}$, $|z| \leq \delta$.

Definition 6 *Let C_0 be a suitable large constant, which satisfies in particular $C_0 > \max\{3, \operatorname{diam}\mathcal{U}\}$, and let*

$$\rho = C_0(|z| + \ell^{-\beta}), \quad \beta \in (\frac{1}{2}, 1). \tag{9}$$

The first bad set *consists of the following lattice points*

$$\mathcal{B}_I = \{x \in \tfrac{1}{\ell}\mathcal{L} \ : \ \operatorname{dist}(x,\Gamma) < 8\rho\}.$$

The second bad set is related to those boundary points of which the normal is almost orthogonal to z. In order to define this set we introduce a projection

$$p_z : A_z \to \partial A$$

which projects each $x \in A_z$ along the direction and orientation of z on ∂A. There might be more than one of such boundary points. If this is the case, we choose that one which is closest to x. Notice that the image of p_z need not be contained in $\partial A \cap \partial B$, see, e.g., Figure 2.

The following technical aside will turn out to be useful later. Let $\partial_+ A_z$ denote the positive part of ∂A_z, i. e. $\{x \in \partial A_z \,:\, n_{A_z}(x) \cdot z > 0\}$, where $n_{A_z}(x)$ is the outer normal to ∂A_z. Notice that there might be points in $\partial_+ A_z$ which do not belong to $\partial_+ A$, the positive part of ∂A, see, e.g., Figure 3.

By construction, $\partial_+ A_z \setminus \partial_+ A$ is a subset of $\partial(B - z)$. Thus it is locally the graph of a Lipschitz continuous function. For small $|z|$, $\partial_+ A_z \setminus \partial_+ A$ is therefore close to the boundary of $(\partial A \cup \partial B)^+$. Hence we may assume that the constant C_0 above is chosen so large that $\{x \in A_z \cap \frac{1}{\ell}\mathcal{L} \,:\, p_z(x) \in \partial_+ A \setminus \partial_+ A_z\}$ is entirely contained in $\mathcal{B}_I$. Then we have $p_z(x) \in \partial A_z$ for all $x \in (A_z \cap \frac{1}{\ell}\mathcal{L}) \setminus \mathcal{B}_I$, which is tacitly used in the proof of Lemma 10.

Moreover, we can treat all $x \in A_z$ whose projection $p_z(x)$ belongs to ∂A but not to ∂B (cf. Figure 3) as elements of $\mathcal{B}_I$. Indeed, by the outer cone property, Assumption $\mathcal{A}_1$ (iii), and the regularity assumptions on ∂A, it follows that $\operatorname{dist}(p_z(x), \Gamma) \le c|z|$ with a constant $c > 0$ depending only on the data related to the regularity assumptions and the cone property. Thus we can choose C_0 so large that $\operatorname{dist}(p_z(x), \Gamma) \le C_0|z| < \rho$ for all $x \in A_z$ with $p_z(x) \in \partial A \setminus \partial B$.

The second bad set and the good set are defined as follows, cf. Figure 3.

Definition 7 *Let ρ be as in* (9) *and let C_1 be a suitable large constant, which satisfies in particular $C_1 > \max\{12 \operatorname{diam} \mathcal{U}, 6 \operatorname{Lip}(n)\}$. Then the* second bad set *is defined as*

$$\mathcal{B}_{II} = \{x \in (A_z \cap \tfrac{1}{\ell}\mathcal{L}) \setminus \mathcal{B}_I \;:\; n(p_z(x)) \cdot \tfrac{z}{|z|} \le C_1(\ell^{\beta-1} + \rho)\}.$$

The good set *is said to be*

$$\mathcal{G} = (A_z \cap \tfrac{1}{\ell}\mathcal{L}) \setminus (\mathcal{B}_I \cup \mathcal{B}_{II}). \tag{10}$$

Since $z \in \frac{1}{\ell}\mathcal{L} \setminus \{0\}$ by assumption, there exists a constant $\tilde{c} > 0$, which depends only on the given Bravais lattice, such that $\frac{\tilde{c}}{\ell} \le |z|$. Moreover it holds $|z| + \frac{1}{\ell}\operatorname{diam} \mathcal{U} < \rho$. We always assume that δ is so small and ℓ_0 so large that $C_1(\ell^{\beta-1} + \rho) \ll 1$ and $\frac{\tilde{c}}{\ell} \le |z| < \delta$ for all $\ell \ge \ell_0$. In particular, we use $|z| < 1$; hence $|z| < |z|^\beta$, $\beta \in (\frac{1}{2}, 1)$ and $\rho < c|z|^\beta$.

The main result of this section is:

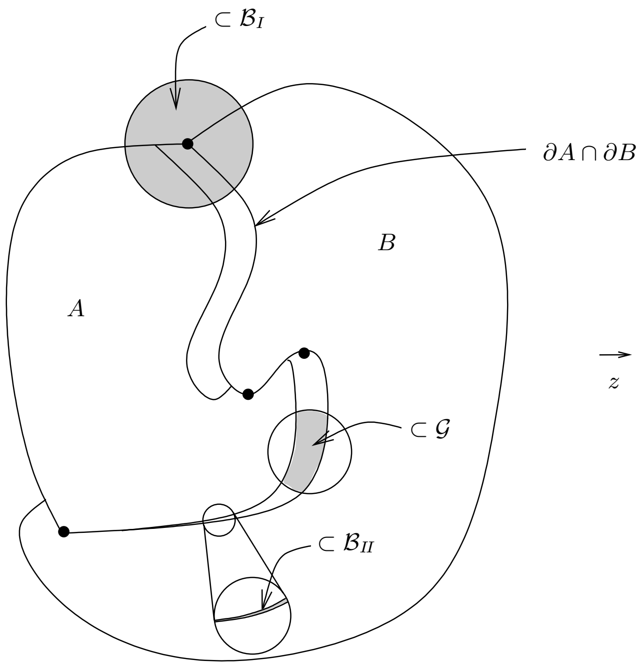

Figure 3: A slice of A and B indicating the good and bad sets as well as A_z. The bullets indicate the set Γ.

Theorem 8 *Let A and B satisfy Assumption $\mathcal{A}_1$ and let f satisfy Assumption $\mathcal{A}_2$. Fix $0 < \delta \ll 1$ and $z \in \frac{1}{\ell}\mathcal{L} \setminus \{0\}$ such that $|z| \leq \delta$. Then there exists an $\ell_0 \in \mathbb{N}$ such that for all $\ell \geq \ell_0$*

$$\Big| \frac{1}{\ell^d} \sum_{x \in A_z \cap \frac{1}{\ell}\mathcal{L}} f(x) - \int_{\partial A \cap \partial B} f(\xi)(n(\xi) \cdot z)_+ \, d\mathcal{H}^{d-1}(\xi) \Big| \leq C(\rho^2 + \ell^{\beta-1}|z|), \quad (11)$$

where $\rho = C_0(|z| + \ell^{-\beta})$ with $\beta \in (\frac{1}{2}, 1)$ as in (9). The constant C only depends on the dimension d, $\sup |f|$, the Lipschitz constant of f and on A and B.

In preparation for the proof of the theorem it is helpful to estimate at first the number of points in the bad sets $\mathcal{B}_{\mathcal{I}}$ and $\mathcal{B}_{II}$, respectively. The proof of the following lemma is along the lines of the proof of Lemma 1 in [10]; it is adapted here to dimensions $d \geq 2$ and is based on the neighborhood estimate (8) as well as on the non-degeneracy condition (S).

Here and in the following, c denotes a generic constant that depends at most on the dimension d, on properties of f and on A and B.

