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Mathematical Derivation of the Continuum Limit of the Magnetic Force between Two Parts of a Rigid Crystalline Material

Anja Schlömerkemper

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Abstract

The topic of this paper is a mathematically rigorous derivation of the continuum limit of the magnetic force between two parts of a rigid magnetized body. For this we start from a discrete setting of magnetic dipoles fixed to a scaled Bravais lattice, $\frac{1}{l}\mathcal{L}$. The limit as $l \to \infty$ corresponds to the passage to the continuum. The magnetic dipole moments are scaled in such a way that we obtain a finite total magnetic moment per unit volume. Under certain regularity assumptions on the magnetization and the boundaries we derive a force formula in the passage from the discrete setting to the continuum. Compared with a corresponding magnetic-force formula which has been previously discussed in the literature, the limiting force consists of an additional explicit local surface term, which is due to short-range effects and which reflects the lattice approximation of the underlying hypersingular integral.

1. Introduction

In this paper we derive a formula for the magnetic force within a rigid magnetized body. We start from a configuration of magnetic dipoles on a Bravais lattice and consider the magnetic force between two parts of a bounded region. Then we calculate the limit for a vanishing lattice parameter. The limiting force consists of a nonlocal volume term and local surface contributions, which we will discuss in detail below.

There have been several approaches to a magnetoelastic theory for ferromagnetic materials also in recent years. An overview, which is interesting with respect to this work, and related references can be found in [19]. For a more general treatment of magnetoelasticity we refer to [12]. The approach in this article is mainly motivated by the work of Brown [5] and is restricted to rigid bodies. Further books in which magnetic forces in continuous settings are studied include [10, 22, 26] and the recent book by Bobbio [4].

In this article we will not discuss the different force formulae which can be found in the literature. Instead we focus on an approach which is based on magnetic dipoles and compare our new formula with the one which is discussed in detail by BROWN [5, especially p. 57]. We will call the latter Brown's formula for short and review it briefly in the following. For this we represent a continuous body by Ω, an open and bounded subset of $\mathbb{R}^3$, and consider a subregion $\tau \subset \Omega$. We assume in general that τ, $\Omega \setminus \bar{\tau}$ and Ω have a C^2 boundary. The outer normal to $\partial\tau$ is denoted by n. Moreover, we introduce the magnetization $M : \Omega \to \mathbb{R}^3$ and write H_Ω for the magnetic field which is generated by the magnetic material in the whole body Ω and is given by Maxwell's equations $\operatorname{curl} H_\Omega = 0$ and $\operatorname{div}(\gamma M_{|\Omega} + H_\Omega) = 0$. Here, γ is a constant which only depends on the choice of the physical units. For Gaussian units, $\gamma = 4\pi$. The value of γ for other physical units can be found in, e.g., [5, p. 6]. In Section 4 we also consider domains with piecewise C^2 boundary.

Brown's formula for the magnetic force which is exerted on τ by its surrounding region $\Omega \setminus \bar{\tau}$ then reads

$$F^{(\mathrm{Br})} = \int_\tau (M(x) \cdot \nabla) H_\Omega(x)\, d^3x + \frac{\gamma}{2} \int_{\partial\tau} (M^- \cdot n)^2(x) n(x)\, d\mathcal{H}^2(x), \tag{1}$$

where M^- denotes the inner trace of M with respect to τ. Several authors discussed this and equivalent formulae for the magnetic force between two parts of a macroscopic magnetic material (see, e.g., [4, 9, 12, 19] and references therein).

A proof of Brown's formula, for which C^2-regularity of the sets and $W^{1,2}$-regularity of the magnetization in τ and in $\Omega \setminus \bar{\tau}$ is assumed, is given in [27, Chapter 2]. The main difficulties appear in the calculation of the term $\int_\tau (M(x) \cdot \nabla) H_\tau(x)\, d^3x$, where H_τ denotes the magnetic field generated by the magnetic material in τ. If this term is rewritten as a double integral using the normal integral representation of H_τ, the kernel is of order $|x - y|^{-4}$ and hence the double integral is hypersingular. This difficulty can be tackled by general methods for singular integrals (see, e.g., [28]), which are closely related to those which we use in the derivation of the continuum limit of the long-range part of the discrete force, see Section 3.2 below.

Brown's force formula describes the long-range contributions of the magnetic force between two parts of a continuous magnetized body, which is a consequence of the way in which this formula is derived, [5, Section 5] or cf. [27, Chapter 2 and 5]. Formula (1) consists of a volume term and of a surface term, which shows a nonlinear dependence on the normal. This dependence also remains if the magnetization is smooth in the whole magnetic body (cf. also [11, p. 177] for a discussion of this). This is worth noting since Cauchy's Theorem (cf. e.g. [18, p. 101]) in continuum mechanics states that surface force densities, which are smooth in the whole body, can be represented as a tensor applied to the normal, i.e., that surface force densities depend linearly on the normal. Brown proposes therefore the existence of further surface terms to the surface term in (1), which yield a linear surface force density.

In order to understand better the structure of the surface term in (1) and the influence of possible discreteness effects, we derive a force formula from a discrete setting of magnetic dipoles. Such an atomistic approach has already been suggested by Brown [5, p. 52]. For this we assign magnetic moments to the points ("atoms") of a scaled Bravais lattice, $\frac{1}{l}\mathcal{L}$. The limit as $l \to \infty$ corresponds to the passage to the continuum. The magnetic moment of an atom is scaled in such a way that we obtain a finite total magnetization (see (2) below). The discrete force is given as the superposition of all dipole-dipole forces between the magnetic dipoles of the two subparts τ and $\Omega \setminus \bar{\tau}$, respectively. Under certain regularity assumptions on the magnetization and the occurring boundaries we derive a force formula in the passage from the discrete setting to the continuum. As we will explain in detail in Section 3, this is done by splitting the discrete force into long-range and short-range contributions.

In Theorem 3 we state that the continuum limit of the kth component of the long-range term of the magnetic force in the discrete setting is

$$\int_\tau (M(x) \cdot \nabla)(H_\Omega)_k(x)\, d^3x \\ + \frac{\gamma}{2} \int_{\partial\tau} (M^- \cdot n)(x)\big((M^- - M^+) \cdot n\big)(x) n_k(x)\, d\mathcal{H}^2(x),$$

where M^+ and M^- denote the outer and inner traces of M with respect to τ, respectively. The volume term agrees with the one in Brown's formula. Compared with Brown's formula we obtain an additional surface term in the limit of the long-range part of the discrete force if $M^+ \neq 0$ and $M^+ \neq M^-$. This additional term also shows a nonlinear dependence on the normal to $\partial\tau$. It vanishes if the magnetization does not jump at the boundary of the sub-body τ, on which the force is exerted. Thus the continuum limit of the discrete force yields a better understanding of the magnetic force in a continuous body in view of Cauchy's Theorem. It can be regarded as a contribution to the additional term which Brown proposed. We note that DESIMONE PODIO-GUIDUGLI [9] have shown in a careful analysis within a continuum setting that (1) is consistent with the usual setting of continuum mechanics if the relevant self-forces are properly taken into account.

In contrast to the nonlinear surface term which comes out of the long-range part of the discrete force, the limit of the kth component of the short-range term of the discrete force

$$\frac{1}{2} \int_{\partial\tau} \sum_{i,j,p=1}^{3} M_i^-(x) M_j^+(x) S_{ijkp} n_p(x)\, d\mathcal{H}^2(x)$$

is linear in the normal (cf. Theorem 2). Here, S_{ijkp} is a singular lattice sum (cf. (6)), which only depends on the underlying lattice structure. This sum is discussed and evaluated in Lemma 5 and Appendix 6.1, where we show that $S = (S_{ijkp})_{i,j,k,p=1,2,3}$ is not zero in general.

This additional local surface term originates from the lattice approximation of a hypersingular integral. A similar phenomenon occurs in the study of the limiting energy of a lattice of dipoles (see [1, pp. 142–145], [6, p. 33], [23, pp. 137–139] and [20]). The study of forces is more delicate since it involves hypersingular kernels (of order $|z|^{-4}$ in three dimensions) rather than singular kernels of order $|z|^{-3}$. One crucial ingredient in the proof is an estimate for Riemann sums in thin domains (see Proposition 1).

A study of forces rather than energy is of particular interest in the context of the recently discovered ferromagnetic shape-memory alloys as for instance Ni_2MnGa (cf., e.g., [19] and references therein). These alloys have interfaces at which large jumps of the magnetization and the deformation gradient occur. Due to motion of the interfaces, ferromagnetic shape-memory alloys exhibit large changes of their macroscopic shape, which can be about 50 times larger than in any previously known material. The motion of the interfaces is driven by external magnetic fields. For making use of this magnetostrictive effect for new micro-devices, a detailed analysis of the dynamic behavior of the interfaces is of interest. Investigations of the forces appearing are a first step towards this. The results reported here form part of [27] and have been partially announced in [25].

The outline of the rest of this paper is as follows. In the subsequent section we introduce the model of the magnetic force in the discrete setting in detail and state the theorem about the existence of the continuum limit and the limiting force formula. The proof of the theorem is given in the third section. Section 4 is about a generalization of the theorem to piecewise C^2 domains. In the fifth section we discuss the limiting-force formula and Brown's formula comparatively, and we mention some open problems.

2. The discrete model and its continuum limit

We consider a Bravais lattice $\mathcal{L} = \{x \in \mathbb{R}^3 \ : \ x = \sum_{i=1}^{3} \mu_i e_i,\ \mu_i \in \mathbb{Z}\}$, where (e_1, e_2, e_3) is a basis of $\mathbb{R}^3$, and we assume that the unit cell $\mathcal{U} = \{x \in \mathbb{R}^3 \ : \ x = \sum_{i=1}^{3} \lambda_i e_i,\ \lambda_i \in [0, 1)\}$ has unit volume. For the passage from the discrete to the continuous setting we consider scaled Bravais lattices $\frac{1}{l}\mathcal{L}$, $l \in \mathbb{N}$. To each lattice point $x \in \frac{1}{l}\mathcal{L}$, which we will also call atom for short, we assign a magnetic moment $m^{(l)}(x) \in \mathbb{R}^3$. For the calculation of the force that one part of the lattice exerts on another part we consider the magnetic moments to be given. Computing the magnetic moments, e.g., by minimization of the quantum-mechanical energy, is a separate problem, which we do not address here.

In particular, let a background magnetization $M : \mathbb{R}^3 \to \mathbb{R}^3$ be given, which is Lipschitz continuous in τ and $\Omega \setminus \bar{\tau}$. For simplicity we assume that M has zero trace at $\partial\Omega$. Further we suppose that

$$m^{(l)}(x) = \frac{1}{l^3} M(x) \tag{2}$$

holds for a magnetic moment at $x \in \frac{1}{l}\mathcal{L}$. This scaling ensures that we obtain a finite total magnetic moment per unit volume. It is based on the physical observation that the magnetization is an intensive quantity, i.e., that the magnetization is independent of the volume. Hence the magnetic moment divided by the volume is constant. For other ways to relate the dipole moments on different lattices and to define a limiting continuous magnetization see [20].

The magnetic field, H_y, generated by the magnetic moment of an atom at $y \in \frac{1}{l}\mathcal{L}$ is given by Maxwell's equations, of which the solution reads for the ith component $(H_y)_i(x) = K_{ij}(x - y) m_j^{(l)}(y)$. Here $m_j^{(l)}(y)$ denotes the jth component of the magnetic moment $m^{(l)}(y)$. We use the convention that the sum is taken over two equal indices from 1 to 3. Furthermore

$$K_{ij}(z) := \partial_i \partial_j N(z) \quad \text{and} \quad N(z) := \frac{\gamma}{4\pi} \frac{1}{|z|}, \quad z \neq 0,$$

where γ denotes, as before, a constant which only depends on the choice of the physical units. We have $K_{ij}(z) = K_{ij}(-z)$ and $K_{ij}(z) = K_{ji}(z)$ and moreover

$$K_{ij}(z) = \partial_i \frac{\gamma}{4\pi} \frac{-z_j}{|z|^3} = -\frac{\gamma}{4\pi |z|^3} (\mathbb{1} - 3 \frac{z}{|z|} \otimes \frac{z}{|z|})_{ij}.$$

A magnetic moment at $y \in \frac{1}{l}\mathcal{L}$ exerts a force on a magnetic moment at $x \in \frac{1}{l}\mathcal{L}$, $x \neq y$. The kth component of this force is given by $f_k = m_i^{(l)}(x)\partial_i (H_y)_k(x)$ (cf., e.g., [5, p. 13]). Since $\partial_i \partial_j \partial_k N(z)$ is independent of the order of the partial derivatives, the kth component of the force can equivalently be written as $f_k = m_i^{(l)}(x)\partial_k (H_y)_i(x)$.

Here we are interested in the magnetic force between two sub-bodies of a magnetic body. Let Ω be a bounded domain in $\mathbb{R}^3$ and τ a subset of Ω such that $\partial\,\Omega \cap \partial\tau = \emptyset$. We consider the force which magnetic moments in $(\Omega \setminus \bar{\tau}) \cap \frac{1}{l}\mathcal{L}$ exert on magnetic moments in $\bar{\tau} \cap \frac{1}{l}\mathcal{L}$. The magnetic force between several moments is the superposition of the forces between all pairs of moments. Since Maxwell's equations are linear, the ith component of the magnetic field generated by the magnetic moments in $(\Omega \setminus \bar{\tau}) \cap \frac{1}{l}\mathcal{L}$ is given by $(H_{(\Omega\setminus\bar{\tau})\cap\frac{1}{l}\mathcal{L}})_i(x) = \sum_{y\in(\Omega\setminus\bar{\tau})\cap\frac{1}{l}\mathcal{L}} K_{ij}(x - y)m_j^{(l)}(y)$. Hence the kth component of the force in the discrete setting reads

$$\begin{aligned} F_k^{(l)} &= \sum_{x\in\bar{\tau}\cap\frac{1}{l}\mathcal{L}} m_i^{(l)}(x)\partial_{x_k}(H_{(\Omega\setminus\bar{\tau})})_i(x) \\ &= \sum_{x\in\bar{\tau}\cap\frac{1}{l}\mathcal{L}} \; \sum_{y\in(\Omega\setminus\bar{\tau})\cap\frac{1}{l}\mathcal{L}} \partial_{x_k} K_{ij}(x-y) m_i^{(l)}(x) m_j^{(l)}(y). \end{aligned} \tag{3}$$

Note that here and in the following the partial derivative ∂_{x_k} only acts on K_{ij} and not on $m_i^{(l)}$ – unless it is marked differently. We also use ∂_k as a shorthand for ∂_{x_k} eventually.

For the passage from the discrete model to the continuum model we introduce a regularized kernel. Let $\varphi^{(1)} \in C_0^\infty(\mathbb{R}^3)$ be such that $\varphi^{(1)}(z) = 1$ if $|z| \leq \frac{1}{2}$ and 0 if $|z| \geq 1$, and let $0 \leq \varphi^{(1)}(z) \leq 1$ else. Moreover, we set $\varphi^{(\delta)}(z) = \varphi^{(1)}(\frac{z}{\delta})$ for $\delta > 0$. With this we define

$$K_{ij}^{(\delta)}(z) = \partial_i \partial_j \Big(\big(1 - \varphi^{(\delta)}(z)\big) N(z) \Big), \tag{4}$$

which we call a regularized kernel as it is not singular, as opposed to $K_{ij}(z)$.

The continuum limit of the force in the discrete setting as the lattice tends to the continuum is given as follows.

Theorem 1. *Suppose that τ is a C^2 domain and $\partial\tau$ satisfies the non-degeneracy condition (S) below. Suppose that $M_{|\tau} \in W^{1,\infty}(\tau,\mathbb{R}^3)$ and $M_{|\Omega\setminus\bar\tau} \in W^{1,\infty}(\Omega\setminus\bar\tau,\mathbb{R}^3)$. Then the limit $\lim_{l\to\infty} F_k^{(l)} = F_k^{(\mathrm{lim})}$ exists and*

$$\begin{aligned} F_k^{(\mathrm{lim})} &= \int_\tau (M(x)\cdot\nabla)(H_\Omega)_k(x)\,d^3x \\ &\quad+\frac{\gamma}{2}\int_{\partial\tau}(M^-\cdot n)(x)\big((M^- - M^+)\cdot n\big)(x)n_k(x)\,d\mathcal{H}^2(x) \\ &\quad+\frac{1}{2}\int_{\partial\tau} M_i^-(x)M_j^+(x)S_{ijkp}n_p(x)\,d\mathcal{H}^2(x). \end{aligned} \tag{5}$$

Here the S_{ijkp} depend only on the lattice $\mathcal{L}$ (and γ) and are given by the singular sum

$$S_{ijkp} := -\lim_{\delta\to 0}\lim_{l\to\infty}\sum_{z\in B_\delta\cap\frac{1}{l}\mathcal{L}^*}\partial_k(K-K^{(\delta)})_{ij}(z)z_p\frac{1}{l^3}, \tag{6}$$

where $\mathcal{L}^* = \mathcal{L}\setminus\{0\}$ and where $K^{(\delta)}$ is the regularized kernel defined in (4). The tensor S is symmetric in i, j and k and it is not identically zero in general, which we show for the case of a cubic lattice in the appendix. Note that there is a sum over $p = 1, 2, 3$ hidden in (27) by the summation convention. The existence of the limits in (6) is proved in Lemma 5.

We say that $\partial\tau$ satisfies the non-degeneracy condition (S) if τ is a Lipschitz domain, $\partial\tau$ can be covered by the closure of finitely many $C^{1,1}$ submanifolds U_i of $\mathbb{R}^3$ (such that ∂U_i is a finite union of rectifiable curves) and the boundary of the set

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

is a finite union of rectifiable curves, where the number and the length of the curves are bounded independently of z. This condition is for example satisfied by polyhedra or by uniformly convex sets. We will give further details in Section 3.1 and Appendix 6.2.

In Section 4 we discuss a generalization of this result to the case of a τ that is a piecewise C^2 domain instead of a C^2 domain.

3. Proof of Theorem 1

To prove the theorem, we use the regularized kernel in (4) and split the force in (3) into a long-range part and a short-range part, i.e.,

$$\begin{aligned} F_k^{(l)} &= \sum_{x\in\bar\tau\cap\frac{1}{l}\mathcal{L}}\ \sum_{y\in(\Omega\setminus\bar\tau)\cap\frac{1}{l}\mathcal{L}} \partial_k K_{ij}^{(\delta)}(x-y)m_i^{(l)}(x)m_j^{(l)}(y) \\ &\quad+\sum_{x\in\bar\tau\cap\frac{1}{l}\mathcal{L}}\ \sum_{y\in(\Omega\setminus\bar\tau)\cap\frac{1}{l}\mathcal{L}} \partial_k(K-K^{(\delta)})_{ij}(x-y)m_i^{(l)}(x)m_j^{(l)}(y) \\ &=: F_k^{(l,\delta)} + \mathcal{F}_k^{(l,\delta)}. \end{aligned}$$

In view of the behavior of the regularizing function $\varphi^{(\delta)}$, we call the first term the long-range part, and the second term the short-range part of the force. To obtain the limiting force we perform first the limit as $l \to \infty$ and then the limit as $\delta \to 0$. The kth component of the limiting force is given by

$$F_k^{(\lim)} := \lim_{l\to\infty} F_k^{(l)} = \lim_{\delta\to 0}\lim_{l\to\infty} F_k^{(l)} = \lim_{\delta\to 0}\left(\lim_{l\to\infty} F_k^{(l,\delta)} + \lim_{l\to\infty} \mathcal{F}_k^{(l,\delta)}\right)$$
$$= \lim_{\delta\to 0}\lim_{l\to\infty} F_k^{(l,\delta)} + \lim_{\delta\to 0}\lim_{l\to\infty} \mathcal{F}_k^{(l,\delta)}$$

provided the limits on the right-hand side exist. We will prove this separately for both terms in the following subsections.

