Magnetic forces in discrete and continuous systems

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Contents

Chapter 1

Introduction

The topic of this thesis is a mathematically rigorous treatment of formulae for the magnetic force between two parts of a macroscopic magnetized body. Firstly, a classical force formula is proven in a continuum setting under nearly optimal regularity assumptions on the magnetization. This formula is called Brown's force formula referring to W. F. Brown, who gave a mainly physically motivated discussion of this formula in 1966 [Br]. Our argument uses a suitable regularization of a hypersingular integral. Secondly, we derive a force formula by a different approach in order to understand better the influence of such a regularization and of possible discreteness effects. 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 moment of an atom is scaled in such a way that we obtain a finite total magnetization per unit volume. Under certain regularity assumptions on the magnetization and the appearing boundaries we derive a force formula in the passage from the discrete setting to the continuum. The limiting force shows a dependence on the shape of a part of the body which is different from that in Brown's force. This is due to short range effects. The corresponding term depends on the symmetry of the crystal lattice.

Before we give a more detailed outline of this thesis, we focus on the motivation for this work. The force formulae are of particular interest in the context of the recently discovered ferromagnetic shape memory alloys as for instance Ni_2MnGa (cf. e.g. [Ja] 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-scale devices, a detailed analysis of the dynamic behaviour of the interfaces is of interest. Investigations of the forces appearing are a first step towards this.

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 [Ja]. For a more general treatment of magneotelasticity we refer to [ErMa]. The approach in this thesis follows the work of Brown [Br].

The magnetostrictive effect is based on elasticity as well as magnetism. A theoretical description of the forces which occur can be split into one of elastic forces and another one of magnetic forces (cf. e.g. [Br]). In this thesis we give a detailed mathematical examination of the magnetic force. This is done firstly in a continuous setting and secondly in an atomistic approach. Books which emphasize rather physical aspects than a precise mathematical treatment of magnetic forces in continuous settings are [LaLiPi], [PeHa] and [Br] and the recent book by Bobbio [Bo].

The jumps of the magnetization, which occur in ferromagnetic shape memory alloys, are believed to be atomically sharp. Thus it is sensible to model the interfaces as idealised sharp interfaces (cf. [Ja]) and not to use the usual approach of micromagnetics via Bloch or Néel walls (cf. e.g. [HuSc]).
In micromagnetism it is often assumed that the magnetization is saturated, i.e. the modulus of the magnetization is a constant which only depends on temperature. This restriction is not needed in this work.

As technical devices become smaller, surface terms become more important compared to volume terms, because of scaling. A good understanding of surface terms is therefore of great interest for the development of devices at microscales. Brown's force formula consists of a volume term and of a surface term which shows a nonlinear dependence on the normal (cf. (1.1) or (2.2)). This dependence also arises if the magnetization is smooth in the whole magnetic body. This is remarkable since Cauchy's Theorem (cf. Theorem 5.3) 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 forces depend linearly on the normal. We discuss this point in Section 5.2. The interest in a detailed analysis of the surface terms motivated the derivation of a force formula in the limit of an atomistic model. Such an atomistic approach was suggested in [Br, p. 52] in order to obtain short range contributions to the magnetic force in addition to the terms in Brown's formula, and thus to understand better the magnetic force in a continuous body in view of Cauchy's Theorem.

That one can obtain additional terms in the continuum limit of an atomistic ansatz is shown for instance in the work by James and Müller [JaMü], in which they consider the field energy of micromagnetics. They compute the continuum limit of the energy starting from a lattice of dipoles. Depending on the convergence properties of the magnetization, they obtain different limiting energies. In the case of dipoles oscillating on the scale of the lattice one has an additional local term to the classical micromagnetic energy. This term contains a lattice sum of a singular kernel.

A more detailed outline of this thesis is as follows.

In Chapter 2 a mathematically rigorous derivation of Brown's formula [Br, p. 57] for the magnetic force between two parts of a magnetized continuous body is given. Here, we work entirely in a continuum setting. The main result of Chapter 2 is Theorem 2.1, which corresponds to Brown's force formula. The force exerted on a subregion, τ, of a magnetized body, Ω, by its surrounding region is formulated in terms of the magnetic field, H_Ω, of the whole body and the magnetization, M_τ, in the subregion τ. The formula reads (see (2.2))

$$F^{(\mathrm{Br})} = \int_\tau (M_\tau(x)\cdot\nabla)H_\Omega(x)\,d^3x + \frac{\gamma}{2}\int_{\partial\tau}(M_\tau^-\cdot n)^2(x)n(x)\,d\mathcal{H}^2(x), \qquad (1.1)$$

where γ is a constant which only depends on the choice of the physical units, n is the outer normal to $\partial\tau$ and M_τ^- denotes the inner trace of M_τ with respect to τ.

In the proof of Brown's formula the main difficulties appear in the calculation of the so-called self-force, $\int_\tau (M_\tau(x)\cdot\nabla)H_\tau(x)\,d^3x$, since the force between two magnetic dipoles involves singularities which are of hypersingular order, i.e. of order $|z|^{-4}$ in three dimensions. This can be tackled with general methods for singular integrals (see e.g. [St]), which are closely related to those which we use for the passage from the discrete to the continuum setting.

Chapter 3 is devoted to the calculation of the limit of the magnetic force between two parts of a magnetized body in the passage from a lattice to a continuum setting. Let again Ω, a bounded and open subset of $\mathbb{R}^3$, be the magnetized body, and τ a subregion. More precisely we consider the magnetic force which is exerted by the magnetized matter in $\Omega\setminus\bar{\tau}$ on that in a subbody $\bar{\tau}$. For the main result in Chapter 3 it is assumed that the shape of the subbody satisfies a mild additional condition (the non-degeneracy condition (S), Definition 3.4), which for instance is satisfied if τ is a convex set with C^2-boundary or if τ is a polyhedron.

The discrete system is given as a configuration of magnetic moments, $m^{(l)}$, on the points of a scaled Bravais lattice, $\frac{1}{l}\mathcal{L}$, $l\in\mathbb{N}$, and the force which is exerted on a part of a bounded region by its complement is the superposition of the magnetic forces between all pairs of magnetic moments in the two parts. In the limit as $l\to\infty$, the scaled lattice tends to the continuum. The scaling of the lattice requires a scaling of the magnetic moments, namely $m^{(l)}(x) = \frac{1}{l^3}m(x)$ (cf. (3.1)), where $m(x)$ is a given background magnetization.

First the discrete force which is exerted by the magnetic moments in $\Omega\setminus\bar{\tau}\cap\frac{1}{l}\mathcal{L}$ on the magnetic moments in $\bar{\tau}\cap\frac{1}{l}\mathcal{L}$ is derived. We then introduce a regularizing function in order to split the discrete force into a short range part and a long range part. Then the limit procedure is performed separately for both parts. We first take the limit $l\to\infty$ and then the limit $\delta\to 0$.

The limit of the kth component of the long range term is (Theorem 3.1)

$$\int_\tau (m(x)\cdot\nabla)(H_\Omega)_k(x)\,d^3x+ \\ +\frac{\gamma}{2}\int_{\partial\tau}(m^-\cdot n)(\xi)\big((m^- - m^+)\cdot n\big)(\xi)n_k(\xi)\,d\mathcal{H}^2(\xi), \tag{1.2}$$

where m^+ and m^- denote the outer and inner traces of m with respect to τ, respectively. 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 $\partial\tau$. In contrast, the limit of the kth component of the short range term of the discrete force (Theorem 3.6)

$$\frac{1}{2}\int_{\partial\tau}\sum_{i,j,p=1}^{3} m_i^-(\xi)m_j^+(\xi)S_{ijkp}n_p(\xi)\,d\mathcal{H}^2(\xi) \tag{1.3}$$

is linear in the normal. Here, S_{ijkp} is a lattice sum which contains a hypersingular kernel (Definition 3.5). This sum is discussed and evaluated in Lemma 3.17 and Chapter 4. In Lemma 3.17 we show that the lattice sum is well defined. The main result of Chapter 4 is that $S=(S_{ijkp})_{i,j,k,p=1,2,3}$ is not zero in the case of a cubic lattice, $\mathbb{Z}^3$.

In Chapter 5 we compare the two force formulae particularly with respect to their surface terms. For this we state the corresponding formulae for the force between two separated magnetized regions to analyze how the surface terms depend on the contact between the two considered parts. If the two parts of the body are separated, i.e. especially $m^+=0$, the limiting force formula coincides with Brown's formula.
In view of Cauchy's Theorem we formulate the force formulae for regions in contact also for magnetizations which are smooth in the whole body. In this case the nonlinear surface term in (1.2) vanishes, while the nonlinear surface term $\frac{\gamma}{2}\int_{\partial\tau}(m\cdot n)^2n$ in Brown's formula remains. As mentioned above this disagrees with the result of Cauchy's Theorem that surface forces depend linearly on the normal as a consequence of balance of momentum. Being aware that his formula describes only the long range contributions of the total magnetic force, Brown [Br, Section 5] tackles the discrepancy by assuming the existence of an additional surface term which cancels the nonlinearity. This can now be

seen as a consequence of the derivation of the magnetic force from an atomistic setting. One can regard the surface term $-\frac{\gamma}{2}\int_{\partial\mathcal{T}}(m^- \cdot n)(m^+ \cdot n)n$ in the limiting force, which is $-\frac{\gamma}{2}\int_{\partial\mathcal{T}}(m \cdot n)^2 n$ if m is smooth in Ω, as the additional term which Brown introduced.

Finally, we mention some open problems in connection with the derived force formulae in Chapter 6.

Chapter 2

Magnetic force formula in the continuum picture

In this chapter magnetic long range forces on a part of a magnetized body in a continuum setting are considered. This work follows the monograph *Magnetoelastic Interactions* [Br] by W. F. Brown. The formula which is developed there (p. 57) consists of a volume term and a surface term. The latter shows a nonlinear dependence on the normal to the boundary of the subbody. This is interesting since surface forces are linear in the normal in Cauchy's Theorem (cf. Theorem 5.3) in continuum mechanics. This discrepancy is discussed in Chapter 5.
In this chapter we focus on a proof of Brown's formula using singular integral methods. The advantage of this approach is that results from this chapter can also be used in Chapter 3 for the magnetic force calculation from an atomistic to a continuous setting. A derivation using purely methods for partial differential equations is given in [Ja].

2.1 Derivation of Brown's force formula

In this thesis Ω always denotes an open and bounded subset of $\mathbb{R}^3$ with C^2-boundary. Let $\tau \subset \Omega$, open, and $\Omega\setminus\bar{\tau}$ be two parts of the body with $\partial\tau\cap\partial\Omega = \emptyset$ (see Figure 2.1). The magnetization $M : \Omega \to \mathbb{R}^3$ is a vector-valued function which may jump at the interface between τ and $\Omega\setminus\bar{\tau}$. Here we are interested in the force which is exerted by the magnetized subbody $\Omega\setminus\bar{\tau}$ on the magnetized subbody τ. For the calculations it is convenient to denote the magnetization in τ by M_τ, i.e. $M_\tau = M\chi_\tau$, where χ_E is the characteristic function of a set E. Similarly, $M_{\Omega\setminus\bar{\tau}} = M\chi_{\Omega\setminus\bar{\tau}}$ is the magnetization in $\Omega\setminus\bar{\tau}$.

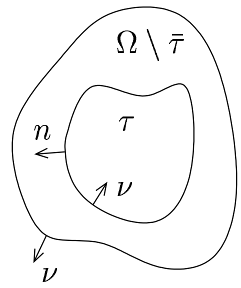

Figure 2.1: The sets Ω, τ and $\Omega \setminus \bar{\tau}$, and the outer normals.

The boundary values of the magnetization are defined as weak boundary values, also called traces. A definition of these and some related facts, which are used later on, are summarized in Appendix A on page 79. For definiteness we make the convention that the interface, $\partial\tau$, belongs to the 'inner' subbody $\bar{\tau}$. It holds $M = M_{\bar{\tau}} + M_{\Omega\setminus\bar{\tau}}$ and $M = M_\tau + M_{\Omega\setminus\bar{\tau}}$ almost everywhere. For the traces one has $(M_{\bar{\tau}} \cdot n)^- = (M_\tau \cdot n)^- = M_\tau^- \cdot n$, where n denotes the outer normal to $\partial\tau$. Notice that $M_\tau \in W^{1,2}(\tau)$ implies that the inner trace of M_τ at $\partial\tau$ belongs to $L^2(\partial\tau)$ by Theorem A.1.
If it is clear from the context that a function has values in $\mathbb{R}^3$, we often use $W^{1,2}(\tau)$ as a shorthand for $W^{1,2}(\tau;\mathbb{R}^3)$. An analogous notation applies to other function spaces.
Note that we do not restrict the modulus of M to a constant as is done in micromagnetism to model a saturation of the magnetization. To simplify the formulae we assume that the boundary value of M at $\partial\Omega$ is zero. It will become clear from the following how a non-zero trace at $\partial\Omega$ has to be implemented.

Moreover the notion of magnetic fields is needed. The magnetic field is related to the magnetization by Maxwell's equations. These and some related facts can be found in Appendix A on page 80. The magnetic fields which are generated by the magnetization in τ, $\Omega\setminus\bar{\tau}$ and Ω, respectively, are denoted by $H_{\bar{\tau}}$, $H_{\Omega\setminus\bar{\tau}}$, and H_Ω, respectively. Similarly to above the boundary values of the magnetic fields are defined as traces. For instance the inner trace of $H_{\Omega\setminus\bar{\tau}}$ with respect to τ is denoted by $H^-_{\Omega\setminus\bar{\tau}}$.

Assume that τ has Lipschitz boundary and that $M_\tau \in W^{1,2}(\tau)$ and $H_{\Omega\setminus\bar{\tau}} \in W^{1,2}(\tau)$. The force which is exerted by the (outer) magnetic field $H_{\Omega\setminus\bar{\tau}}$ on the (inner) magnetic body τ is assumed to be

$$F = \int_\tau (M_\tau(x) \cdot \nabla) H_{\Omega\setminus\bar{\tau}}(x)\, d^3x. \tag{2.1}$$

We take this force formula as the starting point for the derivation of Brown's formula. It corresponds to those contributions to the force, which Brown calls

long range contributions [Br, p. 55].
One could also regard the Lorentz force has the natural starting point. In the appendix (p. 81) we show that (2.1) follows from Lorentz' force formula.

In the following theorem the magnetic force formula which corresponds to Brown's formula (cf. [Br, p. 57]) is stated. Here γ denotes a constant which only depends on the chosen physical units (see [Br, p. 6] for details).

Theorem 2.1 *Let $\tau \subset \Omega$ be open with C^2-boundary and let $M_\tau \in W^{1,2}(\tau)$ and $M_{\Omega\setminus\bar{\tau}} \in W^{1,2}(\Omega\setminus\bar{\tau})$. Then the force exerted by the complement of the magnetic subbody τ on τ is given by*

$$F^{(\mathrm{Br})} = \int_\tau (M_\tau(x)\cdot\nabla)H_\Omega(x)\,d^3x + \frac{\gamma}{2}\int_{\partial\tau}(M_\tau^-\cdot n)^2(x)n(x)\,d\mathcal{H}^2(x). \tag{2.2}$$

Remark 2.2 By Maxwell's equations, the regularity of the magnetization M implies regularity of the magnetic field. If ∂U is of class $C^{1,1}$, then $M \in W^{1,2}(U)$ implies $H \in W^{1,2}(U)$. On page 83 we recall a proof for this result. Note that the three magnetic fields we are dealing with, i.e. $H_{\bar{\tau}}$, $H_{\Omega\setminus\bar{\tau}}$ and H_Ω, belong to $W^{1,2}(\tau)$ under the assumptions of Theorem 2.1.

Proof: The magnetization $M_\tau \in W^{1,2}(\tau)$ can be approximated by smooth functions, i.e. there exist $M_\tau^{(k)} \in C^\infty(\tau)$, $k \in \mathbb{N}$, such that

$$M_\tau^{(k)} \longrightarrow M_\tau \quad \text{in} \quad W^{1,2}(\tau)$$

as $k \to \infty$. By standard regularity (cf. (A.3)) one has that the corresponding magnetic field converges in $W^{1,2}(\tau)$ as well. The trace theorem (cf. Theorem A.1) yields that

$$(M_\tau^{(k)})^- \longrightarrow (M_\tau)^- \quad \text{in} \quad L^2(\partial\tau).$$

Hence, if (2.2) holds for smooth magnetizations and magnetic fields, one can pass to the limit in (2.2) as $k \to \infty$. Therefore we can assume in the following without loss of generality that M_τ and H_Ω belong to $C^\infty(\tau)$.

The starting point for $F^{(\mathrm{Br})}$ is formula (2.1). Notice that one has

$$H_{\Omega\setminus\bar{\tau}} = H_\Omega - H_{\bar{\tau}} \tag{2.3}$$

since Maxwell's equations are linear. Thus one can replace $H_{\Omega\setminus\bar{\tau}}$ with $H_\Omega - H_{\bar{\tau}}$ in (2.1). Hence proving the theorem is equivalent to verifying

$$F_0 := \int_\tau (M_\tau(x)\cdot\nabla)H_{\bar{\tau}}(x)\,d^3x = -\frac{\gamma}{2}\int_{\partial\tau}(M_\tau^-\cdot n)^2(x)n(x)\,d\mathcal{H}^2(x). \tag{2.4}$$

The magnetic field $H_{\bar{\tau}}$ is given by Maxwell's equations, which are discussed in the appendix (p. 80). In particular there exists a scalar field u such that $H_{\bar{\tau}} = -\nabla u$, and u is a solution of the Poisson equation

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

with transition condition

$$[\nabla u \cdot n] := (\nabla u \cdot n)^+ - (\nabla u \cdot n)^- = -\gamma (M_\tau \cdot n)^- \quad \text{on} \quad \partial\tau.$$

One can also write this equation in form of

$$-\Delta u = -\gamma(\nabla \cdot M_\tau)\mathcal{L}^3 \lfloor_\tau + \gamma (M_\tau \cdot n)^- \mathcal{H}^2 \lfloor_{\partial\tau} \quad \text{in} \quad \mathbb{R}^3.$$

The solution is given by

$$u(x) = \frac{\gamma}{4\pi} \left\{ \int_\tau \frac{(-\nabla \cdot M_\tau)(y)}{|x-y|} \, d^3y + \int_{\partial\tau} \frac{(M_\tau \cdot n)^-(y)}{|x-y|} \, d\mathcal{H}^2(y) \right\}$$

for all $x \in \mathbb{R}^3$.

From the solution u one obtains a representation for the magnetic field $H_{\bar{\tau}}$ for every $x \in \mathbb{R}^3$. At first we consider points $x \in \mathbb{R}^3 \setminus \partial\tau$. Since $\nabla \cdot M_\tau$ and $(M_\tau \cdot n)^-$ are bounded on τ and $\partial\tau$ respectively, the integrands in the formula for $u(x)$ are in $L^1(\tau)$ and $L^1(\partial\tau)$, respectively, and the partial derivatives of the integrands with respect to the components of x exist and have integrable majorant functions. Hence one can commute differentiation and integration. So the magnetic field arising from the magnetization in τ is given by

$$\begin{aligned} H_{\bar{\tau}}(x) &= -\nabla_x u(x) \\ &= \frac{\gamma}{4\pi} \Big\{ \int_\tau (-\nabla \cdot M_\tau)(y) \frac{x-y}{|x-y|^3} \, d^3y + \int_{\partial\tau} (M_\tau \cdot n)^-(y) \frac{x-y}{|x-y|^3} \, d\mathcal{H}^2(y) \Big\} \end{aligned} \tag{2.5}$$

for all $x \in \mathbb{R}^3 \setminus \partial\tau$.

Now we consider the case $x \in \partial\tau$. The integrand of the first term of $u(x)$ also satisfies the above conditions. Again one is allowed to commute differentiation and integration, which leads to $\frac{\gamma}{4\pi} \int_\tau (-\nabla \cdot M_\tau)(y) \frac{x-y}{|x-y|^3} \, d^3y$.

If $x \in \partial\tau$, difficulties arise if one wants to differentiate the second term of $u(x)$. We call this term $u^{(2)}(x)$ and treat it on $\partial\tau$ by the following regularization. Let $\eta \in C^\infty(\mathbb{R})$ be such that $\eta(r) = 0$ if $r \le \frac{1}{2}$ and $\eta(r) = 1$ if $r \ge 1$, see Figure 2.2. And set

$$u_\epsilon^{(2)}(x) := \frac{\gamma}{4\pi} \int_{\partial\tau} \eta\Big(\frac{|x-y|}{\epsilon}\Big) \frac{\phi(y)}{|x-y|} \, d\mathcal{H}^2(y) \tag{2.6}$$

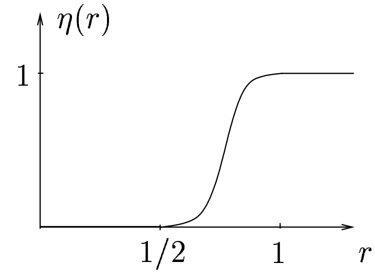

Figure 2.2: A regularizing function η.

with $\phi := (M_\tau \cdot n)^- = M_\tau^- \cdot n$ as a shorthand. As is verified in Section 2.2 it holds

$$u^{(2)}(x) = \lim_{\epsilon \to 0} \frac{\gamma}{4\pi} \int_{\partial\tau} \eta(\frac{|x-y|}{\epsilon}) \frac{\phi(y)}{|x-y|} \, d\mathcal{H}^2(y) \tag{2.7}$$

uniformly in x.

The calculation of the derivative is done separately for the normal derivative and the tangential derivative.
The tangential component of a vector is indicated by the index t; and the tangential derivative is denoted by ∇_t. By the assumptions on the magnetization, the tangential derivative of u is continuous across the interface, i.e. $[\nabla_t u^{(2)}] = 0$ on $\partial\tau$.

Lemma 2.3 *Let τ and M_τ fulfil the same conditions as in Theorem 2.1. 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

$$(\mathcal{T}\phi)(x) := \lim_{\epsilon \to 0} \frac{\gamma}{4\pi} \int_{\partial\tau} \eta(\frac{|x-y|}{\epsilon}) \phi(y) \frac{(x-y)_t}{|x-y|^3} \, d\mathcal{H}^2(y). \tag{2.8}$$

The convergence is uniform.

This is proved in Section 2.2.

In total, the tangential component of $H_{\bar{\tau}}$ on $\partial\tau$, which is the negative of the tangential derivative of u on $\partial\tau$, is given by

$$(H_{\bar{\tau}})_t(x) = (-\nabla_t u)(x) = \frac{\gamma}{4\pi} \int_\tau (-\nabla \cdot M_\tau)(y) \frac{(x-y)_t}{|x-y|^3} \, d^3y \; + \; (\mathcal{T}\phi)(x). \tag{2.9}$$

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

Lemma 2.4 *Let τ and M_τ fulfil the same conditions as in Theorem 2.1. 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 $u^{(2)}(x)$, i.e. of the second term of $u(x)$, are given by*

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

where

$$(\mathcal{N}\phi)(x) := \lim_{\epsilon\to 0}\frac{\gamma}{4\pi}\int_{\partial\tau}\eta(\frac{|x-y|}{\epsilon})\phi(y)\frac{(x-y)\cdot n(x)}{|x-y|^3}\,d\mathcal{H}^2(y). \tag{2.10}$$

The proof of this lemma is given in Section 2.3.