Lemma 9 *If Assumption $\mathcal{A}_1$ holds, the number of points in $\mathcal{B}_I$ is controlled by*

$$\#\mathcal{B}_I \le c\ell^d \rho^2.$$

Proof: (i) If $d = 2$, Γ is a collection of single points x_i, of which the number is uniformly bounded by the non-degeneracy condition (S). Let $B(x_i, \rho)$ be the disc with center $x_i \in \Gamma$ and radius ρ. Then $\mathcal{B}_I \subset \bigcup_i B(x_i, 8\rho)$. Thus $\bigcup_{x\in\mathcal{B}_I} \frac{1}{\ell}\mathcal{U}(x) \subset \bigcup_i B(x_i, 9\rho)$. The number of points in $\mathcal{B}_I$ can be estimated by the volume of $\bigcup_{x\in\mathcal{B}_I} \frac{1}{\ell}\mathcal{U}(x)$ divided by the volume of a scaled unit cell $\frac{1}{\ell}\mathcal{U}$, i.e., divided by $\frac{1}{\ell^2}$. Thus $\#\mathcal{B}_I \le c\rho^2\ell^2$.

(ii) Now let $d > 2$. By the non-degeneracy condition (S), Γ is a finite union of connected $C^{1,1}$ submanifolds of $\mathbb{R}^d$ of which the number and the total $\mathcal{H}^{d-2}$ measure is uniformly bounded. Thus it suffices to consider a single of these submanifolds of Γ, which are, as before, denoted by Γ_i, $i = 1, \ldots, k$.

We cover Γ_i by d dimensional balls $B(x_j, \rho)$, $x_j \in \mathbb{R}^d$, such that $\Gamma_i \subset \bigcup_j B(x_j, \rho)$. The smallest number of such balls of radius ρ needed to cover Γ_i is

$$N(\Gamma_i, \rho) = \min\left\{ m \,:\, \Gamma_i \subset \bigcup_{j=1}^{m} B(x_j, \rho) \text{ for some } x_j \in \mathbb{R}^d \right\}.$$

Then, cf. [6, Eqns. (5.4), (5.5)],

$$N(\Gamma_i, \rho) \le \frac{|\Gamma_i(\frac{\rho}{2})|}{\omega_d \left(\frac{\rho}{2}\right)^d},$$

where ω_d is the volume of the d dimensional unit ball and $\Gamma_i(\frac{\rho}{2})$ denotes the $\frac{\rho}{2}$-neighbourhood of Γ_i, cf. (7). By assumption, the neighbourhood estimate (8) holds, i.e., $|\Gamma_i(\frac{\rho}{2})| \le c\rho^2$. Hence

$$N(\Gamma_i, \rho) \le \frac{c}{\rho^{d-2}}, \tag{12}$$

where c is a constant which only depends on d, A and B.

The number of points in $\mathcal{B}_I$ can be estimated by the volume of $\bigcup_{x\in\mathcal{B}_I}\frac{1}{\ell}\mathcal{U}(x)$ divided by the volume of the scaled unit cell, $\frac{1}{\ell^d}$. We have

$$\bigcup_{x\in\mathcal{B}_I}\frac{1}{\ell}\mathcal{U}(x)\subset\bigcup_{i=1}^{k}\bigcup_{j=1}^{N(\Gamma_i,\rho)}B(x_j,10\rho).$$

By (12) and the non-degeneracy condition (S), we obtain $\#\mathcal{B}_I\leq ck\frac{1}{\rho^{d-2}}\rho^d\ell^d$ and thus the statement. □

Lemma 10 *Let Assumption $\mathcal{A}_1$ hold. Then*

$$\#\mathcal{B}_{II}\leq c\ell^d|z|(\ell^{\beta-1}+\rho).$$

The proof of this lemma essentially follows the proof of Lemma 2 in [10], in which the analogous statement is given for $d=3$. Notice that z is fixed in the beginning. The vector z thus distinguishes one direction, say the e_1-direction in some coordinate system which is used to parameterize the boundary. The other directions, $e_2,\ldots,e_d$, however, do not play an important role. This allows to generalize the proof in [10] easily to dimensions $d\geq 2$.

Proof: By the technical aside before Definition 7, we can assume here that the projection $p_z(x)$ belongs to $\partial A\cap\partial B$ for all $x\in\mathcal{B}_{II}$. Let $x\in\mathcal{B}_{II}$ and consider the $\mathcal{H}^{d-1}$-measure of the set

$$B_x:=B(p_z(x),\rho)\cap(\partial A\cap\partial B),$$

where $\rho=C_0(|z|+\ell^{-\beta})$ as above and $B(p_z(x),\rho)$ is the ball of radius ρ about $p_z(x)$. For sufficiently large ℓ_0 and sufficiently small δ, the set B_x is connected for all $\ell\geq\ell_0$. Since $x\in\mathcal{B}_{II}$ and $\partial A\cap\partial B$ is piecewise $C^{1,1}$ by assumption, the set B_x and even the set $B(p_z(x),5\rho)\cap(\partial A\cap\partial B)$ are contained in a single chart U_i and in $(\partial A\cap\partial B)^+$. (Recall Definition 2 for the definition of U_i.)

As U_i is $C^{1,1}$ by assumption, the area of B_x can be estimated from below by the $\mathcal{H}^{d-1}$-measure of a $d-1$-dimensional ball of radius ρ. Thus $\mathcal{H}^{d-1}(B_x)\geq c\rho^{d-1}$ for some constant $c>0$. Hence

$$\#\mathcal{B}_{II}\leq c\frac{\sum_{y\in\mathcal{B}_{II}}\mathcal{H}^{d-1}(B_y)}{\rho^{d-1}}.$$

To prove the lemma, it remains to show that $\sum_{y\in\mathcal{B}_{II}} \mathcal{H}^{d-1}(B_y) \leq c\ell^d|z|(\ell^{\beta-1}+\rho)\rho^{d-1}$. Let χ_y denote the characteristic function of B_y. Then

$$\begin{aligned}\sum_{y\in\mathcal{B}_{II}} \mathcal{H}^{d-1}(B_y) &= \sum_{y\in\mathcal{B}_{II}} \int_{\partial A\cap\partial B} \chi_y(x)\, d\mathcal{H}^{d-1}(x) \\ &= \int_{\partial A\cap\partial B} \sum_{y\in\mathcal{B}_{II}} \chi_y(x)\, d\mathcal{H}^{d-1}(x) \\ &\leq \mathcal{H}^{d-1}(\partial A\cap\partial B) \sup_{x\in\mathcal{B}_{II}} \sum_{y\in\mathcal{B}_{II}} \chi_y(p_z(x)).\end{aligned}$$

Next we choose an orthonormal coordinate system $e_1,\dots,e_d$ such that $z = |z|e_1$ and $n(p_z(x))\cdot e_i = 0$ for all $i = 2,\dots,d-1$. Then $\partial A\cap\partial B$ is locally represented as a $C^{1,1}$ graph over the $e_1,\dots,e_{d-1}$-hyperplane.

The remainder of the proof is based on a (lengthy) exploitation of the condition on $n(p_z(z))\cdot\frac{z}{|z|}$ in the definition of $\mathcal{B}_{II}$. This calculation can be easily adapted from [10, pp. 239–240] by replacing the 3-component of the vectors with the d-component and is therefore not repeated here in detail for brevity. A further small change in the proof concerns the volume of the scaled unit cell which is now $\frac{1}{\ell^d}$. Moreover note that the $d-1$ dimensional ball about the point $p_z(x)'$, which is the projection of $p_z(x)$ on the hyperplane $e_1,\dots,e_{d-1}$, has volume $c\rho^{d-1}$. With these replacements in the proof in [10], Lemma 10 follows. □

Next we study properties of the good set. Let $x\in\mathcal{G}$ and notice that the translated scaled unit cell $\frac{1}{\ell}\mathcal{U}(x) = x + \frac{1}{\ell}\mathcal{U}$ does not need to be contained in A_z, entirely, cf. Figure 4. We therefore construct a *modified unit cell* $\mathcal{V}(x)\subset A_z$ with similar properties as $\frac{1}{\ell}\mathcal{U}(x)$. In particular we show that $|\mathcal{V}(x)| = |\frac{1}{\ell}\mathcal{U}(x)| = \frac{1}{\ell^d}$ and $\mathcal{V}(x)\cap\mathcal{V}(\tilde{x}) = \emptyset$ if $x,\tilde{x}\in\mathcal{G}$, $x\neq\tilde{x}$.

