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Discrete-to-continuum limits of magnetic forces  
in dependence on the distance between bodies

by

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# Discrete-to-continuum limits of magnetic forces in dependence on the distance between bodies

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## Abstract

We investigate force formulae for two rigid magnetic bodies in dependence on their mutual distance. These formulae are derived as continuum limits of atomistic dipole-dipole interactions. For bodies that are far apart in terms of the typical lattice spacing we recover a classical formula for magnetic forces. For bodies whose distance is comparable to the atomistic lattice spacing, however, we discover a new term that explicitly depends on the distance, measured in atomic units, and the underlying crystal lattice structure. This new term links the classical force formula and a limiting force formula obtained earlier in the case of two bodies being in contact on the atomistic scale.

## 1 Introduction

Multiscale models of materials have recently attracted a lot of interest in the engineering and mathematical literature. Many interesting phenomena in materials science can be understood only when taking into account effects that are due to an intricate interplay between various models at different length scales. To understand such behavior better one relates the models at different scales. In particular, bridging the scales from atomistic models to continuum theory is an

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active area of research. In this article we consider discrete-to-continuum limits for magnetic forces.

Formulae for the magnetic force between rigid magnetic bodies in contact have been under discussion for quite some time, cf. [Bro66, DPG96, Dör68, EM90] and in particular [Bob00]. All those formulae are obtained from models in a continuum setting, i.e. from a macroscopic point of view. This neglects contributions to the force from dipoles close to the interface of the bodies as was already pointed out by W.F. Brown [Bro66, p. 53] and mathematically studied in [MS02, Sch05, PPSa, PPSb]. In these studies a lattice of magnetic dipole moments is considered and the discrete-to-continuum limit of the force between two connected parts of the lattice is calculated, which yields an additional lattice-dependent force term, called  $\mathbf{F}^{\text{short}}$ .

Whereas the discrete-to-continuum results in [Sch05] and [PPSa] deal with the discussion of magnetic forces between bodies being in contact on the lattice as well as on the macroscopic scale, the main focus of the present paper is to study the discrete-to-continuum limit of the magnetic force formula in various distance regimes between two bodies being separated on the scale of the lattice, but being in contact on the macroscopic scale. It turns out that the previous results have to be extended by an additional term that depends on the microscopic distance and reflects the discrete nature of the underlying atomic lattice, cf. Section 3, in particular Theorem 3.4.

More precisely, suppose the lattice spacing is equal to  $\ell^{-1}$ ,  $\ell \in \mathbb{N}$ , and consider two bodies (sets of lattice points) whose mutual distance is given by  $\varepsilon = \frac{a}{\ell}$ , where  $a$  is a measure for the microscopic distance in terms of atomistic units. We study the discrete-to-continuum limit for magnetic forces for fixed  $a \in \mathbb{N}$  in detail in Section 3. As  $\ell \rightarrow \infty$ ,  $\varepsilon$  tends to 0 and thus the macroscopic distance between the two bodies vanishes, i.e., the bodies are macroscopically in contact.

For  $a = 0$  we recover the discrete-to-continuum formula  $\mathbf{F}^{\text{lim}}$  derived in [Sch05, PPSa]. For  $a > 0$  we obtain an additional  $a$ -dependent term, which has not been included in any force formula so far and which might be particularly interesting with regard to nanoscale experiments. In Example 4.4 we prove that this additional term decreases exponentially in  $a$  and give some numerical values.

In Section 4 we discuss properties of the additional  $a$ -dependent force term. In particular we study the limit as  $a \rightarrow \infty$ , which corresponds to two bodies that are in contact on the macroscale but are infinitely far apart on the microscale. It turns out (Theorem 4.3) that the force converges to a force formula which was extensively analyzed by Brown [Bro66] in the continuum setting and which is called Brown's formula  $\mathbf{F}^{\text{Br}}$  for short in the following, cf. (24). In other words,

we give a discrete-to-continuum derivation for  $\mathbf{F}^{\text{Br}}$ . Thereby we flesh out a claim by Brown [Bro66, p. 53] who expected—phrased in the notions of our multi-scale setting—that the force contribution from dipole-dipole interactions close to the (macroscopic) interface decreases rapidly as the (microscopic) distance between the bodies increases.

Furthermore we study the case  $a \sim \ell$ , which corresponds to two bodies being microscopically as well as macroscopically separated. This case yields a classical well-known force formula for separated bodies as  $\ell \rightarrow \infty$ , see Proposition 5.1.

To give a complete multiscale picture of all the possible distance regimes, we also include a study in which the micro-distance  $a = a(\ell)$  scales with  $\ell$  such that  $1 \ll a(\ell) \ll \ell$  (Section 5.2).

In Section 6 we summarize the force formulae obtained for the different scaling regimes in a table. The question arises which formula one should work with in applications if the distance between the bodies is small. To answer this question, one needs to know which scaling regime models the physical situation considered best. The numerical experiments in [PPSb] as well as related real-life experiments [Eim06] will hopefully yield further insight into this issue.

## 2 Preliminaries

Our discrete-to-continuum calculations start from an underlying Bravais lattice  $\mathcal{L}$  of magnetic dipole moments. We sometimes regard the lattice points as atoms. A precise definition of  $\mathcal{L}$  is as follows:  $\mathcal{L} = \{x \in \mathbb{R}^d \mid x = \sum_{i=1}^d \mu_i \mathbf{e}_i, \mu_i \in \mathbb{Z}\}$ , where  $\mathbf{e}_1, \dots, \mathbf{e}_d$  is a basis of  $\mathbb{R}^d$ ,  $d \geq 2$ . For definiteness we suppose that the unit cell  $\{x \in \mathbb{R}^d \mid x = \sum_{i=1}^d \lambda_i \mathbf{e}_i, \lambda_i \in [0, 1)\}$  has volume one. For instance,  $\mathcal{L} = \mathbb{Z}^d$ . In order to pass from the discrete model to the continuum, we consider the scaled Bravais lattice  $\frac{1}{\ell} \mathcal{L} = \{z \in \mathbb{R}^d \mid \ell z \in \mathcal{L}\}$ , for  $\ell \in \mathbb{N}$ .