We now continue with the proof of the theorem. A consequence of the jump of the normal derivative of $u^{(2)}$ is that the normal component of the magnetic field $H_{\bar\tau}$ jumps at $\partial\tau$. If $x\in\partial\tau$, the traces are given by

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

Summarizing the results for the normal and tangential derivatives on the boundary one obtains

$$\begin{aligned}H^+_{\bar\tau}(x) &= (H_{\bar\tau})_t(x)+(H_{\bar\tau}\cdot n)^+(x)n(x)\\ &= \frac{\gamma}{4\pi}\int_\tau(-\nabla\cdot M_\tau)(y)\frac{x-y}{|x-y|^3}\,d^3y\;+(\mathcal{T}\phi)(x)+\frac{\gamma}{2}\phi(x)n(x)+\\ &\quad+(\mathcal{N}\phi)(x)n(x)\\ &= \frac{\gamma}{4\pi}\int_\tau(-\nabla\cdot M_\tau)(y)\frac{x-y}{|x-y|^3}\,d^3y\;+\;(\mathcal{B}\phi)(x)+\frac{\gamma}{2}\phi(x)n(x), \qquad (2.11)\\ H^-_{\bar\tau}(x) &= \frac{\gamma}{4\pi}\int_\tau(-\nabla\cdot M_\tau)(y)\frac{x-y}{|x-y|^3}\,d^3y\;+\;(\mathcal{B}\phi)(x)-\frac{\gamma}{2}\phi(x)n(x), \qquad (2.12)\end{aligned}$$

where

$$\begin{aligned}(\mathcal{B}\phi)(x) &:= (\mathcal{T}\phi)(x)+(\mathcal{N}\phi)(x)n(x)\\ &= \lim_{\epsilon\to 0}\frac{\gamma}{4\pi}\int_{\partial\tau}\eta(\frac{|x-y|}{\epsilon})\phi(y)\frac{x-y}{|x-y|^3}\,d\mathcal{H}^2(y), \qquad (2.13)\end{aligned}$$

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

By substituting the above formulae for the magnetic field $H_{\bar{\tau}}$ into the defining equation (2.4) for F_0 after an integration by parts one gets

$$\begin{aligned} F_0 &= \frac{\gamma}{4\pi}\Big\{\int_\tau (-\nabla\cdot M_\tau)(x) H_{\bar{\tau}}(x)\,d^3x + \int_{\partial\tau}\phi(x)H_{\bar{\tau}}^-(x)\,d\mathcal{H}^2(x)\Big\} \\ &= \frac{\gamma}{4\pi}\Big\{\int_\tau(-\nabla\cdot M_\tau)(x)\int_\tau(-\nabla\cdot M_\tau)(y)\frac{x-y}{|x-y|^3}\,d^3y\,d^3x + \\ &\qquad + \int_\tau(-\nabla\cdot M_\tau)(x)\int_{\partial\tau}\phi(y)\frac{x-y}{|x-y|^3}\,d\mathcal{H}^2(y)\,d^3x + \\ &\qquad + \int_{\partial\tau}\phi(x)\int_\tau(-\nabla\cdot M_\tau)(y)\frac{x-y}{|x-y|^3}\,d^3y\,d\mathcal{H}^2(x)\Big\} + \\ &\quad + \int_{\partial\tau}\phi(x)(\mathcal{B}\phi)(x)\,d\mathcal{H}^2(x) - \frac{\gamma}{2}\int_{\partial\tau}\phi^2(x)n(x)\,d\mathcal{H}^2(x). \end{aligned}$$

Recall that $\nabla\cdot M_\tau$ and $\phi = (M_\tau\cdot n)^-$ are bounded functions on τ and $\partial\tau$, respectively. For an application of Fubini's Theorem we remark that $\frac{x-y}{|x-y|^3}$ is Borel-measurable with respect to $\tau\times\tau$ and $\partial\tau\times\tau$. As $\int_\tau \frac{1}{|x-y|^2}\,d^3y < \infty$ for all $x\in\mathbb{R}^3$, also $\int_{\partial\tau}(\int_\tau\frac{1}{|x-y|^2}\,d^3y)d\mathcal{H}^2(x)$ and $\int_\tau(\int_\tau\frac{1}{|x-y|^2}\,d^3y)d^3x$ are finite. So Fubini's Theorem is applicable to the first, second and third term of F_0. The first term then reads

$$\begin{aligned} &\int_\tau(-\nabla\cdot M_\tau)(x)\int_\tau(-\nabla\cdot M_\tau)(y)\frac{x-y}{|x-y|^3}\,d^3y\,d^3x \\ &= \int_\tau(-\nabla\cdot M_\tau)(y)\int_\tau(-\nabla\cdot M_\tau)(x)\frac{x-y}{|x-y|^3}\,d^3x\,d^3y \\ &= -\int_\tau(-\nabla\cdot M_\tau)(x)\int_\tau(-\nabla\cdot M_\tau)(y)\frac{x-y}{|x-y|^3}\,d^3y\,d^3x, \end{aligned}$$

where the last equation follows by exchanging the variables x and y. Thus the first term in F_0 is zero.

The third term is the negative of the second term, which can be seen similarly with the help of Fubini's Theorem and by exchanging the variables x and y.

Fubini's Theorem can also be applied to the fourth term. For $\epsilon > 0$ the term $\eta(\frac{|x-y|}{\epsilon})\frac{x-y}{|x-y|^3}$ is $\partial\tau\times\partial\tau$-Borel-measurable and $\int_{\partial\tau}\eta(\frac{|x-y|}{\epsilon})\frac{1}{|x-y|^2}\,d\mathcal{H}^2(y)$ is uniformly bounded for all $x\in\partial\tau$. So one can proceed as with the first term. Since $\mathcal{B}\phi$ is the limit of a uniformly convergent sequence one has, using again

Fubini's Theorem and then exchanging x and y,

$$\begin{aligned}
&\int_{\partial\tau} \phi(x)(\mathcal{B}\phi)(x)\, d\mathcal{H}^2(x) \\
&= \lim_{\epsilon\to 0} \frac{\gamma}{4\pi} \int_{\partial\tau} \phi(x) \int_{\partial\tau} \eta(\frac{|x-y|}{\epsilon})\phi(y) \frac{x-y}{|x-y|^3}\, d\mathcal{H}^2(y)\, d\mathcal{H}^2(x) \\
&= \lim_{\epsilon\to 0} \frac{\gamma}{4\pi} \int_{\partial\tau} \phi(y) \int_{\partial\tau} \eta(\frac{|x-y|}{\epsilon})\phi(x) \frac{x-y}{|x-y|^3}\, d\mathcal{H}^2(x)\, d\mathcal{H}^2(y) \\
&= -\int_{\partial\tau} \phi(x)(\mathcal{B}\phi)(x)\, d\mathcal{H}^2(x).
\end{aligned}$$

Hence F_0 reduces to

$$F_0 = -\frac{\gamma}{2} \int_{\partial\tau} \phi^2(x) n(x)\, d\mathcal{H}^2(x),$$

which proves (2.4) and yields the desired force formula

$$F^{(\mathrm{Br})} = \int_\tau (M_\tau(x)\cdot\nabla) H_\Omega(x) + \frac{\gamma}{2} \int_{\partial\tau} \phi^2(x) n(x)\, d\mathcal{H}^2(x).$$

□

We discuss Brown's force formula in Chapter 5. This includes a comparison with the magnetic force formula which is derived in Chapter 3 starting from a discrete setting.
In the remaining sections of this chapter the proofs of Lemmas 2.3 and 2.4 are given. Here and in the following C stands for generic constants which do not always have to be the same.

2.2 The tangential component of the magnetic field

The task of this section is to prove (2.7), i.e. the convergence of the regularization of u, and to prove that the tangential derivative of the second term of the magnetic potential u exists and is given by the uniform limit

$$(-\nabla_t u^{(2)})(x) = \lim_{\epsilon\to 0} \frac{\gamma}{4\pi} \int_{\partial\tau} \eta(\frac{|x-y|}{\epsilon})\phi(y) \frac{(x-y)_t}{|x-y|^3}\, d^3y$$

as stated in Lemma 2.3.

Let $x \in \partial\tau$ and let $\mathcal{U} \subset \mathbb{R}^3$ be a neighbourhood of x. Then

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

For all ϵ smaller than the minimal distance between x and $\partial\mathcal{U}$, one has by definition of η

$$\int_{\partial\tau\setminus\mathcal{U}} \frac{\phi(y)}{|x-y|}\, d\mathcal{H}^2(y) = \int_{\partial\tau\setminus\mathcal{U}} \eta(\frac{|x-y|}{\epsilon})\frac{\phi(y)}{|x-y|}\, d\mathcal{H}^2(y). \qquad (2.14)$$

For the estimate of the other integral, i.e. $\frac{\gamma}{4\pi}\int_{\partial\tau\cap\mathcal{U}} \frac{\phi(y)}{|x-y|}\, d\mathcal{H}^2(y)$, we parametrize the boundary. Let $\psi : \tilde{\mathcal{U}} \subset \mathbb{R}^2 \to \mathbb{R}^3$ be a parametrization of $\partial\tau \cap \mathcal{U}$ such that $\psi(\tilde{x}) = x$, compare Figure 2.3. Without any effect on the derivation of (2.14),

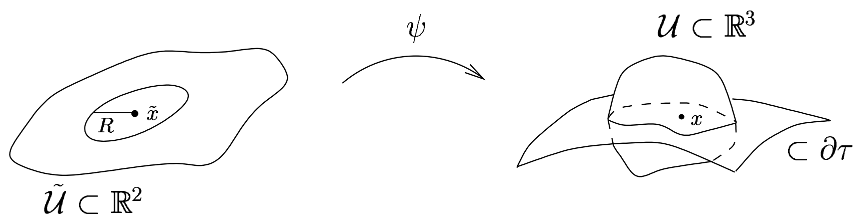

Figure 2.3: Parametrization of $\partial\tau \cap \mathcal{U}$.

one 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. As in Theorem A.5 (area and change of variable formula) the Jacobian of ψ is denoted by $J_\psi(\cdot)$. A transformation of variables leads to

$$\begin{aligned} u^{(2,1)}(x) &:= \frac{\gamma}{4\pi}\int_{\partial\tau\cap\mathcal{U}} \frac{\phi(y)}{|x-y|}\, d\mathcal{H}^2(y) \\ &= \frac{\gamma}{4\pi}\int_{B_R(\tilde{x})} \frac{\phi(\psi(\tilde{y}))}{|\psi(\tilde{x})-\psi(\tilde{y})|} J_\psi(\tilde{y})\, d^2\tilde{y} \\ &=: Q(\tilde{x}). \end{aligned} \qquad (2.15)$$

To show (2.7) denote by $u_\epsilon^{(2,1)}$ the corresponding regularized function of $u^{(2,1)}$. 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 $1-\eta(\frac{|x|}{\epsilon})$ is supported in $B_\epsilon(0)$, one obtains that $1-\eta(\frac{|\psi(\tilde{x})-\psi(\tilde{y})|}{\epsilon})$ is supported in $B_{C\epsilon}(\tilde{x})$. By the boundedness of $\phi(\psi(\cdot))$ and $J_\psi(\cdot)$ in $B_R(\tilde{x})$ one thus has

$$
\begin{aligned}
&|(u^{(2,1)} - u_\epsilon^{(2,1)})(x)| \\
&= \ \Big|\frac{\gamma}{4\pi}\int_{\partial\tau\cap\mathcal{U}} \big(1-\eta(\frac{|x-y|}{\epsilon})\big)\frac{\phi(y)}{|x-y|}\,d\mathcal{H}^2(y)\Big| \\
&= \ \Big|\frac{\gamma}{4\pi}\int_{B_R(\tilde{x})} \big(1-\eta(\frac{|\psi(\tilde{x})-\psi(\tilde{y})|}{\epsilon})\big)\frac{\phi(\psi(\tilde{y}))}{|\psi(\tilde{x})-\psi(\tilde{y})|}J_\psi(\tilde{y})\,d^2\tilde{y}\Big| \qquad (2.16) \\
&\leq \ C\int_{B_R(\tilde{x})} \big(1-\eta(\frac{|\psi(\tilde{x})-\psi(\tilde{y})|}{\epsilon})\big)\frac{1}{|\psi(\tilde{x})-\psi(\tilde{y})|}\,d^2\tilde{y} \qquad (2.17) \\
&\leq \ C\int_{B_{C\epsilon}(\tilde{x})} \frac{1}{|\tilde{x}-\tilde{y}|}\,d^2\tilde{y}. \qquad (2.18)
\end{aligned}
$$

Using polar coordinates one obtains

$$|(u^{(2,1)} - u_\epsilon^{(2,1)})(x)| \ \leq \ C\epsilon, \qquad (2.19)$$

which tends to zero uniformly in x as $\epsilon \to 0$. So (2.7) follows.

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

$$\nabla_x u^{(2)}(x)\cdot D\psi(\tilde{x})v \ = \ \lim_{\epsilon\to 0}\frac{-\gamma}{4\pi}\int_{\partial\tau}\eta(\frac{|x-y|}{\epsilon})\phi(y)\frac{x-y}{|x-y|^3}\cdot D\psi(\tilde{x})v\,d\mathcal{H}^2(y)$$

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

$$\nabla(u_\epsilon^{(2)}\circ\psi) \longrightarrow \nabla(u^{(2)}\circ\psi) \qquad \text{uniformly} \qquad (2.20)$$

as $\epsilon \to 0$, and then we verify that

$$
\begin{aligned}
&\Big|\nabla_{\tilde{x}}(u_\epsilon^{(2)}\circ\psi)(\tilde{x})\cdot v - \frac{-\gamma}{4\pi}\int_{\partial\tau}\eta(\frac{|x-y|}{\epsilon})\phi(y)\frac{x-y}{|x-y|^3}\cdot D\psi(\tilde{x})v\,d\mathcal{H}^2(y)\Big| \\
&\leq C\epsilon. \qquad (2.21)
\end{aligned}
$$

For (2.20) it suffices to consider the convergence of the local term. Notice that $u_\epsilon^{(2,1)}$ equals the regularized function of Q,

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

with η as above. The estimates (2.15)–(2.19) yield that $\lim_{\epsilon\to 0} Q_\epsilon(\tilde{x}) = Q(\tilde{x})$ uniformly in $\tilde{x}$. Next we show that the derivative of Q_ϵ converges uniformly

to $\nabla_{\tilde{x}} Q(\tilde{x})$ as $\epsilon > 0$. For this we prove that $\nabla_{\tilde{x}} Q_\epsilon(\tilde{x})$ is a Cauchy net in C^0 as $\epsilon \to 0$. Thus it follows that Q is C^1 and $\nabla_{\tilde{x}} Q_\epsilon \to \nabla_{\tilde{x}} Q$.
To prove that $\nabla_{\tilde{x}} Q_\epsilon(\tilde{x})$ is a Cauchy net in C^0 as $\epsilon \to 0$ it suffices to show this for $\delta \in [\epsilon/2, \epsilon)$ since the general case follows then by summing a geometric series. We have

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

where

$$g(t) := \frac{\gamma}{4\pi}\big(\eta(\frac{t}{\delta}) - \eta(\frac{t}{\epsilon})\big)\frac{1}{t}.$$

The support of g is contained in $[\epsilon/4, \epsilon]$, and one has $|g'(t)| \leq Ct^{-2}$ and $g \in C^\infty$. In particular, $g(|\psi(\tilde{x}) - \psi(\tilde{y})|)$ vanishes for $\tilde{y}$ in a neighbourhood of $\partial B_R(\tilde{x})$. Thus we can commute differentiation and integration in

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

and obtain

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

Moreover we have

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

since

$$|D\psi(\tilde{x}) - D\psi(\tilde{y})| \leq C|\tilde{x} - \tilde{y}| \leq C|\psi(\tilde{x}) - \psi(\tilde{y})|.$$

Thus

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

The first term can be estimated as in (2.17)–(2.19). 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 one has that $\nabla_{\tilde{y}}\big(\phi(\psi(\tilde{y}))J_\psi(\tilde{y})\big)$ is bounded on $B_R(\tilde{x})$. Thus one can again apply an estimate as in (2.17)–(2.19) and one obtains that $\nabla_{\tilde{x}}Q_\epsilon(\tilde{x})$ is a Cauchy net as $\epsilon \to 0$. Hence ∇Q_ϵ and therefore $\nabla(u_\epsilon^{(2)} \circ \psi)$ converge uniformly. Together with the uniform convergence $u_\epsilon^{(2)} \to u^{(2)}$ this proves (2.20).

Regarding (2.21), we have

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

Since $x = \psi(\tilde{x})$, the proof of (2.21) reduces to estimating the first integral by $C\epsilon$. Since the integral vanishes unless $|y - x| \leq \epsilon$, we can rewrite the integral using the change of variables $y = \psi(\tilde{y})$. With the abbreviations

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

we have to estimate

$$I := \int_{B_{C\epsilon}(\tilde{x})} h(\psi(\tilde{x}) - \psi(\tilde{y})) \cdot D\psi(\tilde{x})v\, j(\tilde{y})\, d^2\tilde{y}.$$

Now $\operatorname{Lip} h \leq \frac{C}{\epsilon^3}$ for $|w| \leq C\epsilon$ and $\operatorname{Lip} j \leq C$. 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

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

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 $|I| \leq C\epsilon$ and (2.21) is proved, which finishes the proof of Lemma 2.3.

2.3 The normal component of the magnetic field

In Lemma 2.4 the behaviour of the normal derivative of $u^{(2)}$ is considered. A detailed treatment of a similar statement can be found e.g. in [Fo, Theorem (3.28)]. There the normal derivative of the so-called single layer potential is derived. The assumption that the boundary is a compact C^2-boundary is used in the proof of a central estimate:

Lemma 2.5 (Lemma (3.15) in [Fo]) *Let τ be a bounded subset of $\mathbb{R}^3$ with C^2-boundary. Then there is a constant $C > 0$ such that for all $x, y \in \partial\tau$,*

$$|(x-y)\cdot n(y)| \le C|x-y|^2.$$

Proof: By a translation and rotation of coordinates one may assume that $y = 0$ and $n(y) = (0,0,1)$, i.e. $(x-y)\cdot n(y) = x_3$. Near y, the boundary $\partial\tau$ can be described by a C^2-function f such that $f(0) = 0$ and $\nabla f(0) = 0$. A Taylor expansion leads to

$$|(x-y)\cdot n(y)| = |x_3| = |f(x_1,x_2)| \le C|(x_1,x_2)|^2 \le C|x|^2 \le C|x-y|^2.$$

Since $\partial\tau$ is C^2 and $\mathcal{H}^2(\partial\tau) < \infty$, there is a uniform bound for all $y \in \partial\tau$. □

Lemma 2.4 of this thesis differs from the corresponding framework in [Fo] only in the differently chosen regularization. While Folland cuts off a ball B_ϵ about the singularity sharply, i.e. by a characteristic function, we use a smooth function η. Thus we have to compare the integral with the sharp cut-off with

$$\begin{aligned}
&\int_{\partial\tau} \nabla_x\big(\eta(\frac{|x-y|}{\epsilon})\phi(y)\frac{1}{|x-y|}\big)\cdot n(x)\,d\mathcal{H}^2(y)\\
&= \int_{\partial\tau} \eta(\frac{|x-y|}{\epsilon})\phi(y)\frac{-(x-y)\cdot n(x)}{|x-y|^3}\,d\mathcal{H}^2(y) + \\
&\quad + \int_{\partial\tau} \nabla_x\big(\eta(\frac{|x-y|}{\epsilon})\big)\cdot n(x)\phi(y)\frac{1}{|x-y|}\,d\mathcal{H}^2(y).
\end{aligned} \tag{2.22}$$

The second integral tends to zero as $\epsilon \to 0$ since with Lemma 2.5

$$\begin{aligned}
&\Big|\int_{\partial\tau} \nabla_x\big(\eta(\frac{|x-y|}{\epsilon})\big)\cdot n(x)\phi(y)\frac{1}{|x-y|}\,d\mathcal{H}^2(y)\Big|\\
&= \Big|\int_{\partial\tau\cap(B_\epsilon(x)\setminus B_{\epsilon/2}(x))} \eta'(\frac{|x-y|}{\epsilon})\frac{1}{\epsilon}\frac{(x-y)\cdot n(x)}{|x-y|}\phi(y)\frac{1}{|x-y|}\,d\mathcal{H}^2(y)\Big|\\
&\le \int_{\partial\tau\cap(B_\epsilon(x)\setminus B_{\epsilon/2}(x))} \frac{C}{\epsilon}\,d\mathcal{H}^2(y) \le C\epsilon,
\end{aligned}$$

where the last inequality follows by using polar coordinates. Thus it suffices to compare the first integral in (2.22) with Folland's regularization. Since

$\phi(y)\frac{(x-y)\cdot n(x)}{|x-y|^3}$ is of order $\frac{1}{|x-y|}$, one obtains

$$\begin{aligned} & |\int_{\partial\tau} \eta(\frac{|x-y|}{\epsilon})\phi(y)\frac{(x-y)\cdot n(x)}{|x-y|^3}\, d\mathcal{H}^2(y) + \\ & \quad - \int_{\partial\tau\setminus(\partial\tau\cap B_\epsilon(x))} \phi(y)\frac{(x-y)\cdot n(x)}{|x-y|^3}\, d\mathcal{H}^2(y)| \\ = & \ |\int_{\partial\tau\cap(B_\epsilon(x)\setminus B_{\epsilon/2})} \eta(\frac{|x-y|}{\epsilon})\phi(y)\frac{(x-y)\cdot n(x)}{|x-y|^3}\, d\mathcal{H}^2(y)| \\ \leq & \ C\int_{\partial\tau} \chi_{B_\epsilon(x)\setminus B_{\epsilon/2}(x)}(x-y)\frac{1}{|x-y|}\, d\mathcal{H}^2(y) \\ \leq & \ C\epsilon. \end{aligned}$$

Hence both regularizations lead to the same limit, and one can reduce the proof of Lemma 2.4 to the proofs in Folland's book.

This finishes the derivation of Brown's formula. This formula is discussed in Chapter 5. There we also compare Brown's formula with the force formula which is derived in the next chapter. The starting point of that force formula is a magnetic force in a discrete setting, i.e. a lattice. From this the limiting force is calculated as the distance between lattice points tends to zero.

Chapter 3

Magnetic force calculation atomistic to continuum

In this chapter we discuss magnetic forces between two subbodies of a magnetic body from a different point of view. We start the derivation of the force formula from an atomistic setting, i.e. from a lattice of magnetic moments. The assigned lattice constants describe the distance between lattice points, and the limit as the lattice constants tend to zero leads to a continuum setting. Here we focus on the behaviour of the magnetic force formula in this limiting procedure. To avoid any confusion we point out that we use the notions atomistic, microscopic and discrete as properties of a physical model synonymously in this work. Also macroscopic and continuous setting mean the same.
Before calculating the force in Section 3.2 we fix the notation for magnetic moments and magnetic fields in the next section.

3.1 Magnetic moment and magnetic field in a lattice of atoms

We consider a Bravais lattice

$$\mathcal{L} = \{x \in \mathbb{R}^3 \ : \ x = \sum_{i=1}^{3} \mu_i e_i, \ \mu_i \in \mathbb{Z}\}$$

of atoms, where (e_1, e_2, e_3) is a basis of $\mathbb{R}^3$. The unit cell $\mathcal{U}$ is given by

$$\mathcal{U} = \{y \in \mathbb{R}^3 \ : \ y = \sum_{i=1}^{3} \lambda_i e_i, \ \lambda_i \in [0, 1)\}.$$

Next we fix some general notation. Let $a, b \in \mathbb{R}^3$ and let A, B be sets. Then we define the segment

$$[a, b) = \{ta + (1 - t)b \ : \ t \in (0, 1]\},$$

the translated set

$$a + A = \{a + x \ : \ x \in A\}$$

and the sum

$$A + B = \{x + y \ : \ x \in A, \ y \in B\}.$$

Moreover we write $|A| = \mathcal{L}^3(A)$ for the three dimensional Lebesgue measure of A.

For $x \in \mathcal{L}$ the (translated) unit cell with base point x is denoted by

$$\mathcal{U}(x) = x + \mathcal{U}.$$

For the passage from the atomistic to the continuous setting we consider scaled Bravais lattices $\frac{1}{l}\mathcal{L}$, $l \in \mathbb{N}$. The unit cells are scaled accordingly, i.e. $\frac{1}{l}\mathcal{U}$, with $|\frac{1}{l}\mathcal{U}| = \frac{1}{l^3}|\mathcal{U}|$. For convenience the volume of the unit cell is normalized to 1. Hence $|\frac{1}{l}\mathcal{U}| = \frac{1}{l^3}$. Moreover we set $\frac{1}{l}\mathcal{U}(x) = x + \frac{1}{l}\mathcal{U}$ and write as a shorthand $\mathcal{L}^* = \mathcal{L} \setminus \{0\}$.

To each atom we assign a magnetic moment. If $x \in \frac{1}{l}\mathcal{L}$ is the position of an atom, then $m^{(l)}(x) \in \mathbb{R}^3$ denotes its magnetic moment. For the calculation of the force that one part of the lattice exerts on another part we consider the magnetic moment of each atom 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 more on background magnetizations see e.g. [JaMü]. The scaling law for a magnetic moment at $x \in \frac{1}{l}\mathcal{L}$ is

$$m^{(l)}(x) = \frac{1}{l^3} m(x), \tag{3.1}$$

i.e. the magnetic moment of an atom is scaled in such a way that we obtain a finite total magnetization per unit volume.

The magnetic field, H_y, corresponding to a magnetic moment of an atom at $y \in \frac{1}{l}\mathcal{L}$ is given by Maxwell's equations. The solution of Maxwell's equations reads for the ith component

$$(H_y)_i(x) = K_{ij}(x - y) m_j^{(l)}(y),$$

where $m_j^{(l)}(y)$ denotes the jth component of the magnetic moment and

$$K_{ij}(z) := \partial_i \partial_j N(z) \quad \text{and} \quad N(z) := \frac{\gamma}{4\pi}\frac{1}{|z|}, \quad z \neq 0, \tag{3.2}$$

i.e.

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

Here γ is a constant which depends only on the chosen physical units. For Gaussian units $\gamma = 4\pi$. The value of γ for other physical units can be found in e.g. [Br, p. 6].

For later use we remark that

$$K_{ij}(z) = K_{ij}(-z) \quad \text{and} \quad K_{ij}(z) = K_{ji}(z). \tag{3.3}$$

Note that we use a summation convention here and in the following. If an index appears twice, one has to sum over this index from 1 to 3.

Let A be a bounded subset of $\mathbb{R}^3$. Since Maxwell's equations are linear, the magnetic field, H_A, of all atoms in $A \cap \frac{1}{l}\mathcal{L}$ is a superposition of the magnetic fields of the single atoms. Thus

$$(H_A)_i(x) = \sum_{y \in A \cap \frac{1}{l}\mathcal{L}} K_{ij}(x-y) m_j^{(l)}(y).$$

3.2 The discrete force and its continuum limit

In this section we consider the magnetic force between two parts of a lattice, and we calculate the limiting force in the passage from the discrete to the continuous system.

A magnetic moment of an atom at $y \in \frac{1}{l}\mathcal{L}$ exerts a force on a magnetic moment of an atom at $x \in \frac{1}{l}\mathcal{L}$, $x \neq y$. The kth component of the force is given by

$$f_k = m_i^{(l)}(x) \partial_i (H_y)_k(x)$$

(cf. e.g. [Br, 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 is also given by

$$\begin{aligned} f_k &= m_i^{(l)}(x) \partial_{x_i} \partial_{x_j} \partial_{x_k} N(x-y) m_j^{(l)}(y) \\ &= m_i^{(l)}(x) \partial_{x_k} \partial_{x_i} \partial_{x_j} N(x-y) m_j^{(l)}(y) \\ &= m_i^{(l)}(x) \partial_k (H_y)_i(x). \end{aligned}$$

The magnetic force between several atoms is the superposition of the forces between all pairs of atoms.