If the unit cell $\frac{1}{\ell}\mathcal{U}(x)$ is entirely contained in A_z, we simply set $\mathcal{V}(x) = \frac{1}{\ell}\mathcal{U}(x)$. In general we define (see Figure 4)

$$\mathcal{V}(x) := \bigcup_{k=-K}^{K} \frac{1}{\ell}\mathcal{U}(x+kz)\cap A_z, \tag{13}$$

where $K := \lfloor\frac{\rho}{|z|}\rfloor$. This notion as well as the following Lemma 11 and its proof are based on [7, 9, 10] for $d = 3$. Here we generalize the results to arbitrary dimensions $d\geq 2$. Note that we make use of the fact that z is a lattice vector in the proof below.

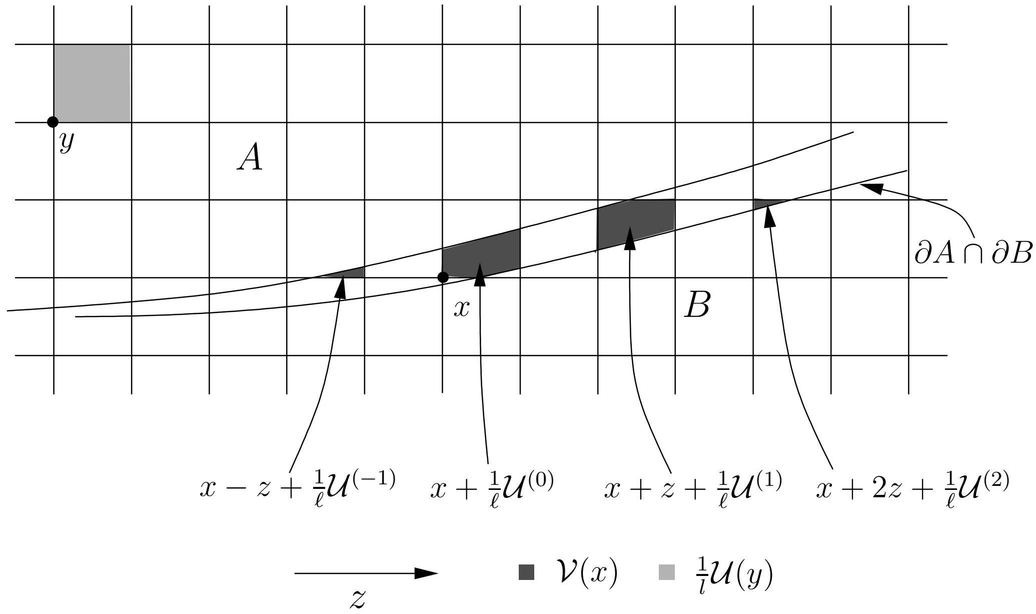

Figure 4: An example of a modified unit cell $\mathcal{V}(x)$. For the definition of $\mathcal{U}^{(k)}$, $k = -1, 0, 1, 2$ see (16).

Lemma 11 *Let $\mathcal{V}(x)$, $x \in \mathcal{G}$, be the modified unit cell defined in (13) and let Assumption $\mathcal{A}_1$ hold. Then*

$$|\mathcal{V}(x)| = \frac{1}{\ell^d} \tag{14}$$

and

$$\mathcal{V}(x) \cap \mathcal{V}(\tilde{x}) = \emptyset \qquad \text{if} \quad x, \tilde{x} \in \mathcal{G} \quad \text{and} \quad x \neq \tilde{x}. \tag{15}$$

Proof: To show (14), we introduce the truncated unit cells (cf. Figure 4)

$$\mathcal{U}^{(k)} := \{y \in \mathcal{U} \ : \ x + kz + \tfrac{1}{\ell} y \in A_z\}. \tag{16}$$

Notice that the x-dependence is suppressed in the notation. Since z is a lattice vector, $\mathcal{U}^{(k)} \cap \mathcal{U}^{(\tilde{k})} = \emptyset$ if $k \neq \tilde{k}$. Thus, if we know that

$$\bigcup_{k=-K}^{K} \mathcal{U}^{(k)} = \mathcal{U}, \tag{17}$$

we have

$$\mathcal{V}(x) = \bigcup_{k=-K}^{K} \left(x + kz + \tfrac{1}{\ell}\mathcal{U}^{(k)}\right)$$

and hence (14) follows. To prove (17), we first consider the case $n(x) \cdot \frac{z}{|z|} \leq 1/2$ and choose the same coordinate system as in the proof of Lemma 10. That is, $\partial A \cap \partial B$ is locally represented as a $C^{1,1}$ graph over the $e_1, \ldots, e_{d-1}$ plane. Set $x' = (x_1, \ldots, x_{d-1})$ and let $u : \mathbb{R}^{d-1} \to \mathbb{R}$ be a parameterization of the boundary.

By making use of the assumption $x \in \mathcal{G}$, i.e., in particular, $x \notin \mathcal{B}_{II}$, we can show in a close analogy to the proof of equation (19) in [10] (with the 3-component replaced with the d-component) that the map

$$\lambda \mapsto u(x' + \lambda z' + \frac{1}{\ell} y') \tag{18}$$

is strictly increasing. Moreover one can show analogously that there exists a unique $\tilde{\lambda}(y) \in (-K, K)$ such that

$$u(x' + \lambda z' + \tfrac{1}{\ell} y') - (x + \tfrac{1}{\ell} y)_d \begin{cases} > 0 & \text{if} \quad \lambda > \tilde{\lambda}(y) \\ = 0 & \text{if} \quad \lambda = \tilde{\lambda}(y) \\ < 0 & \text{if} \quad \lambda < \tilde{\lambda}(y) \end{cases} .$$

Thus

$$x + kz + \tfrac{1}{\ell} y \in A_z \quad \Longleftrightarrow \quad k = \tilde{k}(y) := \lfloor \tilde{\lambda}(y) \rfloor, \tag{19}$$

which yields (17) and thus (14).

The statement in (15) is proved by contradiction: If $\mathcal{V}(x) \cap \mathcal{V}(\tilde{x}) \neq \emptyset$ for $x \neq \tilde{x}$, then there would exist $k \neq \tilde{k}(y) \in \{-K, \ldots, K\}$ such that $x, \tilde{x} \in \mathcal{G}$ and $x + kz = \tilde{x} + \tilde{k}(y)z$, i. e. $\tilde{x} = x + (k - \tilde{k}(y))z$. But the map in (18) is strictly increasing. Thus $k \neq \tilde{k}(y)$ cannot hold in view of the definition of A_z.

If $n(x) \cdot \frac{z}{|z|} > \frac{1}{4}$, similar arguments apply. In this case we choose the coordinate system such that $\frac{z}{|z|} = e_d$ and such that $\partial A \cap \partial B$ is locally a graph over the $e_1, \ldots, e_{d-1}$ plane. $\square$

As a final preparation for the proof of Theorem 8, we estimate the number of points in the good set.

Lemma 12 *Let Assumption $\mathcal{A}_1$ hold. Then the number of points in $\mathcal{G}$ is bounded by*

$$\#\mathcal{G} \le c\ell^d |z|.$$

Proof: The proof is in the lines of [10, p. 244] and is based on the notion of modified unit cells and Lemma 11. Define

$$\mathcal{V} := \bigcup_{x \in \mathcal{G}} \mathcal{V}(x). \tag{20}$$

By construction, $\#\mathcal{G} = \ell^d |\mathcal{V}|$. Thus it remains to estimate $|\mathcal{V}|$, which we do with the help of the coarea formula, see, e.g., [2, Theorem 3.2.12].