3.1. The limit of the short-range part

In this section we consider the short-range part of the discrete magnetic force and we compute the limit $l \to \infty$ and then the limit $\delta \to 0$ of

$$\mathcal{F}_k^{(l,\delta)} = \sum_{x\in\bar\tau\cap\frac{1}{l}\mathcal{L}} \sum_{y\in(\Omega\setminus\bar\tau)\cap\frac{1}{l}\mathcal{L}} \partial_k (K - K^{(\delta)})_{ij}(x-y) m_i^{(l)}(x) m_j^{(l)}(y).$$

We show that the following theorem holds true.

Theorem 2. *Let $\Omega \subset \mathbb{R}^3$ be open and bounded and let $\tau \subset \Omega$ be such that $\partial\tau \cap \partial\Omega = \emptyset$. Assume that $\partial\tau$ satisfies the non-degeneracy condition* (S). *Moreover, let $M_{|\tau} \in W^{1,\infty}(\tau, \mathbb{R}^3)$ and $M_{|\Omega\setminus\bar\tau} \in W^{1,\infty}(\Omega\setminus\bar\tau, \mathbb{R}^3)$. Then*

$$\lim_{\delta\to 0}\lim_{l\to\infty} \mathcal{F}_k^{(l,\delta)} = \frac{1}{2}\int_{\partial\tau} M_i^-(x) M_j^+(x) S_{ijkp} n_p(x)\, d\mathcal{H}^2(x), \tag{7}$$

where S_{ijkp} is defined in (6).

From the required regularity we find that the inner and outer traces of M with respect to τ, M^- and M^+, respectively, belong to $L^\infty(\partial\tau, \mathbb{R}^3)$. For $M \in W^{1,\infty}(\tau, \mathbb{R}^3)$ there is a representative of the same equivalence class which is in $C^{0,1}(\bar\tau, \mathbb{R}^3)$. Similarly there is a representative for $M \in W^{1,\infty}(\Omega\setminus\bar\tau, \mathbb{R}^3)$ in $C^{0,1}(\overline{\Omega\setminus\bar\tau}, \mathbb{R}^3)$. In the following we will work with these representatives. Note that their traces are in $C^{0,1}(\partial\tau, \mathbb{R}^3)$.

Since the support of $(K - K^{(\delta)})_{ij} = \partial_i\partial_j(\varphi^{(\delta)} N)$ is contained in $B_\delta(0)$, we control the short-range behavior, i.e., the occurring singularities of the hypersingular kernel. In the following we suppose that $\delta < \operatorname{dist}(\tau, \partial\Omega)$, which is possible in view of the assumption $\partial\Omega \cap \partial\tau = \emptyset$.

For the evaluation of the sum, the change of variables $y \mapsto x + z$ is useful. This idea goes back to Cauchy's work on the derivation of elasticity from a discrete setting [8]. Notice that for $\delta > 0$ and l finite, the double sum in $\mathcal{F}_k^{(l,\delta)}$ does not depend on the order of summation. As $x \in \bar\tau \cap \frac{1}{l}\mathcal{L}$ and $y \in (\Omega\setminus\bar\tau) \cap \frac{1}{l}\mathcal{L}$ we always have $x \neq y$ which becomes $z \neq 0$ under the transformation. We set $\mathcal{L}^* = \mathcal{L} \setminus \{0\}$

and $B_\delta = B_\delta(0)$. Observe that the sum of two lattice vectors is again a lattice vector. We obtain

$$\begin{aligned}
\mathcal{F}_k^{(l,\delta)} &= -\sum_{x\in\bar\tau\cap\frac{1}{l}\mathcal{L}} \sum_{\substack{z\in B_\delta\cap\frac{1}{l}\mathcal{L}^* \\ x+z\in\Omega\setminus\bar\tau}} \partial_k(K-K^{(\delta)})_{ij}(z) m_i^{(l)}(x) m_j^{(l)}(x+z) \\
&= -\sum_{z\in B_\delta\cap\frac{1}{l}\mathcal{L}^*} \sum_{\substack{x\in\bar\tau\cap\frac{1}{l}\mathcal{L} \\ x+z\in\Omega\setminus\bar\tau}} \partial_k(K-K^{(\delta)})_{ij}(z) m_i^{(l)}(x) m_j^{(l)}(x+z) \\
&= -\sum_{z\in B_\delta\cap\frac{1}{l}\mathcal{L}^*} \partial_k(K-K^{(\delta)})_{ij}(z) \sum_{x\in\tau_z\cap\frac{1}{l}\mathcal{L}} m_i^{(l)}(x) m_j^{(l)}(x+z),
\end{aligned}$$

where

$$\tau_z := \{x \in \bar\tau \,:\, x+z \in \Omega\setminus\bar\tau\},$$

cf. Fig. 1.

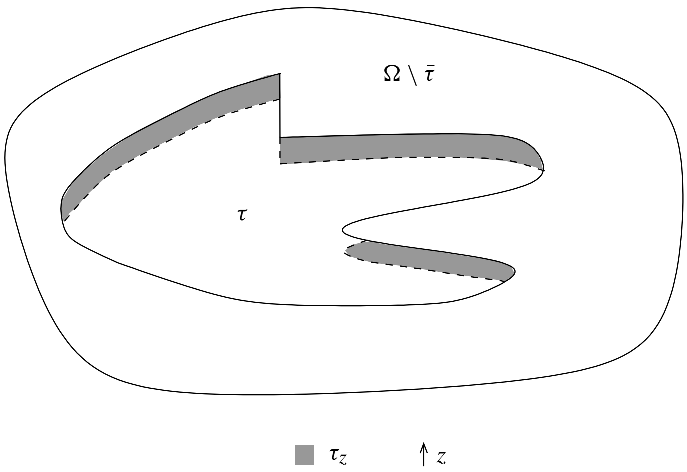

Fig. 1. A slice of the sets indicating τ_z.

Before going into the details of the proof of the limiting force, we outline the main ideas of the following estimates. Notice that c stands for generic positive constants which do not always have to be the same.

The essential idea is to split the set of lattice points in τ_z into a subset which yields the surface integral in (7) and to its complement which gives higher-order terms, which do not contribute to the limiting force. The precise definitions of these sets are given in Definitions 3 and 4 below.

We call the subset which leads to higher-order terms a "bad" set and denote it by $\mathcal{B}$. By Lemma 1 and Lemma 2 below (with for instance $\beta = \frac{2}{3}$ as in (24)), the number of lattice points in $\mathcal{B}$ is estimated by a term of order $l^3|z|^{1+\alpha}$ for an $\alpha > 0$.

With $|\partial_k(K-K^{(\delta)})_{ij}(z)| \le \frac{c}{|z|^4}$ and (2) as well as with the estimate on the number of points in $\mathcal{B}$ and the boundedness of M, we obtain

$$\begin{aligned}
&\Big| \sum_{z\in B_\delta \cap \frac{1}{l}\mathcal{L}^*} \partial_k(K-K^{(\delta)})_{ij}(z) \sum_{x\in\mathcal{B}} m_i^{(l)}(x) m_j^{(l)}(x+z)\Big| \\
&\quad \le \sum_{z\in B_\delta \cap \frac{1}{l}\mathcal{L}^*} \frac{c}{|z|^4} \sum_{x\in\mathcal{B}} |M_i(x)M_j(x+z)| \frac{1}{l^6} \\
&\quad \le c \sum_{z\in B_\delta \cap \frac{1}{l}\mathcal{L}^*} \frac{1}{|z|^4}|z|^{1+\alpha}\frac{1}{l^3} = c \sum_{z\in B_\delta \cap \frac{1}{l}\mathcal{L}^*} \frac{1}{|z|^{3-\alpha}}\frac{1}{l^3}.
\end{aligned} \tag{8}$$

For $\alpha > 0$ this is a Riemann sum, which tends to $\int_{B_\delta} \frac{1}{|z|^{3-\alpha}}\, d^3z$ in the limit $l \to \infty$. By introducing polar coordinates, we find that this integral is bounded by a constant times δ^α, which tends to zero as $\delta \to 0$. Hence the bad points do not contribute to the limiting force.

The other subset is called a "good" set and is denoted by $\mathcal{G}$ (cf. (9)). The number of lattice points which belong to $\mathcal{G}$ can be estimated by a constant times $l^3|z|$ (cf. Lemma 4). As follows by Proposition 1 below, the sum over the good points can be approximated by a certain surface integral. More precisely, we will prove that there is a constant c and a constant $\alpha > 0$ such that

$$\Big| \sum_{x\in\mathcal{G}} M_i(x)M_j(x+z)\frac{1}{l^3} - \int_{\partial\tau} M_i^-(\xi)M_j^+(\xi)(n(\xi)\cdot z)_+\, d\mathcal{H}^2(\xi)\Big| \le c|z|^{1+\alpha}$$

uniformly in l, where n denotes the outward normal to $\partial\tau$ and $(n(\xi)\cdot z)_+$ the positive part of $n(\xi)\cdot z$. With the same arguments which yield (8) it thus remains to consider the force term

$$-\sum_{z\in B_\delta \cap \frac{1}{l}\mathcal{L}^*} \partial_k(K-K^{(\delta)})_{ij}(z)\frac{1}{l^3}\int_{\partial\tau} M_i^-(\xi)M_j^+(\xi)(n(\xi)\cdot z)_+\, d\mathcal{H}^2(\xi).$$

For $\delta > 0$ and l finite, it is possible to commute summation and integration and obtain

$$-\int_{\partial\tau} M_i^-(\xi)M_j^+(\xi) \sum_{z\in B_\delta \cap \frac{1}{l}\mathcal{L}^*} \partial_k(K-K^{(\delta)})_{ij}(z)(n(\xi)\cdot z)_+\frac{1}{l^3}\, d\mathcal{H}^2(\xi).$$

The final step will be to show the convergence of the lattice sum as $l \to \infty$ and $\delta \to 0$ (cf. Lemma 5). With this we will then take the limits and obtain the desired force formula in Theorem 2.

Next we go into the details of the procedure described above. For this we firstly give a precise definition of the non-degeneracy condition (S). Let τ be a bounded Lipschitz domain, that is, the boundary of τ is locally the graph of a Lipschitz continuous function and τ is on one side of the boundary only.

Definition 1. The boundary $\partial\tau$ is said to be *piecewise* $C^{1,1}$ if there exist finitely many pairwise disjoint sets $U_i \subset \partial\tau$ which are relatively open in $\partial\tau$ and have the following properties:
(i) U_i is an orientable $C^{1,1}$ submanifold of $\mathbb{R}^3$ and the normal is Lipschitz continuous up to the boundary,
(ii) $\partial\tau \subset \bigcup_i \bar{U}_i$ and
(iii) ∂U_i is a finite union of rectifiable curves.

Definition 2. We say that $\partial\tau$ *satisfies the non-degeneracy condition* (S) if it is piecewise $C^{1,1}$ and if for all $z \in \mathbb{R}^3 \setminus \{0\}$, the boundary of the set

$$\partial^+\tau = \{x \in \partial\tau \cap \Big(\bigcup_i U_i\Big) \ : \ n(x)\cdot z > 0\}$$

is a finite union of rectifiable curves, of which the number and the total length are bounded independently of z.

The non-degeneracy condition (S) is for instance satisfied for polyhedra (that are on one side of the boundary only, cf., e.g., [17, p. 1]). The sets U_i are the faces, and the boundary of $\partial^+\tau$ is a subset of the edges. More generally, piecewise $C^{1,1}$ boundaries, of which the number of indentations and protrusions is bounded, satisfy condition (S). More examples of sets which satisfy the non-degeneracy condition (S) can be found in the appendix.

Condition (S) is violated in particular if the boundary has the same tangent in infinitely many isolated points. A typical example is a boundary of a two-dimensional set that is locally given by $x^k \sin\frac{1}{x}$, $k > 3$. From this, an example of a set in three dimensions that does not satisfy condition (S) can be constructed by defining a cylinder over the two-dimensional set.

We may assume in the following calculations that $|z|$ is greater than or equal to the minimal distance between any two points of the scaled lattice, i.e., $\frac{\tilde{c}}{l} \le |z|$ for a constant $\tilde{c} > 0$ depending only on the given Bravais lattice, since otherwise the short-range part of the microscopic force is zero.

We split the set τ_z into a bad set $\mathcal{B}$ and a good set $\mathcal{G}$ (cf. Fig. 2). To define these sets we fix a lattice vector $z \in B_\delta$ and set

$$\Gamma := \partial(\partial^+\tau) \cup \bigcup_i \partial U_i$$

with $\partial^+\tau$ as in Definition 2.

The bad set $\mathcal{B}$ is split into the bad sets $\mathcal{B}_I$ and $\mathcal{B}_{II}$. The first bad set contains lattice points which are close to Γ, i.e., it contains those lattice points which are close to edges and corners of τ or close to those boundary points at which z is tangential. In the estimate of the number of these lattice points we use the non-degeneracy condition (S).

The second bad set contains those lattice points in $\tau_z \setminus \mathcal{B}_I$ at which z is almost tangential. This set is of special interest when z and $\frac{1}{l}$ are of the same order.

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

$$\rho = C_0(|z| + l^{-\beta}) \quad \text{and} \quad \beta \in (\tfrac{1}{2}, 1).$$

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

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

Note that in particular $|z| + \frac{1}{l}\operatorname{diam}\mathcal{U} < \rho$ holds. We also define a function $p_z : \tau_z \to \partial\tau$ which projects each $x \in \tau_z$ along the direction and orientation of z on $\partial\tau$. If there happens to be more than one of such boundary points, we choose that one which is closest to x.

Let $\partial_+\tau_z$ denote the positive part of $\partial\tau_z$, i.e., $\{\xi \in \partial\tau_z \ : \ n_{\tau_z}(\xi) \cdot z > 0\}$, where $n_{\tau_z}(\xi)$ is the outer normal to $\partial\tau_z$. If τ has indentations, i.e., if τ is not convex, $\partial_+\tau_z$ can contain elements which do not belong to $\partial_+\tau$, the positive part of $\partial\tau$. Since we require τ to have Lipschitz boundary, we may assume in the following that the constant C_0 is so large that $\mathcal{B}_I$ contains $\{x \in \tau_z \cap \frac{1}{l}\mathcal{L} \ : \ p_z(x) \in \partial_+\tau \setminus (\partial_+\tau \cap \partial_+\tau_z)\}$. We then have $p_z(x) \in \partial\tau_z$ for all $x \in (\tau_z \cap \frac{1}{l}\mathcal{L}) \setminus \mathcal{B}_I$, and this will be used in the proof of Lemma 2.

Definition 4. Let ρ be as before 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

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

Finally, the *good set* is said to be

$$\mathcal{G} = (\tau_z \cap \tfrac{1}{l}\mathcal{L}) \setminus (\mathcal{B}_I \cup \mathcal{B}_{II}). \tag{9}$$

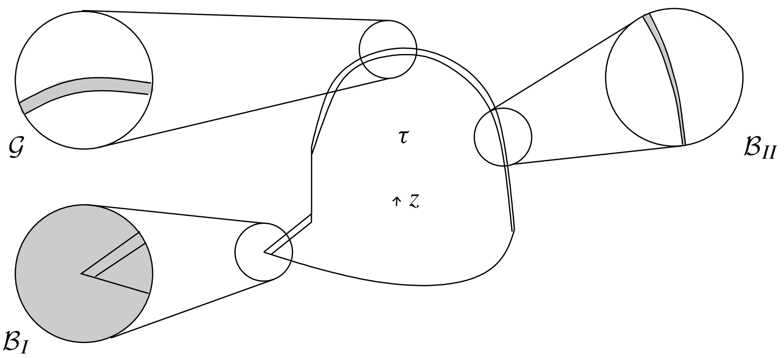

Fig. 2. A slice of τ indicating the good and bad sets and τ_z.

In the following we assume that δ is so small and l so large that $C_1(l^{\beta-1}+\rho) \ll 1$ and $\frac{\tilde{c}}{l} \le |z| < \delta$. In particular, we will use $|z| < 1$ and hence $|z| < |z|^\beta$, $\beta \in (\frac{1}{2}, 1)$ and $\rho < c|z|^\beta$.

For later use we estimate the number of points in $\mathcal{B}_I$.

Lemma 1. *The number of points in $\mathcal{B}_I$ is $\#\mathcal{B}_I \leq cl^3|z|^{2\beta}$.*

Proof. By the non-degeneracy condition (S), Γ is a union of a uniformly bounded number of curves of finite length. Thus it suffices to consider the case where Γ is just a single curve. Let L be the length of this curve and let $\lfloor a \rfloor$ denote the integer part of a. Then we can find balls $B(x_i, \rho)$, $x_i \in \Gamma$, such that $\Gamma \subset \bigcup_i B(x_i, \rho)$ and the number of points x_i on Γ is at most $\lfloor \frac{L}{2\rho} \rfloor + 2$. Let δ be so small and l so large that 4ρ is less than the length of the shortest curve, i.e., in particular $4\rho \leq L$. Then the number of points x_i is bounded by $\frac{L}{\rho}$.

Moreover, $\mathcal{B}_I \subset \bigcup_i B(x_i, 9\rho)$ and $\bigcup_{x \in \mathcal{B}_I} \frac{1}{l}\mathcal{U}(x) \subset \bigcup_i B(x_i, 10\rho)$, where $\frac{1}{l}\mathcal{U}(x) = x + \frac{1}{l}\mathcal{U}$ denotes a translated unit cell. The number of points in $\mathcal{B}_I$ can be estimated by the volume of $\bigcup_{x \in \mathcal{B}_I} \frac{1}{l}\mathcal{U}(x)$ divided by the volume of the scaled unit cell $\frac{1}{l}\mathcal{U}$, i.e., divided by $\frac{1}{l^3}$. Hence we obtain $\#\mathcal{B}_I \leq c\frac{L}{\rho}\rho^3 l^3 = cLl^3\rho^2 \leq cl^3|z|^{2\beta}$ as stated. □

Since $2\beta > 1$ by assumption, the points in $\mathcal{B}_I$ yield terms in the sum which are of higher order, as discussed above. As we will show next, the number of points in the bad set $\mathcal{B}_{II}$ is of order $|z|$ to the power of $2 - \beta$, which is greater than 1 as well because β is assumed to be less than 1.

Lemma 2. *The number of points in $\mathcal{B}_{II}$ is $\#\mathcal{B}_{II} \leq cl^3|z|^{2-\beta}$.*

Proof. For each $x \in \mathcal{B}_{II}$ consider the set

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

with $\rho = C_0(|z| + l^{-\beta})$ and p_z as above. Note that since $\partial\tau$ is a $C^{1,1}$ manifold, the set B_x is connected if $l \geq l_0$ and $|z| < \delta \leq \delta_0$, where l_0 and δ_0 only depend on $\partial\tau$.