Here we are interested in the magnetic force between two subbodies of a magnetic body. Let Ω be a bounded domain in $\mathbb{R}^3$ and τ a subset of Ω such that $\partial\Omega \cap \partial\tau = \emptyset$ as in Figure 2.1 on page 8.
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 kth component of this force reads

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

where $m^{(l)}(x) = (\frac{1}{l})^3 m(x)$ is the magnetic moment of an atom at $x \in \frac{1}{l}\mathcal{L}$ as introduced in Section 3.1. The background magnetization m is a given Lipschitz continuous function in τ and $\Omega \setminus \bar{\tau}$, which has support in $\overline{\Omega}$ and which is bounded on the whole body. For simplicity we assume that m has zero trace at $\partial\Omega$.

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

For the passage from the atomistic model to the continuum model we introduce a regularized kernel. Let $\varphi^{(1)} \in C_0^\infty(\mathbb{R}^3)$ be such that

$$\varphi^{(1)}(z) = \begin{cases} 1 & : \quad |z| \le \frac{1}{2}, \\ 0 & : \quad |z| \ge 1 \end{cases}$$

and $0 \le \varphi^{(1)}(z) \le 1$ else. Set $\varphi^{(\delta)}(z) = \varphi^{(1)}(\frac{z}{\delta})$ for $\delta > 0$. A possible choice is indicated in Figure 3.1.

For later use we also remark that for every multi-index $s = (s_1, s_2, s_3)$, $s_i \ge 0$, there exists a constant C_s such that

$$|\partial^s \varphi^{(\delta)}| = |\partial_1^{s_1} \partial_2^{s_2} \partial_3^{s_3} \varphi^{(\delta)}| \le C_s \frac{1}{\delta^{|s|}},$$

where $|s| = \sum_{i=1}^3 s_i$. Note that the regularizing function η of Chapter 2 can be chosen to be $1 - \varphi^{(1)}$, which is useful in the proofs of Section 3.3 as the results of Chapter 2 can be transferred to the current setting.

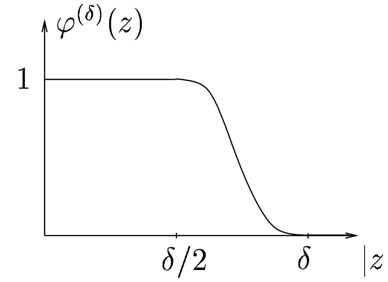

Figure 3.1: A cut-off function $\varphi^{(\delta)}$.

The kernel appearing in the magnetic field is regularized by

$$K_{ij}^{(\delta)}(z) = \partial_i \partial_j \Big(\big(1 - \varphi^{(\delta)}(z)\big) N(z) \Big). \tag{3.4}$$

Using the regularized kernel we split the double sum of the force into a long range part and a short range part.

$$\begin{aligned} F_k^{(l)} &= \sum_{x \in \bar{\tau} \cap \frac{1}{l}\mathcal{L}} \; \sum_{y \in (\Omega \setminus \bar{\tau}) \cap \frac{1}{l}\mathcal{L}} \partial_k K_{ij}^{(\delta)}(x-y) m_i^{(l)}(x) m_j^{(l)}(y) + \\ &\quad + \sum_{x \in \bar{\tau} \cap \frac{1}{l}\mathcal{L}} \; \sum_{y \in (\Omega \setminus \bar{\tau}) \cap \frac{1}{l}\mathcal{L}} \partial_k (K - K^{(\delta)})_{ij}(x-y) m_i^{(l)}(x) m_j^{(l)}(y) \\ &=: F_k^{(l,\delta)} + \mathcal{F}_k^{(l,\delta)}. \end{aligned} \tag{3.5}$$

In view of the behaviour of the regularizing function we call the first term long range term, and the second term the short range term. 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

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

In the following two sections the two terms are considered separately. In the subsequent section we prove the following theorem on the limit of the long range part of the force.

Theorem 3.1 *Let $\Omega \subset \mathbb{R}^3$ be open and bounded and let $\tau \subset \Omega$ with C^2-boundary such that $\Omega \setminus \bar{\tau}$ has C^2-boundary as well. Further let m belong to $W^{1,2}(\tau)$ and $W^{1,2}(\Omega \setminus \bar{\tau})$. Then the long range part of the force satisfies*

$$\begin{aligned} \lim_{\delta \to 0} F_k^{(\infty,\delta)} &:= \lim_{\delta \to 0} \lim_{l \to \infty} F_k^{(l,\delta)} \\ &= \int_\tau (m(x) \cdot \nabla)(H_\Omega)_k(x)\, d^3x + \\ &\quad + \frac{\gamma}{2} \int_{\partial\tau} (m^- \cdot n)(\xi) \big((m^- - m^+) \cdot n\big)(\xi) n_k(\xi)\, d\mathcal{H}^2(\xi). \end{aligned} \tag{3.6}$$

Before stating the theorem for the limit of the short range part of the force we set some notations and introduce a technical notion which regards the shape of the sets under consideration. We suppose that $\delta < \mathrm{dist}(\tau, \partial\Omega)$, which is possible in view of $\partial\Omega \cap \partial\tau = \emptyset$, which is assumed in the theorem on the limit of the short range part of the discrete force (Theorem 3.6).

Definition 3.2 *Let $B_\delta \subset \mathbb{R}^3$ denote the ball with radius δ centred at* 0. *For $z \in B_\delta$ we set*

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

An example of this set is given in Figure 3.2.

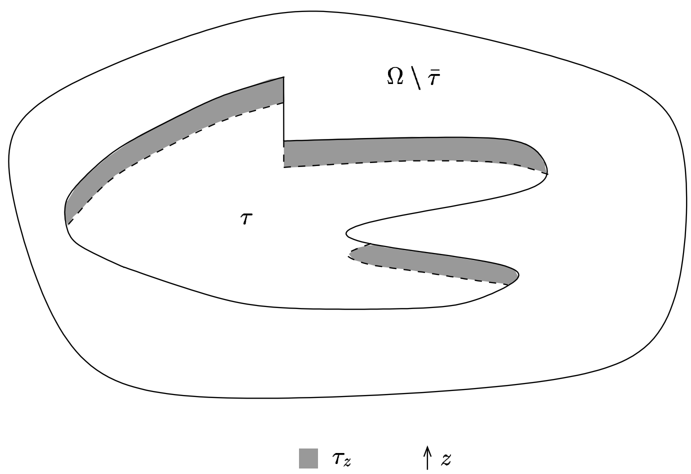

Figure 3.2: A slice of the sets showing τ_z.

Moreover we make use of a non-degeneracy condition on the shape of τ, which we define for $C^{1,1}$-boundaries. Here and in the following we assume that τ is a bounded Lipschitz domain.

Definition 3.3 *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 3.4 *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*

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

is a finite union of rectifiable curves, of which the number and the total length are bounded independently of z. We denote the bound on the number of these curves by $\bar{N}$ and the bound on the length of them by L.

The non-degeneracy condition (S) is for instance satisfied by $C^{1,1}$-boundaries, of which the number of indentations and protrusions is bounded. More concrete examples of boundaries which satisfy condition (S) are given at the end of this section.

The limit of the short range part of the force involves certain regularized lattice sums, for which we give a definition in the following. The existence of the relevant limits is proved in Section 3.4 and further properties are discussed in Chapter 4.

Definition 3.5 *Let $B_\delta \subset \mathbb{R}^3$ denote the ball with radius δ centred at 0. Set*

$$S_{ijkp} := - \lim_{\delta \to 0} \lim_{l \to \infty} \sum_{z \in B_\delta \cap \frac{1}{l}\mathcal{L}^*} \partial_k (K - K^{(\delta)})_{ij}(z) z_p (\frac{1}{l})^3. \tag{3.7}$$

With this we can now state the formula for the limit of the short range part of the microscopic force.

Theorem 3.6 *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 belong to $W^{1,\infty}(\tau)$ and $W^{1,\infty}(\Omega \setminus \bar{\tau})$. Then*

$$\lim_{\delta \to 0} \lim_{l \to \infty} \mathcal{F}_k^{(l,\delta)} = \frac{1}{2} \int_{\partial\tau} m_i^-(\xi) m_j^+(\xi) S_{ijkp} n_p(\xi) \, d\mathcal{H}^2(\xi). \tag{3.8}$$

The proof of this theorem is given in Section 3.4.

By bringing Theorem 3.1 and Theorem 3.6 together we obtain the force formula for the magnetic force between two subbodies of a macroscopic magnetic material as the limit of the corresponding microscopic force.

Theorem 3.7 *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 τ and $\Omega \setminus \bar{\tau}$ have C^2-boundaries and that $\partial\tau$ satisfies the non-degeneracy condition (S). Further let m belong to $W^{1,\infty}(\tau)$ and $W^{1,\infty}(\Omega \setminus \bar{\tau})$. Then*

$$\begin{aligned} F_k^{(\lim)} &= \int_\tau (m(x)\cdot\nabla)(H_\Omega)_k(x)\, d^3x + \\ &+ \frac{\gamma}{2}\int_{\partial\tau} (m^- \cdot n)(\xi)\big((m^- - m^+)\cdot n\big)(\xi) n_k(\xi)\, d\mathcal{H}^2(\xi) + \\ &+ \frac{1}{2}\int_{\partial\tau} m_i^-(\xi) m_j^+(\xi) S_{ijkp} n_p(\xi)\, d\mathcal{H}^2(\xi). \end{aligned} \tag{3.9}$$

The limiting force contains in general other surface integrals than Brown's force does (Theorem 2.1). In Chapter 5 we discuss this in detail. For this we consider the formulae also in the case of separated regions (Section 5.1) and in the case of a magnetization that is smooth in Ω (Section 5.2).

Before going into the proofs of the above theorems in the following two sections, we give some examples of sets which satisfy the non-degeneracy condition (S).

1. Polyhedra.

The sets U_i are the faces and the boundary of $\partial^+\tau$ is a subset of the edges.

2. 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.
Instead of uniformly convex surfaces one can more generally consider surfaces with Gauss curvature bounded away from zero.

3. 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 $\mathcal{A} + [0,\xi]$, where $\xi \in \mathbb{R}^3$ is orthogonal to $\mathcal{A}$.

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

3.3 The long range term

The aim of this section is to prove Theorem 3.1, which provides a formula for the limit of the long range part of the atomistic magnetic force.

In the beginning of the proof of Brown's force formula on page 9 we explain that one can approximate the magnetization, which belongs to $W^{1,2}(\tau)$, by functions, which are smooth in τ. It is sufficient to show the force formula for smooth magnetizations rather than for general magnetizations in $W^{1,2}(\tau)$. The same arguments apply here as well and one has a similar approximation for $m \in W^{1,2}(\Omega \setminus \bar{\tau})$, i.e. we may assume in the following that m is a smooth function on τ and on $\Omega \setminus \bar{\tau}$.

The long range term $F_k^{(l,\delta)}$ of the atomistic force is defined in (3.5). Observe that for $\delta > 0$ the function $\partial_k K_{ij}^{(\delta)}(x-y)$ is continuous and bounded. Since m is continuous and bounded on τ and on $\Omega \setminus \bar{\tau}$, the terms of the double sum are continuous and bounded for $\delta > 0$. Hence the double sum can be viewed as a Riemann sum and converges to

$$F_k^{(\infty,\delta)} = \lim_{l\to\infty} F_k^{(l,\delta)} = \int_\tau \int_{\Omega\setminus\bar{\tau}} \partial_k K_{ij}^{(\delta)}(x-y) m_i(x) m_j(y)\, d^3y\, d^3x$$

as $l \to \infty$. Similarly to the approach in Chapter 2, we split the inner integral into an integral over Ω minus an integral over $\bar{\tau}$. We thus have for $\delta > 0$

$$\begin{aligned} F_k^{(\infty,\delta)} &= \int_\tau \int_\Omega \partial_k K_{ij}^{(\delta)}(x-y) m_i(x) m_j(y)\, d^3y\, d^3x + \\ &\quad - \int_\tau \int_\tau \partial_k K_{ij}^{(\delta)}(x-y) m_i(x) m_j(y)\, d^3y\, d^3x. \end{aligned} \tag{3.10}$$

The latter integral is zero, which is proven in the following. Since $K_{ij}^{(\delta)}(x-y)$ is symmetric in its argument and in the indices (cf. (3.3)) one has

$$\begin{aligned} \partial_k K_{ij}^{(\delta)}(x-y) &\equiv \frac{\partial}{\partial x_k} K_{ij}^{(\delta)}(x-y) = -\frac{\partial}{\partial y_k} K_{ij}^{(\delta)}(x-y) \\ &= -\frac{\partial}{\partial y_k} K_{ij}^{(\delta)}(y-x) = -\frac{\partial}{\partial y_k} K_{ji}^{(\delta)}(y-x). \end{aligned}$$

Hence the second integral in (3.10) reads

$$
\begin{aligned}
&\int_\tau\int_\tau \partial_k K_{ij}^{(\delta)}(x-y)m_i(x)m_j(y)\,d^3y\,d^3x \\
&\quad= \quad -\int_\tau\int_\tau \frac{\partial}{\partial y_k}K_{ji}^{(\delta)}(y-x)m_i(x)m_j(y)\,d^3y\,d^3x \\
&\quad\overset{x\leftrightarrow y}{=} \quad -\int_\tau\int_\tau \frac{\partial}{\partial x_k}K_{ji}^{(\delta)}(x-y)m_i(y)m_j(x)\,d^3x\,d^3y \\
&\quad\overset{\text{Fubini}}{=} \quad -\int_\tau\int_\tau \frac{\partial}{\partial x_k}K_{ji}^{(\delta)}(x-y)m_i(y)m_j(x)\,d^3y\,d^3x \\
&\quad\overset{i\leftrightarrow j}{=} \quad -\int_\tau\int_\tau \partial_k K_{ij}^{(\delta)}(x-y)m_j(y)m_i(x)\,d^3y\,d^3x
\end{aligned}
$$

and is therefore zero for all $\delta > 0$, i.e. this term does not contribute in the limit. Hence

$$
F_k^{(\infty,\delta)} = \int_\tau\int_\Omega \partial_k K_{ij}^{(\delta)}(x-y)m_i(x)m_j(y)\,d^3y\,d^3x. \tag{3.11}
$$

This can be written in terms of $H_\Omega^{(\delta)}$, the regularized version of the magnetic field H_Ω. One has

$$
\begin{aligned}
&\int_\tau\int_\Omega \partial_k K_{ij}^{(\delta)}(x-y)m_i(x)m_j(y)\,d^3y\,d^3x \\
&= \int_\tau m_i(x)\int_\Omega \underbrace{\partial_{x_k}K_{ij}^{(\delta)}(x-y)}_{=\partial_{x_i}K_{kj}^{(\delta)}(x-y)}\,m_j(y)\,d^3y\,d^3x \\
&= \int_\tau m_i(x)\partial_{x_i}\underbrace{\Big(\int_\Omega K_{kj}^{(\delta)}(x-y)m_j(y)\,d^3y\Big)}_{=(K_{kj}^{(\delta)}*m_j\chi_\Omega)(x)=:(H_\Omega^{(\delta)})_k(x)}\,d^3x \\
&= \int_\tau(-\nabla\cdot m)(x)(H_\Omega^{(\delta)})_k(x)\,d^3x + \int_{\partial\tau}(m\cdot n)^-(x)(H_\Omega^{(\delta)})_k^-(x)\,d\mathcal{H}^2(x),
\end{aligned} \tag{3.12}
$$

where we used that the trace of m at $\partial\Omega$ is zero to simplify the formula. When this trace is not zero, one obtains an additional boundary integral over $\partial\Omega$. In the following we always assume that m is zero at $\partial\Omega$ for simplicity. The proof in the general case is similar. Several of the analogous formulae in the general case can be found in Appendix B.

To prove that $F_k^{(\infty,\delta)}$ converges to the desired formula in (3.6) as $\delta \to 0$, we show the convergence of the two integrals in (3.12) separately. For this notice that $H_\Omega^{(\delta)}$ is here defined according to the definition of the magnetic field in the continuum setting. H_Ω is the field generated by the magnetic material m in Ω

and it is given by Maxwell's equations. Since Maxwell's equations are linear, H_Ω is the sum of $H_{\bar\tau}$ and $H_{\Omega\setminus\bar\tau}$. If one sets $H_\Omega = -\nabla u$, the corresponding Maxwell's equations can be written as a Poisson equation (cf. p. 80)

$$-\Delta u = -\gamma \nabla \cdot (m\chi_\Omega) \quad \text{in} \quad \mathbb{R}^3 \setminus \partial\tau$$

with transition condition

$$[\nabla u \cdot n] = \gamma [m \cdot n] \quad \text{on} \quad \partial\tau.$$

(If $(m \cdot \nu)^-$ is not assumed to be zero on $\partial\Omega$ one has $-\Delta u = -\gamma\nabla \cdot (m\chi_\Omega)$ in $\mathbb{R}^3 \setminus (\partial\Omega \cup \partial\tau)$ and $[\nabla u \cdot \nu] = -\gamma(m \cdot \nu)^-$ on $\partial\Omega$ in addition.)

With (3.4) one obtains from the defining equation of $H_\Omega^{(\delta)}$

$$\begin{aligned}
&(H_\Omega^{(\delta)})_k(x) \\
&= -\int_\Omega (-\nabla \cdot m)(y)\partial_k\big((1-\varphi^{(\delta)}(x-y))N(x-y)\big)\, d^3y + \\
&\quad -\int_{\partial\tau} \big((m^- - m^+)\cdot n\big)(y)\partial_k\big((1-\varphi^{(\delta)}(x-y))N(x-y)\big)\, d\mathcal{H}^2(y).
\end{aligned}$$

We first consider the volume integral. Here and in the following c denotes positive generic constants, which do not always have to be the same. Since $\nabla \cdot m$ is bounded on τ and $\Omega \setminus \bar\tau$ and since $\varphi^{(\delta)}$ has support in the ball $B_\delta(x)$ and its derivative has support in $B_\delta(x) \setminus B_{\delta/2}(x)$, one obtains

$$\begin{aligned}
&\Big|\int_\Omega (-\nabla \cdot m)(y)\partial_k\big(\varphi^{(\delta)}(x-y)N(x-y)\big)\, d^3y\Big| \\
&\le c\int_\Omega \big|\big(\partial_k\varphi^{(\delta)}(x-y)\big)N(x-y)\big|\, d^3y + c\int_\Omega \big|\varphi^{(\delta)}(x-y)\partial_k N(x-y)\big|\, d^3y \\
&\le \frac{c}{\delta}\int_{B_\delta(x)\setminus B_{\delta/2}(x)} \frac{1}{|x-y|}\, d^3y + c\int_{B_\delta(x)} \frac{|(x-y)_k|}{|x-y|^3}\, d^3y \\
&\le \frac{c}{\delta}\int_{\delta/2}^{\delta} r\, dr + c\int_0^\delta 1\, dr \\
&\le c\delta.
\end{aligned}$$

Hence the volume term converges uniformly in x to the volume term of H_Ω, i.e.

$$\frac{\gamma}{4\pi}\int_\Omega (-\nabla \cdot m)(y)\frac{x-y}{|x-y|^3}\, d^3y.$$

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 that $x \in \tau$. To pass to the limit in the first term in (3.12) we need

$$(H_\Omega^{(\delta,2)})_k \longrightarrow (H_\Omega^{(2)})_k \qquad \text{in} \quad L^1(\tau) \quad \text{as} \quad \delta \to 0, \tag{3.13}$$

where

$$\begin{aligned} (H_\Omega^{(2)})_k(x) &= -\int_{\partial\tau} \phi^*(y)\partial_k N(x-y)\, d\mathcal{H}^2(y) \\ &= \frac{\gamma}{4\pi}\int_{\partial\tau} \phi^*(y)\frac{(x-y)_k}{|x-y|}\, d\mathcal{H}^2(y). \end{aligned}$$

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

$$\int_{\tau\setminus U_\alpha} |H_\Omega^{(\delta,2)}(x)|\, d^3x < \frac{\epsilon}{2} \tag{3.14}$$

and

$$\int_{\tau\setminus U_\alpha} |H_\Omega^{(2)}(x)|\, d^3x < \frac{\epsilon}{2}, \tag{3.15}$$

since this yields by

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

the desired convergence in (3.13).

To show (3.14) note that one has $|\partial_k\varphi^{(\delta)}(z)| \le \frac{c}{|z|}$ by the fact that $|\partial_k\varphi^{(\delta)}(z)| \le \frac{c}{\delta}$ and $\partial_k\varphi^{(\delta)}(z) = 0$ if $|z| > \delta$. Hence

$$\begin{aligned} &\Big|\partial_k\Big(\big(1-\varphi^{(\delta)}(x-y)\big)N(x-y)\Big)\Big| \\ &\le \big|\partial_k\varphi^{(\delta)}(x-y)\big|N(x-y) + |\partial_k N(x-y)| \le c\frac{1}{|x-y|^2}. \end{aligned}$$

Thus by the boundedness of ϕ^*

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

The integral $\int_{\tau\setminus U_\alpha} \frac{1}{|x-y|^{5/2}}\, d^3x$ is bounded independent 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 (3.14). Similarly one gets (3.15).

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

$$\bar{H}_\Omega(x) = \frac{\gamma}{4\pi}\int_\Omega(-\nabla\cdot m)(y)\frac{x-y}{|x-y|^3}\, d^3y + (\mathcal{B}\phi^*)(x), \tag{3.16}$$

where

$$(\mathcal{B}\phi^*)(x) := \lim_{\delta\to 0}\frac{\gamma}{4\pi}\int_{\partial\tau}(1-\varphi^{(\delta)}(x-y))\phi^*(y)\frac{x-y}{|x-y|^3}\, d\mathcal{H}^2(y), \tag{3.17}$$

similarly to (2.13). The convergence is uniform in $x\in\partial\tau$.

In this case the results in Chapter 2 can be used. For this we replace the regularizing function $1-\varphi^{(1)}$ with η; see (2.1) for a definition of η. The parameter δ plays the role of ϵ. Thus

$$\begin{aligned}&-\int_{\partial\tau}\phi^*(y)\partial_k\Big(\big(1-\varphi^{(\delta)}(x-y)\big)N(x-y)\Big)\, d\mathcal{H}^2(y)\\ &\equiv -\int_{\partial\tau}\phi^*(y)\partial_k\Big(\eta(\frac{|x-y|}{\delta})N(x-y)\Big)\, d\mathcal{H}^2(y)\\ &= -\int_{\partial\tau}\phi^*(y)\big(\partial_k\eta(\frac{|x-y|}{\delta})\big)N(x-y)\, d\mathcal{H}^2(y) +\\ &\quad -\int_{\partial\tau}\phi^*(y)\eta(\frac{|x-y|}{\delta})\partial_k N(x-y)\, d\mathcal{H}^2(y).\end{aligned} \tag{3.18}$$

Note that $\phi^* = (m^- - m^+)\cdot n$ is continuous on $\partial\tau$ and fulfils the same conditions as $M_\tau^-\cdot n$ in Chapter 2. By Lemma 2.3 and Lemma 2.4, the limit of the second integral in (3.18) as $\delta\to 0$ exists and the convergence is uniform for all $x\in\partial\tau$. From the proofs of these lemmas it follows that the first term does not contribute in the limit. Analogously to (2.13) and (3.17) one has

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

uniformly in $x\in\partial\tau$. Hence (3.16) follows.

Similarly to the formulae of H_τ^+ and H_τ^- in (2.11) and (2.12), respectively, one obtains the inner and outer traces of H_Ω at $\partial\tau$. For $x \in \partial\tau$ one has

$$H_\Omega^\pm(x) = \frac{\gamma}{4\pi}\int_\Omega (-\nabla\cdot m)(y)\frac{x-y}{|x-y|^3}\,d^3y \;+\; (\mathcal{B}\phi^*)(x) \pm \frac{\gamma}{2}\phi^*(x)n(x). \quad (3.19)$$

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, one has, by the transition condition for the normal component of H_Ω,

$$\begin{aligned}\bar{H}_\Omega(x) &= \frac{1}{2}(H_\Omega^+ - H_\Omega^-)(x) + H_\Omega^-(x)\\ &= -\frac{\gamma}{2}\Big((m^+\cdot n)(x) - (m^-\cdot n)(x)\Big)n(x) + H_\Omega^-(x)\\ &= \frac{\gamma}{2}\Big((m^- - m^+)\cdot n\Big)(x)n(x) + H_\Omega^-(x). \qquad (3.20)\end{aligned}$$

Next we apply the convergence results to obtain the limit of (3.11) and (3.12), respectively. Notice that $(H_\Omega^{(\delta)})^-(x) = H_\Omega^{(\delta)}(x)$ for $\delta > 0$. In summary one obtains

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

where the last equation follows with (3.20). 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 3.1.

While several results from Chapter 2 could be transferred to this section on the limit of the long range part of the discrete force, the methods which are developed for the short range term in the next section are different from the continuum approach.

3.4 The short range term

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 (3.8) in Theorem 3.6 holds. For this we suppose that the assumptions of Theorem 3.6 hold throughout this section. In particular we assume that $\partial\tau$ satisfies the non-degeneracy condition (S) and that m belongs to $W^{1,\infty}(\tau)$ and $W^{1,\infty}(\Omega \setminus \bar{\tau})$.