If $x \in \mathcal{G}$, then $p_z(x) =: \xi$ is the projection of x on $\partial A \cap \partial B$ along the direction and orientation of z. Let $\mathcal{T}$ denote the image of $\mathcal{V}$ under p_z. Since $\partial A \cap \partial B$ can locally be represented as a $C^{1,1}$ graph, the lines $t \mapsto x + tz$ intersect $\partial A \cap \partial B$ locally at most once. Let $F : \mathcal{V} \to \mathbb{R}$ be the map $x \mapsto t$. Then $\nabla F(x)$ is parallel to $n(p_z(x))$ and it holds $z \cdot \nabla F(x) = -1$. Thus $\nabla F(x) = -\frac{1}{n(p_z(x)) \cdot z} n(p_z(x))$ and the Jacobian of F equals $|\nabla F|$, i.e., $|n(\xi) \cdot z|^{-1}$. Hence the coarea formula yields

$$\begin{aligned} |\mathcal{V}| &= \int_0^1 \int_{F(x)=t} \frac{1}{|\nabla F(x)|} \, d\mathcal{H}^{d-1}(x)\, dt = \int_0^1 \Big(\int_{\mathcal{T}} |n(\xi) \cdot z| \, d\mathcal{H}^{d-1}(\xi) \Big)\, dt \\ &= \int_{\mathcal{T}} |n(\xi) \cdot z| \, d\mathcal{H}^{d-1}(\xi) \le |z| \mathcal{H}^{d-1}(\partial A \cap \partial B). \end{aligned}$$

Thus $\#\mathcal{G} = c\ell^d |z|$ as asserted. □

We are now ready to prove Theorem 8.

Proof of Theorem 8: By Lemma 9 and Lemma 10, we have

$$\#\mathcal{B}_I + \#\mathcal{B}_{II} \le c\ell^d(\rho^2 + |z|(\ell^{\beta-1} + \rho)) \le c\ell^d(\rho^2 + |z|\ell^{\beta-1}) \tag{21}$$

as $|z| < \rho$ by assumption. Thus

$$\begin{aligned} \Big| \sum_{x \in \mathcal{B}_I \cap A_z} f(x) \frac{1}{\ell^d} + \sum_{x \in \mathcal{B}_{II}} f(x) \frac{1}{\ell^d} \Big| &\le c\ell^d \sup |f(x)| \, (\rho^2 + |z|\ell^{\beta-1}) \frac{1}{\ell^d} \\ &\le c(\rho^2 + \ell^{\beta-1}|z|). \end{aligned}$$

Therefore, in (11), it remains to consider the sum over the points $x \in \mathcal{G}$. To estimate this sum, we make use of the modified unit cell $\mathcal{V}(x)$, cf. (13). Let $x \in \mathcal{G}$, then $\mathcal{V}(x)$ is contained in $B(x, 2\rho)$ as $K|z| + \frac{\operatorname{diam}\mathcal{U}}{\ell} \leq \frac{\rho}{|z|}|z| + \frac{\operatorname{diam}\mathcal{U}}{\ell} \leq 2\rho$. By (14), (15), (20), the Lipschitz continuity of f and Lemma 12, we obtain

$$\begin{aligned}\Big|\sum_{x\in\mathcal{G}} f(x)\frac{1}{\ell^d} - \int_{\mathcal{V}} f(y)\,dy\Big| &= \Big|\sum_{x\in\mathcal{G}}\Big(\int_{\mathcal{V}(x)} f(x)\,dy - \int_{\mathcal{V}(x)} f(y)\,dy\Big)\Big| \\ &\leq c\sum_{x\in\mathcal{G}} |\mathcal{V}(x)|\operatorname{Lip}(f)\rho \leq c\#\mathcal{G}\frac{1}{\ell^d}\rho \\ &\leq c|z|\rho \leq c|z|^{1+\beta} \qquad (22)\end{aligned}$$

since $\rho \leq c|z|^\beta$. It thus remains to show that the integral approximation $\int_{\mathcal{V}} f(x)\,dx$ of the lattice sum can itself be estimated by a surface integral of the asserted form.

As before, we denote the image of the projection of $\mathcal{V} = \cup_{x\in\mathcal{G}}\mathcal{V}(x)$ along z on $\partial A \cap \partial B$ by $\mathcal{T}$. We obtain with the help of the coarea formula (cf. the proof of Lemma 12)

$$\begin{aligned}\int_{\mathcal{V}} f(x)\,dx &= \int_0^1\int_{\mathcal{T}} f(\xi - tz)|n(\xi)\cdot z|\,d\mathcal{H}^{d-1}(\xi)\,dt \\ &= \int_0^1\int_{\mathcal{T}} f(x)|n(\xi)\cdot z|\,d\mathcal{H}^{d-1}(\xi)\,dt \\ &\quad + \int_0^1\int_{\mathcal{T}} \big(f(\xi - tz) - f(x)\big)|n(\xi)\cdot z|\,d\mathcal{H}^{d-1}(\xi)\,dt.\end{aligned}$$

By the Lipschitz continuity of f, the second term on the right-hand side can be bounded by a constant times $|z|^2$ times $\mathcal{H}^{d-1}(\partial A \cap \partial B)$. Thus it remains to estimate

$$\begin{aligned}&\Big|\int_{\mathcal{T}} f(\xi)|n(\xi)\cdot z|\,d\mathcal{H}^{d-1}(\xi) - \int_{\partial A\cap\partial B} f(\xi)(n(\xi)\cdot z)_+\,d\mathcal{H}^{d-1}(\xi)\Big| \\ &\leq \Big|\int_{(\partial A\cap\partial B)\setminus\mathcal{T}} f(\xi)(n(\xi)\cdot z)_+\,d\mathcal{H}^{d-1}(\xi)\Big| \\ &\leq \int_{(\partial A\cap\partial B)\setminus\mathcal{T}} |f(\xi)|(n(\xi)\cdot z)_+\,d\mathcal{H}^{d-1}(\xi).\end{aligned}$$

Recall that we deal with the good set $\mathcal{G}$ here. For $\xi \in (\partial A \cap \partial B) \setminus \mathcal{T}$ we therefore either have $n(\xi)\cdot z \leq C_1(\ell^{\beta-1} + \rho)|z|$ or $\operatorname{dist}(x, \Gamma) < 8\rho$ for all

$x \in p_z^{-1}(\xi) \cap A_z$. Since $|x - p_z(x)| \leq \rho$, the latter case can be estimated by $\mathrm{dist}(\xi, \Gamma) < 9\rho$ for all $\xi \in (\partial A \cap \partial B) \setminus \mathcal{T}$.