Since $|x - p_z(x)| \leq |z| \leq \rho$ and since $x \notin \mathcal{B}_I$ and $n(p_z(x)) \cdot \frac{z}{|z|} \leq C_1(l^{\beta-1} + \rho)$, we know that $B(p_z(x), 5\rho) \cap \partial\tau$ is contained in a single chart U_i and in $\partial^+\tau$ (cf. Definitions 1 and 2). Since U_i is $C^{1,1}$, we can estimate the area of B_x by the area of a flat two-dimensional disc, i.e., there exists a $c > 0$ such that $\mathcal{H}^2(B_x) \geq c\pi\rho^2$. With this we can estimate $\#\mathcal{B}_{II}$ as follows. Let χ_y be the characteristic function of B_y. Then

$$\begin{aligned} c\pi\rho^2 \#\mathcal{B}_{II} &\leq \sum_{y \in \mathcal{B}_{II}} \mathcal{H}^2(B_y) = \sum_{y \in \mathcal{B}_{II}} \int_{\partial\tau} \chi_y(\xi)\, d\mathcal{H}^2(\xi) \\ &= \int_{\partial\tau} \sum_{y \in \mathcal{B}_{II}} \chi_y(\xi)\, d\mathcal{H}^2(\xi), \end{aligned}$$

which can be estimated by $\sup_{x \in \mathcal{B}_{II}} \sum_{y \in \mathcal{B}_{II}} \chi_y(p_z(x))$, since $\mathcal{H}^2(\partial\tau)$ is bounded by assumption. Hence, if we show that

$$\sup_{x \in \mathcal{B}_{II}} \sum_{y \in \mathcal{B}_{II}} \chi_y(p_z(x)) \leq cl^3|z|(l^{\beta-1} + \rho)\rho^2, \qquad (10)$$

we obtain $\#\mathcal{B}_{II} \leq cl^3|z|(l^{\beta-1} + \rho)$. Using the fact that $1 > \beta > \frac{1}{2}$ and thus $\rho \leq c(|z| + l^{-\beta}) \leq c(|z| + l^{\beta-1})$, this finally yields $\#\mathcal{B}_{II} \leq cl^3(l^{\beta-1}|z| + |z|^2) \leq cl^3|z|^{2-\beta}$, i.e., the proposed estimate for $\#\mathcal{B}_{II}$. Hence it remains to prove (10). We have

$$\begin{aligned}\sup_{x\in\mathcal{B}_{II}} \sum_{y\in\mathcal{B}_{II}} \chi_y(p_z(x)) &= \sup_{x\in\mathcal{B}_{II}} \#\{y \in \mathcal{B}_{II} \ : \ p_z(x) \in B_y\} \\ &\leq \sup_{x\in\mathcal{B}_{II}} \#\{y \in \mathcal{B}_{II} \ : \ B_y \cap B_x \neq \emptyset\} \\ &\leq \sup_{x\in\mathcal{B}_{II}} \#\{y \in \mathcal{B}_{II} \ : \ p_z(y) \in B(p_z(x), 2\rho)\}.\end{aligned}$$

To estimate the right-hand side, we fix $x \in \mathcal{B}_{II}$ and set

$$\tilde{\mathcal{B}}_{II} := \{y \in \mathcal{B}_{II} \ : \ p_z(y) \in B(p_z(x), 2\rho)\},$$

whereby the dependence on x is suppressed in the notation. In a suitable orthonormal coordinate system $z = |z|e_1$ and $n(p_z(x)) \cdot e_2 = 0$. By assumption,

$$n(p_z(x)) \cdot e_1 = n(p_z(x)) \cdot \frac{z}{|z|} \leq C_1(l^{\beta-1} + \rho).$$

Since $U_i \subset \partial\tau$ is a $C^{1,1}$ manifold, this implies in particular

$$n(\xi) \cdot e_1 \leq c(l^{\beta-1} + \rho) \qquad \forall \xi \in B(p_z(x), 5\rho) \cap \partial\tau. \tag{11}$$

Moreover,

$$n(\xi) \cdot e_1 > 0 \qquad \forall \xi \in B(p_z(x), 5\rho) \cap \partial\tau \tag{12}$$

since $B(p_z(x), 5\rho) \cap \partial\tau \subset \partial^+\tau$ as observed above.

Thus $\partial\tau$ is locally represented as a $C^{1,1}$ graph over the e_1, e_2 plane (see Fig. 3). Set $x' = (x_1, x_2)$ and let $u : \mathbb{R}^2 \to \mathbb{R}$ be a $C^{1,1}$ function which

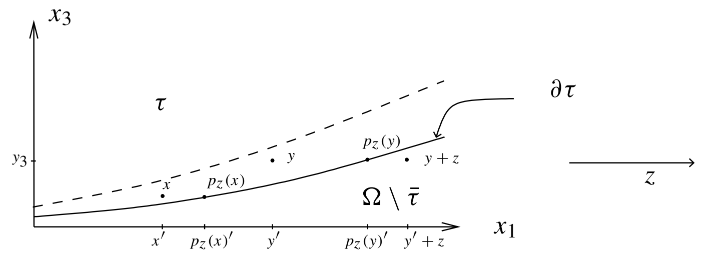

Fig. 3. A local representation of the boundary.

parametrizes the boundary in $B(p_z(x), 5\rho)$. Then

$$\begin{aligned}B(p_z(x), 4\rho) \cap \partial\tau &\subset \{(x', u(x')) \ : \ x' \in B(p_z(x)', 4\rho)\} \\ &\subset B(p_z(x), 5\rho) \cap \partial\tau.\end{aligned}$$

The normal is given by $n = \big(1 + \big(\frac{\partial u}{\partial x_1}\big)^2\big)^{-1/2}\big(\frac{\partial u}{\partial x_1}, 0, -1\big)$. Thus, if some positive constants α_1, α_2 are such that $\alpha_1 < |n \cdot e_1| \le \alpha_2$, then

$$\alpha_1^2 \le \frac{\alpha_1^2}{1-\alpha_1^2} \le \Big(\frac{\partial u}{\partial x_1}\Big)^2 \le \frac{\alpha_2^2}{1-\alpha_2^2}. \tag{13}$$

Hence we obtain by (11) and (12)

$$0 < \frac{\partial u}{\partial x_1}(x') \le c(l^{\beta-1} + \rho) \ll 1 \tag{14}$$

for all $x' \in B(p_z(x)', 4\rho)$ and some constant c.

Let $y \in \tilde{\mathcal{B}}_{II}$. We assert that

$$y + kz \notin \tilde{\mathcal{B}}_{II} \qquad \forall k \in \mathbb{Z} \setminus \{0\},\ |k| \le K := \Big\lfloor \frac{\rho}{|z|} \Big\rfloor. \tag{15}$$

To see this, consider first $k \ge 1$. By definition of $p_z(y)$ we have $p_z(y)' = y' + \lambda z'$, for some $\lambda \in [0, 1)$ and $y_3 = (p_z(y))_3 = u(p_z(y)')$. Since $y' + kz' \in B(y', \rho) \subset B(p_z(y)', \rho + |z|) \subset B(p_z(x)', 3\rho + |z|)$ and thus $y' + kz' \subset B(p_z(x)', 4\rho)$, we obtain by the monotonicity of u for $k \ge 1$,

$$u(y' + kz') > u(p_z(y)') = y_3 = (y + kz)_3.$$

Thus $y + kz \notin \bar{\tau}$ for $k = 1, \dots, K$. So $y + kz \notin \tilde{\mathcal{B}}_{II}$ as asserted.

For $-K \le k \le 0$ we obtain similarly $y + kz \in \bar{\tau}$. Hence $y + kz \notin \tau_z$ for $k = -1, \dots, -K$ since $y + kz + z \notin \Omega \setminus \bar{\tau}$. This proves (15).

In order to estimate $\#\tilde{\mathcal{B}}_{II}$ by computing volumes we introduce the set $V := \bigcup_{y \in \tilde{\mathcal{B}}_{II}} \frac{1}{l}\mathcal{U}(y)$, where $\frac{1}{l}\mathcal{U}(y) = y + \frac{1}{l}\mathcal{U}$ denotes a translated scaled unit cell. The sets $kz + V$ defined for $k = 0, 1, \dots, K$ are disjoint, since otherwise there would exist $y, \tilde{y} \in \tilde{\mathcal{B}}_{II}$ and $k \ne \tilde{k}$ such that $y + kz = \tilde{y} + \tilde{k}z$. Hence $y = (\tilde{k} - k)z + \tilde{y} \ne \tilde{y}$. But this contradicts (15).

Let $W := \bigcup_{k=0}^{K}(kz + V)$. Then, using the definition of $\tilde{\mathcal{B}}_{II}$, the upper bound in (14) and the estimate $|z| + \operatorname{diam}\frac{1}{l}\mathcal{U} \le \rho$, we see that

$$W \subset B(p_z(x)', 4\rho) \times \Big((p_z(x))_3 - H, (p_z(x))_3 + H\Big),$$

where $H \le c(l^{\beta-1} + \rho)\rho + \frac{\operatorname{diam}\mathcal{U}}{l} \le c(l^{\beta-1} + \rho)\rho$. The last step follows with $\frac{\operatorname{diam}\mathcal{U}}{l} \le C_0 l^{\beta-1} l^{-\beta} + C_0 l^{\beta-1}|z| + c\rho^2 \le c(l^{\beta-1} + \rho)\rho$.

We finally obtain

$$\begin{aligned} \#\tilde{\mathcal{B}}_{II} &\le cl^3|V| \le cl^3 \frac{1}{K+1}|W| \le cl^3 \frac{1}{K+1}|B(p_z(x)', 4\rho)|H \\ &\le cl^3 \frac{|z|}{\rho}\rho^2(l^{\beta-1} + \rho)\rho = cl^3|z|\rho^2(l^{\beta-1} + \rho) \end{aligned}$$

uniformly in $x \in \mathcal{B}_{II}$. Hence (10) is proved, which finishes the proof of the Lemma. □

Next we consider the good set. As already mentioned in the sketch of the procedure on page 9, our aim is to show that summation over the points in the good set $\mathcal{G}$ is essentially the same as integration of τ_z (up to sets of measure less than $|z|^{1+\alpha}$, $\alpha > 0$), which leads to the desired surface integral in the limiting force formula. To achieve this, we associate with each $x \in \mathcal{G}$ a "modified unit cell" $\mathcal{V}(x) \subset \tau_z$, for which we show that $|\mathcal{V}(x)| = |\frac{1}{l}\mathcal{U}(x)| = \frac{1}{l^3}$ and $\mathcal{V}(x) \cap \mathcal{V}(\tilde{x}) = \emptyset$ if $x, \tilde{x} \in \mathcal{G}$, $x \neq \tilde{x}$. Moreover we find that $\bigcup_{x\in\mathcal{G}} \mathcal{V}(x)$ is a good approximation of τ_z.

If the usual unit cell $\frac{1}{l}\mathcal{U}(x)$ is contained in τ_z, we can simply take $\mathcal{V}(x) = \frac{1}{l}\mathcal{U}(x)$. More generally we define (see Fig. 4)

$$\mathcal{V}(x) := \bigcup_{k=-K}^{K} \tfrac{1}{l}\mathcal{U}(x + kz) \cap \tau_z, \tag{16}$$

where $K = \left\lfloor \frac{\rho}{|z|} \right\rfloor$ as above.

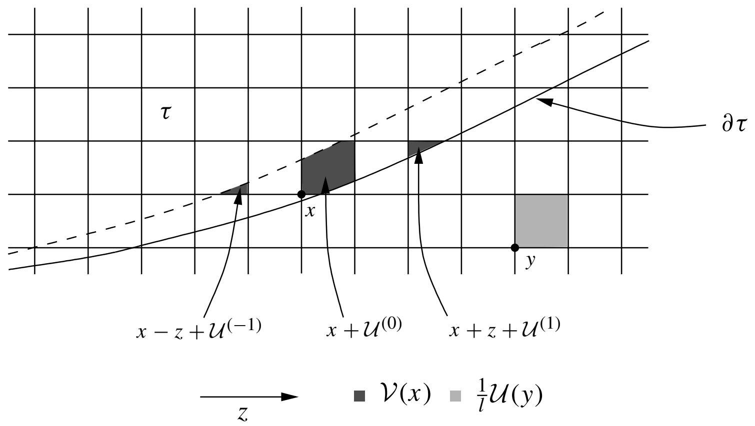

Fig. 4. An example of a modified unit cell $\mathcal{V}(x)$.

Lemma 3. *Let $\mathcal{V}(x)$, $x \in \mathcal{G}$, be the modified unit cell defined in* (16)*. Then*

$$|\mathcal{V}(x)| = \frac{1}{l^3} \tag{17}$$

and

$$\mathcal{V}(x) \cap \mathcal{V}(\tilde{x}) = \emptyset \qquad \text{if} \quad x, \tilde{x} \in \mathcal{G} \quad \text{and} \quad x \neq \tilde{x}. \tag{18}$$

Proof. We first assume in addition that $n(p_z(x)) \cdot \frac{z}{|z|} \leq \frac{1}{2}$. Then we can represent $\partial\tau$ locally as a graph as in the proof of Lemma 2, where some of the following notation is defined.

To prove (17), we define the sets (cf. Fig. 4)

$$\mathcal{U}^{(k)} := \{y \in \mathcal{U} \ : \ x + kz + \tfrac{1}{l} y \in \tau_z\},$$

where the x-dependence is suppressed in the notation. Since $|z| \geq \operatorname{diam} \frac{1}{l}\mathcal{U}$, we have $\mathcal{U}^{(k)} \cap \mathcal{U}^{(k')} = \emptyset$ if $k \neq k'$. Next we show that

$$\bigcup_{k=-K}^{K} \mathcal{U}^{(k)} = \mathcal{U}. \tag{19}$$

Since the translated sets $x + kz + \frac{1}{l}\mathcal{U}^{(k)}$ are trivially disjoint and

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

this implies (17). To prove (19), note that $p_z(x) = x + \bar{\lambda} z$ for some $\bar{\lambda} \in [0, 1)$, thus $p_z(x)' = x' + \bar{\lambda} z'$. Let $y \in \mathcal{U}$ and suppose $|\lambda z| \leq \rho$, then

$$\begin{aligned} |p_z(x)' - (x' + \lambda z' + \tfrac{1}{l} y')| &\leq |\lambda z'| + |\bar{\lambda} z'| + \frac{\operatorname{diam} \mathcal{U}}{l} \\ &\leq \rho + |z| + \frac{\operatorname{diam} \mathcal{U}}{l} \leq 2\rho \end{aligned}$$

as $C_0 > \operatorname{diam} \mathcal{U}$. Moreover, $\operatorname{Lip}(Du) 2\rho \leq \frac{1}{2} C_1 (l^{\beta-1} + \rho)$ for C_1 larger than $4 \operatorname{Lip}(Du)$. Since u is $C^{1,1}$ and $x \in \mathcal{G}$, we thus have

$$\begin{aligned} \frac{\partial u}{\partial x_1}(x' + \lambda z' + \tfrac{1}{l} y') &\geq \frac{\partial u}{\partial x_1}(p_z(x)') - \operatorname{Lip}(Du) |p_z(x)' - (x' + \lambda z' + \tfrac{1}{l} y')| \\ &\geq \frac{\partial u}{\partial x_1}(p_z(x)') - \operatorname{Lip}(Du) 2\rho \geq \frac{1}{2} C_1 (l^{\beta-1} + \rho) > 0. \end{aligned} \tag{20}$$

Hence

$$\lambda \ \mapsto \ u(x' + \lambda z' + \tfrac{1}{l} y') \tag{21}$$

is strictly increasing. Notice that $(K - \bar{\lambda})|z| \geq (K-1)|z| \geq \rho - 2|z| \geq \frac{1}{4}\rho$ as $K \geq \frac{\rho}{|z|} - 1$ and $C_0 > 3$. Moreover we have

$$\begin{aligned} u(p_z(x)' + \tfrac{1}{l} y') - (x + \tfrac{1}{l} y)_3 &= u(p_z(x)' + \tfrac{1}{l} y') - u(p_z(x)') - \tfrac{1}{l} y_3 \\ &\geq -\frac{1}{2}\frac{1}{l}|y'| - \frac{\operatorname{diam} \mathcal{U}}{l} \geq -\frac{3}{2}\frac{\operatorname{diam} \mathcal{U}}{l} \end{aligned}$$

and hence obtain by (20)

$$\begin{aligned} & u(x' + Kz' + \tfrac{1}{l} y') - (x + \tfrac{1}{l} y)_3 \\ &\quad = u(x' + Kz' + \tfrac{1}{l} y') - u(x' + \bar{\lambda} z' + \tfrac{1}{l} y') + u(x' + \bar{\lambda} z' + \tfrac{1}{l} y') - (x + \tfrac{1}{l} y)_3 \\ &\quad \geq \frac{1}{2} C_1 (l^{\beta-1} + \rho)(K - \bar{\lambda})|z| + u(p_z(x)' + \tfrac{1}{l} y') - (x + \tfrac{1}{l} y)_3 \\ &\quad \geq \frac{1}{8} C_1 (l^{\beta-1} + \rho)\rho - \frac{3}{2}\frac{\operatorname{diam} \mathcal{U}}{l} \geq \frac{1}{8}\frac{C_1}{l} - \frac{3}{2}\frac{\operatorname{diam} \mathcal{U}}{l}. \end{aligned}$$

The last step follows with $(l^{\beta-1}+\rho)\rho \geq l^{\beta-1}\rho = l^{\beta-1}C_0(|z|+l^{-\beta}) \geq l^{-1}$. Since $C_1 > 12\,\mathrm{diam}\,\mathcal{U}$ by assumption, we obtain

$$u(x' + Kz' + \tfrac{1}{l}y') - (x + \tfrac{1}{l}y)_3 > 0,$$

and similarly $u(x' - Kz' + \frac{1}{l}y') - (x + \frac{1}{l}y)_3 < 0$. Hence there exists a unique $\tilde{\lambda}(y) \in (-K, K)$ such that

$$u(x' + \lambda z' + \tfrac{1}{l}y') - (x + \tfrac{1}{l}y)_3 \begin{cases} > 0 & \text{if} \quad \lambda > \tilde{\lambda}(y), \\ = 0 & \text{if} \quad \lambda = \tilde{\lambda}(y), \\ < 0 & \text{if} \quad \lambda < \tilde{\lambda}(y). \end{cases}$$

This shows that

$$x + kz + \tfrac{1}{l}y \in \tau_z \quad \Longleftrightarrow \quad k = \tilde{k}(y) := \lfloor \tilde{\lambda}(y) \rfloor, \tag{22}$$

which proves (19) and thus (17). See also Fig. 5.

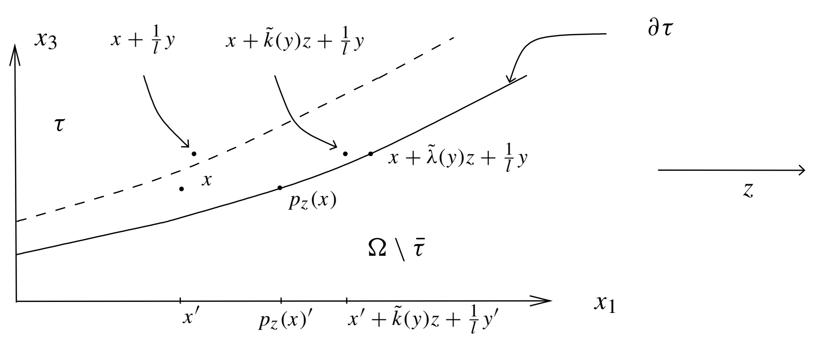

Fig. 5. This is related to (22).

We next show (18). If $\mathcal{V}(x) \cap \mathcal{V}(\tilde{x}) \neq \emptyset$ for $x \neq \tilde{x}$, then there would exist $k \neq \tilde{k}(y) \in \{-K, \dots, K\}$ such that $x, \tilde{x} \in \mathcal{G}$ and $x + kz = \tilde{x} + \tilde{k}(y)z$, i.e., $\tilde{x} = x + (k - \tilde{k}(y))z$. This is impossible in view of the fact that the map in (21) is strictly increasing and in view of the definition of τ_z.

If $n(p_z(x)) \cdot \frac{z}{|z|} > \frac{1}{4}$, the arguments are similar but simpler. In this case it is more convenient to choose a coordinate system such that $\frac{z}{|z|} = e_3$ and $\partial\tau$ is locally a graph over the e_1, e_2 plane (see Fig. 6). It is then obvious that each line $\lambda \mapsto x + \lambda z$ intersects $\partial\tau$ locally exactly once. Moreover, can be represented $\partial\tau$ by a $C^{1,1}$ function u such that $p_z(x) = (x', u(x'))$. $\square$

Next we estimate the number of points in the good set. This estimate will be used in the proof of Proposition 1 below.

Lemma 4. *The number of points in the good set in given by* $\#\mathcal{G} \leq cl^3|z|$.

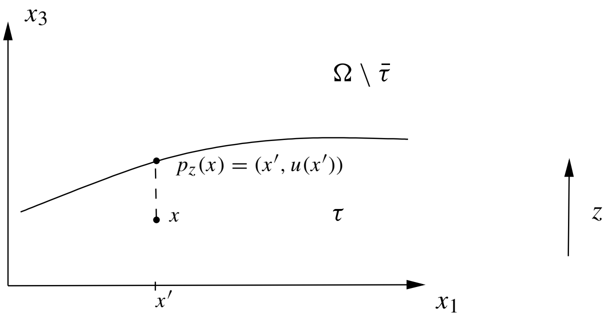

Fig. 6. A local representation of $\partial\tau$ for the case $n(p_z(x)) \cdot \frac{z}{|z|} > \frac{1}{4}$.