From this regularity one has by the theorem on traces (cf. Theorem A.1) that $m^- \in L^\infty(\partial\tau)$ and $m^+ \in L^\infty(\partial\tau)$, where m^- is the inner trace with respect to τ and m^+ denotes the outer trace with respect to τ. By Theorem A.4 there exists to $m \in W^{1,\infty}(\tau)$ a representative of the same equivalence class which is in $C^{0,1}(\bar{\tau})$. Similarly there is a representative to $m \in W^{1,\infty}(\Omega \setminus \bar{\tau})$ in $C^{0,1}(\overline{\Omega \setminus \bar{\tau}})$. In the following we deal with these representatives. Note that their traces are in $C^{0,1}(\partial\tau)$.

Since the support of $(K - K^{(\delta)})_{ij} = \partial_i \partial_j (\varphi^{(\delta)} N)$ is contained in $B_\delta(0)$, we now have to control the short range behaviour, i.e. the occurring singularities of the hypersingular kernel.

For this the change of variables $y \mapsto x + z$ is useful. For $\delta > 0$ 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 $y \in (\Omega \setminus \bar{\tau}) \cap \frac{1}{l}\mathcal{L}$ one always has $x \neq y$ which becomes $z \neq 0$ under the transformation. Recall that 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. Then

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

where $\tau_z = \{x \in \bar{\tau} \, : \, x + z \in \Omega \setminus \bar{\tau}\}$ as in Definition 3.2.

Before going into the details of the proof of the limiting force we summarize 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 (3.8) and to its complement which gives higher order terms, which do not contribute in the limiting force. The precise definitions of these sets are given in Definitions 3.8 and 3.9.

We call the subset which leads to higher order terms 'bad' set and denote it by $\mathcal{B}$. By Lemma 3.10 and Lemma 3.11 (with for instance $\beta = \frac{2}{3}$ as in (3.45)), 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 (3.1) one obtains

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

By the estimate on the number of points in $\mathcal{B}$ and the boundedness of m one has

$$T \le c \sum_{z \in B_\delta \cap \frac{1}{l}\mathcal{L}^*} \frac{1}{|z|^4} |z|^{1+\alpha} (\frac{1}{l})^3 = c \sum_{z \in B_\delta \cap \frac{1}{l}\mathcal{L}^*} \frac{1}{|z|^{3-\alpha}} (\frac{1}{l})^3. \tag{3.21}$$

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

The other subset is called 'good' set and is denoted by $\mathcal{G}$ (cf. (3.22)). The number of lattice points which belong to $\mathcal{G}$ can be estimated by a constant times $l^3|z|$ (cf. Lemma 3.16). As follows by Proposition 3.14, the sum over the good points can be approximated by a certain surface integral. More precisely, we prove that there is a constant c and an $\alpha > 0$ such that

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

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 (3.21) 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 $\delta > 0$ one can commute summation and integration and obtains

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

The final step is to show the convergence of the lattice sum as $l \to \infty$ and $\delta \to 0$ (cf. Lemma 3.17). With this we then take the limits and obtain the desired force formula in Theorem 3.6.

Next we go into the details of the procedure described above. 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. $\frac{\tilde{c}}{l} \leq |z|$ 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.

The set τ_z is split into a bad set $\mathcal{B}$ and a good set $\mathcal{G}$ (cf. Figure 3.3). 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 3.4.

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 the normal is orthogonal to z. 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 the normal is almost orthogonal to z. This set is of special interest when z and $\frac{1}{l}$ are of the same order.

Definition 3.8 *Let C_0 be a suitable large constant, which satisfies in particular $C_0 > \max\{3, \mathrm{diam}\,\mathcal{U}\}$, and let*

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

The first bad set consists of the following lattice points

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

We also define a function $r_z : \tau_z \to \partial\tau$ 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 $\partial\tau$, as is indicated in Figure 3.2. 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 $\{x \in \tau_z \cap \frac{1}{l}\mathcal{L} \,:\, r_z(x) \in \partial^+\tau \setminus (\partial^+\tau \cap \partial^+\tau_z)\}$. One then has that $r_z(x) \in \partial\tau_z$ for all lattice points, which do not belong to $\mathcal{B}_I$. This will be used in the proof of Lemma 3.11.

Definition 3.9 *Let ρ be as before and let C_1 be a suitable large constant, which satisfies in particular $C_1 > \max\{12\,\mathrm{diam}\,\mathcal{U}, 6\,\mathrm{Lip}(n)\}$. Then the second bad set is defined as*

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

Finally, the good set is said to be

$$\mathcal{G} = (\tau_z \cap \frac{1}{l}\mathcal{L}) \setminus (\mathcal{B}_I \cup \mathcal{B}_{II}). \tag{3.22}$$

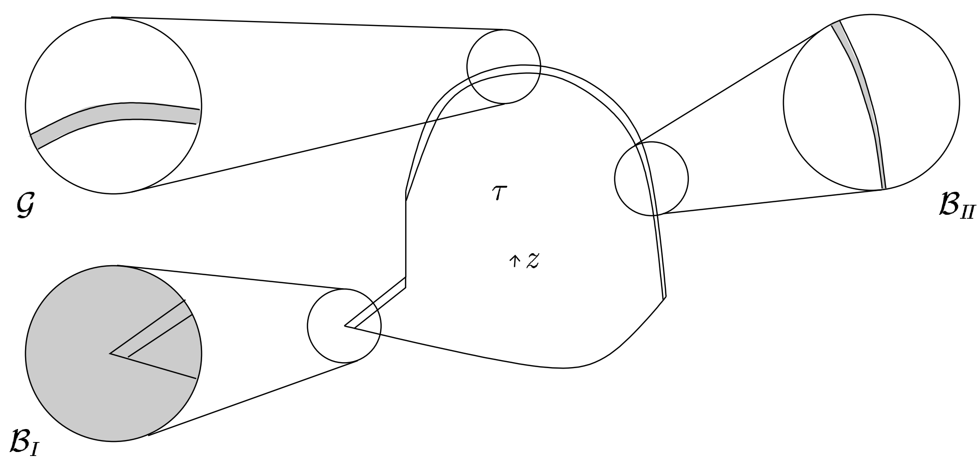

Figure 3.3: A slice of τ indicating the good and bad sets and τ_z.

In the following we assume that δ is so small and l so large that $C_1(l^{\beta-1}+\rho) \ll 1$ and $\frac{\tilde{c}}{l} \leq |z| < \delta$.

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

Lemma 3.10

$$\#\mathcal{B}_I \leq cl^3|z|^{2\beta}.$$

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. Let $\lfloor a \rfloor$ denote the integer part of a. There exist at most $\lfloor \frac{L}{2\rho} \rfloor + 2$ points x_i on Γ such that $\Gamma \subset \bigcup_i B(x_i, \rho)$. Let 4ρ be 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 one has $\mathcal{B}_I \subset \bigcup_i B(x_i, 9\rho)$ and

$$\bigcup_{x \in \mathcal{B}_I} \frac{1}{l}\mathcal{U}(x) \subset \bigcup_i B(x_i, 10\rho).$$

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 one obtains

$$\begin{aligned} \#\mathcal{B}_I &\leq c\frac{L}{\rho}\rho^3 l^3 = cLl^3\rho^2 \\ &\leq cLl^3 C_0^2(|z| + l^{-\beta})^2 \leq cl^3|z|^{2\beta} \end{aligned}$$

as stated. □

Since $2\beta > 1$ by assumption, the points in $\mathcal{B}_I$ yield higher order terms, as discussed on page 36. 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 3.11

$$\#\mathcal{B}_{II} \leq cl^3|z|^{2-\beta}.$$

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

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

with $\rho = C_0(|z| + l^{-\beta})$ and r_z as above. Since $|x - r_z(x)| \leq |z| \leq \rho$ as $C_0 > 1$ and since $x \notin \mathcal{B}_I$ and $n(r_z(x))\cdot\frac{z}{|z|} \leq C_1(l^{\beta-1}+\rho)$, one has that $B(r_z(x), 5\rho)\cap\partial\tau$ is contained in a single chart U_i and in $\partial^+\tau$ (cf. Definitions 3.3 and 3.4). Since U_i is $C^{1,1}$, one 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

$$\mathcal{H}^2(B_x) \geq c\pi\rho^2.$$

Let χ_y be the characteristic function of B_y. Then

$$\begin{aligned}\int_{\partial\tau}\sum_{y\in\mathcal{B}_{II}}\chi_y(\xi)\,d\mathcal{H}^2(\xi) &= \sum_{y\in\mathcal{B}_{II}}\int_{\partial\tau}\chi_y(\xi)\,d\mathcal{H}^2(\xi)=\sum_{y\in\mathcal{B}_{II}}\mathcal{H}^2(B_y)\\ &\geq c\pi\rho^2\#\mathcal{B}_{II}. \end{aligned}\tag{3.23}$$

If we can show that

$$\sup_{x\in\mathcal{B}_{II}}\sum_{y\in\mathcal{B}_{II}}\chi_y(r_z(x))\leq N, \tag{3.24}$$

then

$$\#\mathcal{B}_{II}\leq\frac{cN}{\rho^2} \tag{3.25}$$

since, by (3.24), the left hand side of (3.23) is bounded from above by $N\mathcal{H}^2(\partial\tau)$ and $\mathcal{H}^2(\partial\tau)$ is bounded by assumption.

We have

$$\begin{aligned}\sup_{x\in\mathcal{B}_{II}}\sum_{y\in\mathcal{B}_{II}}\chi_y(r_z(x)) &\leq \sup_{x\in\mathcal{B}_{II}}\#\{y\in\mathcal{B}_{II}\ :\ B_y\cap B_x\neq\emptyset\}\\ &\leq \sup_{x\in\mathcal{B}_{II}}\#\{y\in\mathcal{B}_{II}\ :\ r_z(y)\in B(r_z(x),2\rho)\}. \end{aligned}\tag{3.26}$$

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

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

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

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

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

$$n(\xi)\cdot e_1\leq C_1(l^{\beta-1}+\rho)\qquad\forall\xi\in B(r_z(x),5\rho)\cap\partial\tau. \tag{3.27}$$

Moreover

$$n(\xi)\cdot e_1>0\qquad\forall\xi\in B(r_z(x),5\rho)\cap\partial\tau \tag{3.28}$$

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

Thus $\partial\tau$ is locally represented as a $C^{1,1}$-graph over the e_1,e_2 plane (see Figure 3.4). Set $x'=(x_1,x_2)$ and let $u:\mathbb{R}^2\to\mathbb{R}$ be a $C^{1,1}$-function which

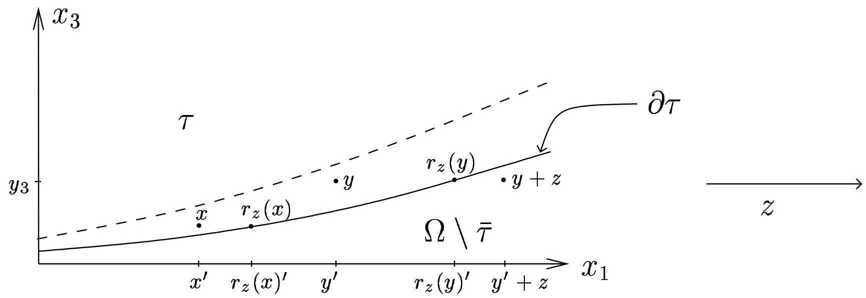

Figure 3.4: A local representation of the boundary.

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

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

and by (3.27) and (3.28)

$$0<\frac{\partial u}{\partial x_1}(x')\le c(l^{\beta-1}+\rho)\ll 1 \tag{3.29}$$

for all $x'\in B(r_z(x)',4\rho)$.

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

$$y+kz\notin\tilde{\mathcal{B}}_{II}\qquad \forall k\in\mathbb{Z}\setminus\{0\},\ |k|\le K:=\lfloor\frac{\rho}{|z|}\rfloor. \tag{3.30}$$

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

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

Thus $y+kz\notin\bar\tau$ for $k=1,\dots,K$. So $y+kz\notin\tilde{\mathcal{B}}_{II}$ as asserted.
For $-K\le k\le 0$ one obtains 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 (3.30).

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 (cf. p. 22). 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 $k \neq \tilde{k}$ such that $y + kz = \tilde{y} + \tilde{k}z$. Hence $y = (\tilde{k} - k)z + \tilde{y} \neq \tilde{y}$. But this contradicts (3.30).

Let

$$W := \bigcup_{k=0}^{K} (kz + V).$$

Then, using the definition of $\tilde{\mathcal{B}}_{II}$, the upper bound in (3.29) and the estimate $|z| + \operatorname{diam} \frac{1}{l}\mathcal{U} \leq \rho$ one sees that

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

where

$$H \leq c(l^{\beta-1} + \rho)\rho + \frac{\operatorname{diam} \mathcal{U}}{l} \leq c(l^{\beta-1} + \rho)\rho.$$

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

We finally obtain

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

uniformly in $x \in \mathcal{B}_{II}$. Thus by (3.24)–(3.26)

$$\#\mathcal{B}_{II} \leq cl^3|z|(l^{\beta-1} + \rho).$$

Using that $1 > \beta > \frac{1}{2}$ and thus $\rho \leq c(|z| + l^{-\beta}) \leq c(|z| + l^{\beta-1})$, this finally yields

$$\#\mathcal{B}_{II} \leq cl^3(l^{\beta-1}|z| + |z|^2) \leq cl^3|z|^{2-\beta},$$

which finishes the proof of Lemma 3.11. □

Next we consider the good set. As already mentioned in the sketch of the procedure on page 36 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 to 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 obtain that $\bigcup_{x \in \mathcal{G}} \mathcal{V}(x)$ is a very 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 Figure 3.5)

$$\mathcal{V}(x) := \bigcup_{k=-K}^{K} \frac{1}{l}\mathcal{U}(x+kz) \cap \tau_z, \tag{3.31}$$

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

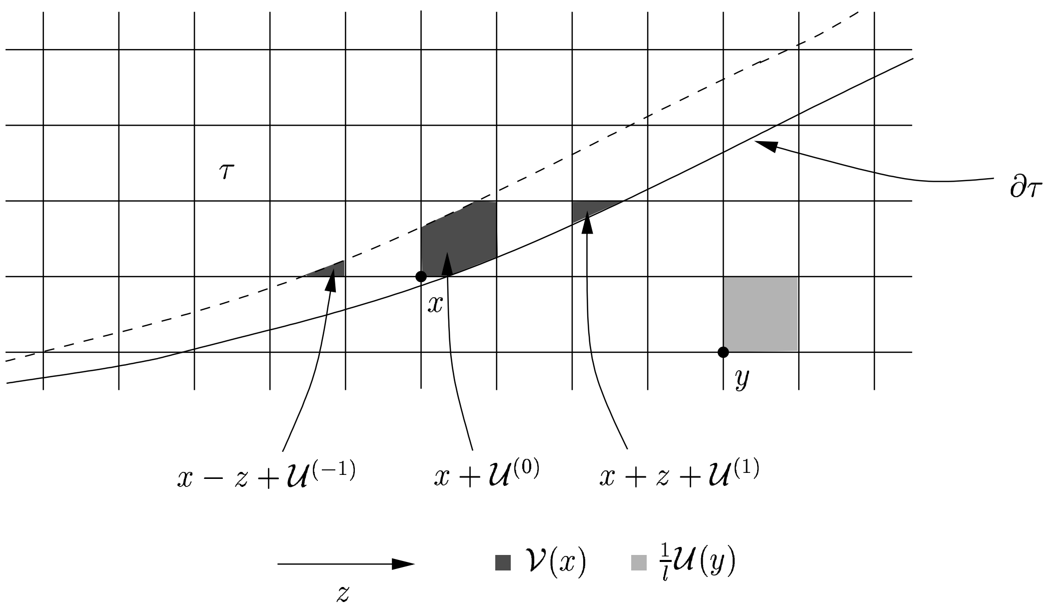

Figure 3.5: An example of a modified unit cell $\mathcal{V}(x)$.

Lemma 3.12 *Let $\mathcal{V}(x)$, $x \in \mathcal{G}$, be the modified unit cell defined in (3.31). Then*

$$|\mathcal{V}(x)| = \frac{1}{l^3} \tag{3.32}$$

and

$$\mathcal{V}(x) \cap \mathcal{V}(\tilde{x}) = \emptyset \qquad \text{if} \quad x, \tilde{x} \in \mathcal{G} \quad \text{and} \quad x \neq \tilde{x}. \tag{3.33}$$

Proof: We first assume in addition that $n(r_z(x)) \cdot \frac{z}{|z|} \leq \frac{1}{2}$. Then we can represent $\partial\tau$ locally as a graph as in the proof of Lemma 3.11.

To prove (3.32) we define the sets (cf. Figure 3.5)

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

where the x-dependence is suppressed in the notation. Next we show that

$$\bigcup_{k=-K}^{K} \mathcal{U}^{(k)} = \mathcal{U} \quad \text{and} \quad \mathcal{U}^{(k)} \cap \mathcal{U}^{(k')} = \emptyset \quad \text{if} \quad k \neq k'. \tag{3.34}$$

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

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

this implies (3.32). To prove (3.34) note that $r_z(x) = x + \bar{\lambda} z$ with $\bar{\lambda} \in [0,1)$, thus $r_z(x)' = x' + \bar{\lambda} z$. Let $y \in \mathcal{U}$ and suppose $|\lambda z| \leq \rho$, then

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

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

$$\begin{aligned} \frac{\partial u}{\partial x_1}(x' + \lambda z + \frac{1}{l}y') &\geq \frac{\partial u}{\partial x_1}(r_z(x)') - \operatorname{Lip}(Du)|r_z(x)' - (x' + \lambda z + \frac{1}{l}y')| \\ &\geq \frac{\partial u}{\partial x_1}(r_z(x)') - \operatorname{Lip}(Du) 2\rho \\ &\geq \frac{1}{2} C_1 (l^{\beta-1} + \rho) > 0. \end{aligned} \tag{3.35}$$

Hence

$$\lambda \mapsto u(x' + \lambda z + \frac{1}{l}y') \tag{3.36}$$

is strictly increasing. Since

$$\begin{aligned} |x' + Kz + \frac{1}{l}y' - (x' + \bar{\lambda} z + \frac{1}{l}y')| &= (K - \bar{\lambda})|z| \geq (K-1)|z| \\ &\geq \rho - 2|z| \geq \frac{1}{4}\rho \end{aligned}$$

as $K \geq \frac{\rho}{|z|} - 1$ and $C_0 > 3$ and since

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

one obtains by (3.35)

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

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 $C_1 > 12 \operatorname{diam}\mathcal{U}$ by assumption, one obtains

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

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

$$u(x' + \lambda z + \frac{1}{l}y') - (x + \frac{1}{l}y)_3 \begin{cases} > 0 & \text{if} \quad \lambda > \tilde{\lambda}(y), \\ = 0 & \text{if} \quad \lambda = \tilde{\lambda}(y), \\ < 0 & \text{if} \quad \lambda < \tilde{\lambda}(y). \end{cases} \tag{3.37}$$

This shows that

$$x + kz + \frac{1}{l}y \in \tau_z \quad \Longleftrightarrow \quad k = \tilde{k}(y) := \lfloor \tilde{\lambda}(y) \rfloor, \tag{3.38}$$

which proves (3.34) and thus (3.32). See also Figure 3.6.

We next show (3.33). If $\mathcal{V}(x) \cap \mathcal{V}(\tilde{x}) \neq \emptyset$ for $x \neq \tilde{x}$, then there would exist $k \neq \tilde{k}(y) \in \{-K, \ldots, K\}$ such that $x, \tilde{x} \in \mathcal{G}$ and $x + kz = \tilde{x} + \tilde{k}(y)z$, i.e.

$$\tilde{x} = x + (k - \tilde{k}(y))z.$$

This is impossible in view of the fact that the map in (3.36) is strictly increasing and in view of the definition of τ_z.

If $n(r_z(x)) \cdot \frac{z}{|z|} > \frac{1}{4}$, 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 Figure 3.7). In this case it is obvious

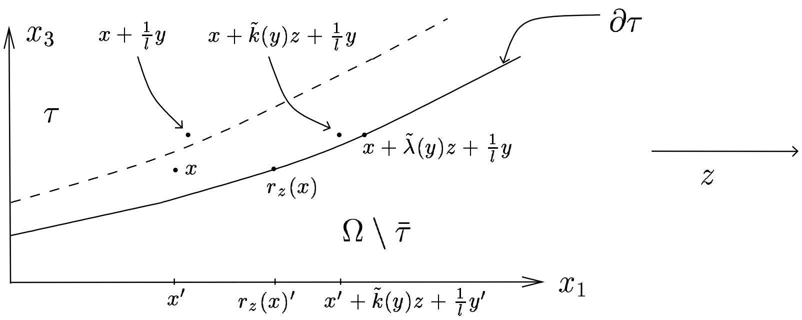

Figure 3.6: This is related to (3.38).

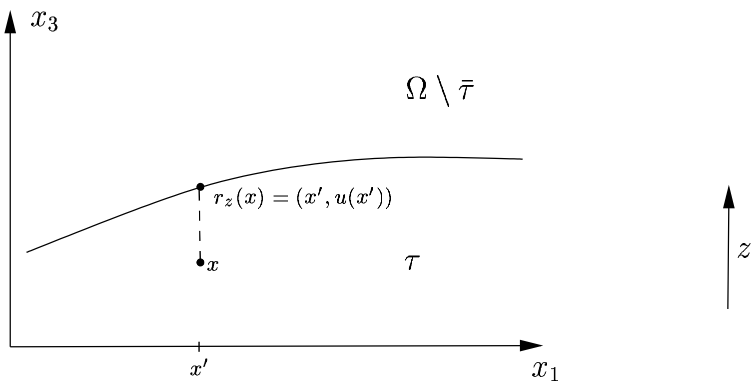

Figure 3.7: A local representation of $\partial\tau$ for the case $n(r_z(x)) \cdot \frac{z}{|z|} > \frac{1}{4}$.

that each line $\lambda \mapsto x + \lambda z$ intersects $\partial\tau$ locally exactly once. Moreover one can represent $\partial\tau$ by a $C^{1,1}$-function u such that $r_z(x) = (x', u(x'))$. □

For later estimates we introduce two sets, for which we prove inclusions regarding the modified unit cells and the good set $\mathcal{G}$. Let

$$\mathcal{T}^+ := \{\xi \in \partial\tau \;:\; n(\xi) \cdot \frac{z}{|z|} \geq \frac{1}{2} C_1(l^{\beta-1} + \rho),\ \mathrm{dist}(\xi, \Gamma) > 2\rho\}$$

and

$$\mathcal{T}^- := \{\xi \in \partial\tau \;:\; n(\xi) \cdot \frac{z}{|z|} \geq 2C_1(l^{\beta-1} + \rho),\ \mathrm{dist}(\xi, \Gamma) > 10\rho\}.$$

Lemma 3.13 *Let* $\mathcal{V} := \bigcup_{x\in\mathcal{G}} \mathcal{V}(x)$. *Set* $\mathcal{V}^+ := \mathcal{T}^+ + [0, -z)$ *and* $\mathcal{V}^- := \mathcal{T}^- + [0, -z)$. *Then*

$$\mathcal{V}^- \subset \mathcal{V} \subset \mathcal{V}^+. \tag{3.39}$$

Proof: As in the proof of Lemma 3.12 we assume first that $n(r_z(x)) \cdot \frac{z}{|z|} \leq \frac{1}{2}$. The arguments in the case $n(r_z(x)) \cdot \frac{z}{|z|} > \frac{1}{4}$ are obtained similarly by choosing a different coordinate system.

Let $x \in \mathcal{G}$. Notice that $K|z| + \frac{\operatorname{diam}\mathcal{U}}{l} \leq \frac{\rho}{|z|}|z| + \frac{\operatorname{diam}\mathcal{U}}{l} \leq 2\rho$ and thus

$$\mathcal{V}(x) \subset B(x, 2\rho). \tag{3.40}$$

The second inclusion in (3.39) follows from (3.40) and the Lipschitz continuity of the normal. Indeed for $\tilde{x} \in B(x, 2\rho) \cap \mathcal{G}$ we have $\tilde{x} \in r_z(\tilde{x}) + [0, -z)$ and $|r_z(\tilde{x}) - r_z(x)| \leq 2\rho + 2|z| \leq 3\rho$ as $C_0 > 2$. Hence

$$\Big| n(r_z(\tilde{x})) \cdot \frac{z}{|z|} - n(r_z(x)) \cdot \frac{z}{|z|} \Big| \leq 3 \operatorname{Lip}(n) \rho.$$

With $C_1 > 6 \operatorname{Lip}(n)$ one obtains

$$\begin{aligned} n(r_z(\tilde{x})) \cdot \frac{z}{|z|} &\geq n(r_z(x)) \cdot \frac{z}{|z|} - 3 \operatorname{Lip}(n) \rho \\ &\geq C_1(l^{\beta-1} + \rho) - \frac{1}{2} C_1 \rho \\ &\geq \frac{1}{2} C_1 (l^{\beta-1} + \rho). \end{aligned}$$

Together with the estimate

$$\operatorname{dist}(r_z(\tilde{x}), \Gamma) \geq \operatorname{dist}(\tilde{x}, \Gamma) - \rho \geq \operatorname{dist}(x, \Gamma) - 3\rho > 5\rho$$

this implies the second inclusion in (3.39).