We write $\Gamma = \bigcup_{i=1}^k \Gamma_i$, as in the comment following (6). The neighbourhood estimate (8) implies $|\Gamma_i(9\rho)| \leq c\rho^2$. Thus $\mathcal{H}^{d-1}(\Gamma(9\rho) \cap (\partial A \cap \partial B)) \leq k\mathcal{H}^{d-1}(\Gamma_i(9\rho) \cap (\partial A \cap \partial B)) \leq k|\Gamma_i(9\rho)| \leq c\rho^2$. Hence we have

$$\begin{aligned}
&\int_{(\partial A \cap \partial B)\setminus \mathcal{T}} |f(\xi)|(n(\xi) \cdot z)_+ \, d\mathcal{H}^{d-1}(\xi) \\
&\leq \sup |f| \Big(\int_{\Gamma(9\rho)\cap(\partial A \cap \partial B)} |z| \, d\mathcal{H}^{d-1}(\xi) + \int_{\partial A \cap \partial B} C_1(\ell^{\beta-1} + \rho)|z| \, d\mathcal{H}^{d-1}(\xi) \Big) \\
&\leq c\rho^2 |z| + c(\ell^{\beta-1} + \rho)|z|. \qquad (23)
\end{aligned}$$

In summary, (21), (22) and (23) yield

$$\begin{aligned}
&\Big| \frac{1}{\ell^d} \sum_{x \in A_z \cap \frac{1}{\ell}\mathcal{L}} f(x) - \int_{\partial A \cap \partial B} f(\xi)(n(\xi) \cdot z)_+ \, d\mathcal{H}^{d-1}(\xi) \Big| \\
&\qquad \leq c(\rho^2 + \ell^{\beta-1}|z| + \rho|z| + \rho^2|z|) \leq c(\rho^2 + \ell^{\beta-1}|z|),
\end{aligned}$$

since $|z| < \rho < 1$. □

It remains to prove Proposition 1. As mentioned before, this proof is an easy consequence of Theorem 8.

Proof of Proposition 1: We recall from above: There exists a constant $\tilde{c} > 0$ such that $\frac{\tilde{c}}{\ell} \leq |z|$. Moreover, $|z| < 1$ and hence $\rho < c|z|^\beta$ for some constant $c > 0$ by definition. Thus the right-hand side of (11) is bounded as follows

$$\rho^2 + \ell^{\beta-1}|z| \leq c(|z|^{2\beta} + |z|^{2-\beta}) \leq c|z|^{4/3},$$

where the last step follows by setting $\beta = \frac{2}{3}$. This together with Theorem 8 gives Proposition 1. □

In this section we proved an approximation of certain surface integrals by lattice sums which are taken over lattice points close to the surface (Proposition 1 and Theorem 8). As mentioned before, these results generalize previous results [10] to arbitrary dimension $d \geq 2$ and to more general geometrical settings. Now, the above approximations can be applied also to non-nested sets, which is of interest in [8] and also for instance for domains as they typically occur in micromagnetism.

Despite this progress, there remains an open problem which is of interest both for applications and for mathematical analysis. This concerns the non-degeneracy condition (S), which is a mild assumption on the shape of the domains. However, as already pointed out after Definition 3, the non-degeneracy condition (S) excludes 'rough' surfaces, i.e., surfaces which have infinitely many wiggles. A generalization of Theorem 8 and Proposition 1 to domains which have infinitely many indentations and protrusions remains an open problem.

3 Convergence of a singular lattice sum

In this section we prove the convergence of a singular lattice sum as the lattice spacing tends to zero. The sum consists of the expressions $\partial_i \partial_j P_k^{(\delta)}(z)$, where $P_k^{(\delta)}(z)$ is essentially a derivative of the fundamental solution of Laplace's equation, see (24) for a precise definition. Thus $\partial_i \partial_j P_k^{(\delta)}(z)$ is of order $|z|^{-d-1}$. In the terms of the sum studied below, $\partial_i \partial_j P_k^{(\delta)}(z)$ is multiplied by z_p, the pth component of the lattice vector z. Note that $\partial_i \partial_j P_k^{(\delta)}(z) z_p$ is of singular order. Due to the singularity, the sum in (25) does not converge absolutely; it only converges due to cancellations, which makes the convergence proof subtle. Theorem and proof below are inspired by an analogous one for $d = 3$ in [10, Lemma 5]. See [10] also for an application and the derivation of this sum in the context of magnetostatics. Here we generalize the result to $d = 2$ and $d \geq 4$. For an application of Theorem 13 to magnetic forces in $d = 2$ see [8].

Fix a point $y \in \mathbb{R}^d$. Then the normalized fundamental solution of Laplace's equation $-\Delta u = 0$ is given by (see, e.g., [3, p. 17])

$$N(x-y) = \begin{cases} -\frac{1}{2\pi} \ln |x-y|, & \text{if } d = 2 \\ \frac{1}{d(d-2)\omega_d} |x-y|^{2-d}, & \text{if } d \geq 3 \end{cases} \quad \text{for all } x \in \mathbb{R}^d, x \neq y,$$

where ω_d denotes the volume of the unit ball in $\mathbb{R}^d$ (with $\omega_d = \frac{2\pi^{d/2}}{d\Gamma(d/2)}$, where $\Gamma(\cdot)$ is the Gamma-function—unlike in Definition 4).

The sum we study here is a sum over a scaled lattice $\frac{1}{\ell}\mathcal{L}$, $\ell \in \mathbb{N}$, restricted to a ball, B_δ, of radius δ about 0. The sum becomes a series by letting the lattice spacing tend to zero, i.e., $\ell \to \infty$. Subsequently, we take the limit $\delta \to 0$.

It turns out to be useful not to work with a sharp cut-off but a smooth cut-off $\varphi^{(\delta)}$, cf. the derivation of (29) below. Let $\varphi^{(1)} : \mathbb{R}^d \to [0,1]$ be a C_0^∞ function such that

$$\varphi^{(1)}(z) = \begin{cases} 1, & \text{if } |z| < \frac{1}{2} \\ 0, & \text{if } |z| > 1 \end{cases}.$$

Moreover, let $\delta > 0$ and set $\varphi^{(\delta)}(z) = \varphi^{(1)}(\frac{z}{\delta})$. Notice that $|\partial^\alpha \varphi^{(\delta)}(z)| \le \frac{c}{\delta^{|\alpha|}}$ for some constant $c > 0$ and any multi-index α. We set

$$P_k^{(\delta)}(x-y) = \begin{cases} (\varphi^{(\delta)} \partial_k N)(x-y), & \text{if } d = 2 \\ \partial_k(\varphi^{(\delta)} N)(x-y), & \text{if } d \ge 3 \end{cases}. \tag{24}$$

Note that for all dimensions $d \ge 2$, the cut-off function $\varphi^{(\delta)}$ is multiplied by a 1-homogeneous function. This fact is used in a scaling argument in the proof below. Moreover, it is crucial that the cut-off function $\varphi^{(\delta)}$ enters in the definition of $P_k^{(\delta)}$. If we would simply multiply the hypersingular kernel $\partial_i \partial_j \partial_k N(x-y)$ with the cut-off function, we did not get (29) below, which is a key step in the proof of Theorem 13.

The lattice $\mathcal{L}$ is defined as in (2). We set $\mathcal{L}^* = \mathcal{L} \setminus \{0\}$. The main result of this section is

Theorem 13 *Let $a \in \mathbb{R}^d$. Then the limit*

$$S_{ijkp} = - \lim_{\delta \to 0} \lim_{\ell \to \infty} \sum_{z \in B_\delta \cap \frac{1}{\ell}\mathcal{L}^*} \big(\partial_i \partial_j P_k^{(\delta)}\big)(z)\; z_p \frac{1}{\ell^d} \tag{25}$$

exists in $\mathbb{R}$ and it holds

$$\frac{1}{2} \sum_{p=1}^{d} S_{ijkp} a_p = - \lim_{\delta \to 0} \lim_{\ell \to \infty} \sum_{z \in B_\delta \cap \frac{1}{\ell}\mathcal{L}^*} \big(\partial_i \partial_j P_k^{(\delta)}\big)(z)\; (a \cdot z)_+ \frac{1}{\ell^d}. \tag{26}$$

The link between this Theorem and the study in the previous section can be seen in brief as follows. Recall that the integrand in the surface integral in (11) is $f(\xi)(n(\xi) \cdot z)_+$. In the application of Theorem 13 to magnetic forces in $d = 2, 3$, the term $(a \cdot z)_+$ in (26) becomes $(n(\xi) \cdot z)_+$. In turn, $(n(\xi) \cdot z)_+$ is related to the height/thickness of the set A_z in equation (3). For details we again refer to [8, 10] (the notations in [10] and this article are related by $(\partial_i \partial_j P_k^{(\delta)})(z) = \partial_k (K - K^{(\delta)})_{ij}(z)$ if $d = 3$).