Proof. We give a proof using the coarea formula (cf., e.g., [13, 15]) since a similar argument is used in the proof of Proposition 1 below.

Set $\mathcal{V} := \bigcup_{x\in\mathcal{G}} \mathcal{V}(x)$ and notice that $\#\mathcal{G} = l^3|\mathcal{V}|$ by (17) and (18). To estimate $|\mathcal{V}|$, we project $\mathcal{V}$ along z on $\partial\tau$ by $\mathcal{T}$ so that for each $x \in \mathcal{V}$ there exists a unique $\xi \in \mathcal{T}$ and a $t \in [0, 1)$ such that $x = \xi - tz = p_z(x) - tz$. This projection of $\mathcal{V}$ along z on $\partial\tau$ is denoted by $\mathcal{T}$.

Here we use again the fact that $\partial\tau$ can locally be expressed as a graph. The lines $t \mapsto x + tz$ can intersect $\partial\tau$ 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 we have $z \cdot \nabla F(x) = -1$. Thus $\nabla F(x) = -\frac{1}{n(p_z(x))\cdot z} n(p_z(x))$ and the Jacobian of F equals $|\nabla F|$. Hence the coarea formula yields

$$|\mathcal{V}| = \int_0^1 \int_{F(x)=t} \frac{1}{|\nabla F(x)|}\, d\mathcal{H}^2(x)\, dt = \int_0^1 \Big(\int_{\mathcal{T}} |n(\xi)\cdot z|\, d\mathcal{H}^2(\xi) \Big)\, dt$$
$$= \int_{\mathcal{T}} |n(\xi)\cdot z|\, d\mathcal{H}^2(\xi) \le |z|\mathcal{H}^2(\partial\tau).$$

As $\#\mathcal{G} = l^3|\mathcal{V}|$ by (17) and (18), we obtain Lemma 4. □

Having estimated the number of points in the good and the bad sets we next approximate the sum over all lattice points in τ_z by a certain surface integral. We state the proposition for a general function f which is Lipschitz continuous in τ_z. For an application to the force formula we essentially set $f(x) = M_i(x)M_j(x+z)$. The details are discussed after the proof of the following proposition.

Proposition 1. *Let* $z \in \frac{1}{l}\mathcal{L}^*$ *with* $|z| \le \delta \ll 1$. *Suppose that* $\partial\tau$ *satisfies the non-degeneracy condition* (*S*) *and assume that* f *is Lipschitz continuous on* τ_z. *Then*

$$\Big| \frac{1}{l^3} \sum_{x\in\tau_z\cap\frac{1}{l}\mathcal{L}} f(x) - \int_{\partial\tau} f(\xi)(n(\xi)\cdot z)_+\, d\mathcal{H}^2(\xi) \Big| \le C|z|^{4/3}. \tag{23}$$

The constant C *only depends on* $\sup|f|$, *the Lipschitz constant of* f *and the geometric data of* τ *and of those in the formulation of the non-degeneracy condition* (*S*).

Remark 1. It is possible to derive sharper error estimates involving $|z|$ and l. Since for our purposes any estimate by $|z|^{1+\alpha}$, $\alpha > 0$, is sufficient, we do not strive for optimal exponents.

Proof of Proposition 1: Recall the decomposition of $\tau_z \cap \frac{1}{l}\mathcal{L}$ in $(\mathcal{B}_I \cap \tau_z) \cup \mathcal{B}_{II} \cup \mathcal{G}$ (Definitions 3 and 4). In the following we take $\beta = \frac{2}{3}$. By Lemma 1 and Lemma 2 we have

$$\#\mathcal{B}_I + \#\mathcal{B}_{II} \le cl^3(|z|^{2\beta} + |z|^{2-\beta}) \le cl^3|z|^{4/3}. \tag{24}$$

Hence in (23) it suffices to consider the sum over $x \in \mathcal{G}$ as discussed on page 9.

The modified unit cell $\mathcal{V}(x)$, which is associated with $x \in \mathcal{G}$, is contained in $B(x, 2\rho)$ as $K|z| + \frac{\operatorname{diam}\mathcal{U}}{l} \le \frac{\rho}{|z|}|z| + \frac{\operatorname{diam}\mathcal{U}}{l} \le 2\rho$. Since $|\mathcal{V}(x)| = \frac{1}{l^3}$ and $\mathcal{V} = \bigcup_{x\in\mathcal{G}} \mathcal{V}(x)$, we get by (18), the Lipschitz continuity of f and Lemma 4,

$$\begin{aligned}\Big|\sum_{x\in\mathcal{G}} \frac{1}{l^3} f(x) - \int_{\mathcal{V}} f(y)\, d^3y\Big| &= \Big|\sum_{x\in\mathcal{G}} \Big(\int_{\mathcal{V}(x)} f(x)\, d^3y - \int_{\mathcal{V}(x)} f(y)\, d^3y\Big)\Big| \\ &\le c\sum_{x\in\mathcal{G}} |\mathcal{V}(x)|\, \mathrm{Lip}(f)\rho \le c\#\mathcal{G}\frac{1}{l^3}\rho \\ &\le c|z|\rho \le c|z|^{1+\beta} = c|z|^{5/3} \le c|z|^{4/3}.\end{aligned}$$

It thus remains to show that

$$\Big|\int_{\mathcal{V}} f(x)\, d^3x - \int_{\partial\tau} f(\xi)(n(\xi)\cdot z)_+\, d\mathcal{H}^2(\xi)\Big| \le c|z|^{4/3}. \tag{25}$$

As before we denote the projection of $\mathcal{V} = \cup_{x\in\mathcal{G}}\mathcal{V}(x)$ along z on $\partial\tau$ by $\mathcal{T}$. We use the coarea formula as in the proof of Lemma 4 and the Lipschitz continuity of f to obtain

$$\begin{aligned}\int_{\mathcal{V}} f(x)\, d^3x &= \int_0^1 \int_{\mathcal{T}} f(\xi - tz)|n(\xi)\cdot z|\, d\mathcal{H}^2(\xi)\, dt \\ &= \int_0^1 \int_{\mathcal{T}} f(\xi)|n(\xi)\cdot z|\, d\mathcal{H}^2(\xi)\, dt \\ &\quad + \int_0^1 \int_{\mathcal{T}} \big(f(\xi - tz) - f(\xi)\big)|n(\xi)\cdot z|\, d\mathcal{H}^2(\xi)\, dt \\ &= \int_{\mathcal{T}} f(\xi)|n(\xi)\cdot z|\, d\mathcal{H}^2(\xi) + \mathcal{O}\big(\mathcal{H}^2(\partial\tau)|z|^2\big).\end{aligned}$$

Thus, finally, we need to estimate

$$\begin{aligned}&\Big|\int_{\mathcal{T}} f(\xi)|n(\xi)\cdot z|\, d\mathcal{H}^2(\xi) - \int_{\partial\tau} f(\xi)(n(\xi)\cdot z)_+\, d\mathcal{H}^2(\xi)\Big| \\ &\le \Big|\int_{\partial\tau\setminus\mathcal{T}} f(\xi)(n(\xi)\cdot z)_+\, d\mathcal{H}^2(\xi)\Big| \le \int_{\partial\tau\setminus\mathcal{T}} |f(\xi)|(n(\xi)\cdot z)_+\, d\mathcal{H}^2(\xi).\end{aligned}$$

By the definition of $\mathcal{G}$, $\xi \in \partial\tau\setminus\mathcal{T}$ implies $n(\xi)\cdot z \le C_1(l^{\beta-1}+\rho)|z|$ or $\operatorname{dist}(x, \Gamma) < 8\rho$ for all $x \in p_z^{-1}(\xi) \cap \tau_z$. That is, $\operatorname{dist}(\xi, \Gamma) < 9\rho$ since $|x - p_z(x)| \le \rho$. Using the fact that $\partial\tau$ is piecewise $C^{1,1}$ and covering Γ by balls as in the estimate for $\#\mathcal{B}_I$, we obtain $\mathcal{H}^2(B(\Gamma, 9\rho) \cap \partial\tau) \leq c\rho^2$. Thus we have

$$\begin{aligned}
&\int_{\partial\tau\setminus\mathcal{T}} |f(\xi)|(n(\xi)\cdot z)_+ \, d\mathcal{H}^2(\xi) \\
&\qquad \leq \sup|f| \Big(\int_{B(\Gamma,9\rho)\cap\partial\tau} |z| \, d\mathcal{H}^2(\xi) + \int_{\partial\tau} C_1(l^{\beta-1}+\rho)|z| \Big) \\
&\qquad \leq c\rho^2|z| + c(l^{\beta-1}+\rho)|z| \leq c|z|^{4/3}
\end{aligned}$$

and obtain (25), which finishes the proof. □

For an application of Proposition 1 to the short-range part of the discrete force, we set $f(x) = M_i(x)M_j(x+z)$ in the interior of τ_z. On the positive part of the boundary, $\partial_+\tau$, we have $f(\xi) = M_i^-(\xi)M_j(\xi+z)$, where M_i^- denotes as before the inner trace of M_i with respect to τ. To obtain the desired surface integral we make use of the Lipschitz continuity of M in $\Omega \setminus \bar{\tau}$ and separate another term of higher order, i.e., $|f(\xi) - M_i^-(\xi)M_j^+(\xi)| \leq |M_i^-(\xi)||M_j(\xi+z) - M_j^+(\xi)| \leq c|z|$, and we obtain an analogous estimate to (23). Thus the short-range part of the discrete force reads

$$\begin{aligned}
&\mathcal{F}_k^{(l,\delta)} \\
&\quad = -\sum_{z\in B_\delta\cap\frac{1}{l}\mathcal{L}^*} \partial_k(K-K^{(\delta)})_{ij}(z)\frac{1}{l^3}\int_{\partial\tau} M_i^-(\xi)M_j^+(\xi)(n(\xi)\cdot z)_+ \, d\mathcal{H}^2(\xi) \\
&\qquad + \mathcal{O}\Big(\sum_{z\in B_\delta\cap\frac{1}{l}\mathcal{L}^*} \frac{1}{|z|^4}\frac{1}{l^3}|z|^{4/3} \Big).
\end{aligned}$$

As discussed in (8), the second term tends to zero if we first take the limit $l \to \infty$ and then the limit $\delta \to 0$.

To estimate the first term, notice that it is possible to commute summation and integration in this term as long as $\delta > 0$. Thus

$$\begin{aligned}
&-\sum_{z\in B_\delta\cap\frac{1}{l}\mathcal{L}^*} \partial_k(K-K^{(\delta)})_{ij}(z)\frac{1}{l^3}\int_{\partial\tau} M_i^-(\xi)M_j^+(\xi)(n(\xi)\cdot z)_+ \, d\mathcal{H}^2(\xi) \qquad (26) \\
&\quad = -\int_{\partial\tau} M_i^-(\xi)M_j^+(\xi) \sum_{z\in B_\delta\cap\frac{1}{l}\mathcal{L}^*} \partial_k(K-K^{(\delta)})_{ij}(z)(n(\xi)\cdot z)_+\frac{1}{l^3} \, d\mathcal{H}^2(\xi).
\end{aligned}$$

Next the convergence of the sum which occurs in the right-hand side of (26) is considered.

Lemma 5. *Let $a \in \mathbb{R}^3$. Then the limit*

$$S_{ijkp} = -\lim_{\delta\to 0}\lim_{l\to\infty} \sum_{z\in B_\delta\cap\frac{1}{l}\mathcal{L}^*} \partial_k(K-K^{(\delta)})_{ij}(z)z_p\frac{1}{l^3} \in \mathbb{R}$$

exists and

$$-\lim_{\delta\to 0}\lim_{l\to\infty}\sum_{z\in B_\delta\cap\frac{1}{l}\mathcal{L}^*}\partial_k(K-K^{(\delta)})_{ij}(z)(a\cdot z)_+\frac{1}{l^3}=\frac{1}{2}S_{ijkp}a_p \tag{27}$$

holds true. Furthermore, S_{ijkp} is symmetric in the indices i, j and k.

Proof. Notice that $\partial_k(K-K^{(\delta)})_{ij}(z)$ and $a\cdot z$ are antisymmetric in z, their product is symmetric in z. Thus we obtain, with the definition of the kernel and a change of variables,

$$\begin{aligned}\sum_{z\in B_\delta\cap\frac{1}{l}\mathcal{L}^*}&\partial_k(K-K^{(\delta)})_{ij}(z)(a\cdot z)_+\frac{1}{l^3}\\ &=\frac{1}{2}\sum_{z\in B_\delta\cap\frac{1}{l}\mathcal{L}^*}\partial_k(K-K^{(\delta)})_{ij}(z)(a\cdot z)\frac{1}{l^3}.\\ &=\frac{1}{2}\sum_{z\in B_{l\delta}\cap\mathcal{L}^*}\Big(\partial_k\partial_i\partial_j\big(\varphi^{(l\delta)}N\big)(z)\Big)z_pa_p=:-\frac{1}{2}S^{(l\delta)}_{ijkp}a_p.\end{aligned} \tag{28}$$

We will show that the limit $l\to\infty$ of $S^{(l\delta)}_{ijkp}$ exists for fixed $\delta>0$. For convenience we restrict the proof of this to natural numbers. It works in the same way for nets. In the following we will prove that the limit of $S^{(n)}_{ijkp}$ exists as $n\to\infty$ by showing that $S^{(n)}_{ijkp}$ is a Cauchy sequence in $\mathbb{R}$. For this let $n,m\in\mathbb{N}$ with $m\le n<\infty$. The support of $\varphi^{(n)}-\varphi^{(m)}$ is contained in $B_n\setminus B_{m/2}$. Therefore

$$|S^{(n)}_{ijkp}-S^{(m)}_{ijkp}|=\Big|\sum_{z\in(B_n\setminus B_{m/2})\cap\mathcal{L}^*}\Big(\partial_k\partial_i\partial_j\big((\varphi^{(n)}-\varphi^{(m)})N\big)(z)\Big)z_p\Big|. \tag{29}$$

The idea is to replace this sum by the following integral, which is in fact zero. Let ν denote the outer normal to $\partial(B_n\setminus B_{m/2})$. Then,

$$\begin{aligned}\int_{B_n\setminus B_{m/2}}&\Big(\partial_k\partial_i\partial_j\big((\varphi^{(n)}-\varphi^{(m)})N\big)(\zeta)\Big)\zeta_p\,d\zeta\\ &=\int_{\partial(B_n\setminus B_{m/2})}\big(\partial_i\partial_j\big((\varphi^{(n)}-\varphi^{(m)})N\big)(\zeta)\big)\zeta_p\nu_k(\zeta)\,d\mathcal{H}^2(\zeta)\\ &\quad-\int_{\partial(B_n\setminus B_{m/2})}\partial_j\big((\varphi^{(n)}-\varphi^{(m)})N\big)(\zeta)\delta_{kp}\nu_i(\zeta)\,d\mathcal{H}^2(\zeta)\\ &=0\end{aligned} \tag{30}$$

because $\varphi^{(n)}-\varphi^{(m)}$ and all its derivatives are zero on $\partial(B_n\setminus B_{m/2})$ by definition. To estimate the sum in (29) by the above integral, let y_x denote the base point of the unit cell to which x belongs and introduce the sets

$$\begin{aligned}\mathcal{U}^{\text{out}}&:=\{x\in(B_n\setminus B_{m/2})\ :\ y_x\in\mathbb{R}^3\setminus(B_n\setminus B_{m/2})\},\\ \mathcal{U}^{\text{in}}&:=\{x\notin(B_n\setminus B_{m/2})\ :\ y_x\in(B_n\setminus B_{m/2})\}.\end{aligned}$$

Moreover, let step(f) denote the step-function of f which has the same value as f on lattice points and which is constantly extended on unit cells. We then have

$$
\begin{aligned}
|S^{(n)}_{ijkp} - S^{(m)}_{ijkp}| = \Big| \int_{B_n \setminus B_{m/2}} &\operatorname{step}\Big(\Big(\partial_k \partial_i \partial_j \big((\varphi^{(n)} - \varphi^{(m)})N\big)(\zeta)\Big)\zeta_p\Big)\, d\zeta \\
+ \int_{\mathcal{U}^{\text{in}}} &\operatorname{step}\Big(\Big(\partial_k \partial_i \partial_j \big((\varphi^{(n)} - \varphi^{(m)})N\big)(\zeta)\Big)\zeta_p\Big)\, d\zeta \\
- \int_{\mathcal{U}^{\text{out}}} &\operatorname{step}\Big(\Big(\partial_k \partial_i \partial_j \big((\varphi^{(n)} - \varphi^{(m)})N\big)(\zeta)\Big)\zeta_p\Big)\, d\zeta \Big|.
\end{aligned}
$$

Since $\varphi^{(n)} - \varphi^{(m)}$ and all its derivatives are zero in the complement of $B_n \setminus B_{m/2}$, the third integral vanishes. For the estimate of the second term notice that $\mathcal{U}^{\text{in}} \subset (B_{n+d} \setminus B_n) \cup (B_{m/2} \setminus B_{m/2-d})$ as indicated in Fig. 7, where d denotes the diameter of the unit cell. So $|\mathcal{U}^{\text{in}}| \leq c\big((n+d)^3 - n^3 + (\frac{m}{2})^3 - (\frac{m}{2} - d)^3\big) \leq cd\big(n^2 + (m/2)^2\big) \leq cn^2$. Moreover, the value of the step-function in the second term is small since the lattice points of interest are close to the boundary of $B_n \setminus B_{m/2}$, i.e., if z_ζ is the lattice point corresponding to $\zeta \in \mathcal{U}^{\text{in}}$, then either $m/2 \leq |z_\zeta| \leq m/2 + d$ or $n - d \leq |z_\zeta| \leq n$. By applying the product rule, the definition of $\varphi^{(n)}$ and $\varphi^{(m)}$ and Young's inequality, we obtain

$$
\begin{aligned}
&\Big|\Big(\partial_k \partial_i \partial_j \big((\varphi^{(n)} - \varphi^{(m)})N\big)(z_\zeta)\Big)(z_\zeta)_p\Big| \\
&\quad \leq c\bigg(\Big(\frac{1}{n^3} + \frac{1}{m^3}\chi_{B_m}\Big)\frac{1}{|z_\zeta|} + \Big(\frac{1}{n^2} + \frac{1}{m^2}\chi_{B_m}\Big)\frac{1}{|z_\zeta|^2} + \Big(\frac{1}{n} + \frac{1}{m}\chi_{B_m}\Big)\frac{1}{|z_\zeta|^3} \\
&\qquad\quad + \frac{1}{|z_\zeta|^4}\bigg)|(z_\zeta)_p| \\
&\quad \leq c\Big(\frac{1}{n^3} + \frac{1}{m^3}\chi_{B_m} + \frac{1}{|z_\zeta|^3}\Big).
\end{aligned}
$$

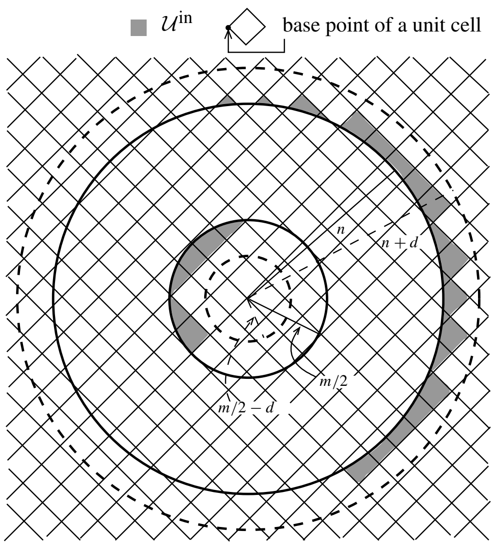

Fig. 7. The set $\mathcal{U}^{\text{in}}$ as a subset of $(B_{n+d} \setminus B_n) \cup (B_{m/2} \setminus B_{m/2-d})$.