To establish the first inclusion in (3.39) let $\tilde{\xi} \in \partial^+\tau$ such that $n(\tilde{\xi}) \cdot \frac{z}{|z|} \geq 2C_1(l^{\beta-1} + \rho)$ and let $\tilde{x} = \tilde{\xi} - \tilde{\lambda} z$, $\tilde{\lambda} \in [0, 1)$ with $\operatorname{dist}(\tilde{\xi}, \Gamma) > 10\rho$, i.e. $\tilde{\xi} \in \mathcal{T}^-$. Then we can write $\partial\tau$ as a graph in a neighbourhood of $\tilde{\xi}$. There exists $\hat{x} \in \frac{1}{l}\mathcal{L}$ and $y \in \mathcal{U}$ such that $\tilde{x} = \hat{x} + \frac{1}{l} y$. We have

$$|\hat{x} - \tilde{\xi}| \leq |z| + \frac{\operatorname{diam}\mathcal{U}}{l} \leq \rho \quad \text{and} \quad \operatorname{dist}(\hat{x}, \Gamma) > 9\rho.$$

Arguing as in the proof of the fact that the map in (3.36) is strictly increasing and of (3.37) we see that the function

$$\lambda \mapsto u(\hat{x}' + \lambda z)$$

is strictly increasing and

$$u(\hat{x}' + Kz) - \hat{x}_3 > 0, \quad u(\hat{x}' - Kz) - \hat{x}_3 < 0.$$

Hence there exists a unique $k \in \{-K, \dots, K\}$ and a unique $\lambda \in [k, k+1)$ such that

$$x := \hat{x} + kz \in \tau_z \quad \text{and} \quad \xi := r_z(\hat{x}) = r_z(x) = \hat{x} + \lambda z \in \partial\tau.$$

In particular, $|\xi - \tilde{\xi}| \leq |\xi - \hat{x}| + |\hat{x} - \tilde{\xi}| \leq 2\rho$. Hence $\operatorname{dist}(\xi, \Gamma) \geq \operatorname{dist}(\tilde{\xi}, \Gamma) - 2\rho > 8\rho$. The Lipschitz continuity of the normal and $C_1 > 2\operatorname{Lip}(n)$ imply similarly to above that $n(\xi) \cdot \frac{z}{|z|} > C_1(l^{\beta-1} + \rho)$. Hence $x \in \mathcal{G}$ and $\tilde{x} = x - kz + \frac{1}{l}y \in \mathcal{V}(x)$. □

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 one essentially sets $f(x) = m_i(x)m_j(x+z)$. The details are discussed after the proof of the following proposition on page 51.

Proposition 3.14 *Let $z \in \frac{1}{l}\mathcal{L}^*$ with $|z| \leq \delta \ll 1$. Suppose that $\partial\tau$ satisfies the non-degeneracy condition (S) and assume that f is Lipschitz continuous on τ_z. Then*

$$\left| \frac{1}{l^3} \sum_{x \in \tau_z \cap \frac{1}{l}\mathcal{L}} f(x) - \int_{\partial\tau} f(\xi)(n(\xi) \cdot z)_+ \, d\mathcal{H}^2(\xi) \right| \leq C|z|^{4/3}. \tag{3.41}$$

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 3.15 One can derive sharper error estimates involving $|z|$ and l. Since for our purposes any estimate by $|z|^{1+\alpha}$, $\alpha > 0$, is sufficient (cf. p. 36), we do not strive for optimal exponents.

To prove the proposition we first show some more preliminary estimates for the number of lattice points in τ_z.

Lemma 3.16 *Under the assumptions of Proposition 3.14 one has*

$$|\mathcal{V}^+| \leq c|z|, \tag{3.42}$$

$$|\mathcal{V}^+ \setminus \mathcal{V}^-| \leq c|z|^{2-\beta}, \tag{3.43}$$

$$\#\mathcal{G} \leq cl^3|z|. \tag{3.44}$$

Proof: We give a proof using the coarea formula (cf. Theorem A.6) since a similar argument is used in the proof of Proposition 3.14.
For each $x \in \mathcal{V}^+$ there exists a unique $\xi \in \mathcal{T}^+$ and a $t \in [0,1)$ such that

$$x = \xi - tz = r_z(x) - tz.$$

Here we use again 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 $n(r_z(x))$ and one has $z \cdot \nabla F(x) = -1$. Thus

$$\nabla F(x) = -\frac{1}{n(r_z(x)) \cdot z} n(r_z(x))$$

and the Jacobian of F equals $|\nabla F|$. Hence the coarea formula yields

$$\begin{aligned}
|\mathcal{V}^+| &= \int_{\mathcal{V}^+} 1\, d^3x = \int_{\mathcal{V}^+} \frac{1}{|\nabla F(x)|} |\nabla F(x)|\, d^3x \\
&= \int_0^1 \int_{F(x)=t} \frac{1}{|\nabla F(x)|}\, d\mathcal{H}^2(x)\, dt \\
&= \int_0^1 \Big(\int_{\mathcal{T}^+} |n(\xi) \cdot z|\, d\mathcal{H}^2(\xi) \Big)\, dt \\
&= \int_{\mathcal{T}^+} |n(\xi) \cdot z|\, d\mathcal{H}^2(\xi) \le |z| \mathcal{H}^2(\partial\tau).
\end{aligned}$$

This proves estimate (3.42), and estimate (3.44) follows from (3.32), (3.33) and the second inclusion in (3.39). Indeed, $\#\mathcal{G} \le l^3 |\mathcal{V}^+| \le c l^3 |z|$.

Similarly one obtains

$$|\mathcal{V}^+ \setminus \mathcal{V}^-| = \int_{\mathcal{T}^+ \setminus \mathcal{T}^-} |n(\xi) \cdot z|\, d\mathcal{H}^2(\xi).$$

If $\xi \in \mathcal{T}^+ \setminus \mathcal{T}^-$, then $\operatorname{dist}(\xi, \Gamma) \le 10\rho$ or $n(\xi) \cdot z < 2C_1(l^{\beta-1} + \rho)|z|$. Using the fact that $\partial\tau$ is piecewise $C^{1,1}$ and covering Γ by balls of radius 20ρ, one obtains as in the estimate for $\#\mathcal{B}_I$ that

$$\mathcal{H}^2(B(\Gamma, 10\rho) \cap \partial\tau) \le c\rho.$$

Thus

$$\begin{aligned}
|\mathcal{V}^+ \setminus \mathcal{V}^-| &= \int_{\mathcal{T}^+ \setminus \mathcal{T}^-} |n(\xi) \cdot z|\, d\mathcal{H}^2(\xi) \\
&\le \int_{B(\Gamma,10\rho) \cap \partial\tau} |n(\xi) \cdot z|\, d\mathcal{H}^2(\xi) + \int_{\mathcal{T}^+ \setminus B(\Gamma,10\rho)} |n(\xi) \cdot z|\, d\mathcal{H}^2(\xi) \\
&\le c\rho|z| + \int_{\mathcal{T}^+ \setminus B(\Gamma,10\rho)} 2C_1(l^{\beta-1} + \rho)|z|\, d\mathcal{H}^2(\xi) \\
&\le c|z|^{2-\beta},
\end{aligned}$$

which finishes the proof of Lemma 3.16. □

Proof of Proposition 3.14: 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 3.8 and 3.9). In the following we take $\beta = \frac{2}{3}$. By Lemma 3.10 and Lemma 3.11 we have

$$\#\mathcal{B}_I + \#\mathcal{B}_{II} \le cl^3(|z|^{2\beta} + |z|^{2-\beta}) \le cl^3|z|^{4/3}. \tag{3.45}$$

Hence in (3.41) it suffices to consider the sum over $x \in \mathcal{G}$ as discussed on page 36.
The modified unit cell $\mathcal{V}(x)$, which is associated to $x \in \mathcal{G}$, is contained in $B(x, 2\rho)$ by (3.40). Since $|\mathcal{V}(x)| = \frac{1}{l^3}$ and $\mathcal{V} = \bigcup_{x\in\mathcal{G}} \mathcal{V}(x)$, one gets by (3.33), the Lipschitz continuity of f and (3.44)

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

It thus remains to show that

$$\Big|\int_{\mathcal{V}} f(x)\,d^3x - \int_{\partial\tau} f(\xi)(n(\xi)\cdot z)_+\,d\mathcal{H}^2(\xi)\Big| \le c|z|^{4/3}. \tag{3.46}$$

Since $\mathcal{V}^- \subset \mathcal{V} \subset \mathcal{V}^+$, (3.43) yields

$$\begin{aligned}
\Big|\int_{\mathcal{V}} f(x)\,d^3x - \int_{\mathcal{V}^-} f(x)\,d^3x\Big| &\le |\mathcal{V}^+ \setminus \mathcal{V}^-|\,\sup|f| \\
&\le c|z|^{4/3}.
\end{aligned} \tag{3.47}$$

Using the coarea formula as in the proof of Lemma 3.16 and the Lipschitz continuity of f we obtain

$$\begin{aligned}
\int_{\mathcal{V}^-} f(x)\,d^3x &= \int_0^1 \int_{\mathcal{T}^-} f(\xi - tz)|n(\xi)\cdot z|\,d\mathcal{H}^2(\xi)\,dt \\
&= \int_0^1 \int_{\mathcal{T}^-} f(\xi)|n(\xi)\cdot z|\,d\mathcal{H}^2(\xi)\,dt + \\
&\quad + \int_0^1 \int_{\mathcal{T}^-} \big(f(\xi - tz) - f(\xi)\big)|n(\xi)\cdot z|\,d\mathcal{H}^2(\xi)\,dt \\
&= \int_{\mathcal{T}^-} f(\xi)|n(\xi)\cdot z|\,d\mathcal{H}^2(\xi) + \mathcal{O}\big(\mathcal{H}^2(\partial\tau)|z|^2\big).
\end{aligned} \tag{3.48}$$

Finally, by the definition of $\mathcal{T}^-$

$$\begin{aligned}
&\Big|\int_{\mathcal{T}^-} f(\xi)|n(\xi)\cdot z|\,d\mathcal{H}^2(\xi) - \int_{\partial\tau} f(\xi)(n(\xi)\cdot z)_+\,d\mathcal{H}^2(\xi)\Big| \\
&= \Big|\int_{\partial\tau\setminus\mathcal{T}^-} f(\xi)|n(\xi)\cdot z|\,d\mathcal{H}^2(\xi)\Big| \\
&\leq \sup|f|\Big(\int_{B(\Gamma,10\rho)\cap\partial\tau} |z|\,d\mathcal{H}^2(\xi) + \int_{\partial\tau} 2C_1(l^{\beta-1}+\rho)|z|\Big) \\
&\leq c(l^{\beta-1}+\rho)|z| \leq c|z|^{4/3}. \qquad (3.49)
\end{aligned}$$

Combining (3.47)–(3.49) we obtain (3.46) and the proof is finished. □

For an application of Proposition 3.14 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 (3.41). Thus the short range part of the atomistic force reads

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

As discussed in (3.21), the second term tends to zero if one first takes the limit $l\to\infty$ and then the limit $\delta\to 0$.

To estimate the first term, notice that one can commute summation and integration in this term as long as $\delta > 0$. Thus

$$\begin{aligned} & -\sum_{z\in B_\delta\cap\frac{1}{l}\mathcal{L}^*} \partial_k(K-K^{(\delta)})_{ij}(z)(\frac{1}{l})^3 \int_{\partial\tau} m_i^-(\xi)m_j^+(\xi)(n(\xi)\cdot z)_+\, d\mathcal{H}^2(\xi) \quad (3.50) \\ = & -\int_{\partial\tau} m_i^-(\xi)m_j^+(\xi) \sum_{z\in B_\delta\cap\frac{1}{l}\mathcal{L}^*} \partial_k(K-K^{(\delta)})_{ij}(z)(n(\xi)\cdot z)_+(\frac{1}{l})^3\, d\mathcal{H}^2(\xi). \end{aligned}$$

Next the convergence of the sum which occurs on the right hand side of (3.50) is considered.

Lemma 3.17 *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 it holds

$$-\lim_{\delta\to 0}\lim_{l\to\infty} \sum_{z\in B_\delta\cap\frac{1}{l}\mathcal{L}^*} \partial_k(K-K^{(\delta)})_{ij}(z)(a\cdot z)_+(\frac{1}{l})^3 = \frac{1}{2}S_{ijkp}a_p. \quad (3.51)$$

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

Note that there is a sum over $p = 1, 2, 3$ hidden in (3.51) by the summation convention.

Proof: Since $\partial_k(K-K^{(\delta)})_{ij}(z)$ and $a\cdot z$ are antisymmetric in z, their product is symmetric in z, and one obtains

$$\begin{aligned} & \sum_{z\in B_\delta\cap\frac{1}{l}\mathcal{L}^*} \partial_k(K-K^{(\delta)})_{ij}(z)(a\cdot z)_+(\frac{1}{l})^3 \\ = & \sum_{\substack{z\in B_\delta\cap\frac{1}{l}\mathcal{L}^* \\ a\cdot z>0}} \partial_k(K-K^{(\delta)})_{ij}(z)(a\cdot z)(\frac{1}{l})^3 \\ \overset{z=-\tilde{z}}{=} & \sum_{\substack{\tilde{z}\in B_\delta\cap\frac{1}{l}\mathcal{L}^* \\ a\cdot\tilde{z}<0}} \partial_k(K-K^{(\delta)})_{ij}(\tilde{z})(a\cdot\tilde{z})(\frac{1}{l})^3. \end{aligned}$$

Hence the definition of the kernel and a change of variables yield

$$\begin{aligned}
&\sum_{z\in B_\delta\cap\frac{1}{l}\mathcal{L}^*} \partial_k(K-K^{(\delta)})_{ij}(z)(a\cdot z)_+(\frac{1}{l})^3 \\
&= \frac{1}{2}\sum_{z\in B_\delta\cap\frac{1}{l}\mathcal{L}^*} \partial_k \underbrace{(K-K^{(\delta)})_{ij}}_{=\partial_i\partial_j(\varphi^{(\delta)}N)}(z)(a\cdot z)(\frac{1}{l})^3 \\
&\overset{z'=lz}{=} \frac{1}{2}\sum_{z'\in B_{l\delta}\cap\mathcal{L}^*} \Big(\partial_k\partial_i\partial_j(\varphi^{(\delta)}N)\Big)(\frac{z'}{l})(a\cdot\frac{z'}{l})(\frac{1}{l})^3 \\
&= \frac{1}{2}\sum_{z\in B_{l\delta}\cap\mathcal{L}^*} \Big(\partial_k\partial_i\partial_j\big(\underbrace{(\varphi^{(\delta)}N)(\frac{z}{l})}_{=\varphi^{(l\delta)}(z)lN(z)}\big)l^3\Big)(a\cdot\frac{z}{l})(\frac{1}{l})^3 \\
&= \frac{1}{2}\sum_{z\in B_{l\delta}\cap\mathcal{L}^*} \Big(\partial_k\partial_i\partial_j\big(\varphi^{(l\delta)}N\big)(z)\Big)(a\cdot z) \\
&= \underbrace{\frac{1}{2}\sum_{z\in B_{l\delta}\cap\mathcal{L}^*} \Big(\partial_k\partial_i\partial_j\big(\varphi^{(l\delta)}N\big)(z)\Big)z_p}_{=:-S^{(l\delta)}_{ijkp}}\, a_p.
\end{aligned} \tag{3.52}$$

The aim is to show that the limit $l\to\infty$ of $S^{(l\delta)}_{ijkp}$ exists. For convenience we restrict the proof of this to natural numbers. It works in the same way for nets.

In the following we show that the limit of $S^{(n)}_{ijkp}$ exists as $n\to\infty$. This is done by proving that $S^{(n)}_{ijkp}$ is a Cauchy sequence as $n\to\infty$. 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

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

Let y_x denote the base point of the unit cell to which x belongs. To replace the sum with an integral we introduce the sets

$$\mathcal{U}^{\text{out}} := \{x\in\mathcal{U}(y_x)\cap(B_n\setminus B_{m/2})\;:\;y_x\in\mathbb{R}^3\setminus(B_n\setminus B_{m/2})\}$$

and

$$\mathcal{U}^{\text{in}} := \{x\in\mathcal{U}(y_x)\setminus(B_n\setminus B_{m/2})\;:\;y_x\in(B_n\setminus B_{m/2})\}.$$

Moreover let $\text{step}(f)$ denote the step-function of f which has the same value as f on lattice points and which is constantly extended on unit cells. One has

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

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

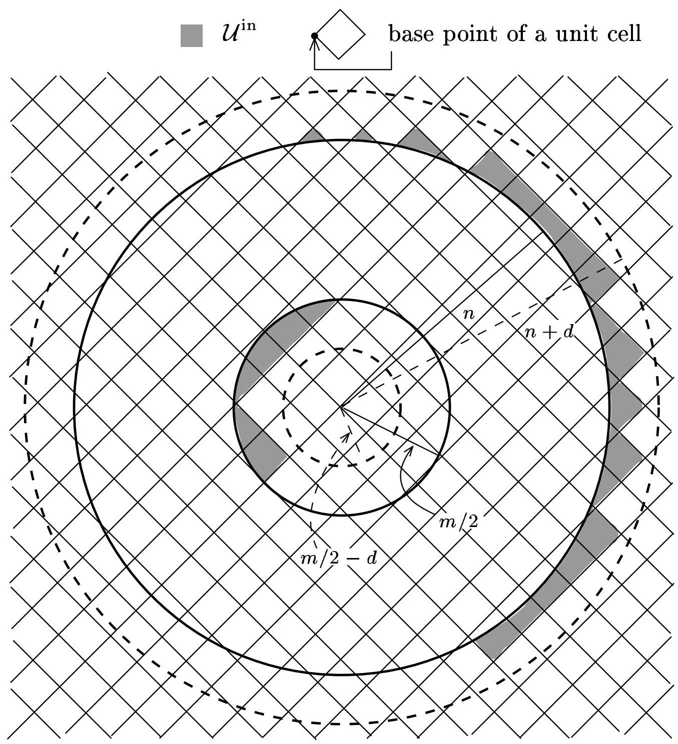

Figure 3.8: $\mathcal{U}^{\text{in}}$ as a subset of $(B_{n+d} \setminus B_n) \cup (B_{m/2} \setminus B_{m/2-d})$.

$\mathcal{U}^{\text{in}} \subset (B_{n+d} \setminus B_n) \cup (B_{m/2} \setminus B_{m/2-d})$ as indicated in Figure 3.8, where d denotes the diameter of the unit cell. So $|\mathcal{U}^{\text{in}}| \leq c((n+d)^3 - n^3 + (\frac{m}{2})^3 - (\frac{m}{2} - d)^3) \leq cd(n^2 + (m/2)^2) \leq cn^2$. Moreover, the value of the step-function in the second term is small since the interesting lattice points 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 (A.15) one obtains

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

So

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

which tends to zero as n and m tend to ∞. Hence it remains to estimate the first integral. We obtain

$$
\begin{aligned}
&\Big|\int_{B_n\setminus B_{m/2}}\text{step}\Big(\Big(\partial_k\partial_i\partial_j\big((\varphi^{(n)}-\varphi^{(m)})N\big)(\zeta)\Big)\zeta_p\Big)\,d\zeta\Big| \\
&\le \Big|\int_{B_n\setminus B_{m/2}}\Big(\partial_k\partial_i\partial_j\big((\varphi^{(n)}-\varphi^{(m)})N\big)(\zeta)\Big)\zeta_p\,d\zeta\Big|+ \\
&\qquad +\Big|\int_{B_n\setminus B_{m/2}}\text{step}\Big(\Big(\partial_k\partial_i\partial_j\big((\varphi^{(n)}-\varphi^{(m)})N\big)(\zeta)\Big)\zeta_p\Big)+ \\
&\qquad\qquad -\Big(\partial_k\partial_i\partial_j\big((\varphi^{(n)}-\varphi^{(m)})N\big)(\zeta)\Big)\zeta_p\,d\zeta\Big| \\
&\le \Big|\int_{B_n\setminus B_{m/2}}\Big(\partial_k\partial_i\partial_j\big((\varphi^{(n)}-\varphi^{(m)})N\big)(\zeta)\Big)\zeta_p\,d\zeta\Big|+ \\
&\qquad +c\int_{B_n\setminus B_{m/2}}\sup_{\eta\in U(z_\zeta)}\Big|D\big[\big(\partial_k\partial_i\partial_j\big((\varphi^{(n)}-\varphi^{(m)})N\big)(\eta)\big)\eta_p\big]\Big|\,d\zeta. \qquad (3.53)
\end{aligned}
$$

In the latter inequality we used Lemma A.7. As before $\mathcal{U}(z_\zeta)$ denotes the unit cell to which ζ belongs. The first term is zero since an integration by parts yields

$$\begin{aligned}
&\int_{B_n\setminus B_{m/2}} \Big(\partial_k\partial_i\partial_j\big((\varphi^{(n)}-\varphi^{(m)})N\big)(\zeta)\Big)\zeta_p\,d\zeta \\
&= \int_{B_n\setminus B_{m/2}} \Big\{\partial_k\Big(\big(\partial_i\partial_j\big((\varphi^{(n)}-\varphi^{(m)})N\big)(\zeta)\big)\zeta_p\Big) + \\
&\qquad - \Big(\partial_i\partial_j\big((\varphi^{(n)}-\varphi^{(m)})N\big)\Big)(\zeta)\delta_{kp}\Big\}\,d\zeta \\
&= \int_{\partial(B_n\setminus B_{m/2})} \big(\partial_i\partial_j\big((\varphi^{(n)}-\varphi^{(m)})N\big)(\zeta)\big)\zeta_p n_k(\zeta)\,d\mathcal{H}^2(\zeta) + \\
&\quad - \int_{\partial(B_n\setminus B_{m/2})} \partial_j\big((\varphi^{(n)}-\varphi^{(m)})N\big)(\zeta)\delta_{kp}n_i(\zeta)\,d\mathcal{H}^2(\zeta) \\
&= 0 \qquad (3.54)
\end{aligned}$$

because $\varphi^{(n)}-\varphi^{(m)}$ and all its derivatives are zero on $\partial(B_n\setminus B_{m/2})$ by definition.

For the estimate of the supremum in the second term of (3.53) we use again the fact that $|\partial^s\varphi^{(n)}| \le C_s\frac{1}{n^{|s|}}$ for all multi-indices s. By the product rule one obtains

$$\begin{aligned}
&\big|D[\big(\partial_k\partial_i\partial_j\big((\varphi^{(n)}-\varphi^{(m)})N\big)(\eta)\big)\eta_p]\big| \qquad (3.55)\\
&\le \big|D\big(\partial_k\partial_i\partial_j\big((\varphi^{(n)}-\varphi^{(m)})N\big)(\eta)\big)\big||\eta| + |\partial_k\partial_i\partial_j\big((\varphi^{(n)}-\varphi^{(m)})N\big)(\eta)||D\eta| \\
&\le c\Big(\big(\frac{1}{n^4}+\frac{1}{m^4}\chi_{B_m}\big)\frac{1}{|\eta|} + \big(\frac{1}{n^3}+\frac{1}{m^3}\chi_{B_m}\big)\frac{1}{|\eta|^2} + \big(\frac{1}{n^2}+\frac{1}{m^2}\chi_{B_m}\big)\frac{1}{|\eta|^3} + \\
&\qquad + \big(\frac{1}{n}+\frac{1}{m}\chi_{B_m}\big)\frac{1}{|\eta|^4} + \frac{1}{|\eta|^5}\Big)|\eta| + \\
&\quad + c\Big(\big(\frac{1}{n^3}+\frac{1}{m^3}\chi_{B_m}\big)\frac{1}{|\eta|} + \big(\frac{1}{n^2}+\frac{1}{m^2}\chi_{B_m}\big)\frac{1}{|\eta|^2} + \big(\frac{1}{n}+\frac{1}{m}\chi_{B_m}\big)\frac{1}{|\eta|^3} + \frac{1}{|\eta|^4}\Big).
\end{aligned}$$

This can be simplified with the help of Young's inequality (A.15) to

$$\big|D[\big(\partial_k\partial_i\partial_j\big((\varphi^{(n)}-\varphi^{(m)})N\big)(\eta)\big)\eta_p]\big| \le c\big(\frac{1}{n^4}+\frac{1}{m^4}\chi_{B_m}+\frac{1}{|\eta|^4}\big).$$

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 $m > 2d+2$. By summarizing the above estimates one then obtains

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

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 one obtains

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

In the definition of $S^{(l\delta)}_{ijkp}$ (cf. (3.52)) one can commute the occurring partial derivatives. 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. □

Notice that the way in which the regularization is chosen is crucial in (3.54). The cut-off function $\varphi^{(n)}$ is multiplied directly by the potential N and is therefore 'inside' of all the derivatives and not 'outside', which allows one 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 (3.51). Differentiating the second factor, i.e. ξ_p, yields a Kronecker δ_{kp}, and one can apply the Divergence Theorem to the corresponding integral. If the second factor depended nonlinearly on ξ, one could not apply the Divergence Theorem.
Besides we remark that one can also show Lemma 3.17 by applying the methods which we discuss in Chapter 4.

For a final discussion of the convergence of the short range part $\mathcal{F}_k^{(l,\delta)}$ of the discrete force we apply Lemma 3.17 to (3.50). Since $|S_{ijkp}^{(l\delta)} n_p(\xi)| \leq c|n_p(\xi)| \leq c$ for all $\xi \in \partial\tau$, $0 < l\delta < \infty$ and $p = 1, 2, 3$, the assumptions of Lebesgue's Convergence Theorem are fulfilled. Hence one can commute limiting processes and integration, and one obtains

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

Putting together the estimates of the terms of the short range part of the microscopic force we obtain the result which is stated in Theorem 3.6.