Proof: Notice that $P_k^{(\delta)}(z)$ and therefore $(\partial_i \partial_j P_k^{(\delta)})(z)$ are anti-symmetric in z. Thus $\big(\partial_i \partial_j P_k^{(\delta)}\big)(z)\ a \cdot z$ is symmetric in z. Since $\mathcal{L}$ is a Bravais lattice, $z \in \mathcal{L}$ implies $-z \in \mathcal{L}$. Hence

$$\begin{aligned}\sum_{z \in B_\delta \cap \frac{1}{\ell}\mathcal{L}^*} \big(\partial_i \partial_j P_k^{(\delta)}\big)(z)\ (a \cdot z)_+ \frac{1}{\ell^d} &= \sum_{\substack{z \in B_\delta \cap \frac{1}{\ell}\mathcal{L}^* \\ a \cdot z < 0}} \big(\partial_i \partial_j P_k^{(\delta)}\big)(z)\ a \cdot z \frac{1}{\ell^d} \\ &= \frac{1}{2} \sum_{z \in B_\delta \cap \frac{1}{\ell}\mathcal{L}^*} \big(\partial_i \partial_j P_k^{(\delta)}\big)(z)\ a \cdot z \frac{1}{\ell^d}.\end{aligned}$$

Before we change variables from z to $z' = \ell z$ in the previous formula, we show that

$$\big(\partial_i \partial_j P_k^{(\delta)}\big)(\frac{z'}{\ell}) = \partial_i \partial_j P_k^{(\ell\delta)}(z') \ell^{d+1}. \tag{27}$$

Indeed, if $d = 2$, we obtain

$$\big(\partial_i \partial_j P_k^{(\delta)}\big)(\frac{z'}{\ell}) \ = \ \partial_i \partial_j \Big(\varphi^{(\delta)}(\frac{z'}{\ell}) \partial_k N(\frac{z'}{\ell})\Big) \ell^3$$

by the chain rule. Since $\varphi^{(\delta)}(\frac{z'}{\ell}) = \varphi^{(\ell\delta)}(z')$ by definition and $\partial_k N(\frac{z'}{\ell}) = -\frac{1}{2\pi} \partial_k \ln \big|\frac{z'}{\ell}\big| = \partial_k N(z')$, we obtain (27). In the case $d \geq 3$ we have $N(\frac{z'}{\ell}) = \frac{1}{d(d-2)\omega_d} \big|\frac{z'}{\ell}\big|^{2-d} = \ell^{d-2} N(z')$. Thus

$$\big(\partial_i \partial_j P_k^{(\delta)}\big)(\frac{z'}{\ell}) = \partial_i \partial_j \partial_k \big(\varphi^{(\delta)}(\frac{z'}{\ell}) N(\frac{z'}{\ell})\big) \ell^3 = \ell^{d+1} \partial_i \partial_j \partial_k \big(\varphi^{(\ell\delta)}(z') N(z')\big),$$

which yields (27). Hence

$$\begin{aligned}\frac{1}{2} \sum_{z \in B_\delta \cap \frac{1}{\ell}\mathcal{L}^*} \big(\partial_i \partial_j P_k^{(\delta)}\big)(z)\ a \cdot z \frac{1}{\ell^d} &= \frac{1}{2} \sum_{z' \in B_{\ell\delta} \cap \mathcal{L}^*} \big(\partial_i \partial_j P_k^{(\delta)}\big)(\frac{z'}{\ell})\ a \cdot \frac{z'}{\ell} \frac{1}{\ell^d} \\ &= \frac{1}{2} \sum_{z' \in B_{\ell\delta} \cap \mathcal{L}^*} \big(\partial_i \partial_j P_k^{(\ell\delta)}\big)(z')\ a \cdot z'.\end{aligned}$$

To prove the theorem, we set $S_{ijkp}^{(\ell\delta)} = \sum_{z\in B_{\ell\delta}\cap\mathcal{L}^*} \big(\partial_i\partial_j P_k^{(\ell\delta)}\big)(z)\, z_p$ with z instead of z' by some abuse of notation. First we prove the convergence of $S_{ijkp}^{(\ell\delta)}$ for fixed $\delta > 0$ as $\ell \to \infty$. In order to do so, we can reduce the proof to a convergence proof of $S_{ijkp}^{(n)}$, $n \in \mathbb{N}$, as $n \to \infty$. The idea is to show that $S_{ijkp}^{(n)}$ is a Cauchy sequence in $\mathbb{R}$. Let $m, n \in \mathbb{N}$ with $m \le n < \infty$ and notice that the support of $\varphi^{(n)} - \varphi^{(m)}$ is contained in $B_n \setminus B_{m/2}$. Thus

$$|S_{ijkp}^{(n)} - S_{ijkp}^{(m)}| = \Big| \sum_{z\in(B_n\setminus B_{m/2})\cap\mathcal{L}^*} \Big(\partial_i\partial_j \big(P_k^{(n)} - P_k^{(m)}\big)(z)\Big) z_p \Big|. \tag{28}$$

The remainder of the proof is driven by the following observation about the integral corresponding to the sum in (28). Let ν denote the outer normal to $\partial(B_n \setminus B_{m/2})$ and integrate by parts twice.

$$\begin{aligned}
&\int_{B_n\setminus B_{m/2}} \Big(\partial_i\partial_j \big(P_k^{(n)} - P_j^{(m)}\big)(z)\Big) z_p \, d^d z \\
&= \; -\int_{\partial(B_n\setminus B_{m/2})} \big(P_k^{(n)} - P_k^{(m)}\big)(z)\delta_{ip}\nu_j(z)\, d\mathcal{H}^{d-1}(z) \\
&\qquad + \int_{\partial(B_n\setminus B_{m/2})} \big(\partial_j \big(P_k^{(n)} - P_k^{(m)}\big)(z)\big) z_p \nu_i(z)\, d\mathcal{H}^{d-1}(z) \\
&= \; 0,
\end{aligned} \tag{29}$$

since $P_k^{(n)} = P_k^{(m)}$ on $\partial(B_n \setminus B_{m/2})$.

The observation in (29) suggests to replace the sum in (28) by an integral. We do so by using piecewise constant step-functions. Let y_z denote the base point of the unit cell to which z belongs. We define the sets

$$\begin{aligned}
\mathcal{U}^{\text{out}} &:= \{z \in (B_n \setminus B_{m/2}) \; : \; y_z \in \mathbb{R}^d \setminus (B_n \setminus B_{m/2})\}, \\
\mathcal{U}^{\text{in}} &:= \{z \notin (B_n \setminus B_{m/2}) \; : \; y_z \in (B_n \setminus B_{m/2})\}.
\end{aligned} \tag{30}$$

(See [10, p. 248] for a figure that indicates these sets.) Moreover, let step(f) denote the step-function which has the same value as f on lattice points and which is constantly extended on unit cells. Hence we obtain the equality

$$\begin{aligned}
|S_{ijkp}^{(n)} - S_{ijkp}^{(m)}| \;=\; & \Big| \int_{B_n\setminus B_{m/2}} \text{step}\Big(\Big(\partial_i\partial_j \big(P_k^{(n)} - P_k^{(m)}\big)(z)\Big) z_p\Big)\, d^d z \quad (31) \\
& + \int_{\mathcal{U}^{\text{in}}} \text{step}\Big(\Big(\partial_i\partial_j \big(P_k^{(n)} - P_k^{(m)}\big)(z)\Big) z_p\Big)\, d^d z \\
& - \int_{\mathcal{U}^{\text{out}}} \text{step}\Big(\Big(\partial_i\partial_j \big(P_k^{(n)} - P_k^{(m)}\big)(z)\Big) z_p\Big)\, d^d z \Big|.
\end{aligned}$$

Since $P_k^{(n)} - P_k^{(m)}$ and its derivatives are zero in the complement of $B_n \setminus B_{m/2}$, the third integral is identically zero.