So

$$
\begin{aligned}
&\int_{\mathcal{U}^{\text{in}}} \text{step}\left|\Big(\partial_k\partial_i\partial_j\big((\varphi^{(n)}-\varphi^{(m)})N\big)(\zeta)\Big)\zeta_p\right| \, d\zeta \\
&\quad \le c\int_{\mathcal{U}^{\text{in}}}\Big(\frac{1}{n^3}+\frac{1}{m^3}\chi_{B_m}+\frac{1}{|z_\zeta|^3}\Big)\,d\zeta \\
&\quad \le c\Big(\int_{B_{n+d}\setminus B_n}\underbrace{\Big(\frac{1}{n^3}+\frac{1}{|z_\zeta|^3}\Big)}_{\le\frac{2}{(n-d)^3}}\,d\zeta+\int_{B_{m/2}\setminus B_{m/2-d}}\underbrace{\Big(\frac{1}{n^3}+\frac{1}{m^3}+\frac{1}{|z_\zeta|^3}\Big)}_{\le\frac{3}{(m/2)^3}}\,d\zeta\Big) \\
&\quad \le \frac{c}{(n-d)^3}((n+d)^3-n^3)+\frac{c}{(m/2)^3}((m/2)^3-(m/2-d)^3),
\end{aligned}
$$

which tends to zero as n and m tend to ∞. Hence it remains to estimate the first integral. We obtain, by (30) and the chain rule,

$$
\begin{aligned}
&\Big|\int_{B_n\setminus B_{m/2}}\text{step}\Big(\Big(\partial_k\partial_i\partial_j\big((\varphi^{(n)}-\varphi^{(m)})N\big)(\zeta)\Big)\zeta_p\Big)\,d\zeta\Big| \\
&\qquad \le \int_{B_n\setminus B_{m/2}}\sup_{\eta\in U(z_\zeta)}\big|\nabla\big(\big(\partial_k\partial_i\partial_j\big((\varphi^{(n)}-\varphi^{(m)})N\big)(\eta)\big)\eta_p\big)\big|\,d\zeta, \qquad (31)
\end{aligned}
$$

where $\mathcal{U}(z_\zeta)$ denotes the unit cell to which ζ belongs. For the estimate of the supremum in (31) we use $|\partial^s\varphi^{(n)}|\le C_s\frac{1}{n^{|s|}}$ for all multi-indices s. By the product rule we obtain

$$
\begin{aligned}
&\big|\nabla\big[\big(\partial_k\partial_i\partial_j\big((\varphi^{(n)}-\varphi^{(m)})N\big)(\eta)\big)\eta_p\big]\big| \\
&\le\big|\nabla\big(\partial_k\partial_i\partial_j\big((\varphi^{(n)}-\varphi^{(m)})N\big)(\eta)\big)\big||\eta|+|\partial_k\partial_i\partial_j\big((\varphi^{(n)}-\varphi^{(m)})N\big)(\eta)||\nabla\eta| \\
&\le c\Big(\big(\tfrac{1}{n^4}+\tfrac{1}{m^4}\chi_{B_m}\big)\tfrac{1}{|\eta|}+\big(\tfrac{1}{n^3}+\tfrac{1}{m^3}\chi_{B_m}\big)\tfrac{1}{|\eta|^2}+\big(\tfrac{1}{n^2}+\tfrac{1}{m^2}\chi_{B_m}\big)\tfrac{1}{|\eta|^3} \\
&\qquad+\big(\tfrac{1}{n}+\tfrac{1}{m}\chi_{B_m}\big)\tfrac{1}{|\eta|^4}+\tfrac{1}{|\eta|^5}\Big)|\eta| \\
&\quad+c\Big(\big(\tfrac{1}{n^3}+\tfrac{1}{m^3}\chi_{B_m}\big)\tfrac{1}{|\eta|}+\big(\tfrac{1}{n^2}+\tfrac{1}{m^2}\chi_{B_m}\big)\tfrac{1}{|\eta|^2}+\big(\tfrac{1}{n}+\tfrac{1}{m}\chi_{B_m}\big)\tfrac{1}{|\eta|^3}+\tfrac{1}{|\eta|^4}\Big), \\
&\le c\Big(\tfrac{1}{n^4}+\tfrac{1}{m^4}\chi_{B_m}+\tfrac{1}{|\eta|^4}\Big),
\end{aligned}
$$

where the last step follows with the help of Young's inequality. Notice that $|\eta|=|\zeta|-(|\zeta|-|\eta|)\ge|\zeta|-|\zeta-\eta|\ge|\zeta|-d$, where d denotes, as before, the diameter of the unit cell. Therefore the supremum of $\frac{1}{|\eta|^4}$ over all $\eta\in\mathcal{U}(\zeta)$ for $\zeta\in B_n\setminus B_{m/2}$ is bounded by $\frac{1}{(|\zeta|-d)^4}$. Now let $m>2d+2$. Bringing the above estimates together, we obtain

$$
\begin{aligned}
&|S^{(n)}_{ijkp} - S^{(m)}_{ijkp}| \\
&\quad \le c \int_{B_n \setminus B_{m/2}} \Big(\frac{1}{n^4} + \frac{1}{m^4} \chi_{B_m} + \frac{1}{(|\zeta| - d)^4} \Big)\, d\zeta \\
&\quad \le c \Big\{ \int_{m/2}^{n} \frac{1}{n^4} |\zeta|^2 \, d|\zeta| + \int_{m/2}^{m} \frac{1}{m^4} |\zeta|^2 \, d|\zeta| + \int_{m/2}^{n} \frac{|\zeta|^2}{(|\zeta| - d)^4}\, d|\zeta| \Big\} \\
&\quad \le c \Big\{ \frac{1}{n^4} \underbrace{(n^3 - (m/2)^3)}_{\le n^3} + \frac{1}{m^4} \underbrace{(m^3 - (m/2)^3)}_{\le m^3} \\
&\qquad + \Big[\frac{-1}{|\zeta| - d} + \frac{-d}{(|\zeta| - d)^2} + \frac{-d^2}{3(|\zeta| - d)^3} \Big]_{m/2}^{n} \Big\} \\
&\quad \le c \Big\{ \frac{1}{n} + \frac{1}{m} + \frac{1}{m/2 - d} + \frac{d}{(m/2 - d)^2} + \frac{d^2}{3(m/2 - d)^3} \Big\} \\
&\quad \le c \frac{1}{m/2 - d}.
\end{aligned}
$$

Since $\frac{1}{m/2-d}$ tends to zero as $m \to \infty$, $S^{(n)}_{ijkp}$ is a Cauchy sequence in n. So the limit $l \to \infty$ of $S^{(l\delta)}_{ijkp}$ exists and is moreover independent of δ. Thus we obtain

$$
\begin{aligned}
- \lim_{\delta \to 0} \lim_{l \to \infty} \sum_{z \in B_\delta \cap \frac{1}{l}\mathcal{L}^*} \partial_k (K - K^{(\delta)})_{ij}(z)(a \cdot z)_+ \frac{1}{l^3} &= \frac{1}{2} \lim_{\delta \to 0} \lim_{l \to \infty} S^{(l\delta)}_{ijkp} a_p \\
&=: \frac{1}{2} S_{ijkp} a_p.
\end{aligned}
$$

It is possible to commute the occurring partial derivatives in the definition of $S^{(l\delta)}_{ijkp}$ (cf. (28)). Since the proof of the convergence does not depend on the order of the partial derivatives, S_{ijkp} is symmetric in i, j and k. $\square$

Notice that the way in which the regularization is chosen is crucial in (30). The cut-off function $\varphi^{(n)}$ is multiplied directly by the potential N and is therefore "inside" all the derivatives and not "outside", which allows us to apply the Divergence Theorem in the described manner. Also decisive is that the term $\partial_k \partial_i \partial_j \big((\varphi^{(n)} - \varphi^{(m)})N\big)(\zeta)$ is multiplied by ξ_p in the integrand, which is a consequence of the structure of the term (27). Differentiating the second factor, i.e., ξ_p, yields a Kronecker δ_{kp}, and we can apply the Divergence Theorem to the corresponding integral. If the second factor depended nonlinearly on ξ, it would not be possible to apply the Divergence Theorem.

For a final discussion of the convergence of the short-range part $\mathcal{F}^{(l,\delta)}_k$ of the discrete force we apply Lemma 5 to (26). Since $|S^{(l\delta)}_{ijkp} n_p(\xi)| \le c|n_p(\xi)| \le c$ for all $\xi \in \partial\tau$, $0 < l\delta < \infty$ and $p = 1, 2, 3$, we can commute limiting processes and integration by Lebesgue's Convergence Theorem and obtain, with (26),

$$
\begin{aligned}
&-\lim_{\delta\to 0}\lim_{l\to\infty}\int_{\partial\tau} M_i^-(\xi)M_j^+(\xi)\sum_{z\in B_\delta\cap\frac{1}{l}\mathcal{L}^*}\partial_k(K-K^{(\delta)})_{ij}(z)(n(\xi)\cdot z)_+\frac{1}{l^3}\,d\mathcal{H}^2(\xi)\\
&=\int_{\partial\tau} M_i^-(\xi)M_j^+(\xi)\lim_{\delta\to 0}\lim_{l\to\infty}\frac{1}{2}S_{ijkp}^{(l\delta)}n_p(\xi)\,d\mathcal{H}^2(\xi)\\
&=\frac{1}{2}\int_{\partial\tau} M_i^-(\xi)M_j^+(\xi)S_{ijkp}n_p(\xi)\,d\mathcal{H}^2(\xi).
\end{aligned}
$$

Putting together the estimates of the terms of the short-range part of the discrete force, we obtain the result which is stated in Theorem 2. □

3.2. The limit of the long-range part

In this subsection we prove the existence of the continuum limit of the long-range part of the force in the discrete setting. The assumptions on M and on the sets used for this result, are summarized in the following theorem.

Theorem 3. *Let $\Omega\subset\mathbb{R}^3$, open and bounded, and $\tau\subset\Omega$ have a C^2 boundary. Moreover, let $\Omega\setminus\bar\tau$ have a C^2 boundary as well. Further let $M_{|\tau}\in W^{1,2}(\tau,\mathbb{R}^3)$ and $M_{|\Omega\setminus\bar\tau}\in W^{1,2}(\Omega\setminus\bar\tau,\mathbb{R}^3)$. Then the limit of the long-range part of the discrete force is*

$$
\begin{aligned}
\lim_{\delta\to 0}\lim_{l\to\infty} F_k^{(l,\delta)} &= \int_\tau (M(x)\cdot\nabla)(H_\Omega)_k(x)\,d^3x \qquad (32)\\
&\quad+\frac{\gamma}{2}\int_{\partial\tau}(M^-\cdot n)(x)\big((M^- - M^+)\cdot n\big)(x)n_k(x)\,d\mathcal{H}^2(x).
\end{aligned}
$$

This theorem also holds in the case of piecewise C^2 boundaries as is discussed in Section 4.

To prove Theorem 3, we first note that the magnetization $M_{|\tau}\in W^{1,2}(\tau,\mathbb{R}^3)$ can be globally approximated by smooth functions, i.e., there exists a sequence $M_{|\tau}^{(n)}\in W^{1,2}(\tau,\mathbb{R}^3)\cap C^\infty(\bar\tau,\mathbb{R}^3)$, $n\in\mathbb{N}$, such that $M_{|\tau}^{(n)}\to M_{|\tau}$ in $W^{1,2}(\tau,\mathbb{R}^3)$ as $n\to\infty$, (cf., e.g., [13, p. 127]). Similarly, $M_{|\Omega\setminus\bar\tau}$ can be approximated by smooth functions in $W^{1,2}(\Omega\setminus\bar\tau,\mathbb{R}^3)\cap C^\infty\big(\overline{\Omega\setminus\bar\tau},\mathbb{R}^3\big)$. Regularity for the solutions of Maxwell's equations [7] shows that the corresponding magnetic field converges in $W^{1,2}(\tau,\mathbb{R}^3)$ as well. Moreover, for the traces we have (see e.g. [13]) $(M_{|\tau}^{(n)})^-\to(M_{|\tau})^-$ in $L^2(\partial\tau,\mathbb{R}^3)$. Hence, if (32) holds for smooth magnetizations and magnetic fields, we can pass to the limit in (32) as $n\to\infty$. Therefore we can assume in the following without loss of generality that $M_{|\tau}$ and $M_{|\Omega\setminus\bar\tau}$ belong to $W^{1,2}(\tau,\mathbb{R}^3)\cap C^\infty(\bar\tau,\mathbb{R}^3)$ and $W^{1,2}(\Omega\setminus\bar\tau,\mathbb{R}^3)\cap C^\infty\big(\overline{\Omega\setminus\bar\tau},\mathbb{R}^3\big)$, respectively.

We obtain, since $\partial_k K_{ij}^{(\delta)}(x-y)$ is continuous and bounded for $\delta>0$, that the terms of the double sum in $F_k^{(l,\delta)}$ are continuous and bounded for $\delta>0$. Hence the double sum can be viewed as a Riemann sum, which converges as $l\to\infty$ to

$$
F_k^{(\infty,\delta)} := \lim_{l\to\infty} F_k^{(l,\delta)} = \int_\tau\int_{\Omega\setminus\bar\tau}\partial_k K_{ij}^{(\delta)}(x-y)M_i(x)M_j(y)\,d^3y\,d^3x. \qquad (33)
$$

Since $K_{ij}^{(\delta)}(x-y)$ is symmetric in its argument and in i and j, we have $\partial_k K_{ij}^{(\delta)}(x-y) \equiv \frac{\partial}{\partial x_k} K_{ij}^{(\delta)}(x-y) = -\frac{\partial}{\partial y_k} K_{ji}^{(\delta)}(y-x)$. We obtain, by a change of variables and Fubini's Theorem,

$$\begin{aligned}\int_\tau \int_\tau \partial_k K_{ij}^{(\delta)}(x-y) M_i(x) M_j(y)\, d^3y\, d^3x \\ = -\int_\tau \int_\tau \frac{\partial}{\partial y_k} K_{ji}^{(\delta)}(y-x) M_i(x) M_j(y)\, d^3y\, d^3x \\ = -\int_\tau \int_\tau \partial_k K_{ij}^{(\delta)}(x-y) M_j(y) M_i(x)\, d^3y\, d^3x,\end{aligned}$$

which is therefore zero for all $\delta > 0$, i.e., this term does not contribute in the limit. Hence (33) reads

$$F_k^{(\infty,\delta)} = \int_\tau \int_\Omega \partial_k K_{ij}^{(\delta)}(x-y) M_i(x) M_j(y)\, d^3y\, d^3x.$$

With $\partial_{x_k} K_{ij}^{(\delta)}(x-y) = \partial_{x_i} K_{kj}^{(\delta)}(x-y)$ we obtain, for $\delta > 0$,

$$\begin{aligned}F_k^{(\infty,\delta)} &= \int_\tau M_i(x) \int_\Omega \partial_{x_k} K_{ij}^{(\delta)}(x-y) M_j(y)\, d^3y\, d^3x \\ &= \int_\tau M_i(x) \partial_{x_i} \Big(\int_\Omega K_{kj}^{(\delta)}(x-y) M_j(y)\, d^3y \Big)\, d^3x.\end{aligned}$$

We set $(H_\Omega^{(\delta)})_k(x) := \int_\Omega K_{kj}^{(\delta)}(x-y) M_j(y)\, d^3y$ and get, after an integration by parts,

$$F_k^{(\infty,\delta)} = \int_\tau (-\nabla \cdot M)(x) (H_\Omega^{(\delta)})_k(x)\, d^3x \tag{34}$$

$$+ \int_{\partial\tau} (M \cdot n)^-(x) (H_\Omega^{(\delta)})_k^-(x)\, d\mathcal{H}^2(x), \tag{35}$$

where $^-$ again denotes inner traces.

To prove that $F_k^{(\infty,\delta)}$ converges to the desired formula in (32) as $\delta \to 0$, we show the convergence of the integrals in (34) and (35) separately. For this, notice that H_Ω is the field generated by the magnetization M in Ω and is a solution of Maxwell's equations. If we set $H_\Omega = -\nabla u$, the corresponding Maxwell equations become the Poisson equation

$$-\Delta u = -\gamma \nabla \cdot M_{|\Omega} \quad \text{in} \quad \mathbb{R}^3 \setminus \partial\tau \tag{36}$$

with transition condition $[\nabla u \cdot n] = \gamma [M \cdot n]$ on $\partial\tau$. If $x \in \tau$, the integral representation of H_Ω is given by

$$\begin{aligned}(H_\Omega)_k(x) = (-\partial_k u)(x) = &-\int_{\tau \cup \Omega \setminus \bar\tau} (-\nabla \cdot M)(y) \partial_k N(x-y)\, d^3y \\ &- \int_{\partial\tau} \big((M^- - M^+) \cdot n\big)(y) \partial_k N(x-y)\, d\mathcal{H}^2(y),\end{aligned}$$

where $N(z) = \frac{\gamma}{4\pi}\frac{1}{|z|}$ as before. By definition of $H_\Omega^{(\delta)}$, we have

$$(H_\Omega^{(\delta)})_k(x) = -\int_{\tau\cup\Omega\setminus\bar\tau} (-\nabla\cdot M)(y)\partial_k\big((1-\varphi^{(\delta)}(x-y))N(x-y)\big)\,d^3y$$
$$-\int_{\partial\tau}\big((M^- - M^+)\cdot n\big)(y)\partial_k\big((1-\varphi^{(\delta)}(x-y))N(x-y)\big)\,d\mathcal{H}^2(y).$$

We first consider the volume integral of $(H_\Omega^{(\delta)})_k(x)$ and show that this converges uniformly in $x\in\tau$ to the volume term of $(H_\Omega)_k(x)$. Here and in the following, c denotes again positive generic constants, which do not always have to be the same. By assumption, $\nabla\cdot M$ is bounded on τ and on $\Omega\setminus\bar\tau$, and $\varphi^{(\delta)}$ is supported in the ball $B_\delta(x)$ and its derivative has support in $B_\delta(x)\setminus B_{\delta/2}(x)$. Moreover, $|\partial_k\varphi^{(\delta)}(z)| \le \frac{c}{|z|}$ by the fact that $|\partial_k\varphi^{(\delta)}(z)| \le \frac{c}{\delta}$ and by $\partial_k\varphi^{(\delta)}(z) = 0$ if $|z|>\delta$. Hence

$$\Big|\partial_k\Big(\varphi^{(\delta)}(x-y)N(x-y)\Big)\Big| \le c\frac{1}{|x-y|^2}. \tag{37}$$

Thus

$$\Big|\int_{\tau\cup\Omega\setminus\bar\tau}(-\nabla\cdot M)(y)\partial_k\big(\varphi^{(\delta)}(x-y)N(x-y)\big)\,d^3y\Big|$$
$$\le c\int_{B_\delta(x)}\frac{1}{|x-y|^2}\,d^3y \le c\delta, \tag{38}$$

and the uniform convergence of the volume term follows.

For the boundary integral, i.e.,

$$(H_\Omega^{(\delta,2)})_k(x) := -\int_{\partial\tau}\phi(y)\partial_k\big((1-\varphi^{(\delta)}(x-y))N(x-y)\big)\,d\mathcal{H}^2(y)$$

with $\phi := -[M\cdot n] = (M^- - M^+)\cdot n$, we consider first the case $x\in\tau$. If we can show that

$$(H_\Omega^{(\delta,2)})_k \longrightarrow (H_\Omega^{(2)})_k \qquad \text{in} \quad L^1(\tau) \quad \text{as} \quad \delta\to 0, \tag{39}$$

where

$$(H_\Omega^{(2)})_k(x) := -\int_{\partial\tau}\phi(y)\partial_k N(x-y)\,d\mathcal{H}^2(y)$$
$$= \frac{\gamma}{4\pi}\int_{\partial\tau}\phi(y)\frac{(x-y)_k}{|x-y|^3}\,d\mathcal{H}^2(y),$$

we can pass to the limit in (34).