With this also the proof of Theorem 3.7 is completed. That is, the magnetic force formula (3.9), which is derived from a discrete setting, consists of an additional term which contains the 4-tensor $S := (S_{ijkp})_{i,j,k,p=1,2,3}$. This term is studied in detail in Chapter 4. In particular we show that S is not zero in general.

Chapter 4

Evaluation of the lattice sum S_{ijkp}

In Chapter 3 the passage of the magnetic force in a discrete setting to a continuous setting is discussed. In this chapter we focus on the limiting formula of the short range part of the microscopic force (Theorem 3.6). This is a surface integral which contains the lattice sum

$$S_{ijkp} = -\lim_{\delta \to 0} \lim_{l \to \infty} \sum_{z \in B_\delta \cap \frac{1}{l}\mathcal{L}^*} \partial_k (K - K^{(\delta)})_{ij}(z) z_p (\frac{1}{l})^3. \tag{4.1}$$

That this limit exists is the assertion of Lemma 3.17. Moreover one has that S_{ijkp} is symmetric in i, j, k since

$$\partial_k (K - K^{(\delta)})_{ij}(z) = \partial_k \partial_i \partial_j (\varphi^{(\delta)} N)(z)$$

is symmetric in i, j, k, where $N(z) = \frac{\gamma}{4\pi}\frac{1}{|z|}$ (see (3.2)) and $\varphi^{(\delta)}(z) = \varphi^{(1)}(\frac{z}{\delta})$ being the regularizing function defined on page 24.

We denote the 4-tensor $(S_{ijkp})_{i,j,k,p=1,2,3}$ by S. For a comparison of Brown's formula and the limiting force formula the values of S_{ijkp} are of interest. The main result of this chapter is that S is not identically zero in general. Hence the limit of the short range term of the discrete force gives a non-trivial contribution to the limiting force formula.

In order to evaluate S, we recall the definition of $S^{(n)}_{ijkp}$ for fixed $n \in \mathbb{N}$ (cf. p. 53; recall that one actually has nets, which can be treated analogously). The terms of the sum are given by $\Big(\partial_k \partial_i \partial_j \big(\varphi^{(n)} N\big)(z)\Big) z_p$, which is expanded in the following. 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. One has

$$\begin{aligned}\partial_j\varphi^{(n)}(z) &= \frac{z_j}{|z|}\varphi^{(n)\prime}(z),\\ \partial_i\partial_j\varphi^{(n)}(z) &= (\frac{\delta_{ij}}{|z|} - \frac{z_i z_j}{|z|^3})\varphi^{(n)\prime}(z) + \frac{z_i z_j}{|z|^2}\varphi^{(n)\prime\prime}(z)\end{aligned}$$

and

$$\begin{aligned}\partial_k\partial_i\partial_j\varphi^{(n)}(z) &= \big(-\frac{\delta_{ij}z_k}{|z|^3} - \frac{\delta_{ik}z_j}{|z|^3} - \frac{\delta_{jk}z_i}{|z|^3} + 3\frac{z_i z_j z_k}{|z|^5}\big)\varphi^{(n)\prime}(z) +\\ &\quad + \big(\frac{\delta_{ij}z_k}{|z|^2} + \frac{\delta_{ik}z_j}{|z|^2} + \frac{\delta_{jk}z_i}{|z|^2} - 3\frac{z_i z_j z_k}{|z|^4}\big)\varphi^{(n)\prime\prime}(z) +\\ &\quad + \frac{z_i z_j z_k}{|z|^3}\varphi^{(n)\prime\prime\prime}(z).\end{aligned}$$

As

$$\begin{aligned}\partial_j N(z) &= \frac{\gamma}{4\pi}\frac{-z_j}{|z|^3},\\ \partial_i\partial_j N(z) &= \frac{\gamma}{4\pi}\frac{-1}{|z|^3}\big(\delta_{ij} - 3\frac{z_i z_j}{|z|^2}\big)\end{aligned}$$

and

$$\partial_k\partial_i\partial_j N(z) = \frac{\gamma}{4\pi}\frac{3}{|z|^5}\big(\delta_{ij}z_k + \delta_{ik}z_j + \delta_{jk}z_i - 5\frac{z_i z_j z_k}{|z|^2}\big)$$

one obtains by the product rule

$$\partial_i\partial_j(\varphi^{(n)}N)(z) = \frac{\gamma}{4\pi}\Big(\big(-\frac{\varphi^{(n)}}{|z|^3} + \frac{\varphi^{(n)\prime}(z)}{|z|^2}\big)\big(\delta_{ij} - 3\frac{z_i z_j}{|z|^2}\big) + \varphi^{(n)\prime\prime}(z)\frac{z_i z_j}{|z|^3}\Big)$$

and

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

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.

Up to now each index i, j or k could take all possible values 1, 2 and 3. In what follows different indices within one expression stand for different values, which makes the formulae and statements clearer, i.e. we assume that (i, j, k) is a permutation of $(1, 2, 3)$. For example $S^{(n)}_{iipp}$ is shorthand for $S^{(n)}_{iipp}(1 - \delta_{ip})$. Here we do not use the summation convention.

Because of the symmetry in the first three indices of S_{ijkp} it suffices to consider the following cases:

$$S^{(n)}_{iiip},\ S^{(n)}_{ijjp},\ S^{(n)}_{ijpp},\ S^{(n)}_{ippp}, \tag{4.2}$$

$$S^{(n)}_{iipp} \ \text{ and } \ S^{(n)}_{pppp}. \tag{4.3}$$

For a cubic lattice the sums in (4.2) are zero for every $n \in \mathbb{N}$, which is essentially shown by using symmetry properties of the terms of the sum regarding z. The terms of the sums in (4.3) do not show these symmetries and therefore have to be treated differently. They are not equal to zero. We focus on this in the following sections.

4.1 Antisymmetric terms

Starting with the index-configurations in (4.2) notice that the corresponding terms of the sum are

$$\begin{aligned} &3f(|z|)z_i z_p + g(|z|)\frac{z_i^3 z_p}{|z|^4}, \\ &f(|z|)z_i z_p + g(|z|)\frac{z_i z_j^2 z_p}{|z|^4}, \\ &g(|z|)\frac{z_i z_j z_p^2}{|z|^4} \quad \text{and} \\ &f(|z|)z_i z_p + g(|z|)\frac{z_i z_p^3}{|z|^4}, \end{aligned} \tag{4.4}$$

respectively. All these terms are antisymmetric in z_i. As the terms of the sum are zero for $z_i = 0$, the sum over all $z \in B_n \cap \mathcal{L}^*$ can be split into the sum over all $z \in B_n \cap \mathcal{L}^*$, $z_i > 0$ and $z \in B_n \cap \mathcal{L}^*$, $z_i < 0$. For (4.4) one obtains

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

for every $n \in \mathbb{N}$ if one assumes that the lattice has the property that the sets $\{(z_j, z_p) : z \in B_n \cap \mathcal{L}^*,\ z_i > 0\}$ and $\{(z_j, z_p) : z \in B_n \cap \mathcal{L}^*,\ z_i < 0\}$ are equal. This is valid for the cubic lattice and for other lattices which are symmetric with respect to the chosen coordinate-planes.

The same argument applies to the other terms of the sum which are antisymmetric in z_i. Hence, for sufficiently symmetric lattices, all sums in (4.2) are zero for every $n \in \mathbb{N}$ and do not contribute in the limit as $n \to \infty$.

4.2 Symmetric terms

In this section we consider the symmetric terms of the lattice sum. These terms, which are given in (4.3), are the terms which lead to non-zero elements of the tensor S. The terms of the sum read

$$f(|z|)z_p^2 + g(|z|)\frac{z_i^2 z_p^2}{|z|^4} \quad \text{and} \tag{4.5}$$

$$3f(|z|)z_p^2 + g(|z|)\frac{z_p^4}{|z|^4}, \tag{4.6}$$

respectively. They are not antisymmetric in any component of z but symmetric in every component. Notice moreover that the terms of the sum are zero if $z_p = 0$.

For the evaluation of this terms the sum over all $z \in B_n \cap \mathcal{L}^*$ is split 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 $B_n \setminus \bar{B}_{n/2}$.

4.2.1 The sum over the shell where the regularizing function varies

A similar calculation to that which leads to (3.52) implies that

$$\sum_{z\in(B_n\setminus\bar{B}_{n/2})\cap\mathcal{L}} \Big(\partial_k\partial_i\partial_j\big(\varphi^{(n)}N\big)(z)\Big)z_p = \sum_{z\in(B_1\setminus\bar{B}_{1/2})\cap\frac{1}{n}\mathcal{L}} \Big(\partial_k\partial_i\partial_j\big(\varphi^{(1)}N\big)(z)\Big)z_p\frac{1}{n^3}.$$

As the terms of the sum are continuous and bounded on $B_1 \setminus \bar{B}_{1/2}$, the sum is a Riemann sum. In the limit as $n \to \infty$ it converges to

$$\int_{B_1\setminus B_{1/2}} \Big(\partial_k\partial_i\partial_j\big(\varphi^{(1)}N\big)(z)\Big)z_p\, d^3z.$$

Let ν denote the outer normal to $\partial(B_1 \setminus B_{1/2})$ and n the outer normal to $\partial B_{1/2}$. Next we consider the sum of all symmetric terms, i.e. those terms which correspond to the index configurations with $i = j$ and $k = p$. A permutation of the indices, the product rule and Gauss' Theorem yield

$$\begin{aligned}
&\sum_{\iota=1}^{3}\int_{B_1\setminus B_{1/2}} \Big(\partial_k\partial_\iota\partial_\iota\big(\varphi^{(1)}N\big)(z)\Big)z_k\, d^3z\\
&= \sum_{\iota=1}^{3}\int_{B_1\setminus B_{1/2}} \Big(\partial_\iota\partial_\iota\partial_k\big(\varphi^{(1)}N\big)(z)\Big)z_k\, d^3z\\
&= \sum_{\iota=1}^{3}\int_{B_1\setminus B_{1/2}} \Big\{\partial_\iota\Big(\partial_\iota\partial_k\big(\varphi^{(1)}N\big)(z)z_k\Big) - \partial_\iota\partial_k\big(\varphi^{(1)}N\big)(z)\delta_{\iota k}\Big\}\, d^3z\\
&= \sum_{\iota=1}^{3}\int_{\partial(B_1\setminus B_{1/2})} \Big\{\nu_\iota(z)\partial_\iota\partial_k\big(\varphi^{(1)}N\big)(z)z_k - \nu_\iota(z)\partial_k\big(\varphi^{(1)}N\big)(z)\delta_{\iota k}\Big\}\, d\mathcal{H}^2(z)\\
&= -\sum_{\iota=1}^{3}\int_{\partial B_{1/2}} n_\iota(z)\big(\partial_\iota\partial_kN(z)z_k - \partial_kN(z)\delta_{\iota k}\big)\, d\mathcal{H}^2(z),
\end{aligned} \tag{4.7}$$

where the last equality follows by the definition of $\varphi^{(1)}$. With

$$\begin{aligned}
&\sum_{\iota=1}^{3} n_\iota(z)\big(\partial_\iota\partial_kN(z)z_k - \partial_kN(z)\delta_{\iota k}\big)\\
&= \frac{\gamma}{4\pi}\sum_{\iota=1}^{3}\frac{z_\iota}{|z|}\Big(\frac{-z_k}{|z|^3}\big(\delta_{\iota k} - 3\frac{z_\iota z_k}{|z|^2}\big) - \frac{-z_k}{|z|^3}\delta_{\iota k}\Big) \qquad (4.8)\\
&= \frac{\gamma}{4\pi}\sum_{\iota=1}^{3}3\frac{z_\iota^2z_k^2}{|z|^6} = \frac{\gamma}{4\pi}3\frac{z_k^2}{|z|^4}
\end{aligned}$$

one obtains that

$$\begin{aligned}\sum_{\iota=1}^{3}\int_{B_1\setminus B_{1/2}}\Big(\partial_k\partial_\iota\partial_\iota\big(\varphi^{(1)}N\big)(z)\Big)z_k\,d^3z &= -\frac{3\gamma}{4\pi}\int_{\partial B_{1/2}}\frac{z_k^2}{|z|^4}\,d\mathcal{H}^2(z)\\ &= -\frac{3\gamma}{4\pi}\int_0^{\pi}\int_0^{2\pi}\cos^2\vartheta\sin\vartheta\,d\phi\,d\vartheta\\ &= \frac{3\gamma}{4\pi}2\pi\Big[\frac{1}{3}\cos^3\vartheta\Big]_0^{\pi}\\ &= -\frac{\gamma}{4\pi}4\pi=-\gamma.\end{aligned}$$

Since the two terms with $\iota\neq k$ have the same value, one obtains the relation

$$\begin{aligned}&\int_{B_1\setminus B_{1/2}}\Big(\partial_k\partial_i\partial_i\big(\varphi^{(1)}N\big)(z)\Big)z_k\,d^3z\\ &\quad=\frac{1}{2}\Big(-\frac{\gamma}{4\pi}4\pi-\int_{B_1\setminus B_{1/2}}\Big(\partial_k\partial_k\partial_k\big(\varphi^{(1)}N\big)(z)\Big)z_k\,d^3z\Big).\end{aligned}\tag{4.9}$$

Similarly to (4.7) and (4.8), the sum corresponding to a configuration of four equal indices is given by

$$\begin{aligned}&-\int_{B_1\setminus B_{1/2}}\Big(\partial_k\partial_k\partial_k\big(\varphi^{(1)}N\big)(z)\Big)z_k\,d^3z\\ &\quad=\int_{\partial B_{1/2}}n_k(z)\big(\partial_k\partial_kN(z)z_k-\partial_kN(z)\big)\,d\mathcal{H}^2(z)\\ &\quad=\frac{3\gamma}{4\pi}\int_{\partial B_{1/2}}\frac{z_k^4}{|z|^6}\,d\mathcal{H}^2(z)\\ &\quad=\frac{3\gamma}{4\pi}\int_0^{\pi}\int_0^{2\pi}\cos^4\vartheta\sin\vartheta\,d\phi\,d\vartheta\\ &\quad=-\frac{3\gamma}{4\pi}2\pi\Big[\frac{1}{5}\cos^5\vartheta\Big]_0^{\pi}=\frac{\gamma}{4\pi}\frac{12\pi}{5}=\frac{3\gamma}{5}.\end{aligned}\tag{4.10}$$

Hence we have that by (4.9) and (4.10)

$$\begin{aligned}-\int_{B_1\setminus B_{1/2}}\Big(\partial_k\partial_i\partial_i\big(\varphi^{(1)}N\big)(z)\Big)z_k\,d^3z &= -\frac{1}{2}\Big(-\frac{\gamma}{4\pi}4\pi+\frac{\gamma}{4\pi}\frac{12\pi}{5}\Big)\\ &= \frac{\gamma}{4\pi}\frac{4\pi}{5}=\frac{\gamma}{5}.\end{aligned}\tag{4.11}$$

4.2.2 The sum over the ball with constant regularizing function

In this subsection we assume that the given lattice is a cubic lattice which is centred at the origin. This lattice corresponds to $\mathbb{Z}^3$ if the volume of the unit cell is 1, i.e. $\mathcal{L}^*=\mathbb{Z}^3\setminus(0,0,0)$.

Set

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

The two sums which correspond to the index configurations $iikk$ and $jjkk$ with $i\neq j\neq k$ have the same value (see e.g. (4.12)). Hence

$$s_{iikk}^{(n)} = \frac{1}{2}\big(\sum_{\iota=1}^{3}s_{\iota\iota kk}^{(n)} - s_{kkkk}^{(n)}\big).$$

As

$$\begin{aligned}\sum_{\iota=1}^{3}s_{\iota\iota kk}^{(n)} &= -\sum_{z\in\bar{B}_{n/2}\cap\mathcal{L}^*}\sum_{\iota=1}^{3}\big(\partial_k\partial_\iota\partial_\iota N(z)\big)z_k\\ &= -\frac{\gamma}{4\pi}\sum_{z\in\bar{B}_{n/2}\cap\mathcal{L}^*}\sum_{\iota=1}^{3}\big(\frac{3}{|z|^5}(z_k+2\delta_{\iota k}z_k)-\frac{15}{|z|^3}\frac{z_\iota^2 z_k}{|z|^4}\big)z_k \qquad (4.12)\\ &= -\frac{\gamma}{4\pi}\sum_{z\in\bar{B}_{n/2}\cap\mathcal{L}^*}\big(3\frac{3z_k^2}{|z|^5}+6\frac{z_k^2}{|z|^5}-\frac{15|z|^2z_k^2}{|z|^7}\big)\\ &= 0\end{aligned}$$

we have

$$s_{iikk}^{(n)} = -\frac{1}{2}s_{kkkk}^{(n)} \qquad (4.13)$$

for every $n\in\mathbb{N}$. By Lemma 3.17, we know that $s_{kkkk}^{(n)}$ converges in $\mathbb{R}$ as $n\to\infty$. By setting

$$\mathcal{S} := \lim_{n\to\infty}s_{kkkk}^{(n)} = \lim_{n\to\infty}-\frac{\gamma}{4\pi}\sum_{z\in\bar{B}_{n/2}\cap\mathcal{L}^*}\frac{3z_k^2}{|z|^5}\big(3-5\frac{z_k^2}{|z|^2}\big) \qquad (4.14)$$

one thus has with (4.13)

$$\lim_{n\to\infty}s_{iikk}^{(n)} = -\frac{1}{2}\mathcal{S}. \qquad (4.15)$$

The main aim of this chapter is to prove that the tensor $S=(S_{ijkp})_{i,j,k,p=1,2,3}$ is not identically zero. This is done in the following section.

4.3 Nontrivial lattice sums and a rewritten force formula

In this section we show that $S = (S_{ijkp})_{i,j,k,p=1,2,3}$ is not identically zero in the case of a cubic lattice, $\mathcal{L} = \mathbb{Z}^3$. As discussed in Section 4.1, the antisymmetric terms are in fact zero. Hence the only terms of S which can be nonzero are S_{kkkk} and S_{iikk} with $i \neq k$.

By the definition of S_{kkkk} and by (4.10) and (4.14) we obtain

$$S_{kkkk} = \mathcal{S} + \frac{3\gamma}{5}. \tag{4.16}$$

Similarly, the definition of S_{iikk} and (4.11) and (4.13) yield

$$S_{iikk} = -\frac{1}{2}\mathcal{S} + \frac{\gamma}{5}. \tag{4.17}$$

Thus S_{kkkk} and S_{iikk} cannot be zero at the same time. Hence $S \neq 0$ as asserted.

Using this result we rewrite the surface density in the limiting formula which contains S_{ijkp} (Theorem 3.7). As in (3.9) we consider the kth component of the force. Notice that S_{kkii} has the same value as S_{iikk}. Because of symmetry in the first three indices of S_{ijkp}, also S_{kiki} and S_{ikki} equal S_{iikk}. By the summation convention we obtain

$$\begin{aligned}
m_i^- m_j^+ S_{ijkp} n_p &\equiv \sum_{i=1}^{3}\sum_{j=1}^{3} m_i^- m_j^+ \sum_{p=1}^{3} S_{ijkp} n_p \\
&= m_k^- m_k^+ S_{kkkk} n_k + \sum_{i=1}^{3} m_i^- m_i^+ S_{iikk} n_k (1-\delta_{ik}) + \\
&\quad + \sum_{i=1}^{3} m_k^- m_i^+ S_{kiki} n_i (1-\delta_{ik}) + \sum_{i=1}^{3} m_i^- m_k^+ S_{ikki} n_i (1-\delta_{ik}) \\
&= m_k^- m_k^+ S_{kkkk} n_k + \\
&\quad + \sum_{i=1}^{3} \big(m_i^- m_i^+ n_k + (m_k^- m_i^+ + m_i^- m_k^+) n_i\big) S_{iikk} (1-\delta_{ik}).
\end{aligned}$$

With (4.16) and (4.17) one has

$$\begin{aligned}
m_i^- m_j^+ S_{ijkp} n_p &= (\mathcal{S} + \frac{3\gamma}{5}) m_k^- m_k^+ n_k + \\
&\quad + (-\frac{1}{2}\mathcal{S} + \frac{\gamma}{5}) \sum_{\substack{i=1 \\ i\neq k}}^{3} \big(m_i^- m_i^+ n_k + (m_k^- m_i^+ + m_i^- m_k^+) n_i\big)
\end{aligned}$$

for the integrand of the additional linear surface term in the limiting formula.

Finally, we would like to mention that the lattice series $\mathcal{S}$ is related to a special value of a L-series. Therefore one can convert $\mathcal{S}$ in an exponentially convergent series, which can be evaluated very sufficiently numerically [Za2]. In fact, using the function equation principle for the corresponding theta-series one can also obtain precise information on $\mathcal{S}$ analytically. For further reference see e.g. [Za1] and [KoKr].

The important result of this chapter for the comparison of the force formulae in Chapter 5 is that the tensor S is not identically zero. Thus the corresponding term in the limiting force formula is in general not zero.

Chapter 5

Comparison of the force formulae

In this chapter we compare the two force formulae which we discussed in Chapters 2 and 3. For this we unify the notation and write M for the magnetization M_τ in Chapter 2 and for m in Chapter 3. The points of interest are Brown's force formula (2.2), which is derived in a continuum setting,

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

and the force formula (3.9), which arises in the passage from an atomistic to a continuous setting. The kth component of this limiting force is given by

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

where the lattice sum S_{ijkp} is defined in (3.7) and evaluated in Chapter 4.

Obviously, the two force formulae both contain the same volume term, and they both contain a surface integral which shows a nonlinear dependence on the normal. In the case of separated regions or when the outer trace M^+ is zero, the two force formulae coincide as we will discuss in Section 5.1.

In view of an application of the magnetic force formulae to magnetoelastic materials we consider the formulae with respect to Cauchy's Theorem in continuum mechanics in Section 5.2. In particular we focus on the discrepancy between the appearance of the nonlinear surface term in Brown's formula and Cauchy's statement that surface force densities should be linear in the normal. For this, volume and surface densities are of interest, which are smooth in the whole magnetic body Ω. If M is continuous across $\partial\tau$, i.e. $M^+ = M^-$, the nonlinear surface term in the limiting force vanishes. In this case the only surface term appearing in the limiting force is the one which is linear in the normal. This one agrees with Cauchy's Theorem.

When one derives a new force formula, a first simple check whether the formula is correct, is to show that it satisfies Newton's law of actio equals reactio, which is one of the axioms of classical mechanics. A verification of this for both formulae can be found in Appendix B.

First we consider the force between two regions which are a positive distance apart from each other.

5.1 Magnetic force formulae for separated regions

In Chapter 2 Brown's formula is derived for a body $\Omega \subset \mathbb{R}^3$, which is divided into the regions $\bar{\tau}$ and $\Omega \setminus \bar{\tau}$. In preparation for the discussions in the following section we consider in contrast a set Ω consisting of two proper (i.e. $\bar{A} \cap \bar{B} = \emptyset$) distinct regions, A and B with boundaries ∂A and ∂B and outer normals n_A and n_B, respectively. The force which is exerted by the magnetic field, H_B, of part B on the magnetization in A is given by

$$F = \int_A (M(x) \cdot \nabla) H_B(x)\, d^3x.$$

Proposition 5.1 *Let $\Omega = A \cup B$ such that $\bar{A} \cap \bar{B} = \emptyset$. Suppose that A and B have C^2-boundary and that M belongs to $W^{1,2}(A)$ and $W^{1,2}(B)$. Then the corresponding Brown's formula reads*

$$F^{(\mathrm{Br,\,sep})} = \int_A (M(x) \cdot \nabla) H_\Omega(x)\, d^3x + \frac{\gamma}{2} \int_{\partial A} (M^- \cdot n_A)^2(x) n_A(x)\, d\mathcal{H}^2(x), \quad (5.1)$$

where $H_\Omega = H_A + H_B$.

This formula has the same structure as Brown's formula in the non-separated case. One can adapt the proof of Theorem 2.1 since it is not used there that $\bar{\tau}$ and $\Omega \setminus \bar{\tau}$ are not separated.

The magnetic fields are determined by Maxwell's equations (cf. p. 80). For instance, the magnetic field H_A is given by

$$-\Delta u_A = -\gamma(\nabla \cdot M)\mathcal{L}^3\lfloor_A + \gamma(M^- \cdot n_A)\mathcal{H}^2\lfloor_{\partial A} \quad \text{and} \quad H_A = -\nabla u_A.$$

The difference between the two geometric settings in Theorem 2.1 and Proposition 5.1 is reflected in the magnetic field of the whole body $H_\Omega = -\nabla u_\Omega$. In the separated case, u_Ω is the solution of

$$-\Delta u_\Omega = -\gamma(\nabla \cdot M)\mathcal{L}^3\lfloor_{A\cup B} + \gamma(M \cdot n_A)^-\mathcal{H}^2\lfloor_{\partial A} + \gamma(M \cdot n_B)^-\mathcal{H}^2\lfloor_{\partial B} \quad \text{in} \quad \mathbb{R}^3,$$

while u_Ω is a solution of (B.1) in the non-separated case.

The force obtained in the limit of a discrete setting shows a different appearance in the case of separated regions.

Proposition 5.2 *Let again $\Omega = A \cup B$ such that $\bar{A} \cap \bar{B} = \emptyset$. Assume that A and B have C^2-boundaries and that $M \in W^{1,\infty}(A)$ and $M \in W^{1,\infty}(B)$. Then the limit of the discrete force is*

$$F^{(\mathrm{lim,\,sep})} = \int_A (M(x)\cdot\nabla)H_\Omega(x)\,d^3x + \frac{\gamma}{2}\int_{\partial A}(M^- \cdot n_A)^2(x)n_A(x)\,d\mathcal{H}^2(x) \quad (5.2)$$

with $H_\Omega = H_A + H_B$ as above.