To estimate the second integral, observe that the lattice points of interest are close to the boundary of $B_n \setminus B_{m/2}$. Let γ denote the diameter of the unit cell. Then $\mathcal{U}^{\text{in}} \subset (B_{n+\gamma} \setminus B_n) \cup (B_{m/2} \setminus B_{m/2-\gamma})$ by construction. Thus $|\mathcal{U}^{\text{in}}| \leq c\big((n+\gamma)^d - n^d + (\frac{m}{2})^d - (\frac{m}{2} - \gamma)^d\big) \leq c\gamma\big(n^{d-1} + (m/2)^{d-1}\big) \leq cn^{d-1}$.

Let y_z denote the lattice point corresponding to $z \in \mathcal{U}^{\text{in}}$, then either $m/2 \leq |y_z| \leq m/2 + \gamma$ or $n - \gamma \leq |y_z| \leq n$. By applying the product rule, the definition of $\varphi^{(n)}$ and $\varphi^{(m)}$, and Young's inequality, we obtain in the case $d = 2$

$$
\begin{aligned}
&\Big|\partial_i\partial_j\big(P_k^{(n)} - P_k^{(m)}\big)(y_z)\Big| \\
&\leq\ c\Big(\Big(\frac{1}{n^2} + \frac{1}{m^2}\chi_{B_m}(y_z)\Big)\frac{1}{|y_z|} + \Big(\frac{1}{n} + \frac{1}{m}\chi_{B_m}(y_z)\Big)\frac{1}{|y_z|^2} + \frac{1}{|y_z|^3}\Big) \\
&\leq\ c\Big(\Big(\frac{1}{n^2} + \frac{1}{m^2}\chi_{B_m}(y_z)\Big)\frac{1}{|y_z|} + \frac{1}{|y_z|^3}\Big). \qquad (32)
\end{aligned}
$$

Hence, if $d = 2$,

$$
\begin{aligned}
&\int_{\mathcal{U}^{\text{in}}} \text{step}\,\Big|\Big(\partial_i\partial_j\big(P_k^{(n)} - P_k^{(m)}\big)(z)\Big)z_p\Big|\ d^2z \\
&\leq\ c\int_{\mathcal{U}^{\text{in}}}\Big(\frac{1}{n^2} + \frac{1}{m^2}\chi_{B_m}(z) + \frac{1}{|y_z|^2}\Big)\ d^2z \\
&\leq\ c\Big(\int_{B_{n+\gamma}\setminus B_n}\underbrace{\Big(\frac{1}{n^2} + \frac{1}{|y_z|^2}\Big)}_{\leq\frac{2}{(n-\gamma)^2}}\ d^2z + \int_{B_{m/2}\setminus B_{m/2-\gamma}}\underbrace{\Big(\frac{1}{n^2} + \frac{1}{m^2} + \frac{1}{|y_z|^2}\Big)}_{\leq\frac{3}{(m/2)^2}}\ d\zeta\Big) \\
&\leq\ \frac{c}{(n-\gamma)^2}((n+\gamma)^2 - n^2) + \frac{3c}{(m/2)^2}((m/2)^2 - (m/2-\gamma)^2),
\end{aligned}
$$

which tends to zero as $n, m \to \infty$. Similarly, we obtain for $d \geq 3$

$$
\Big|\partial_i\partial_j\big(P_k^{(n)} - P_k^{(m)}\big)(y_z)\Big| \leq c\Big(\big(\frac{1}{n^3} + \frac{1}{m^3}\chi_{B_m}(y_z)\big)\frac{1}{|y_z|^{d-2}} + \frac{1}{|y_z|^{d+1}}\Big). \qquad (33)
$$

and hence

$$\begin{aligned}
&\int_{\mathcal{U}^{\text{in}}} \text{step}\left|\Big(\partial_i\partial_j\big(P_k^{(n)}-P_k^{(m)}\big)(z)\Big)z_p\right|\,d^dz\\
&\le\; c\Big(\int_{B_{n+\gamma}\setminus B_n}\underbrace{\Big(\frac{1}{n^3}\frac{1}{|y_z|^{d-3}}+\frac{1}{|y_z|^d}\Big)}_{\le\frac{2}{(n-\gamma)^d}}\,d^dz\\
&\qquad+\int_{B_{m/2}\setminus B_{m/2-\gamma}}\underbrace{\Big(\frac{1}{n^3}\frac{1}{|y_z|^{d-3}}+\frac{1}{m^3}\frac{1}{|y_z|^{d-3}}+\frac{1}{|y_z|^d}\Big)}_{\le\frac{3}{(m/2)^d}}\,d^dz\Big)\\
&\le\; \frac{c}{(n-\gamma)^d}\big((n+\gamma)^d-n^d\big)+\frac{c}{(m/2)^d}\big((m/2)^d-(m/2-\gamma)^d\big),
\end{aligned}$$

which tends to zero as m and n tend to ∞. So it remains to estimate the first integral in (31), which we denote by I.

It holds $|\text{step}f(z)-f(z)|=|f(z)-f(y_z)|=\sup_{\eta\in\mathcal{U}(y_z)}|\nabla f(\eta)|$, see, e.g., [9, Appendix A]. Here, $\mathcal{U}(y_z)$ is the unit cell to which z belongs, and y_z is the base point of this unit cell. Hence

$$\begin{aligned}
|I| \;\le\;& c\int_{B_n\setminus B_{m/2}}\sup_{\eta\in\mathcal{U}(y_z)}\left|\nabla\Big(\partial_i\partial_j\big(P_k^{(n)}-P_k^{(m)}\big)(\eta)\eta_p\Big)\right|\,d^dz\\
&+c\left|\int_{B_n\setminus B_{m/2}}\Big(\partial_i\partial_j\big(P_k^{(n)}-P_k^{(m)}\big)(z)\Big)z_p\,d^dz\right|.
\end{aligned}$$

The second term equals zero by (29). To estimate the first term, we consider the cases $d=2$, $d=3$ and $d\ge 4$ separately. Similarly as in (32) and with the help of $|\eta|\ge|z|-(|z|-|\eta|)\ge|z|-|z-\eta|\ge|z|-\gamma$, we obtain if $d=2$ for sufficiently large m

$$\begin{aligned}
|I| \;\le\;& c\int_{B_n\setminus B_{m/2}}\sup_{\eta\in\mathcal{U}(y_z)}\Big(\frac{1}{n^3}+\frac{1}{m^3}\chi_{B_m}(y_z)+\frac{1}{|\eta|^3}\Big)\,d^2z\\
\le\;& c\int_{B_n\setminus B_{m/2}}\sup_{\eta\in\mathcal{U}(y_z)}\Big(\frac{1}{n^3}+\frac{1}{m^3}\chi_{B_m}(y_z)+\frac{1}{(|z|-\gamma)^3}\Big)\,d^2z\\
\le\;& c\Big\{\int_{m/2}^{n}\frac{1}{n^3}r\,dr+\int_{m/2}^{m}\frac{1}{m^3}r\,dr+\int_{m/2}^{n}\frac{r}{(r-\gamma)^3}\,dr\Big\},
\end{aligned}$$

where we introduced polar coordinates. Furthermore we get

$$
\begin{aligned}
|I| &\leq c\Big\{\frac{1}{n^3}\underbrace{(n^2-(m/2)^2)}_{\leq n^2}+\frac{1}{m^3}\underbrace{(m^2-(m/2)^2)}_{\leq m^2} \\
&\quad + \Big[\frac{-1}{|z|-\gamma}+\frac{-\gamma}{2(|z|-\gamma)^2}\Big]_{m/2}^{n}\Big\} \\
&\leq c\Big\{\frac{1}{n}+\frac{1}{m}+\frac{1}{m/2-\gamma}+\frac{\gamma}{2(m/2-\gamma)^2}\Big\} \leq c\frac{1}{m/2-\gamma},
\end{aligned}
$$