To prove (39), set $U_\alpha := \{x\in\tau \,:\, \mathrm{dist}(x,\partial\tau)>\alpha\}$. For $\alpha>0$, $H_\Omega^{(\delta,2)}(x)$ converges uniformly to $H_\Omega^{(2)}(x)$ on the set U_α. Thus it suffices to show that for each $\varepsilon>0$ there exists an $\alpha>0$ such that

$$\int_{\tau\setminus U_\alpha}|(H_\Omega^{(\delta,2)})_k(x)|\,d^3x < \frac{\varepsilon}{2} \tag{40}$$

and

$$\int_{\tau\setminus U_\alpha} |(H_\Omega^{(2)})_k(x)|\, d^3x < \frac{\epsilon}{2}, \tag{41}$$

since this yields by

$$\begin{aligned}\int_\tau |(H_\Omega^{(\delta,2)})_k(x) - (H_\Omega^{(2)})_k(x)|\, d^3x \\ \leq \int_{U_\alpha} |(H_\Omega^{(\delta,2)})_k(x) - (H_\Omega^{(2)})_k(x)|\, d^3x + \int_{\tau\setminus U_\alpha} |(H_\Omega^{(\delta,2)})_k(x)|\, d^3x \\ + \int_{\tau\setminus U_\alpha} |(H_\Omega^{(2)})_k(x)|\, d^3x\end{aligned}$$

the desired convergence in (39).

To show (40), note that by (37) and by the boundedness of $\phi = (M^- - M^+)\cdot n$, we have

$$\begin{aligned}\int_{\tau\setminus U_\alpha} |(H_\Omega^{(\delta,2)})_k(x)|\, d^3x &\leq c\int_{\tau\setminus U_\alpha}\int_{\partial\tau} \frac{1}{|x-y|^2}\, d\mathcal{H}^2(y)\, d^3x \\ &= c\int_{\partial\tau}\int_{\tau\setminus U_\alpha} 1\cdot\frac{1}{|x-y|^2}\, d^3x\, d\mathcal{H}^2(y).\end{aligned}$$

The integral $\int_{\tau\setminus U_\alpha}\frac{1}{|x-y|^{5/2}}\, d^3x$ is bounded independently of α. Hence, by Hölder's inequality,

$$\begin{aligned}\int_{\tau\setminus U_\alpha} |(H_\Omega^{(\delta,2)})_k(x)|\, d^3x \\ \leq c\int_{\partial\tau}\Big(\int_{\tau\setminus U_\alpha} 1\, d^3x\Big)^{\frac{1}{5}}\Big(\int_{\tau\setminus U_\alpha}\frac{1}{|x-y|^{\frac{5}{2}}}\, d^3x\Big)^{\frac{4}{5}}\, d\mathcal{H}^2(y) \\ \leq c\,\mathcal{H}^2(\partial\tau)\,|\tau\setminus U_\alpha|^{\frac{1}{5}}.\end{aligned}$$

Since $|\tau\setminus U_\alpha| \leq c\alpha\mathcal{H}^2(\partial\tau)$ by construction, we obtain (40). Similarly we get (41) and hence (39).

If $x \in \partial\tau$, we show that the limiting magnetic field is given by

$$\bar{H}_\Omega(x) = \frac{\gamma}{4\pi}\int_{\tau\cup\Omega\setminus\bar{\tau}} (-\nabla\cdot M)(y)\frac{x-y}{|x-y|^3}\, d^3y + (\mathcal{B}\phi)(x), \tag{42}$$

where

$$(\mathcal{B}\phi)(x) := \lim_{\delta\to 0}\frac{\gamma}{4\pi}\int_{\partial\tau}(1-\varphi^{(\delta)}(x-y))\phi(y)\frac{x-y}{|x-y|^3}\, d\mathcal{H}^2(y), \tag{43}$$

the convergence being uniform in $x \in \partial\tau$.

The convergence of the volume term of $H_\Omega^{(\delta)}(x)$ follows from (38). Hence it remains to show the convergence of the surface term to $(-\nabla u^{(2)})(x) = (\mathcal{B}\phi)(x)$ for $x \in \partial\tau$. This is done by considering the derivatives in tangential and in normal direction separately. The following two lemmas will be proved in the appendix.

Lemma 6. *Let τ and M fulfill the same conditions as in Theorem 3. Then the tangential derivative of $u^{(2)}$ exists for all $x \in \partial\tau$ and is given by*

$$(-\nabla_t u^{(2)})(x) = (\mathcal{T}\phi)(x),$$

where

$$(\mathcal{T}\phi)(x) := \lim_{\delta\to 0} \frac{\gamma}{4\pi} \int_{\partial\tau} (1 - \varphi^{(\delta)}(x-y))\phi(y) \frac{(x-y)_t}{|x-y|^3}\, d\mathcal{H}^2(y).$$

The convergence is uniform.

Hence the tangential component of H_Ω on $\partial\tau$ is given by

$$(H_\Omega)_t(x) = (-\nabla_t u)(x) = \frac{\gamma}{4\pi} \int_{\tau\cup\Omega\setminus\bar{\tau}} (-\nabla\cdot M)(y) \frac{(x-y)_t}{|x-y|^3}\, d^3y \;+\; (\mathcal{T}\phi)(x). \tag{44}$$

While the tangential derivative is continuous at the boundary, the normal derivative jumps at $\partial\tau$.

Lemma 7. *Let τ and M fulfill the same conditions as in Theorem 3. Then $(-\nabla u^{(2)} \cdot n)(x+\alpha n(x))$ and $(-\nabla u^{(2)} \cdot n)(x-\alpha n(x))$ converge uniformly on $\partial\tau$ to continuous limits $(-\nabla u^{(2)} \cdot n)^+(x)$ and $(-\nabla u^{(2)} \cdot n)^-(x)$, respectively, as $\alpha \to 0$. The normal derivatives of $u^{(2)}(x)$ are given by*

$$(-\nabla u^{(2)} \cdot n)^\pm(x) = \pm\frac{1}{2}\gamma\phi(x) + (\mathcal{N}\phi)(x),$$

where

$$(\mathcal{N}\phi)(x) := \lim_{\delta\to 0} \frac{\gamma}{4\pi} \int_{\partial\tau} (1 - \varphi^{(\delta)}(x-y))\phi(y) \frac{(x-y)\cdot n(x)}{|x-y|^3}\, d\mathcal{H}^2(y).$$

A consequence of the jump of the normal derivative of $u^{(2)}$ is that the normal component of the magnetic field H_Ω jumps at $\partial\tau$. If $x \in \partial\tau$, the traces are given by

$$\begin{aligned}
&(H_\Omega \cdot n)^\pm(x) \\
&\quad= \frac{\gamma}{4\pi} \int_{\tau\cup\Omega\setminus\bar{\tau}} (-\nabla\cdot M)(y) \frac{(x-y)\cdot n(x)}{|x-y|^3}\, d^3y \pm \frac{\gamma}{2}\phi(x) + (\mathcal{N}\phi)(x).
\end{aligned}$$

Summarizing the results for the normal and tangential derivatives on the boundary, we obtain for the traces of the magnetic field at $x \in \partial\tau$,

$$\begin{aligned}
H_\Omega^\pm(x) &= (H_\Omega)_t(x) + (H_\Omega \cdot n)^\pm(x) n(x) \\
&= \frac{\gamma}{4\pi} \int_{\tau\cup\Omega\setminus\bar{\tau}} (-\nabla\cdot M)(y) \frac{x-y}{|x-y|^3}\, d^3y \;+ (\mathcal{T}\phi)(x) \pm \frac{\gamma}{2}\phi(x) n(x) \\
&\quad + (\mathcal{N}\phi)(x) n(x) \\
&= \frac{\gamma}{4\pi} \int_{\tau\cup\Omega\setminus\bar{\tau}} (-\nabla\cdot M)(y) \frac{x-y}{|x-y|^3}\, d^3y \;+\; (\mathcal{B}\phi)(x) \pm \frac{\gamma}{2}\phi(x) n(x),
\end{aligned}$$

where $(\mathcal{B}\phi)(x) := (\mathcal{T}\phi)(x) + (\mathcal{N}\phi)(x)n(x)$ gives (43). Thus $\bar{H}_\Omega(x) = \frac{1}{2}(H_\Omega^+ + H_\Omega^-)(x)$. Since the tangential component of H_Ω is continuous across the interface, we have, by the transition condition for the normal component of H_Ω,

$$\begin{aligned}\bar{H}_\Omega(x) &= \frac{1}{2}(H_\Omega^+ - H_\Omega^-)(x) + H_\Omega^-(x) \\ &= -\frac{\gamma}{2}\Big((M^+ \cdot n)(x) - (M^- \cdot n)(x)\Big)n(x) + H_\Omega^-(x) \\ &= \frac{\gamma}{2}\big((M^- - M^+)\cdot n\big)(x)n(x) + H_\Omega^-(x). \end{aligned} \tag{45}$$

Next we apply the convergence results (39) and (42) to obtain the limits of the terms in (34) and (35). Notice that $(H_\Omega^{(\delta)})^-(x) = H_\Omega^{(\delta)}(x)$ for $\delta > 0$. In summary we get

$$\begin{aligned}&\lim_{\delta\to 0}\int_\tau\int_\Omega \partial_k K_{ij}^{(\delta)}(x-y)M_i(x)M_j(y)\,d^3y\,d^3x \\ &\quad= \lim_{\delta\to 0}\int_\tau -(\nabla\cdot M)(x)(H_\Omega^{(\delta)})_k(x)\,d^3x \\ &\qquad+ \lim_{\delta\to 0}\int_{\partial\tau}(M\cdot n)^-(x)(H_\Omega^{(\delta)})_k^-(x)\,d\mathcal{H}^2(x) \qquad (46)\\ &\quad= \int_\tau -(\nabla\cdot M)(x)(H_\Omega)_k(x)\,d^3x + \int_{\partial\tau}(M\cdot n)^-(x)(\bar{H}_\Omega)_k(x)\,d\mathcal{H}^2(x) \\ &\quad= \int_\tau -(\nabla\cdot M)(x)(H_\Omega)_k(x)\,d^3x + \int_{\partial\tau}(M\cdot n)^-(x)(H_\Omega)_k^-(x)\,d\mathcal{H}^2(x) \\ &\qquad+ \frac{\gamma}{2}\int_{\partial\tau}(M\cdot n)^-(x)\big((M^- - M^+)\cdot n\big)(x)n_k(x)\,d\mathcal{H}^2(x), \qquad (47)\end{aligned}$$

where the last equation follows with (45). Finally, an integration by parts yields

$$\begin{aligned}\lim_{\delta\to 0} F_k^{(\infty,\delta)} &= \int_\tau (M(x)\cdot\nabla)(H_\Omega)_k(x)\,d^3x \\ &\quad+ \frac{\gamma}{2}\int_{\partial\tau}(M\cdot n)^-(x)\big((M^- - M^+)\cdot n\big)(x)n_k(x)\,d\mathcal{H}^2(x),\end{aligned}$$

as is stated in Theorem 3.

If we now combine Theorem 2 and Theorem 3, we obtain Theorem 1. □

4. Magnetic force in piecewise C^2 domains

This section is about a generalization of Theorem 1 to the case of Lipschitz continuous and piecewise C^2 domains. That is, $\partial\tau$ is assumed to be locally the graph of a Lipschitz continuous function and τ is on one side of the boundary only. Moreover, there exist finitely many pairwise disjoint sets $U_i \subset \partial\tau$ which are relatively open in $\partial\tau$ and have the following properties: (i) U_i is an orientable C^2 submanifold of $\mathbb{R}^3$ and its normal is C^1 up to the boundary, (ii) $\partial\tau \subset \cup_i \bar{U}_i$ and (iii) ∂U_i is a finite union of rectifiable curves.

As the normal is no langer defined in every point of the boundary, some of the above equations only hold almost everywhere in $\partial\tau$. Since we are mainly interested in integrals, this does not effect the estimates.

In the proof of the limit of the short-range term (Theorem 2) we did not use the fact that $\partial\tau$ is C^2. We assumed that $\partial\tau$ satisfies the non-degeneracy condition (S), which is also assumed in this section, and is therefore in particular piecewise $C^{1,1}$ and Lipschitz continuous. Hence we only need to focus on the limit of the long range part of the force (Section 3.2) in the following.

In the beginning of the proof of Theorem 3 we argued that it suffices to consider smooth magnetizations instead of general magnetizations in $W^{1,2}$. The estimate is based on a regularity result [7] for solutions of Maxwell's equations, which no longer hold in general if the domain has edges and corners. To circumvent the estimate, we assume in the following that $M_{|\tau} \in W^{1,\infty}(\tau, \mathbb{R}^3)$ and $M_{|\Omega\setminus\bar{\tau}} \in W^{1,\infty}(\Omega\setminus\bar{\tau}, \mathbb{R}^3)$. This is also assumed in Theorem 1 and is a reasonable assumption on the magnetization. As in the proof of Theorem 2 we will work with representatives that are in $C^{0,1}(\bar{\tau}, \mathbb{R}^3)$ and $C^{0,1}(\overline{\Omega\setminus\bar{\tau}}, \mathbb{R}^3)$, respectively.

Under these assumptions we assert that the limit of the long-range part of the discrete force is, as before, given by (32). To prove this, note that the lattice sum $F_k^{(l,\delta)}$ is again a Riemann sum that converges to (33) as $l \to \infty$. In τ, the convergence of the magnetic field as $\delta \to 0$ can be proved analogously to before. To prove (39), note that $|\tau \setminus U_\alpha| \le c\alpha\mathcal{H}^2(\partial\tau)$ still holds under the above assumptions on $\partial\tau$.

The convergence of the volume term of the magnetic field on $\partial\tau$ as $\delta \to 0$ follows again from (38). Regarding the convergence of the surface term of the magnetic field $H_\Omega^{(\delta,2)}$ on $\partial\tau$, note that τ is assumed to be a C^2 domain in Lemma 6 and Lemma 7, which therefore cannot be applied here. In fact, if τ has edges and corners, we no longer have uniform convergence. However, we still obtain uniform convergence on compact subsets of the C^2 submanifolds $U_i \subset \partial\tau$: Let $r_0 > 0$. Set $\Gamma = \cup_i \partial U_i$ and $\mathcal{V}_{r_0} = \{x \in \partial\tau \,:\, \operatorname{dist}(x,\Gamma) < r_0\}$. Then $H_\Omega^{(\delta,2)}(x)$ converges uniformly to $\bar{H}_\Omega^{(2)}(x) := \mathcal{B}\phi(x)$ in $x \in \partial\tau \setminus \mathcal{V}_{r_0}$ as $\delta \to 0$.

If we show in addition that $H_\Omega^{(\delta,2)} \to \bar{H}_\Omega^{(2)}$ in $L^1(\mathcal{V}_{r_0})$ as $\delta \to 0$, we can pass to the limit in (46) as $(M\cdot n)^-$ is bounded almost everywhere. The L^1-convergence can be proved using Lebesgue's Convergence Theorem. Indeed, $H_\Omega^{(\delta,2)}(x)$ converges to $\bar{H}_\Omega^{(2)}(x)$ for almost every $x \in \partial\tau$. Now let $x \in \mathcal{V}_{r_0}$ and $r = \frac{1}{2}\operatorname{dist}(x,\Gamma)$. Then

$$
\begin{aligned}
H_\Omega^{(\delta,2)}(x) = &\int_{\partial\tau\setminus B(x,r)} \phi(y)\nabla N^{(\delta)}(x-y)\, d\mathcal{H}^2(y) \\
&+ \int_{\partial\tau\cap B(x,r)} \phi(y)\nabla N^{(\delta)}(x-y)\, d\mathcal{H}^2(y).
\end{aligned}
$$

As in the proof of Lemma 6 and 7 in the Appendix, it can be shown that the second term converges uniformly in x since $\partial\tau \cap B(x,r)$ is contained in $\cup_i U_i$. The first term is bounded by $\int_{\partial\tau\setminus B(x,r)} \frac{c}{|x-y|^2}\, d\mathcal{H}^2(y)$ and hence by $c\int_r^{\operatorname{diam}(\tau)} \frac{1}{\rho}\, d\rho$. This can be estimated by $c \ln \frac{1}{\operatorname{dist}(x,\Gamma)}$ for all $\delta > 0$, which is an integrable function on $\mathcal{V}_{r_0}$. Hence (47) follows.

Finally, we show $\nabla H_\Omega \in L^1(\tau)$ and integrate (47) by parts as in the end of the proof of Theorem 3. The integrability of the volume term follows by standard singular integral estimates. For the estimate of the surface integral $\nabla H_\Omega^{(2)}$, we split τ into three sets $\tau^{(1)}$, $\tau^{(2)}$ and $\tau^{(3)}$, where for $0 < r_0 < 1$ and $\epsilon > 0$,

$$\begin{aligned}
\tau^{(1)} &:= \{x \in \tau \,:\, \operatorname{dist}(x, \partial\tau) \geq r_0^{1+\epsilon}\},\\
\tau^{(2)} &:= \{x \in \tau \,:\, r_0^{1+\epsilon} \geq \operatorname{dist}(x, \partial\tau) \geq \operatorname{dist}(x, \Gamma)^{1+\epsilon}\},\\
\tau^{(3)} &:= \{x \in \tau \,:\, \operatorname{dist}(x, \partial\tau) \leq \operatorname{dist}(x, \Gamma)^{1+\epsilon},\ \operatorname{dist}(x, \partial\tau) \leq r_0^{1+\epsilon}\}.
\end{aligned}$$

Observe that, for $x \notin \partial\tau$,

$$\begin{aligned}
|\nabla H_\Omega^{(2)}(x)| &\leq c \int_{\partial\tau} \frac{1}{|x-y|^3}\, d\mathcal{H}^2(y) = \int_{\partial\tau} \Big(\int_0^\infty \chi_{|x-y|<\rho} \frac{3}{\rho^4}\, d\rho \Big) d\mathcal{H}^2(y)\\
&= c \int_0^\infty \frac{3}{\rho^4} \mathcal{H}^2(\partial\tau \cap B(x,\rho))\, d\rho \leq c \int_{\operatorname{dist}(x,\partial\tau)}^\infty \frac{1}{\rho^2}\, d\rho\\
&\leq \frac{c}{\operatorname{dist}(x, \partial\tau)}. \qquad (48)
\end{aligned}$$

We will use similar estimates also in the following without explicitly mentioning this. By definition of $\tau^{(1)}$ and (48) we have $\int_{\tau^{(1)}} |\nabla H_\Omega^{(2)}(x)|\, d^3x \leq \frac{c}{r_0^{1+\epsilon}} \leq c$.

To estimate $\nabla H_\Omega^{(2)}$ on $\tau^{(2)}$, note that $|\nabla H_\Omega^{(2)}(x)| \leq \frac{c}{\operatorname{dist}(x,\Gamma)^{1+\epsilon}}$ for all $x \in \tau^{(2)}$ by (48) and the definition of $\tau^{(2)}$. By a covering argument, the volume of $\{x \in \tau \,:\, \operatorname{dist}(x, \Gamma) \leq r_0\}$ can be bounded by cr_0^2, which shows that $\frac{1}{\operatorname{dist}(x,\Gamma)^{1+\epsilon}}$ is integrable on $\tau^{(2)}$.

On $\tau^{(3)}$ we proceed as follows. Set $r = \min\{\operatorname{dist}(x, \Gamma), r_0\}$ and let $x \in \tau^{(3)}$. Then

$$\begin{aligned}
\Big| \int_{\partial\tau \setminus B(x,r)} \phi(y) \nabla^2 N(x-y)\, d\mathcal{H}^2(y) \Big| &\leq c \int_{\partial\tau \setminus B(x,r)} \frac{1}{|x-y|^3}\, d\mathcal{H}^2(y)\\
&\leq c \int_r^\infty \frac{1}{\rho^2}\, d\rho \leq \frac{c}{r} \leq \frac{c}{\operatorname{dist}(x, \partial\tau)^{\frac{1}{1+\epsilon}}},
\end{aligned}$$

which is integrable on $\tau^{(3)}$. It remains to estimate

$$\begin{aligned}
\int_{\partial\tau \cap B(x,r)} \phi(y) \nabla^2 N(x-y)\, d\mathcal{H}^2(y) &= \int_{\partial\tau \cap B(x,r)} \phi(x) \nabla^2 N(x-y)\, d\mathcal{H}^2(y)\\
&\quad + \int_{\partial\tau \cap B(x,r)} \big(\phi(y) - \phi(x)\big) \nabla^2\\
&\quad \times N(x-y)\, d\mathcal{H}^2(y).
\end{aligned}$$

Since ϕ is Lipschitz continuous, the second integral is bounded by $c \int_{\operatorname{dist}(x,\partial\tau)}^r \frac{1}{\rho}\, d\rho$ and hence by $c \ln \frac{1}{\operatorname{dist}(x,\partial\tau)}$, which is integrable on $\tau^{(3)}$. For the estimate of the integral $\int_{\partial\tau \cap B(x,r)} \nabla^2 N(x-y)\, d\mathcal{H}^2(y)$, assume that $\partial\tau \cap B(x, r)$ is connected and contained in one of the C^2 submanifolds U_i, otherwise apply the following arguments to each of the connected components restricted to one of the C^2 submanifolds.