The proof of this follows from that of Theorem 3.7. Indeed, the estimate of the short range part of the discrete force (Section 3.4) applies trivially in the case of separated regions since $(K - K^{(\delta)})_{ij}(x-y) \equiv 0$ if δ is less than the distance between the two regions. Hence the short range part does not lead to an additional surface term in the continuum limit.
The estimates for the long range part of the discrete force (Section 3.3) are not affected by a distance between the two regions — apart from the fact that the outer trace M^+ is zero. Hence in this case the limit of the long range part of the force is (5.2).

Consequently, Brown's formula and the limiting force formula coincide if the subbodies are separated, i.e. not in contact, and they have the same structural appearance as Brown's formula in Theorem 2.1 in the case of regions in contact.

5.2 Cauchy's Theorem and the force formulae

As pointed out in the introduction we are interested in an application of the magnetic force formulae to magnetoelastic materials. In the framework of elasticity, the (sub-)bodies, which are considered in the magnetic force formulae above, correspond to regions in the deformed configuration.

To obtain equations of motion for a magnetoelastic body one can use Cauchy's Theorem which relates momentum balance laws and volume and surface forces. Firstly, we briefly mention Cauchy's Theorem, which can be found in many textbooks on continuum mechanics (see e.g. [Gu, Chapter V]). While the models in this thesis are purely static, time is taken into consideration subsequently. Secondly, we discuss the magnetic force formulae in view of Cauchy's Theorem.

In Cauchy's Theorem a system of forces (s, b) for a body, $\mathcal{B}$, during motion is considered, where s denotes the surface or contact forces and b are the so-called volume or body forces. Let $\mathcal{N}$ be the set of all unit vectors and let $\mathcal{T}$ be the trajectory of the motion. Let $\mathrm{s} : \mathcal{N} \times \mathcal{T} \to \mathbb{R}^3$ and $\mathrm{b} : \mathcal{T} \to \mathbb{R}^3$ be functions with the following properties:
(i) for each $e \in \mathcal{N}$ and $t \in \mathbb{R}$, the surface force $\mathrm{s}(e, x, t)$ is a smooth function of x on $\mathcal{B}_t$;
(ii) for each t, the body force $\mathrm{b}(x, t)$ is a continuous function of x on $\mathcal{B}_t$, where $\mathcal{B}_t$ denotes the body $\mathcal{B}$ at time t.

Let a force $f(\mathcal{P}, t)$ on a part $\mathcal{P}$ of the body at time t be given by

$$f(\mathcal{P}, t) = \int_{\mathcal{P}_t} \mathrm{b}(x, t)\, d^3x + \int_{\partial \mathcal{P}_t} \mathrm{s}(n(x), x, t)\, d\mathcal{H}^2(x),$$

where $n(x)$ is the outer normal to $\partial \mathcal{P}_t$ at x. Similarly, the torque is defined. A connection with motion is given by the momentum balance laws. The balance law of linear momentum reads

$$f(\mathcal{P}, t) = \int_{\mathcal{P}_t} \rho(x, t) \dot{v}(x, t)\, d^3x, \tag{5.3}$$

where ρ is the mass density and v the velocity of the body. Here, $\dot{v}(x, t) = \frac{\partial}{\partial t} v(x, t)$ denotes the material time derivative of v. A similar formula, called balance of angular momentum, gives a link to the torque.

Theorem 5.3 (Cauchy's Theorem) *Let* (s, b) *be a system of forces for* $\mathcal{B}$ *during motion. Then a necessary and sufficient condition that the momentum balance laws are satisfied is that there exists a spatial tensor field* T *(called the Cauchy stress) such that*
(a) for each $e \in \mathcal{N}$,

$$\mathrm{s}(e, x, t) = T(x, t) e \quad \forall (x, t) \in \mathcal{T}; \tag{5.4}$$

(b) T *is symmetric;*
(c) T *satisfies the equation of motion*

$$\nabla \cdot T + \mathrm{b} = \rho \dot{v}.$$

The proof (see e.g. [Gu, p. 101]) is mainly based on the so-called Cauchy tetrahedron argument and on a localization theorem. One has that (a) and (c) are equivalent to balance of linear momentum. If balance of linear momentum is granted, the symmetry of T is equivalent to balance of angular momentum.

For an application of Cauchy's Theorem to Brown's force formula notice that Brown's formula in Theorem 2.1 has the same appearance if the magnetization is smooth in the whole body Ω, i.e.

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

We first mention that the splitting of this force into a volume term and a surface term is not unique. Below we will discuss various equivalent expressions for F. We consider the formula above mathematically the most convenient since it expresses most transparently the dependence of the force on the surface normal n.

An equivalent expression for the force is given by our starting point

$$F = \int_\tau (M(x)\cdot\nabla)H_{\Omega\setminus\bar\tau}(x)\,d^3x,$$

which is purely a volume integral. The integrand, however, depends on τ and thus Cauchy's Theorem cannot be applied to this expression since it requires that the force system (s, b) be independent of the part $\mathcal{P}$ which is considered, i.e. that it is independent of τ in our case.

A further equivalent formulation is obtained if one integrates the first term in Brown's formula by parts, which yields

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

and thus another surface term. This surface term is smooth in Ω and linear in the normal if the magnetization and hence H_Ω is smooth in Ω.

Recalling the proof of Theorem 2.1 (p. 9) one has that the surface term in Brown's formula is actually equal to the negative of the self-force on τ, i.e. that it is equal to the volume integral

$$-\int_\tau (M(x)\cdot\nabla)H_{\bar\tau}(x)\,d^3x.$$

After an integration by parts we get

$$\begin{aligned}&\frac{\gamma}{2}\int_{\partial\tau}(M^-\cdot n)^2(x)n(x)\,d\mathcal{H}^2(x)\\ &\quad=\int_\tau(\nabla\cdot M)(x)H_\tau(x)\,d^3x-\int_{\partial\tau}(M^-\cdot n)(x)H_\tau^-(x)\,d\mathcal{H}^2(x).\end{aligned}$$

The term in the surface integral now appears to be linear in the normal n. One should note that H_τ depends on τ and hence implicitly on n. Moreover one cannot apply Cauchy's Theorem to the system of forces $\mathrm{b}=(M\cdot\nabla)H_\Omega+(M\cdot\nabla)H_\tau$ and $\mathrm{s}=-(M^-\cdot n)H_\tau^-$, since these forces depend on the subbody.

The smoothness assumption of Cauchy's Theorem is satisfied in the formulation of the magnetic force by Brown. The surface density $(M\cdot n)^2n$ in Brown's formula is not linear in the normal and hence disagrees with statement (a) in Cauchy's Theorem under the physical assumption that the momentum balance laws hold. This discrepancy is discussed in [Br, Section 5]. To tackle the discrepancy Brown assumes that there is an additional term in the surface force which cancels the nonlinear surface term. He introduces this additional term in the formulae for the mechanical stress and then works with this new expression.

Brown emphasizes that his force formula is only associated to long range contributions. He expects that the total magnetic force has additional short range contributions. Together with Cauchy's statement this leads to his hypothesis of the existence of the additional surface term which cancels the nonlinearity. He suggests to derive this additional term from an atomistic model [Br, p. 52]. This is what we did in Chapter 3. A careful analysis of Cauchy's Theorem and the derivation of pointwise balance laws such as (5.4) from balance laws for each part of the body such as (5.3) in the context of long range forces was carried out in [DSPG]. These authors conclude (see p. 213) that the pointwise balance laws must take into account self-interactions. Specifically the relevant stress tensor does not account solely for contact interactions exerted on τ by $\mathbb{R}^n\setminus\tau$. This is in agreement with Brown's point of view that the total magnetic force has additional short range contributions.

Notice that the terms 'long range' and 'short range' can be used differently depending on the scale. In a continuum setting it is suggestive to define short range forces as those forces which are due to contact and long range forces as those which are not due to contact. In this sense the force terms in $F^{(\mathrm{Br,sep})}$ and $F^{(\mathrm{lim,sep})}$ in (5.1) and (5.2), respectively, are long range forces, whereas the remaining terms of the limiting force are short range contributions. This coincides with the notions which Brown uses.

On the scale of the discrete setting, we use the terms 'short range' and 'long range' to indicate the range of the interaction considered in the two terms of the discrete force, which we obtain by introducing a regularizing kernel. Notice that we obtain in the limit of the long range part of the discrete force a surface density, $(M^- \cdot n)(M^+ \cdot n)n$, which is due to the fact that τ and $\Omega \setminus \bar{\tau}$ are not separated. For this compare Proposition 5.2 and Theorem 3.7. This surface term can thus be considered in the continuum setting as being a short range contribution.

For smooth magnetizations as considered in Cauchy's Theorem one obtains the following result for the limiting force as a consequence of Theorem 3.7.

Proposition 5.4 *Let τ and Ω satisfy the assumptions in Theorem 3.7 and suppose that M is smooth in Ω. Then the kth component of the limiting force reduces to*

$$F_k^{(\mathrm{lim,\,smooth})} = \int_\tau (M(x) \cdot \nabla)(H_\Omega)_k(x)\, d^3x + \frac{1}{2} \int_{\partial\tau} M_i(x) M_j(x) S_{ijkp} n_p(x)\, d\mathcal{H}^2(x).$$

That is, the nonlinear surface terms in the general limiting force formula in Theorem 3.7 cancel. This suggests to regard the term $-\frac{\gamma}{2}\int_{\partial\tau}(M^-\cdot n)(M^+\cdot n)n$ as exactly that additional contribution which Brown introduces to obtain a linear surface force as mentioned above. Hence one can consider Brown's hypothesis, i.e. the existence of an additional surface term which cancels the nonlinearity, as a consequence of the derivation of the limiting force formula.

The limit of the short range part of the discrete force yields an explicit formula for the short range contribution to the magnetic force. This term,

$$\frac{1}{2} \int_{\partial\tau} M_i^-(x) M_j^+(x) S_{ijkp} n_p(x)\, d\mathcal{H}^2(x), \tag{5.5}$$

is linear in the normal and thus agrees with statement (a) in Cauchy's Theorem. From this one can obtain a formula for the stress which is due to magnetic interaction between two magnetized subregions which are in contact.

Concluding, the limiting force formula supports the ideas of Brown with respect to the discrepancy between his formulation of the magnetic force and Cauchy's Theorem. Moreover it gives an explicit formula for the short range part of the magnetic force.

In the following final chapter we mention some open problems related to the force formulae.

Chapter 6

Outlook

In this thesis we studied magnetic forces in three-dimensional lattice and continuum settings. In Chapter 2 we verified Brown's formula for the magnetic force which is exerted on a subbody τ of a bounded, continuous, magnetized body Ω by its surrounding. For this we assume that the boundary of τ has C^2-regularity and that the magnetization belongs to $W^{1,2}(\tau)$ and $W^{1,2}(\Omega \setminus \bar{\tau})$ (Theorem 2.1). This allows for a jump of the magnetization at the interface of the subbody and its complement.
In order to model also subbodies with edges one could try to sharpen the proof of the force formula to the weaker assumption of piecewise C^1 or Lipschitz continuous boundaries. For appropriate results for boundary layer integrals one can rely on the work of Fabes, Jodeit and Rivière [FaJoRi] for C^1-domains, and on the paper by Verchota [Ve] for Lipschitz domains.

In Chapter 3 we discussed a corresponding force in a discrete system of atoms. In the limit to the continuum we obtain a force formula which is different from Brown's formula. The proof of the limiting force is split into two parts. For the long range part of the discrete force similar methods as for the verification of Brown's force apply if one assumes C^2-regularity for the boundaries and $W^{1,2}$-regularity for the magnetizations (Theorem 3.1). Again it would be interesting to obtain optimal conditions regarding the required regularity.
For the short range part of the force we require that the magnetization is Lipschitz continuous in the two subregions. For the boundary of τ we assume that it satisfies the non-degeneracy condition (S) (cf. Theorem 3.6 and Definition 3.4), which restricts the number of indentations and protrusions of τ.
As discussed in Chapter 5, the difference between the two force formulae concerns surface integrals and the dependence of the surface terms on the normal. While Brown's surface term is nonlinear in the normal, the limiting force shows an additional surface term, which depends linearly on the normal. For further investigations of the force formulae it would be interesting to consider

sequences of boundaries which oscillate around their limit in order to model rough boundaries. A first step towards this would be to prove the formula for the limit of the short range part of the discrete force under a weaker assumption on the shape of the set than the already mild non-degeneracy condition (S).

In Chapter 4 we evaluated the lattice sum which contains the hypersingular kernel, mainly to show that the tensor $S = (S_{ijkp})_{i,j,k,p=1,2,3}$ is in general not identically zero. For some calculations we restricted the lattice structure to a cubic Bravais lattice, namely $\mathbb{Z}^3$, to make use of its symmetry properties. One could now go further and evaluate the lattice sum for other Bravais lattices to estimate the effect of the surface term which contains S_{ijkp} in view of different underlying lattice structures.

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 [Ja], [BaJa1], [BaJa2] and e.g. [Mü]).
In order to take into account different deformation gradients in the discrete setting one could start with a force between two parts of the body which have different lattice structures, i.e. one Bravais lattice in one part of the region and another (maybe just rotated) lattice in the other part. Here one can assume the above mentioned compatibility conditions at the interface. The derivation of the limit of the long rang part of the force in such an extended model is not really affected by a change of the underlying lattices in the sets τ and $\Omega \setminus \bar{\tau}$ since the limit of the Riemann sum does not depend on the chosen partition of the sets. With respect to the limit of the short range part notice that we used the fact that z is a lattice vector in our derivation (cf. p. 35). This does not hold in general in such an extended model. Thus one would have to prove the convergence of the short range part of the discrete force, which involves a proof of the convergence of a modified 'lattice' sum, which contains the hypersingular kernel.

Finally, we return to the problem 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 [Ja] within a continuum setting. One could now try to combine his calculations with our result for the limiting formula derived from the discrete setting. Probably, one would obtain additional terms in the dynamic equations corresponding to the additional linear surface term of the limiting force.

Appendix A

Supplementary Material

Traces

Proofs of the following theorems can be found e.g. in [Al].

Theorem A.1 *Let $\mathcal{U} \subset \mathbb{R}^n$ be open and bounded with Lipschitz boundary, and let $1 \le p \le \infty$. Then there exists a unique continuous linear mapping*

$$\mathrm{Tr} : \mathrm{W}^{1,\mathrm{p}}(\mathcal{U}) \to \mathrm{L}^{\mathrm{p}}(\partial\mathcal{U})$$

such that

$$\mathrm{Tr}\,\mathrm{g} = \mathrm{g}|_{\partial\mathcal{U}} \qquad \textit{if} \quad \mathrm{g} \in \mathrm{W}^{1,\mathrm{p}}(\mathcal{U}) \cap \mathrm{C}^0(\bar{\mathcal{U}}).$$

The weak boundary values $\mathrm{Tr}\,\mathrm{g}$ are called traces of g on $\partial\mathcal{U}$, and the mapping Tr is called trace operator. A trace is nothing else but the limit of the values of g on hypersurfaces, which are shifted copies of $\partial\mathcal{U}$. If nothing else is said, we always regard traces as inner traces, i.e. those which come from hypersurfaces, which are shifted to the inside of $\mathcal{U}$. In this case we also write g^- instead of $\mathrm{Tr}\,\mathrm{g}$. Traces which are given by the limit of the values of g on hypersurfaces from outside $\partial\mathcal{U}$ (supposing g is defined on a superset of $\mathcal{U}$) are called outer traces. They will be denoted by g^+.

The difference between the outer and the inner trace of g is denoted by $[g]$, i.e. $[g] = g^+ - g^-$.

With the notion of traces, weak formulations of Gauss' Theorem and of the integration by parts formula can be derived.

Theorem A.2 *Let $\mathcal{U} \subset \mathbb{R}^n$ be open and bounded with Lipschitz boundary and outer normal ν.*
1) If $u \in W^{1,1}(\mathcal{U})$, then for $i = 1, \dots, n$

$$\int_{\mathcal{U}} \partial_i u = \int_{\partial\mathcal{U}} u\nu_i \, d\mathcal{H}^{n-1}$$

holds.
2) Let $1 \le p \le \infty$. If $u \in W^{1,p}(\mathcal{U})$ and $v \in W^{1,q}(\mathcal{U})$ with $\frac{1}{p} + \frac{1}{q} = 1$, then for $i = 1, \dots, n$ the integration by parts formula reads

$$\int_{\mathcal{U}} (u\partial_i v + v\partial_i u) = \int_{\partial\mathcal{U}} uv\nu_i \, d\mathcal{H}^{n-1}.$$

Maxwell's equations

The magnetization M, the magnetic field H and the magnetic induction B satisfy

$$B - H = \gamma M,$$

where γ depends on the choice of units. In a region without conduction currents Maxwell's equations become

$$\nabla \cdot B = 0, \qquad \nabla \times H = 0$$

(cf. e.g. [Br, p. 18]).
In $\mathbb{R}^3$ the condition $\nabla \times H = 0$ is equivalent to the fact that H admits a potential u with

$$H = -\nabla u.$$

Thus

$$-\Delta u = -\gamma \nabla \cdot M, \tag{A.1}$$

and this equation is understood in the sense of distributions. In particular, if M is smooth (or in $W^{1,p}$) in a bounded region U and its complement $\mathbb{R}^n \setminus \bar{U}$ but may jump at ∂U, one has

$$-\Delta u = -\gamma \nabla \cdot M \qquad \text{in } U \text{ and } \mathbb{R}^n \setminus \bar{U}$$

and

$$[\nabla u \cdot n] = \gamma(M^+ \cdot n - M^- \cdot n),$$

where n denotes the outer normal to U and M^+ and M^- denote the outer and inner traces, respectively.

For $M \in L^2(\mathbb{R}^3)$ equation (A.1) admits a unique (up to constants) solution with $\nabla u \in L^2(\mathbb{R}^3)$, which is characterized by the weak form of (A.1)

$$\int \nabla u \cdot \nabla v = \gamma \int M \cdot \nabla v \qquad \forall\, v \ \text{ with } \ \nabla v \in L^2(\mathbb{R}^3).$$

In particular taking $u = v$ we get

$$\int |\nabla u|^2 = \gamma \int M \cdot \nabla u$$

and by the Cauchy-Schwarz inequality

$$\int |\nabla u|^2 \leq \gamma^2 \int |M|^2.$$

In fact ∇u is (up to a factor γ) the L^2-projection of M onto gradient fields. In Fourier space ∇u and M are related by

$$\widehat{\nabla u}(\xi) = \gamma \frac{\xi \otimes \xi}{|\xi|^2} \widehat{M}(\xi),$$

and passing back to real space one obtains the singular integral representation

$$H_i = -\partial_i u = \int K_{ij}(x-y) M_j(y)\, dy, \tag{A.2}$$

where $K_{ij} = \partial_i \partial_j N$ with $N = \frac{\gamma}{4\pi} \frac{1}{|x|}$. In (A.2) the integral is understood in the sense of principal values. From the L^p-theory for such integrals (see e.g. [St]) or equivalently the L^p-theory for $-\Delta$ one obtains the estimate

$$\|H\|_{L^p} \leq C_p \gamma \|M\|_{L^p} \qquad \forall\, 1 < p < \infty. \tag{A.3}$$

Lorentz' force formula as a starting point

In Chapter 2 we start the derivation of Brown's formula from (2.1), i.e. $F = \int_\tau (M_\tau \cdot \nabla) H_{\Omega \setminus \bar{\tau}}$. One can start alternatively with Lorentz' force formula, which describes the force on a current in an outer field of magnetic induction (see e.g. [Br, p. 19]). Some readers might find this force formula more natural. For their convenience we show that Lorentz' force formula implies (2.1) using the relation between currents and magnetizations, and between magnetic inductions and magnetic fields.

Let $\tau \subset \Omega$ be open and bounded with Lipschitz boundary, and let M_τ and $H_{\Omega\setminus\bar\tau} \in W^{1,2}(\tau)$. Then Lorentz' force, which is exerted by a field of magnetic induction $B_{\Omega\setminus\bar\tau}$ on a current J in τ, is given by

$$F^{(\mathrm{Lo})} = \frac{1}{c}\int_\tau J(x) \times B_{\Omega\setminus\bar\tau}(x)\, d^3x,$$

where c is the velocity of light. If there are no conduction currents,

$$J\lfloor_{\bar\tau} = c(\nabla \times M_\tau)\, d\mathcal{L}^3\lfloor_\tau - c(n \times M_\tau)^-\, d\mathcal{H}^2\lfloor_{\partial\tau},$$

where n denotes the outward normal to $\partial\tau$.

Since $B_{\Omega\setminus\bar\tau} = H_{\Omega\setminus\bar\tau} + \gamma M_{\Omega\setminus\bar\tau}$, $M_{\Omega\setminus\bar\tau} = 0$ on τ and $H_{\Omega\setminus\bar\tau} \in W^{1,2}(\tau)$, we deduce $B_{\Omega\setminus\bar\tau} \in W^{1,2}(\tau)$. Therefore the following integrals are well-defined. With the help of standard vector formulae, namely equations (A.4) and (A.5), one obtains

$$\begin{aligned} F^{(\mathrm{Lo})} &= \int_\tau (\nabla \times M_\tau)(x) \times B_{\Omega\setminus\bar\tau}(x)\, d^3x - \int_{\partial\tau} (n \times M_\tau)^-(x) \times B_{\Omega\setminus\bar\tau}(x)\, d\mathcal{H}^2(x) \\ &= \int_\tau \{-\nabla(B_{\Omega\setminus\bar\tau} \cdot M_\tau) + (B_{\Omega\setminus\bar\tau} \cdot \nabla) M_\tau + (M_\tau \cdot \nabla) B_{\Omega\setminus\bar\tau} + \\ &\qquad + M_\tau \times (\nabla \times B_{\Omega\setminus\bar\tau})\} - \int_{\partial\tau} \{-(B_{\Omega\setminus\bar\tau} \cdot M_\tau)^- n + (B_{\Omega\setminus\bar\tau} \cdot n)^- M_\tau\}. \end{aligned}$$

By Gauss' Theorem (cf. Theorem A.2) the first term of the volume integral and the first term of the surface integral cancel. We integrate the second term of the volume integral by parts. For the last term of the volume integral notice that, by Maxwell's equation, $\nabla \times B_{\Omega\setminus\bar\tau} = \gamma\nabla \times M_{\Omega\setminus\bar\tau}$ holds. Since $M_{\Omega\setminus\bar\tau}$ vanishes in τ and hence has zero inner trace with respect to τ, the last volume term vanishes. Therefore

$$\begin{aligned} F^{(\mathrm{Lo})} &= \int_\tau (-\nabla \cdot B_{\Omega\setminus\bar\tau}) M_\tau + \int_{\partial\tau} (B_{\Omega\setminus\bar\tau} \cdot n)^- M_\tau^- + \int_\tau (M_\tau \cdot \nabla) B_{\Omega\setminus\bar\tau} + \\ &\quad - \int_{\partial\tau} (B_{\Omega\setminus\bar\tau} \cdot n)^- M_\tau^-. \end{aligned}$$

Using Maxwell's equation $\nabla \cdot B_{\Omega\setminus\bar\tau} = 0$, one ends up with

$$F^{(\mathrm{Lo})} = \int_\tau (M_\tau \cdot \nabla) B_{\Omega\setminus\bar\tau} = \int_\tau (M_\tau \cdot \nabla) H_{\Omega\setminus\bar\tau}$$

since $B_{\Omega\setminus\bar\tau} - H_{\Omega\setminus\bar\tau} = M_{\Omega\setminus\bar\tau} = 0$ in τ. By (2.1) one has $F^{(\mathrm{Lo})} = F$.

Vector Formulae

Let a, b and c be vector fields in $\mathbb{R}^3$. Then one proves by direct computation that

$$a \times (b \times c) = (a \cdot c)b - (a \cdot b)c = -(b \times c) \times a \tag{A.4}$$

and

$$\nabla(a \cdot b) = (a \cdot \nabla)b + (b \cdot \nabla)a + a \times (\nabla \times b) + b \times (\nabla \times a) \tag{A.5}$$

if a and b are differentiable.