which tends to zero as $m, n \to \infty$. For $d = 3$ we refer to [10, p. 250]. Now let $d \geq 4$. Then we use a similar statement as in (33) to derive

$$
\begin{aligned}
|I| &\leq c\int_{B_n\setminus B_{m/2}} \sup_{\eta\in\mathcal{U}(y_z)} \Big(\big(\frac{1}{n^4}+\frac{1}{m^4}\chi_{B_m}(y_z)\big)\frac{1}{|\eta|^{d-3}}+\frac{1}{|\eta|^{d+1}}\Big)\, d^dz \\
&\leq c\int_{B_n\setminus B_{m/2}} \sup_{\eta\in\mathcal{U}(y_z)} \Big(\big(\frac{1}{n^4}+\frac{1}{m^4}\chi_{B_m}(y_z)\big)\frac{1}{(|z|-\gamma)^{d-3}}+\frac{1}{(|z|-\gamma)^{d+1}}\Big)\, d^dz \\
&\leq c\Big\{\int_{m/2}^{n}\frac{1}{n^4}\frac{r^{d-1}}{(r-\gamma)^{d-3}}\,dr+\int_{m/2}^{m}\frac{1}{m^4}\frac{r^{d-1}}{(r-\gamma)^{d-3}}\,dr+\int_{m/2}^{n}\frac{r^{d-1}}{(r-\gamma)^{d+1}}\,dr\Big\} \\
&=: c(I_1+I_2+I_3).
\end{aligned}
$$

First we estimate I_3. It holds

$$
\begin{aligned}
I_3 &= \Big[\frac{-1}{\gamma d}\frac{r^d}{(r-\gamma)^d}\Big]_{m/2}^{n} = \frac{1}{\gamma d}\Big(\big(\frac{\frac{m}{2}}{\frac{m}{2}-\gamma}\big)^d-\big(\frac{n}{n-\gamma}\big)^d\Big) \\
&= \frac{1}{\gamma d}\Big(\frac{\frac{m}{2}n-\frac{m}{2}\gamma-n\frac{m}{2}-\gamma n}{(\frac{m}{2}-\gamma)(n-\gamma)}\Big)^d \\
&= \frac{\gamma^d}{\gamma d}\Big(\frac{-\frac{1}{2n}-\frac{1}{m}}{\frac{1}{2}-\frac{\gamma}{2n}-\frac{\gamma}{m}+\frac{\gamma^2}{nm}}\Big)^d,
\end{aligned}
$$

which tends to zero as $m, n \to \infty$. To estimate I_1 and I_2, we first consider the case $d = 4$. Then

$$
\begin{aligned}
I_1 &= \int_{m/2}^{n}\frac{1}{n^4}\frac{r^3}{r-\gamma}\,dr = \frac{1}{n^4}\Big[\gamma^2 r+\gamma\frac{r^2}{2}+\frac{r^3}{3}+\gamma^3\ln(r-\gamma)\Big]_{m/2}^{n} \\
&\leq \frac{1}{n^4}\big(\gamma^2 n+\gamma\frac{n^2}{2}+\frac{n^3}{3}+\gamma^3\ln(n-\gamma)\big) \leq c\frac{1}{n}.
\end{aligned}
$$

If $d > 4$, we obtain, since $r \le n$,

$$\begin{aligned} I_1 &\le \int_{m/2}^{n} \frac{r^{d-5}}{(r-\gamma)^{d-3}}\,dr = \frac{1}{\gamma(4-d)}\Big[\frac{r^{d-4}}{(r-\gamma)^{d-4}}\Big]_{m/2}^{n} \\ &= \frac{1}{\gamma(4-d)}\Big(\frac{(\frac{m}{2}-\gamma)n - \frac{m}{2}(n-\gamma)}{(n-\gamma)(\frac{m}{2}-\gamma)}\Big)^{d-4} \\ &= \frac{\gamma^{d-4}}{\gamma(4-d)}\Big(\frac{\frac{1}{2n}-\frac{1}{m}}{\frac{1}{2}-\gamma(\frac{1}{2n}+\frac{1}{m})+\frac{\gamma^2}{nm}}\Big)^{d-4}, \end{aligned}$$

which converges to zero as m, n tend to ∞. Analogous but simpler estimates hold for I_2. Hence $|I|$ and therefore the sum in (28) tend to zero as $m, n \to \infty$. Thus $S_{ijkp}^{(n)}$ is a Cauchy sequence in n for every dimension d. So $\lim_{\ell\to\infty} S_{ijkp}^{(\ell\delta)}$ exists independently of δ. Hence (25) and also (26) follow. □

Remark 14 (i) If $d \ge 3$, one can commute the partial derivatives in the definition of S_{ijkp}, (25). Moreover, the above proof does not rely on the order of the partial derivatives. Thus S_{ijkp} is symmetric in i, j and k. This is also true if $d = 2$, cf. [8].

(ii) It has been proven in $d = 2$ [8] and in $d = 3$ [9, 10] that the value of S_{ijkp} is in general not equal to zero; moreover, approximate values are given in the case of the square and the cubic lattice, respectively.

Acknowledgment. I would like to thank B. Kirchheim for helpful discussions on the generalization of the estimate in Lemma 9 and of the related definitions to higher dimensions. This work was partially supported by the RTN network MRTN-CT-2004-50522.

References

[1] Cauchy, A.: De la pression ou tension dans un système de points matériels. *Exercices de Mathématique* (1828), In: *Œuvre complètes d'Augustin Cauchy,* publiées sous la direction scientifique de l'Académie des sciences, Paris, II^{E} Séries **8,** 253–277 (1890)

[2] Federer, H.: *Geometric measure theory,* Springer-Verlag, Berlin (1969)

[3] Gilbarg, D., Trudinger, N.S.: *Elliptic Partial Differential Equations of Second Order,* Reprint of the 1998 ed., Springer-Verlag, Berlin (2001)

[4] Gray, A.: *Tubes,* 2nd ed., Birkhäuser Verlag, Basel (2004)

[5] James, R.D., Hane, K.F.: Martensitic transformations and shape-memory materials, *Acta mater.* **48,** 197–222 (2000)

[Lo] Love, A.E.H.: *A treatise on the mathematical theory of elasticity,* Dover Publications, New York (1944)

[6] Mattila, P.: *Geometry of Sets and Measures in Euclidean Spaces,* Cambridge University Press, Cambridge (1995)

[7] Müller, S., Schlömerkemper, A.: Discrete-to-continuum limit of magnetic forces, *C. R. Acad. Sci. Paris, Ser. I* **335,** 393–398 (2002)

[8] Praetorius, D., Popović, N., Schlömerkemper, A.: Analysis and numerical simulation of magnetic forces between rigid polygonal bodies, in preparation

[9] Schlömerkemper, A.: *Magnetic forces in discrete and continuous systems,* Doctoral thesis, University of Leipzig (2002)

[10] Schlömerkemper, A.: Mathematical derivation of the continuum limit of the magnetic force between two parts of a rigid crystalline material, *Arch. Rational Mech. Anal.* **176,** 227–269 (2005)

[11] Tadmor, E.B., Ortiz, M., Phillips, R.: Quasicontinuum analysis of defects in solids, *Philos. Mag. A* **73,** 1529–1563 (1996)

[12] Zagier, D.: Introduction to Modular Forms. In: Waldschmidt, M., Moussa, P., Luck, J.-M., Itzkyson, C. (Eds.): *From Number Theory to Physics,* Springer-Verlag, Berlin (1992)