Now choose a parametrization $\psi : \mathbb{R}^2 \to \mathbb{R}^3$, $y' \mapsto \psi(y') = (y', \psi_3(y')) = y$ of $\partial\tau \cap B(x,r)$ such that there is a $\tilde{c}$ with $0 < \tilde{c} < 1$ and $B(x', \tilde{c}r) \subset \psi^{-1}(\partial\tau \cap B(x,r))$, where x' is the orthogonal projection of x on $\mathbb{R}^2$. Then $\int_{\partial\tau\cap B(x,r)} \nabla^2 N(x-y)\, d\mathcal{H}^2(y)$ equals

$$\begin{aligned}\int_{\psi^{-1}(\partial\tau\cap B(x,r))} &\nabla^2 N(x-\psi(y'))J_\psi(y')\, d^2y' \\ &= \int_{\psi^{-1}(\partial\tau\cap B(x,r))\setminus B(x',\tilde{c}r)} \nabla^2 N(x-\psi(y'))J_\psi(y')\, d^2y' \\ &\quad + \int_{B(x',\tilde{c}r)} \nabla^2 N(x-\psi(y'))J_\psi(y')\, d^2y'.\end{aligned}$$

The first integral can be estimated by $c\int_{B(x',r)\setminus B(x',\tilde{c}r)} \frac{1}{|x-\psi(y')|^3}\, d^2y'$. Since $|x - \psi(y')|^3 \geq |x'-y'|^3$, we can show that the first integral is bounded by $\frac{c}{r}$ and hence by $c\,\mathrm{dist}(x,\partial\tau)^{-\frac{1}{1+\epsilon}}$.

To estimate the second integral, we consider an orthonormal basis (t_1, t_2, ν) at $\psi(y')$ where ν is the normal at $\psi(y')$ to $\partial\tau$. It varies in a C^1 way along $\partial\tau$. Let $\nabla_{t_1}N$, $\nabla_{t_2}N$ and $\nabla_\nu N$ denote the derivative of N in the direction of t_1, t_2 and ν, respectively. We write $\nabla^2 N$ in terms of $\nabla_{t_1}N$, $\nabla_{t_2}N$ and $\nabla_\nu N$. Since $\Delta N = 0$, we have $\nabla_\nu^2 N = -\nabla_{t_1}^2 N - \nabla_{t_2}^2 N$. Thus it suffices to consider the expressions $(\nabla_{t_i}\nabla_{t_j})N$, which we discuss in the following, and $(\nabla_{t_i}\nabla_\nu)N$, which can be dealt with analogously. Here, $i, j \in \{1,2\}$. We have $(\nabla_{t_i}\nabla_{t_j})N = \nabla_{t_i}(\nabla_{t_j}N) - (\nabla N)\nabla_{t_i}t_j$. Since $\partial\tau$ is piecewise C^2, we have $|\nabla_{t_i}t_j| \leq C$. Thus $(\nabla N)\nabla_{t_i}t_j$ is bounded by $c|\nabla N|$.

The tangential derivative can be written in terms of y'. There is an invertible matrix $(a_{ij})_{i,j=1,2}$ such that $t_i = a_{ik}(y')\partial_k\psi(y')$. Moreover, $y' \mapsto a_{ik}(y')$ is C^1. Hence $\big(\nabla_{t_i}(\nabla_{t_j}N)\big)(x-\psi(y')) = \big(a_{ik}(y')(\partial_k\psi)(y')\cdot(\nabla_{t_j}N)\big)(x-\psi(y'))$, which equals $-\big(a_{ik}(y')\partial_k(\nabla_{t_j}N)\big)(x-\psi(y'))$. Thus we can integrate by parts. In total we obtain

$$\begin{aligned}\int_{B(x',\tilde{c}r)} &\nabla^2 N(x-\psi(y'))J_\psi(y')\, d^2y' \\ &\leq c\int_{B(x',\tilde{c}r)} |\nabla N(x-\psi(y'))|\, d^2y' + c\int_{\partial B(x',\tilde{c}r)} |\nabla N(x-\psi(y'))|\, d\mathcal{H}^1(y') \\ &\leq \int_{B(x',\tilde{c}r)} \frac{c}{|x-\psi(y')|^2}\, d^2y' + \int_{\partial B(x',\tilde{c}r)} \frac{c}{|x-\psi(y')|^2}\, d\mathcal{H}^1(y').\end{aligned}$$

Since $|x-\psi(y')| \geq \mathrm{dist}(x,\partial\tau) > 0$, the first integral can be estimated by $c\ln\frac{1}{\mathrm{dist}(x,\partial\tau)} \leq c\,\mathrm{dist}(x,\partial\tau)^{-\frac{1}{1+\epsilon}}$. The boundary integral can be estimated by $\int_{\partial B(x',\tilde{c}r)} \frac{c}{|x'-y'|^2}\, d^2y'$ because $|x-\psi(y')| \geq |x'-y'|$. This integral can be bounded by $\frac{c\tilde{c}r}{\tilde{c}^2r^2} \leq c\,\mathrm{dist}(x,\partial\tau)^{-\frac{1}{1+\epsilon}}$ as $x \in \tau^{(3)}$, which shows that $|\nabla H_\Omega^{(2)}(x)|$ has an integrable bound on $\tau^{(3)}$.

It follows that $\nabla H_\Omega \in L^1(\tau)$. If we now integrate (47) by parts, the stated force formula is obtained. That is, the magnetic-force formula in Theorem 1 also holds in the case of piecewise C^2 domains that satisfy the non-degeneracy condition (S).

5. Closing remarks

In this paper we have derived a limiting force formula (5) from a discrete setting of magnetic moments. The nonlocal volume term of this force formula agrees with the one in Brown's force formula (1). Moreover, both formulae consist of nonlinear surface terms. In view of Cauchy's Theorem in continuum mechanics (cf. also our discussion in the introduction), we compare the force formulae in the case of a smooth magnetization in Ω. If M does not jump at $\partial\tau$, the nonlinear surface term in the limiting force vanishes. In contrast, the nonlinear surface term $\frac{\gamma}{2}\int_{\partial\tau}(M\cdot n)^2 n$ in Brown's formula remains. As already mentioned in the introduction, Brown was aware of this fact [5, Section 5]. In order to obtain a linear surface force density in agreement with Cauchy's Theorem, he proposed the existence of some additional surface term which cancels the nonlinearity, but he did not give an explicit formula. The surface term $-\frac{\gamma}{2}\int_{\partial\tau}(M^-\cdot n)(M^+\cdot n)n$ in the limiting force can now be regarded as (part of) the proposed additional term. This is $-\frac{\gamma}{2}\int_{\partial\tau}(M\cdot n)^2 n$ if M is smooth in Ω. Hence the surface terms of the force are linear in n in the smooth case as stated in Cauchy's Theorem. For a discussion of the surface term in Brown's formula see also [9].

The derivation of the continuum limit of the discrete force yields an additional surface integral that is linear in the normal and that also occurs if the magnetization is smooth in Ω. This term comes from the short-range contributions of the force in the discrete setting and is due to a lattice approximation of a hypersingular integral. It reflects the underlying lattice structure. This phenomenon is also known in other systems of magnetic dipoles, cf. [1, pp. 142–145], [6, p. 33], [23, pp. 137–139] and [20] for studies of the limiting energy of a lattice of dipoles.

Regarding the comparison of the two force formulae we finally mention that the limiting force formula coincides with Brown's formula if the considered "body" consists of two separated subparts. For this let $\Omega = A\cup B\subset\mathbb{R}^3$ with $\bar{A}\cap\bar{B}=\emptyset$. Moreover, let H_Ω be the magnetic field generated by the magnetization in Ω, and let n_A denote the outer normal to ∂A. If A and B have piecewise C^2 boundaries and $M_{|A}\in W^{1,\infty}(A,\mathbb{R}^3)$ and $M_{|B}\in W^{1,\infty}(B,\mathbb{R}^3)$, then we obtain

$$F^{(\mathrm{lim,sep})} = \int_A (M(x)\cdot\nabla)H_\Omega(x)\,d^3x + \frac{\gamma}{2}\int_{\partial A}(M^-\cdot n_A)^2(x)n_A(x)\,d\mathcal{H}^2(x).$$

This can be shown similarly to the derivation of the limiting force, but more easily since the short-range part of the discrete force is zero for δ sufficiently small.

There is a natural analog for the corresponding problem involving electric polarization, if there are no free charges. Indeed, the force between two electric dipoles has the same form as for two magnetic dipoles.

Open problems with respect to the limiting magnetic formula regard the required regularity of the sets and magnetizations. A further step might be to prove the result for piecewise C^1 or Lipschitz continuous boundaries. For appropriate results for boundary layer integrals we can probably go back to [14] for C^1 domains and [29] for Lipschitz domains. To be able to investigate sequences of boundaries which oscillate around their limit, i.e., to model rough boundaries, it would be a first step to weaken the already mild non-degeneracy condition (S) as this restricts the number of indentations and protrusions of τ.

Regarding an application of the magnetic-force formulae to magnetoelastic materials, notice that the sets τ and Ω and the scaled Bravais lattice $\frac{1}{l}\mathcal{L}$ correspond to the deformed configuration of the elastic material. In ferromagnetic shape-memory alloys the deformation gradient jumps at the same interfaces as the magnetization. The deformation gradients satisfy certain compatibility conditions across the interface, which are well known in nonlinear elasticity (see [2, 3, 19] and, e.g., [24]) and will probably be useful if implemented.

Finally, we return to the topic of a dynamic theory for the deformation of a ferromagnetic shape-memory alloy due to an external magnetic field, which we mentioned in the introduction. Based on Brown's force formula and his approach to a magnetoelastic theory, JAMES develops a dynamic theory [19] within a continuum setting. It would be interesting to combine his calculations with our result for the limiting formula derived from the discrete setting.

6. Appendix

6.1. The singular sum in the case of a cubic lattice

The surface integral of the continuum force consists of the lattice sum

$$S_{ijkp} = -\lim_{\delta\to 0}\lim_{l\to\infty}\sum_{z\in B_\delta\cap\frac{1}{l}\mathcal{L}^*}\partial_k(K-K^{(\delta)})_{ij}(z)z_p\frac{1}{l^3}.$$

The existence of the limits is the assertion of Lemma 5. Moreover we know that S_{ijkp} is symmetric in i, j, k. An explicit formula of S_{ijkp} is not known due to the form of the lattice sum, which is only conditionally convergent. Formula (49) seems to be somehow more explicit and will be used in the following. However, the former shows the modelling on which the derivation of the force formula is based explicitly.

We denote the 4-tensor $(S_{ijkp})_{i,j,k,p=1,2,3}$ by S and will show that S is not identically zero in general. In order to evaluate S, we recall that, as discussed in the proof of Lemma 5,

$$\begin{aligned} S_{ijkp} &= -\lim_{n\to\infty}\sum_{z\in B_n\cap\mathcal{L}^*}\Big(\partial_k\partial_i\partial_j\big(\varphi^{(n)}N\big)(z)\Big)z_p \\ &=: -\lim_{n\to\infty}\sum_{z\in B_n\cap\mathcal{L}^*}L^{(n)}_{ijkp}(z). \end{aligned} \tag{49}$$

Notice that $\varphi^{(n)}$ does not denote the nth derivative of φ but the regularizing function, which is $\varphi^{(n)}(z) = \varphi^{(n)}(|z|)$. The exterior derivative of $\varphi^{(n)}(z)$ is denoted by $\varphi^{(n)\prime}(z)$, the second exterior derivative by $\varphi^{(n)\prime\prime}(z)$ etc. The support of all these derivatives is contained in $B_n\setminus B_{n/2}$ by construction. For instance we have $\partial_j\varphi^{(n)}(z) = \frac{z_j}{|z|}\varphi^{(n)\prime}(z)$. With this we obtain

$$\partial_k \partial_i \partial_j (\varphi^{(n)} N)(z)$$
$$= \underbrace{\frac{\gamma}{4\pi}\Big(\frac{3}{|z|^5}\varphi^{(n)}(z) - \frac{3}{|z|^4}\varphi^{(n)\prime}(z) + \frac{1}{|z|^3}\varphi^{(n)\prime\prime}(z)\Big)}_{=:f(|z|)} \big(\delta_{ij} z_k + \delta_{ik} z_j + \delta_{jk} z_i\big)$$
$$+ \underbrace{\frac{\gamma}{4\pi}\Big(\frac{-15}{|z|^3}\varphi^{(n)}(z) + \frac{15}{|z|^2}\varphi^{(n)\prime}(z) - \frac{6}{|z|}\varphi^{(n)\prime\prime}(z) + \varphi^{(n)\prime\prime\prime}(z)\Big)}_{=:g(|z|)} \frac{z_i z_j z_k}{|z|^4}.$$

Observe that f and g do not depend on $\frac{z}{|z|}$ but only on $|z|$. Both functions are zero if $|z| \geq n$. Moreover, if $|z| \leq \frac{n}{2}$, they reduce to $\frac{\gamma}{4\pi}\frac{3}{|z|^5}$ and $\frac{\gamma}{4\pi}\frac{-15}{|z|^3}$, respectively.

Denoting different indices with different letters and using the symmetry of S_{ijkp} in the first three indices, we see that there are only six types of terms:

$$S^{(n)}_{iiip},\ S^{(n)}_{ijjp},\ S^{(n)}_{ijpp},\ S^{(n)}_{ippp}, \tag{50}$$
$$S^{(n)}_{iipp} \text{ and } S^{(n)}_{pppp}. \tag{51}$$

For a cubic lattice, the sums in (50) are zero for every $n \in \mathbb{N}$ since the terms of the sums,

$$3f(|z|)z_i z_p + g(|z|)\frac{z_i^3 z_p}{|z|^4}, \quad f(|z|)z_i z_p + g(|z|)\frac{z_i z_j^2 z_p}{|z|^4},$$
$$g(|z|)\frac{z_i z_j z_p^2}{|z|^4} \quad \text{and} \quad f(|z|)z_i z_p + g(|z|)\frac{z_i z_p^3}{|z|^4},$$

respectively, are antisymmetric in z_i and are zero if $z_i = 0$. Thus we have for instance

$$\sum_{z \in B_n \cap \mathcal{L}^*} \Big(3f(|z|)z_i z_p + g(|z|)\frac{z_i^3 z_p}{|z|^4}\Big)$$
$$= \sum_{\substack{z \in B_n \cap \mathcal{L}^* \\ z_i > 0}} \Big(3f(|z|)z_i z_p + g(|z|)\frac{z_i^3 z_p}{|z|^4}\Big) - \sum_{\substack{z \in B_n \cap \mathcal{L}^* \\ z_i > 0}} \Big(3f(|z|)z_i z_p + g(|z|)\frac{z_i^3 z_p}{|z|^4}\Big)$$
$$= 0.$$

As this holds for every $n \in \mathbb{N}$, the limit is zero as well.

The terms of the sums in (51),

$$f(|z|)z_p^2 + g(|z|)\frac{z_i^2 z_p^2}{|z|^4} \quad \text{and} \quad 3f(|z|)z_p^2 + g(|z|)\frac{z_p^4}{|z|^4},$$

respectively, are symmetric in all components of z. We will show that these terms yield non-zero elements in the tensor S. For this we assume that $\mathcal{L}$ is a cubic lattice and we split the sum over all $z \in B_n \cap \mathcal{L}^*$ into the sum over all $z \in (B_n \setminus \bar{B}_{n/2}) \cap \mathcal{L}$ and the sum over all $z \in \bar{B}_{n/2} \cap \mathcal{L}^*$. This splitting is done correspondingly to the chosen regularization. On $\bar{B}_{n/2}$ the regularizing function is identically 1, while it is in general varying on $B_n \setminus \bar{B}_{n/2}$. Similarly to the calculation which leads to (28), a change of variables yields

$$\sum_{z \in (B_n \setminus \bar{B}_{n/2}) \cap \mathcal{L}} L^{(n)}_{ijkp}(z) = \sum_{z \in (B_1 \setminus \bar{B}_{1/2}) \cap \frac{1}{n}\mathcal{L}} L^{(1)}_{ijkp}(z) \frac{1}{n^3}.$$

As the terms of the sum are continuous and bounded on $B_1 \setminus \bar{B}_{1/2}$, the sum is a Riemann sum, which converges to $\int_{B_1 \setminus B_{1/2}} L^{(1)}_{ijkp}(z)\, d^3z$ as $n \to \infty$. Let ν denote the outer normal to $\partial(B_1 \setminus B_{1/2})$ and $\tilde{\nu}$ the outer normal to $\partial B_{1/2}$. Then we obtain, by Gauss' Theorem and the definition of $\varphi^{(1)}$,

$$\begin{aligned}
\int_{B_1 \setminus B_{1/2}} L^{(1)}_{ijkp}(z)\, d^3z &= \int_{B_1 \setminus B_{1/2}} L^{(1)}_{jkip}(z)\, d^3z \\
&= \int_{B_1 \setminus B_{1/2}} \Big\{ \partial_i \Big(\partial_j \partial_k \big(\varphi^{(1)} N\big)(z) z_p \Big) - \partial_j \partial_k \big(\varphi^{(1)} N\big)(z) \delta_{ip} \Big\}\, d^3z \\
&= \int_{\partial(B_1 \setminus B_{1/2})} \Big\{ \nu_i(z) \partial_j \partial_k \big(\varphi^{(1)} N\big)(z) z_p - \nu_j(z) \partial_k \big(\varphi^{(1)} N\big)(z) \delta_{ip} \Big\}\, d\mathcal{H}^2(z) \\
&= -\int_{\partial B_{1/2}} \Big\{ \tilde{\nu}_i(z) \partial_j \partial_k N(z) z_p - \tilde{\nu}_j(z) \partial_k N(z) \delta_{ip} \Big\}\, d\mathcal{H}^2(z).
\end{aligned}$$

Note that $\tilde{\nu}_k(z) = \frac{z_k}{|z|}$. Hence

$$\begin{aligned}
-\int_{B_1 \setminus B_{1/2}} L^{(1)}_{kkkk}(z)\, d^3z &= \int_{\partial B_{1/2}} \tilde{\nu}_k(z) \big(\partial_k \partial_k N(z) z_k - \partial_k N(z) \big)\, d\mathcal{H}^2(z) \\
&= \frac{3\gamma}{4\pi} \int_{\partial B_{1/2}} \frac{z_k^4}{|z|^6}\, d\mathcal{H}^2(z) \\
&= \frac{3\gamma}{4\pi} \int_0^{\pi} \int_0^{2\pi} \cos^4 \vartheta \sin \vartheta\, d\phi\, d\vartheta = \frac{3\gamma}{5}. \qquad (52)
\end{aligned}$$

Since S_{iikk} and S_{jjkk} have the same value also if $i \neq j$, we have $S_{iikk} = \frac{1}{2}(\sum_{\iota=1}^3 S_{\iota\iota kk} - S_{kkkk})$ and therefore

$$\int_{B_1 \setminus B_{1/2}} L^{(1)}_{iikk}(z)\, d^3z = \frac{1}{2}\Big(\sum_{\iota=1}^{3} \int_{B_1 \setminus B_{1/2}} L^{(1)}_{\iota\iota kk}(z)\, d^3z + \frac{3\gamma}{5} \Big).$$