Regularity

Theorem A.3 *Let $U \subset \mathbb{R}^n$ be bounded and open and suppose that ∂U is of class $C^{1,1}$. Let $1 < p < \infty$. Suppose that $m \in W^{1,p}(U)$ and extend m by zero to $\mathbb{R}^n$. Define u by*

$$-\Delta u = -\nabla \cdot m \qquad \text{in } \mathbb{R}^n. \tag{A.6}$$

Then

$$\nabla u \in W^{1,p}(U), \quad \nabla u \in W^{1,p}(\mathbb{R}^n \setminus \bar{U}). \tag{A.7}$$

Proof: The proof closely follows the usual argument for regularity of solutions of second order elliptic partial differential equations (see e.g. [GiTr]). Since we do not have Dirichlet boundary conditions, we recall the argument for the convenience of the reader.
By standard regularity results (see (A.3))

$$\|\nabla u\|_{L^p} \leq C_p \|m\|_{L^p(\mathbb{R}^n)} = C_p \|m\|_{L^p(U)}.$$

By a partition of unity it suffices to consider the case that m is supported in a small neighbourhood V of a point on ∂U. (If m is compactly supported in U then the assertion follows by differentiating (A.6) once.) By assumption there is a $C^{1,1}$ diffeomorphism Φ (which is C^1 close to a rigid motion) that maps $V \cap U$ to the half-ball $B^+ = \{y \in \mathbb{R}^n : |y| < r, \ y_n > 0\}$. We may extend Φ to a diffeomorphism of $\mathbb{R}^n$ to itself which is a rigid motion outside a compact set. Define $\tilde{m}$ and $\tilde{u}$ by

$$(\operatorname{adj} D\Phi)\tilde{m} \circ \Phi = m, \tag{A.8}$$
$$\tilde{u} \circ \Phi = u. \tag{A.9}$$

The weak form of (A.6) is

$$\int \nabla u \cdot \nabla \eta = \int m \cdot \nabla \eta \qquad \forall\, \eta \;\text{ with }\; \nabla \eta \in L^2 \tag{A.10}$$

and defining $\tilde{\eta} \circ \Phi = \eta$ the right hand side becomes

$$\begin{aligned} \int_{\mathbb{R}^n} m \cdot \nabla \eta &= \int_{\mathbb{R}^n} (\operatorname{adj} D\Phi)(\tilde{m} \circ \Phi) \cdot (\nabla\Phi)^T (\nabla \tilde{\eta}) \circ \Phi \\ &= \int_{\mathbb{R}^n} (\det D\Phi)(\tilde{m} \circ \Phi) \cdot (\nabla \tilde{\eta} \circ \Phi) \\ &= \int_{\mathbb{R}^n} \tilde{m} \cdot \nabla \tilde{\eta} \end{aligned}$$

since $F \operatorname{adj} F = (\det F)\mathrm{Id}$. If we define

$$g(y) = \big((\nabla\Phi)(\nabla\Phi)^T \frac{1}{\det \nabla\Phi} \big) \circ \Phi^{-1}$$

then

$$\begin{aligned} \int \nabla u \cdot \nabla \eta &= \int (\nabla\Phi)^T (\nabla \tilde{u}) \circ \Phi \cdot (\nabla\Phi)^T (\nabla \tilde{\eta}) \circ \Phi \\ &= \int g \circ \Phi (\nabla \tilde{u} \circ \Phi) \cdot \nabla \tilde{\eta} \circ \Phi \det \nabla\Phi \\ &= \int g \circ \Phi (\nabla \tilde{u} \circ \Phi) \cdot \nabla \tilde{\eta} \circ \Phi \det \nabla\Phi \\ &= \int g \nabla \tilde{u} \cdot \nabla \tilde{\eta}. \end{aligned}$$

Hence

$$\int_{\mathbb{R}^n} g \nabla \tilde{u} \cdot \nabla \tilde{\eta} = \int_{\mathbb{R}^n} \tilde{m} \cdot \nabla \tilde{\eta}$$

and by the assumptions on m and Φ we have $\tilde{m} \in W^{1,p}(\mathbb{R}^n_+)$, $\tilde{m} = 0$ on $\mathbb{R}^n_-$, where $\mathbb{R}^n_\pm = \{x \in \mathbb{R}^n : \pm x_n > 0\}$.
The corresponding strong form is

$$\nabla \cdot (g \nabla \tilde{u}) = \nabla \cdot \tilde{m} \qquad \text{in } \; \mathbb{R}^n. \tag{A.11}$$

By the usual difference quotient argument we can differentiate (A.11) in the tangential directions. This yields

$$\nabla \cdot (g \nabla \partial_s \tilde{u}) = \nabla(\partial_s \tilde{m}) - \nabla \cdot ((\partial_s g) \nabla \tilde{u}) \qquad \text{for } \; s \neq n \quad \text{in } \; \mathbb{R}^n$$

and

$$\begin{aligned} \|\nabla \partial_s \tilde{u}\|_{L^p} &\leq \|\partial_s \tilde{m}\|_{L^p} + \|(\partial_s g)\nabla \tilde{u}\|_{L^p} \\ &\leq C\|\tilde{m}\|_{W^{1,p}(\mathbb{R}^n_+)} \leq C\|m\|_{W^{1,p}(U)}. \end{aligned} \tag{A.12}$$

This gives control over all second derivatives of $\tilde{u}$ except $\partial_n^2 \tilde{u}$. To bound this derivative we use (A.11) to obtain

$$\partial_n^2 \tilde{u} = -\frac{1}{g_{nn}} \Big(\sum_{(i,j)\neq(n,n)} g_{ij}\partial_i\partial_j\tilde{u} + \sum_{(i,j)} (\partial_i g_{ij})\partial_j \tilde{u} - \nabla \cdot \tilde{m} \Big).$$

Together with (A.12) and $\nabla \cdot \tilde{m} \in L^p(\mathbb{R}^n_\pm)$ this yields the L^p-bound for $\nabla^2 \tilde{u}$ in the regions $x_n > 0$ and $x_n < 0$. Transforming back to u we obtain the desired assertion. □

Embeddings

The following theorem allows us to identify the Sobolev spaces $W^{k+1,\infty}$ with the space $C^{k,1}$ of functions of which the kth derivatives are Lipschitz continuous. A proof can be found e.g. in [Al, p. 305].

Theorem A.4 *Let $\tau \subset \mathbb{R}^n$ be bounded and open with Lipschitz boundary. For $k \geq 0$ the embedding*

$$\mathrm{Id} : C^{k,1}(\bar{\tau}) \to W^{k+1,\infty}(\tau)$$

is well-defined and an isomorphism in the sense that for every $f \in W^{k+1,\infty}(\tau)$ exists a $\tilde{f} \in C^{k,1}(\bar{\tau})$ such that $\tilde{f} = f$ almost everywhere in τ. So $\tilde{f} = f$ in $W^{k+1,\infty}(\tau)$.

Area and coarea formulae

The area formula is a generalization of the classical change of variables formula for Lipschitz continuous functions instead of C^1-diffeomorphisms. The coarea formula can be regarded as a curvilinear generalization of Fubini's Theorem. For $n = N$ the area and coarea formula are the same. Proofs of the following theorems can be found e.g. in [EvGa], [Fe] or [GiMoSo].

Theorem A.5 (Area and change of variable formulae) *Let $\psi : \mathbb{R}^n \to \mathbb{R}^N$ be a Lipschitz map, $n \le N$, and let $B \subset \mathbb{R}^n$ be a Lebesgue measurable set. Then*

$$\int_B J_\psi(y)\, d^n y = \int_{\psi(B)} \mathcal{H}^0(B \cap \psi^{-1}(\xi))\, d\mathcal{H}^n(\xi)$$

where $J_\psi(y)$ is the Jacobian of ψ

$$J_\psi(y) := \sqrt{\det(D\psi(y)^* D\psi(y))}.$$

If in addition $u : \mathbb{R}^n \to [0,\infty]$ is a Lebesgue measurable map, then

$$\int_{\mathbb{R}^n} u(y) J_\psi(y)\, d^n y = \int_{\mathbb{R}^N} \Big(\sum_{y \in \psi^{-1}(\xi)} u(y) \Big)\, d\mathcal{H}^n(\xi).$$

In particular, for any $\mathcal{H}^n$-measurable function $v : \mathbb{R}^N \to [0,\infty]$ we have

$$\int_B v(\psi(y)) J_\psi(y)\, d^n y = \int_{\psi(B)} v(\xi)\, \#\{y \in B : \psi(y) = \xi\}\, d\mathcal{H}^n(\xi). \tag{A.13}$$

Theorem A.6 (Coarea formula) *Let $f : \mathbb{R}^n \to \mathbb{R}^N$ be a Lipschitz map, $n \ge N$, and let $A \subset \mathbb{R}^n$ be a Lebesgue measurable set. Then*

$$\int_A J_f(x)\, d^n x = \int_{\mathbb{R}^N} \mathcal{H}^{n-N}(A \cap f^{-1}(y))\, d\mathcal{H}^N(y),$$

where $J_f(x)$ is the Jacobian of f

$$J_f(x) := \sqrt{\det Df(x)(Df(x))^*}.$$

If in addition $u : \mathbb{R}^n \to [0,\infty]$ is a Lebesgue measurable map, then

$$\int_{\mathbb{R}^n} u(x) J_f(x)\, d^n x = \int_{\mathbb{R}^N} \Big[\int_{f^{-1}(y)} u\, d\mathcal{H}^{n-N} \Big]\, d\mathcal{H}^N(y). \tag{A.14}$$

Inequalities

Young's inequality For $p > 1$, $\frac{1}{p} + \frac{1}{p'} = 1$ and $A, B \ge 0$ one has

$$AB = \frac{A^p}{p} + \frac{B^{p'}}{p'}.$$

An application with $A = a^{4-k}$, $B = b^k$ and $\frac{1}{p} = \frac{4-k}{4}$ yields

$$a^{4-k}b^k \leq \frac{4-k}{4}(a^{4-k})^{\frac{4}{4-k}} + \frac{k}{4}(b^k)^{\frac{4}{k}} = \frac{4-k}{4}a^4 + \frac{k}{4}b^4 \qquad \text{(A.15)}$$

for $k \in \{1, 2, 3\}$, which is used in Chapter 3.

The following lemma is used in the passage from the lattice to the continuum. Let f be a Lipschitz continuous function, and let a lattice be given. Then the corresponding step-function is defined as that function which equals f on the lattice points and which is constantly extended on the corresponding unit cells.

Lemma A.7 *Let $f \in W^{1,\infty}(\mathbb{R}^3)$ and let $B \subset \mathbb{R}^3$ be a bounded domain. Let $\mathcal{U}(z_\zeta)$ be the unit cell in which ζ is contained. Denote by* step *the corresponding step-function. Then*

$$\left| \int_B \text{step}(f(\zeta)) - f(\zeta)\, d\zeta \right| \leq c \int_B \operatorname*{ess-sup}_{\eta \in \mathcal{U}(z_\zeta)} |Df(\eta)|\, d\zeta.$$

Proof:

$$|\text{step}(f(\zeta)) - f(\zeta)| = |f(z_\zeta) - f(\zeta)| = \left| \int_0^1 \frac{d}{dt}(f(tz_\zeta + (1-t)\zeta)\, dt \right|$$
$$= \left| \int_0^1 D(f(tz_\zeta + (1-t)\zeta) \cdot (z_\zeta - \zeta)\, dt \right| \leq \operatorname*{ess-sup}_{\eta \in \mathcal{U}(z_\zeta)} |Df(\eta)| \sup_{\zeta \in \mathcal{U}(z_\zeta)} |z_\zeta - \zeta|$$
$$\leq c \operatorname*{ess-sup}_{\eta \in \mathcal{U}(z_\zeta)} |Df(\eta)|$$

□

Appendix B

actio equals reactio

In this part of the appendix we verify that Brown's force and the limiting force satisfy Newton's law of actio equals reactio. That is we show that the force exerted by the magnetic field $H_{\Omega\setminus\bar{\tau}}$ on the magnetization in τ, actio, is the negative of the force exerted by the magnetic field $H_{\bar{\tau}}$ on the magnetic material in $\Omega \setminus \bar{\tau}$, which is described by the magnetization $M_{\Omega\setminus\bar{\tau}} : \Omega \setminus \bar{\tau} \to \mathbb{R}^3$, reactio.

For this we suppose that the assumptions of Theorem 2.1 for Brown's formula and of Theorem 3.7 for the limiting force hold. Analogous assumptions are also required for the magnetizations and the sets in the reactio case. The reactio formula which corresponds to Brown's force formula is derived from $\bar{F} := \int_{\Omega\setminus\bar{\tau}} (M_{\Omega\setminus\bar{\tau}}(x) \cdot \nabla) H_{\bar{\tau}}(x)\, d^3x$. By replacing $H_{\bar{\tau}}$ with $H_\Omega - H_{\Omega\setminus\bar{\tau}}$ one obtains

$$\bar{F} = \int_{\Omega\setminus\bar{\tau}} (M_{\Omega\setminus\bar{\tau}}(x) \cdot \nabla) H_\Omega(x)\, d^3x - \int_{\Omega\setminus\bar{\tau}} (M_{\Omega\setminus\bar{\tau}}(x) \cdot \nabla) H_{\Omega\setminus\bar{\tau}}(x)\, d^3x.$$

The second term can be treated in a similar way as F_0 on page 9. Analogously to the derivation of the formulae for H_τ and H_Ω in Sections 2.1 and 3.3, respectively, one obtains a representation of $H_{\Omega\setminus\bar{\tau}}$. If $x \in \mathbb{R}^3 \setminus \partial(\Omega \setminus \bar{\tau})$, one has

$$\begin{aligned} H_{\Omega\setminus\bar{\tau}}(x) &= \frac{\gamma}{4\pi}\Big\{ \int_{\Omega\setminus\bar{\tau}} (-\nabla \cdot M_{\Omega\setminus\bar{\tau}})(y) \frac{x-y}{|x-y|^3}\, d^3y + \\ &\quad + \int_{\partial(\Omega\setminus\bar{\tau})} (M_{\Omega\setminus\bar{\tau}} \cdot \nu)^-(y) \frac{x-y}{|x-y|^3}\, d\mathcal{H}^2(y) \Big\}. \end{aligned}$$

Here $(M_{\Omega\setminus\bar{\tau}} \cdot \nu)^-$ is the inner trace with respect to $\Omega \setminus \bar{\tau}$, to which the outer normal is called ν. Thus the inner traces with respect to $\Omega \setminus \bar{\tau}$ are denoted with the superscript $^-$. This notation is also used for the inner traces with respect to τ. It will be clear from the appearing normal which trace is meant. Set $\tilde{\phi}(x) = (M_{\Omega\setminus\bar{\tau}} \cdot \nu)^-(x)$. For $x \in \partial(\Omega \setminus \bar{\tau})$ the magnetic field is given by

$$H^\pm_{\Omega\setminus\bar{\tau}}(x) \;=\; \frac{\gamma}{4\pi}\int_{\Omega\setminus\bar{\tau}} (-\nabla\cdot M_{\Omega\setminus\bar{\tau}})(y)\frac{x-y}{|x-y|^3}\, d^3y \;+\; (\bar{\mathcal{B}}\tilde{\phi})(x) \pm \frac{\gamma}{2}\tilde{\phi}(x)\nu(x),$$

where, similarly to (2.13),

$$(\bar{\mathcal{B}}\tilde{\phi})(x) \;=\; \lim_{\epsilon\to 0}\frac{\gamma}{4\pi}\int_{\partial(\Omega\setminus\bar{\tau})} \eta(\frac{|x-y|}{\epsilon})\tilde{\phi}(y)\frac{(x-y)}{|x-y|^3}\, d\mathcal{H}^2(y)$$

with η being the regularizing function introduced on page 10. This reduces to $(\mathcal{B}\tilde{\phi})(x)$ if $(M_{\Omega\setminus\bar{\tau}} \cdot \nu)^- \lfloor_{\partial\Omega} = 0$, where $\mathcal{B}$ is defined in (2.13).

One derives analogously to Brown's formula in Chapter 2

$$\bar{F}^{(\mathrm{Br})} = \int_{\Omega\setminus\bar{\tau}} (M_{\Omega\setminus\bar{\tau}}(x)\cdot\nabla)H_\Omega(x)\, d^3x + \frac{\gamma}{2}\int_{\partial(\Omega\setminus\bar{\tau})} \tilde{\phi}^2(x)\nu(x)\; d\mathcal{H}^2(x).$$

Proposition B.1 *Let $\tau \subset \Omega$ be open with C^2-boundary and let $\Omega\setminus\bar{\tau}$ have C^2-boundary as well. Let $M_\tau \in W^{1,2}(\tau)$ and $M_{\Omega\setminus\bar{\tau}} \in W^{1,2}(\Omega\setminus\bar{\tau})$. Then*

$$F^{(\mathrm{Br})} + \bar{F}^{(\mathrm{Br})} = 0.$$

Proof: In the following we omit d^3x and $\mathcal{H}^2(x)$ in some formulae; the domains of integration indicate which measure is meant. With Brown's force formula as stated in Theorem 2.1 and with ϕ as a shorthand for $M_\tau^- \cdot n$ one obtains

$$\begin{aligned} & F^{(\mathrm{Br})} + \bar{F}^{(\mathrm{Br})} \\ &= \int_\tau (M_\tau\cdot\nabla)H_\Omega + \frac{\gamma}{2}\int_{\partial\tau}\phi^2 n + \int_{\Omega\setminus\bar{\tau}}(M_{\Omega\setminus\bar{\tau}}\cdot\nabla)H_\Omega + \frac{\gamma}{2}\int_{\partial(\Omega\setminus\bar{\tau})}\tilde{\phi}^2\nu\; d\mathcal{H}^2 \\ &= \int_\tau(-\nabla\cdot M)H_\Omega + \int_{\partial\tau}\phi H_\Omega^- + \frac{\gamma}{2}\int_{\partial\tau}\phi^2 n + \int_{\Omega\setminus\bar{\tau}}(-\nabla\cdot M)H_\Omega + \\ &\quad + \int_{\partial\Omega}\tilde{\phi}H_\Omega^- + \int_{\partial\tau}\tilde{\phi}H_\Omega^- + \frac{\gamma}{2}\int_{\partial\Omega}\tilde{\phi}^2\nu + \frac{\gamma}{2}\int_{\partial\tau}\tilde{\phi}^2\nu, \end{aligned}$$

where we suppress the indices at M in the last equation. They are clear from the domain of integration.

To show that $F^{(\mathrm{Br})} + \bar{F}^{(\mathrm{Br})} = 0$ we use some formulae for H_Ω and H_Ω^-. In Section 3.3 these formulae are derived under the assumption that the trace of M at $\partial\Omega$ is zero. Now let u_Ω be the magnetic potential such that $H_\Omega = -\nabla u_\Omega$, which solves

$$-\Delta u_\Omega = -\gamma(\nabla\cdot M)\mathcal{L}^3\lfloor_{\tau\cup(\Omega\setminus\bar{\tau})} - \gamma[M\cdot n]\mathcal{H}^2\lfloor_{\partial\tau} + \gamma(M\cdot\nu)^-\mathcal{H}^2\lfloor_{\partial\Omega} \quad \text{in} \quad \mathbb{R}^3. \tag{B.1}$$

From this one derives similarly as in Section 3.3 for $x \in \mathbb{R}^3 \setminus \partial(\Omega \setminus \bar{\tau})$

$$\begin{aligned}
&H_\Omega(x) \\
&= \frac{\gamma}{4\pi}\Big\{ \int_{\tau \cup (\Omega \setminus \bar{\tau})} (-\nabla \cdot M)(y) \frac{x-y}{|x-y|^3}\, d^3y + \\
&\quad + \int_{\partial\tau} -[M \cdot n](y) \frac{x-y}{|x-y|^3}\, d\mathcal{H}^2(y) + \int_{\partial\Omega} (M \cdot \nu)^-(y) \frac{x-y}{|x-y|^3}\, d\mathcal{H}^2(y) \Big\} \\
&=: \mathcal{A} + \mathcal{B} + \mathcal{C}.
\end{aligned}$$

If $x \in \partial\Omega$, one obtains analogously to (3.19)

$$\begin{aligned}
H_\Omega^\pm(x) &= \mathcal{A} + \mathcal{B} + \underbrace{\lim_{\epsilon \to 0} \frac{\gamma}{4\pi} \int_{\partial\Omega} \eta(\frac{|x-y|}{\epsilon})(M \cdot \nu)^-(y) \frac{x-y}{|x-y|^3}\, d\mathcal{H}^2(y) +}_{=:\mathcal{D}} \\
&\quad \pm \frac{\gamma}{2}(M \cdot \nu)^- \nu.
\end{aligned}$$

If $x \in \partial\tau$, the traces of the magnetic field of the whole body Ω are given by

$$\begin{aligned}
H_\Omega^\pm(x) &= \mathcal{A} + \underbrace{\lim_{\epsilon \to 0} \frac{\gamma}{4\pi} \int_{\partial\tau} \eta(\frac{|x-y|}{\epsilon})(-1)[M \cdot n](y) \frac{x-y}{|x-y|^3}\, d\mathcal{H}^2(y)}_{=:\mathcal{E}} + \mathcal{C} + \\
&\quad \pm \frac{\gamma}{2}(-1)[M \cdot n] n.
\end{aligned}$$

Recall that $\phi = (M \cdot n)^-$ and $\tilde{\phi} = (M \cdot \nu)^- = -(M \cdot n)^+$ on $\partial\tau$. One has $[M \cdot n] = (M \cdot n)^+ - (M \cdot n)^- = -(M \cdot \nu)^- - (M \cdot n)^-$. Inserting all these equations into $F^{(\mathrm{Br})} + \bar{F}^{(\mathrm{Br})}$ and using as before Fubini's Theorem and uniform convergence one obtains

$$\begin{aligned}
&F^{(\mathrm{Br})} + \bar{F}^{(\mathrm{Br})} \\
&= \int_{\tau \cup (\Omega \setminus \bar{\tau})} (-\nabla \cdot M)\{\mathcal{A} + \mathcal{B} + \mathcal{C}\} + \int_{\partial\tau} (M \cdot n)^- \{\mathcal{A} + \mathcal{E} + \mathcal{C}\} + \\
&\quad + \frac{\gamma}{2} \int_{\partial\tau} (M \cdot n)^- [M \cdot n] n + \frac{\gamma}{2} \int_{\partial\tau} (M^- \cdot n)^2 n + \\
&\quad + \int_{\partial\Omega} (M \cdot \nu)^- \{\mathcal{A} + \mathcal{B} + \mathcal{D}\} - \frac{\gamma}{2} \int_{\partial\Omega} (M^- \cdot \nu)^2 \nu + \\
&\quad + \int_{\partial\tau} (M \cdot \nu)^- \{\mathcal{A} + \mathcal{E} + \mathcal{C}\} - \frac{\gamma}{2} \int_{\partial\tau} (M \cdot \nu)^- [M \cdot n] n + \\
&\quad + \frac{\gamma}{2} \int_{\partial\Omega} (M^- \cdot \nu)^2 \nu + \frac{\gamma}{2} \int_{\partial\tau} (M^- \cdot \nu)^2 \nu \\
&= \int_{\tau \cup (\Omega \setminus \bar{\tau})} (-\nabla \cdot M) \mathcal{B} + \int_{\partial\tau} -[M \cdot n]\{\mathcal{A} + \mathcal{E} + \mathcal{C}\} + \frac{\gamma}{2} \int_{\partial\Omega} (M \cdot \nu) \mathcal{B} \\
&= 0.
\end{aligned}$$

Hence Brown's force formula satisfies Newton's law of actio equals reactio. □

We now verify Newton's law for the limiting force. Suppose that $\Omega \setminus \bar{\tau}$, Ω and M satisfy analogous assumptions to those in Theorem 3.7. (As in Chapter 5 we write M instead of m to unify notation with that in Brown's formula.) Then the reactio limiting force reads

$$\begin{aligned}\bar{F}^{(\mathrm{lim})} &= \int_{\Omega\setminus\bar{\tau}} (M(x)\cdot\nabla)(H_\Omega)_k(x)\,d^3x + \\ &\quad + \frac{\gamma}{2}\int_{\partial(\Omega\setminus\bar{\tau})} (M^-\cdot\nu)(x)\big((M^- - M^+)\cdot\nu\big)(x)\nu_k(x)\,d\mathcal{H}^2(x) + \\ &\quad + \frac{1}{2}\int_{\partial(\Omega\setminus\bar{\tau})} M_i^-(x)M_j^+(x)S_{ijkp}\nu_p(x)\,d\mathcal{H}^2(x).\end{aligned}$$

Proposition B.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 τ and $\Omega \setminus \bar{\tau}$ have C^2-boundaries and that $\partial\tau$ and $\partial\Omega$ satisfy the non-degeneracy condition (S). Further let M belong to $W^{1,\infty}(\tau)$ and $W^{1,\infty}(\Omega\setminus\bar{\tau})$. Then*

$$F^{(\mathrm{lim})} + \bar{F}^{(\mathrm{lim})} = 0. \tag{B.2}$$

Proof: For the limit of the long range part of the discrete force (Theorem 3.1) one can show (B.2) similarly to the calculations in the proof of Proposition B.1. The additional surface term in the limiting force, $\int_{\partial\tau}(M^-\cdot n)(M^+\cdot n)n$, is contained analogously in the reactio term and thus cancels.

For the discussion of the term of the limiting force which comes from the short range part (Theorem 3.6) we denote the traces with respect to $\Omega\setminus\bar{\tau}$ by the superscripts $\nu^\pm$ and the traces with respect to τ by the superscripts $n^\pm$. One then has

$$\begin{aligned}&\frac{1}{2}\int_{\partial(\Omega\setminus\bar{\tau})} M_i^{\nu^-}(x)M_j^{\nu^+}(x)S_{ijkp}\nu_p(x)\,d\mathcal{H}^2(x)\\ &= \frac{1}{2}\int_{\partial\tau} M_i^{\nu^-}(x)M_j^{\nu^+}(x)S_{ijkp}\nu_p(x)\,d\mathcal{H}^2(x)\\ &= \frac{1}{2}\int_{\partial\tau} M_i^{n^+}(x)M_j^{n^-}(x)S_{ijkp}(-1)n_p(x)\,d\mathcal{H}^2(x)\\ &= -\frac{1}{2}\int_{\partial\tau} M_i^{n^-}(x)M_j^{n^+}(x)S_{ijkp}n_p(x)\,d\mathcal{H}^2(x),\end{aligned}$$

where the last equality follows since there is a sum over all $i = 1,2,3$ and $j = 1,2,3$ hidden in the formula by the summation convention. The last term is the negative of the short range term of the actio limiting force. Hence actio equals reactio holds also for the limiting force. □

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