With

$$\sum_{\iota=1}^{3} \tilde{\nu}_\iota(z) \big(\partial_\iota \partial_k N(z) z_k - \partial_k N(z) \delta_{\iota k} \big) = \frac{\gamma}{4\pi} \sum_{\iota=1}^{3} 3 \frac{z_\iota^2 z_k^2}{|z|^6} = \frac{\gamma}{4\pi} 3 \frac{z_k^2}{|z|^4}$$

we obtain

$$\sum_{\iota=1}^{3} \int_{B_1 \setminus B_{1/2}} L_{\iota\iota kk}(z)\, d^3z = -\frac{3\gamma}{4\pi} \int_0^{\pi} \int_0^{2\pi} \cos^2 \vartheta \sin \vartheta\, d\phi\, d\vartheta = -\gamma$$

and thus

$$\int_{B_1\setminus B_{1/2}} \Big(\partial_k \partial_i \partial_i \big(\varphi^{(1)} N\big)(z)\Big) z_k \, d^3 z = -\frac{\gamma}{5}. \tag{53}$$

It now remains to estimate the terms

$$s^{(n)}_{\iota\iota kk} := - \sum_{z \in \bar{B}_{n/2} \cap \mathcal{L}^*} \big(\partial_k \partial_\iota \partial_\iota N(z)\big) z_k$$

for $\iota = k$ and $\iota \neq k$. Similarly to above we have $s^{(n)}_{iikk} = \frac{1}{2}\big(\sum_{\iota=1}^3 s^{(n)}_{\iota\iota kk} - s^{(n)}_{kkkk}\big)$. Since $\sum_{\iota=1}^3 s^{(n)}_{\iota\iota kk} = 0$, we obtain

$$s^{(n)}_{iikk} = -\frac{1}{2} s^{(n)}_{kkkk} \tag{54}$$

for every $n \in \mathbb{N}$. By Lemma 5, we know that $s^{(n)}_{kkkk}$ converges in $\mathbb{R}$ as $n \to \infty$. We set

$$\mathcal{S} := \lim_{n\to\infty} s^{(n)}_{kkkk} = \lim_{n\to\infty} -\frac{\gamma}{4\pi} \sum_{z \in \bar{B}_{n/2} \cap \mathcal{L}^*} \frac{3 z_k^2}{|z|^5} \Big(3 - 5 \frac{z_k^2}{|z|^2}\Big) \tag{55}$$

and then have with (54) $\lim_{n\to\infty} s^{(n)}_{iikk} = -\frac{1}{2}\mathcal{S}$. Hence we obtain, by the definition of S_{kkkk} and by (52) and (55),

$$S_{kkkk} = \mathcal{S} + \frac{3\gamma}{5}.$$

Similarly, the definition of S_{iikk} and (53) and (54) yield

$$S_{iikk} = -\frac{1}{2}\mathcal{S} + \frac{\gamma}{5}.$$

Thus S_{kkkk} and S_{iikk} cannot be zero at the same time. Hence the tensor $S = (S_{ijkp})_{i,j,k,p=1,2,3}$ is not identically zero.

Finally, we would like to mention that the lattice series $\mathcal{S}$ is related to a special value of an L series. Therefore we can convert $\mathcal{S}$ in an exponentially convergent series, which can be evaluated very efficiently numerically [31]. In fact, using the function equation principle for the corresponding theta-series we can also obtain precise information on $\mathcal{S}$ analytically. For further reference see, e.g., [30] and [21]. Numerically we obtain $\mathcal{S} \approx \frac{\gamma}{4\pi} 9.33\ldots$.

6.2. *Examples of sets which satisfy the non-degeneracy condition* (*S*)

(i) Lipschitz continuous polyhedra: The sets U_i are the faces and the boundary of $\partial^+\tau$ is a subset of the edges.

(ii) Uniformly convex C^2 surfaces: In this case the boundary of $\partial^+\tau$ is the set $\{y \in \partial\tau \,:\, n(y)\cdot z = 0\}$, which is the pre-image of the equator $\{\eta \in S^2 \,:\, \eta \cdot z = 0\}$

under the Gauss map $y \mapsto n(y)$. Since the Gauss map is C^1 and its Jacobian is bounded from below by uniform convexity the boundary of $\partial^+\tau$ is a C^1 curve. More generally, surfaces with Gauss curvature bounded away from zero can be considered instead of uniformly convex surfaces.

(iii) Cylinders over non-degenerate curves: These are defined as follows. Let $\mathcal{A} \subset \mathbb{R}^2$ be a Lipschitz domain with non-degenerate boundary $\tilde{\gamma} = \partial\mathcal{A}$. We say that $\tilde{\gamma}$ is non-degenerate if $\tilde{\gamma}$ is a $C^{1,1}$ curve and for all $\tilde{z} \in \mathbb{R}^2$ the outward normal $\tilde{n} \in \mathbb{R}^2$ to $\mathcal{A}$ satisfies: the set $\{\tilde{y} \in \tilde{\gamma} \,:\, \tilde{n}(\tilde{y}) \cdot \tilde{z} = 0\}$ is a finite union of intervals and the bound on the number is independent of $\tilde{z}$. In particular, piecewise $C^{1,1}$ strictly convex curves are non-degenerate. The cylinder is defined by a translation of $\mathcal{A}$ with a translation vector that is orthogonal to $\mathcal{A}$.

(iv) Moreover, all surfaces which are made by gluing pieces of the above along rectifiable curves satisfy the non-degeneracy condition (S).

6.3. Proof of Lemma 6

Let $x \in \partial\tau$ and let $\mathcal{U} \subset \mathbb{R}^3$ be a neighborhood of x. The surface term of the integral representation of the solution of the Poisson equation (36) is

$$u^{(2)}(x) = \frac{\gamma}{4\pi}\left\{\int_{\partial\tau\cap\mathcal{U}} \frac{\phi(y)}{|x-y|}\, d\mathcal{H}^2(y) + \int_{\partial\tau\setminus\mathcal{U}} \frac{\phi(y)}{|x-y|}\, d\mathcal{H}^2(y)\right\}.$$

For all δ smaller than the minimal distance between x and $\partial\mathcal{U}$, we have by definition of $(1-\varphi^{(\delta)})$

$$\int_{\partial\tau\setminus\mathcal{U}} \frac{\phi(y)}{|x-y|}\, d\mathcal{H}^2(y) = \int_{\partial\tau\setminus\mathcal{U}} (1-\varphi^{(\delta)}(x-y))\frac{\phi(y)}{|x-y|}\, d\mathcal{H}^2(y). \tag{56}$$

For the estimate of the local term, i.e., $u^{(2,1)}(x) := \frac{\gamma}{4\pi}\int_{\partial\tau\cap\mathcal{U}} \frac{\phi(y)}{|x-y|}\, d\mathcal{H}^2(y)$, we parametrize the boundary. Let $\psi : \mathcal{Q} \subset \mathbb{R}^2 \to \mathbb{R}^3$ be a parametrization of $\partial\tau \cap \mathcal{U}$ such that $\psi(\tilde{x}) = x$. Without any effect on the derivation of (56), we can choose $\mathcal{U}$ and ψ such that $\psi^{-1}(\partial\tau \cap \mathcal{U}) = B_R(\tilde{x})$ with some constant $R > 0$. Since $\partial\tau$ is assumed to be C^2, the same holds for ψ. We apply the area formula (see, e.g., [13] or [15]) and denote the Jacobian of ψ by $J_\psi(\cdot)$. A transformation of variables then leads to $u^{(2,1)}(x) = \frac{\gamma}{4\pi}\int_{B_R(\tilde{x})} \frac{\phi(\psi(\tilde{y}))}{|\psi(\tilde{x})-\psi(\tilde{y})|} J_\psi(\tilde{y})\, d^2\tilde{y} =: Q(\tilde{x})$. Next we consider the corresponding regularized function $u_\delta^{(2,1)}(x) = \int_{\partial\tau\cap\mathcal{U}} (1-\varphi^{(\delta)}(x-y))\frac{\phi(y)}{|x-y|}\, d\mathcal{H}^2(y)$ and show that this converges to $u^{(2,1)}$ as $\delta \to 0$. Observe that there is a $C > 0$ such that $\frac{1}{C}|\tilde{x}-\tilde{y}| \le |\psi(\tilde{x})-\psi(\tilde{y})| \le C|\tilde{x}-\tilde{y}|$. Since $\varphi^{(\delta)}(x)$ is supported in $B_\delta(0)$, we find that $\varphi^{(\delta)}(\psi(\tilde{x})-\psi(\tilde{y}))$ is supported in $B_{C\delta}(\tilde{x})$. By the boundedness of $\phi(\psi(\cdot))$ and $J_\psi(\cdot)$ in $B_R(\tilde{x})$, we thus have

$$
\begin{aligned}
&|(u^{(2,1)} - u_\delta^{(2,1)})(x)| \\
&\quad = \Big| \frac{\gamma}{4\pi} \int_{\partial\tau \cap \mathcal{U}} \varphi^{(\delta)}(x-y) \frac{\phi(y)}{|x-y|} \, d\mathcal{H}^2(y) \Big| \\
&\quad = \Big| \frac{\gamma}{4\pi} \int_{B_R(\tilde{x})} \varphi^{(\delta)}(\psi(\tilde{x}) - \psi(\tilde{y})) \frac{\phi(\psi(\tilde{y}))}{|\psi(\tilde{x}) - \psi(\tilde{y})|} J_\psi(\tilde{y}) \, d^2\tilde{y} \Big| \\
&\quad \le c \int_{B_{C\delta}(\tilde{x})} \frac{1}{|\tilde{x} - \tilde{y}|} \, d^2\tilde{y} \le c\delta,
\end{aligned} \tag{57}
$$

which tends to zero uniformly in x as $\delta \to 0$.

Next we establish the desired formula for the tangential derivative. Since $D\psi(\tilde{x})$ maps $\mathbb{R}^2$ on the tangent space at $x = \psi(\tilde{x})$, this is equivalent to showing

$$
\begin{aligned}
&\nabla_x u^{(2)}(x) \cdot D\psi(\tilde{x}) v \\
&\quad = \lim_{\delta \to 0} \frac{-\gamma}{4\pi} \int_{\partial\tau} (1 - \varphi^{(\delta)}(x-y)) \phi(y) \frac{x-y}{|x-y|^3} \cdot D\psi(\tilde{x}) v \, d\mathcal{H}^2(y)
\end{aligned}
$$

for all $v \in \mathbb{R}^2$. Since $\nabla_{\tilde{x}}(u^{(2)} \circ \psi)(\tilde{x}) v = \nabla_x u^{(2)}(x) \cdot D\psi(\tilde{x}) v$, we first show that

$$
\nabla(u_\delta^{(2)} \circ \psi) \longrightarrow \nabla(u^{(2)} \circ \psi) \tag{58}
$$

uniformly as $\delta \to 0$, and then we verify that

$$
\begin{aligned}
&\Big| \nabla_{\tilde{x}}(u_\delta^{(2)} \circ \psi)(\tilde{x}) \cdot v - \frac{-\gamma}{4\pi} \int_{\partial\tau} (1 - \varphi^{(\delta)}(x-y)) \phi(y) \frac{x-y}{|x-y|^3} \cdot D\psi(\tilde{x}) v \, d\mathcal{H}^2(y) \Big| \\
&\le c\delta.
\end{aligned} \tag{59}
$$

For (58) it suffices to consider the convergence of the local term. Notice that $u_\delta^{(2,1)}$ is equal to the regularized function of Q, i.e.,

$$
Q_\delta(\tilde{x}) := \frac{\gamma}{4\pi} \int_{B_R(\tilde{x})} (1 - \varphi^{(\delta)}(\psi(\tilde{x}) - \psi(\tilde{y}))) \frac{\phi(\psi(\tilde{y}))}{|\psi(\tilde{x}) - \psi(\tilde{y})|} J_\psi(\tilde{y}) \, d^2\tilde{y}.
$$

Estimate (57) shows that $\lim_{\delta \to 0} Q_\delta(\tilde{x}) = Q(\tilde{x})$ uniformly in $\tilde{x}$. Next we show that the derivative of Q_δ converges uniformly to $\nabla_{\tilde{x}} Q(\tilde{x})$ as $\delta \to 0$. For this we prove that $\nabla_{\tilde{x}} Q_\delta(\tilde{x})$ is a Cauchy sequence in C^0 as $\delta \to 0$. Thus it follows that Q is C^1 and $\nabla_{\tilde{x}} Q_\delta \to \nabla_{\tilde{x}} Q$.

To prove that $\nabla_{\tilde{x}} Q_\delta(\tilde{x})$ is a Cauchy sequence in C^0 as $\delta \to 0$, it suffices to show this for $\epsilon \in [\delta/2, \delta)$ since the general case follows then by summing a geometric series. We have

$$
Q_\epsilon(\tilde{x}) - Q_\delta(\tilde{x}) = \int_{B_R(\tilde{x})} g(|\psi(\tilde{x}) - \psi(\tilde{y})|) \phi(\psi(\tilde{y})) J_\psi(\tilde{y}) \, d\tilde{y}, \tag{60}
$$

where $g(t) := \frac{\gamma}{4\pi}\big((1 - \varphi^{(\epsilon)}(t)) - (1 - \varphi^{(\delta)}(t))\big)\frac{1}{t}$. The support of g is contained in $[\delta/4, \delta]$, and we have $|g'(t)| \le ct^{-2}$ and $g \in C^\infty$. In particular, $g(|\psi(\tilde{x}) - \psi(\tilde{y})|)$ vanishes for $\tilde{y}$ in a neighborhood of $\partial B_R(\tilde{x})$. Thus we can commute differentiation and integration when we differentiate (60) and obtain

$$
\nabla_{\tilde{x}} Q_\epsilon(\tilde{x}) - \nabla_{\tilde{x}} Q_\delta(\tilde{x}) = \int_{B_R(\tilde{x})} \nabla_{\tilde{x}} g(|\psi(\tilde{x}) - \psi(\tilde{y})|) \phi(\psi(\tilde{y})) J_\psi(\tilde{y}) \, d^2\tilde{y}.
$$

Moreover, we have

$$\begin{aligned}
&\big|\nabla_{\tilde x}\, g(|\psi(\tilde x)-\psi(\tilde y)|)+\nabla_{\tilde y}\, g(|\psi(\tilde x)-\psi(\tilde y)|)\big|\\
&\quad=\Big|g'(|\psi(\tilde x)-\psi(\tilde y)|)\frac{\psi(\tilde x)-\psi(\tilde y)}{|\psi(\tilde x)-\psi(\tilde y)|}(D\psi(\tilde x)-D\psi(\tilde y))\Big|\\
&\quad\le c\frac{1}{|\psi(\tilde x)-\psi(\tilde y)|}\chi_{[\delta/4,\delta]}(|\psi(\tilde x)-\psi(\tilde y)|)
\end{aligned}$$

since $|D\psi(\tilde x)-D\psi(\tilde y)|\le c|\tilde x-\tilde y|\le c|\psi(\tilde x)-\psi(\tilde y)|$. Thus

$$\begin{aligned}
&\big|\nabla_{\tilde x} Q_\epsilon(\tilde x)-\nabla_{\tilde x} Q_\delta(\tilde x)\big|\\
&\quad\le c\int_{B_R(\tilde x)}\frac{1}{|\psi(\tilde x)-\psi(\tilde y)|}\chi_{[\delta/4,\delta]}(|\psi(\tilde x)-\psi(\tilde y)|)\,d^2\tilde y\\
&\qquad+\Big|\int_{B_R(\tilde x)}\nabla_{\tilde y} g(|\psi(\tilde x)-\psi(\tilde y)|)\phi(\psi(\tilde y))J_\psi(\tilde y)\,d^2\tilde y\Big|.
\end{aligned}$$

The first term can be estimated as in (57). For an estimate of the second term we integrate by parts, whereby the boundary term vanishes since g is zero on the boundary. By the assumptions on τ and ϕ, we have that $\nabla_{\tilde y}\big(\phi(\psi(\tilde y))J_\psi(\tilde y)\big)$ bounded on $B_R(\tilde x)$. Thus we can again apply an estimate as in (57) and show that $\nabla_{\tilde x} Q_\delta(\tilde x)$ is a Cauchy sequence as $\delta\to 0$. Hence ∇Q_δ and therefore $\nabla(u_\delta^{(2)}\circ\psi)$ converge uniformly. Together with the uniform convergence $u_\delta^{(2)}\to u^{(2)}$ this proves (58).

Regarding (59), we have

$$\begin{aligned}
&\nabla_{\tilde x}(u_\delta^{(2)}\circ\psi)(\tilde x)\cdot v\\
&\quad=\frac{\gamma}{4\pi}\int_{\partial\tau}\big(\nabla_{\tilde x}(1-\varphi^{(\delta)}(\psi(\tilde x)-y))\big)\cdot v\frac{1}{|\psi(\tilde x)-y|}\phi(y)\,d\mathcal{H}^2(y)\\
&\qquad+\frac{\gamma}{4\pi}\int_{\partial\tau}(1-\varphi^{(\delta)}(\psi(\tilde x)-y))\Big(\frac{-(\psi(\tilde x)-y)}{|\psi(\tilde x)-y|^3}\cdot D\psi(\tilde x)v\Big)\phi(y)\,d\mathcal{H}^2(y).
\end{aligned}$$

Since $x=\psi(\tilde x)$, the proof of (59) reduces to estimating the first integral by $c\delta$. Since the integral vanishes if $|y-x|>\delta$, we can rewrite the integral using the change of variables $y=\psi(\tilde y)$. With the abbreviations

$$\begin{aligned}
h(w)&=\frac{\gamma}{4\pi}\frac{1}{\delta}(1-\varphi^{(\delta)})'(w)\frac{w}{|w|^2}=-\frac{\gamma}{4\pi}\frac{1}{\delta}\varphi^{(\delta)\prime}(w)\frac{w}{|w|^2},\\
j(\tilde y)&=\phi(\tilde y)J_\psi(\tilde y)
\end{aligned}$$

we then have to estimate $I:=\int_{B_{c\delta}(\tilde x)}h(\psi(\tilde x)-\psi(\tilde y))\cdot D\psi(\tilde x)v\, j(\tilde y)\,d^2\tilde y$. Now, $\operatorname{Lip} h\le\frac{c}{\delta^3}$ since $|w|\le c\delta$, and $\operatorname{Lip} j\le c$. Setting $\tilde z=\tilde x-\tilde y$ we have $\psi(\tilde x)-\psi(\tilde y)=D\psi(\tilde x)\tilde z+\mathcal{O}(|\tilde z|^2)$ and obtain

$$I=\int_{B_{c\delta}(0)}h(D\psi(\tilde x)\tilde z)\cdot D\psi(\tilde x)v\, j(\tilde x)\,d^2\tilde z+\mathcal{O}(\delta).$$

The integral on the right-hand side vanishes since h is antisymmetric and the domain of integration is invariant under $\tilde z\mapsto-\tilde z$. Hence $|I|\le c\delta$ and (59) is proved, which finishes the proof of Lemma 6.

6.4. Proof of Lemma 7

In Lemma 7 the behavior of the normal derivative of $u^{(2)}$ is considered. A detailed treatment of a similar statement, viz on the normal derivative of the so-called single-layer potential, can be found for instance in [16, Theorem (3.28)]. Lemma 7 differs from the corresponding framework in [16] only in the differently chosen regularization. While Folland cuts off a ball B_δ about the singularity sharply, i.e., by a characteristic function, we use a smooth function $(1 - \varphi^{(\delta)})$. By using the central estimate $|(x - y) \cdot n(y)| \le c|x - y|^2$ for all $x, y \in \partial\tau$ (which requires the assumption that τ has C^2 boundary, cf. Lemma (3.15) in [16]), we can show that both regularizations lead to the same limit. Thus the proof of Lemma 7 reduces to the one in [16].

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Institut für Analysis, Dynamik und Modellierung
Universität Stuttgart
Pfaffenwaldring 57
D-70569 Stuttgart
Germany
e-mail: schloeme@mathematik.uni-stuttgart.de

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