In Figure 1 we give an example for the domains considered in the following assumption.

**Assumption  $\mathcal{A}$ .** Let  $d \in \mathbb{N}$  be fixed.

1.  $A$  and  $B$  are bounded Lipschitz domains in  $\mathbb{R}^d$ .  $A$  and  $B$  have polygonal boundaries and finitely many corners or edges such that  $A \cap B = \emptyset$ . Moreover,  $A$  and  $B$  are in contact, i.e., the surface measure of  $\partial A \cap \partial B \subset \partial A$  is positive. The set

$$B_\varepsilon = B + \varepsilon \nu, \tag{1}$$

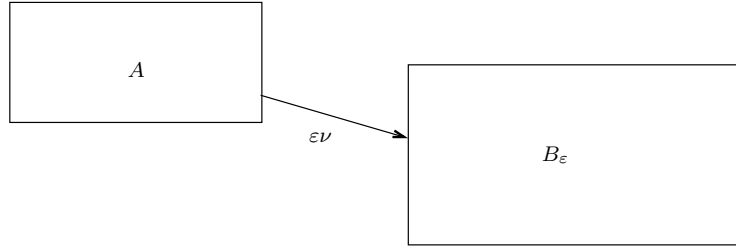


Figure 1: Sketch of the sets  $A$  and  $B_\varepsilon$ .

where  $\nu \in \mathcal{L}$  is fixed and  $\varepsilon = \frac{a}{\ell}$  with  $a \in \mathbb{N}$ , satisfies  $\overline{A} \cap \overline{B_\varepsilon} = \emptyset$  for all  $\varepsilon > 0$ .

2. The corresponding magnetizations  $\mathbf{m}_A : A \rightarrow \mathbb{R}^d$  and  $\mathbf{m}_B : B \rightarrow \mathbb{R}^d$  are Lipschitz continuous and are supported on  $\overline{A}$  and  $\overline{B}$ , respectively, i.e., there holds  $\mathbf{m}_A \in W^{1,\infty}(A)$  and  $\mathbf{m}_B \in W^{1,\infty}(B)$ . Moreover, the magnetization  $\mathbf{m}_{B_\varepsilon} : B_\varepsilon \rightarrow \mathbb{R}^d$  satisfies

$$\mathbf{m}_{B_\varepsilon}(x) = \mathbf{m}_B(x - \varepsilon\nu) \quad \text{for all } x \in B_\varepsilon. \quad (2)$$

All magnetization fields are extended by zero to the entire space  $\mathbb{R}^d$ .

Later we will use the following implication of the above assumptions: Let  $\mathbf{n}_A$  denote the outer normal to  $\partial A$ . Then  $\mathbf{n}_A(x) \cdot \nu > 0$  for all  $x \in \partial A \cap \partial B$  (if  $\mathbf{n}_A$  exists).

Assumption  $\mathcal{A}$  is natural in view of applications. However, in Remark 1, we briefly indicate how the assumptions on the domains can be relaxed.

The magnetization is related to the magnetic dipole moments on the lattice points of  $\frac{1}{\ell}\mathcal{L}$  through the scaling law

$$\mathbf{m}_A^{(\ell)}(x) := \frac{1}{\ell^d} \mathbf{m}_A(x) \text{ if } x \in A \cap \frac{1}{\ell}\mathcal{L}, \quad \mathbf{m}_{B_\varepsilon}^{(\ell)}(x) := \frac{1}{\ell^d} \mathbf{m}_{B_\varepsilon}(x) \text{ if } x \in B_\varepsilon \cap \frac{1}{\ell}\mathcal{L}. \quad (3)$$

The  $k$ th component of the magnetic force that all dipole moments in  $B_\varepsilon$  exert on all dipole moments in  $\overline{A}$  is given by (see e.g. [Sch05])

$$\mathbf{F}_k^{(\ell)}(A, B) := \gamma \sum_{x \in \overline{A} \cap \frac{1}{\ell}\mathcal{L}} \sum_{y \in B_\varepsilon \cap \frac{1}{\ell}\mathcal{L}} \partial_i \partial_j \partial_k N(x - y) (\mathbf{m}_A^{(\ell)})_i(x) (\mathbf{m}_{B_\varepsilon}^{(\ell)})_j(y), \quad (4)$$

where  $\gamma$  is a constant which only depends on the choice of physical units. For instance,  $\gamma = 4\pi$  in Gaussian units, cf. [Bro66, p. 6]. Note that we use the Einstein summation convention, i.e., the above expression contains sums over  $i, j = 1, \dots, d$  as these indices occur twice. The function  $N$  denotes the fundamental solution of Laplace's equation, which is given by

$$N(x) := \begin{cases} -\frac{1}{2\pi} \log |x| & \text{for } d = 2, \\ \frac{\Gamma(\frac{d}{2})}{(d-2)2\pi^{d/2}} |x|^{2-d} & \text{for } d \geq 3, \end{cases}$$

where  $\Gamma(\cdot)$  denotes the Gamma-function. In particular,  $N(x) = \frac{1}{4\pi} \frac{1}{|x|}$  for  $d = 3$ .

Let  $\varphi$  be a smooth, radially symmetric function such that

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

and, for  $\varphi^{(\delta)}(z) := \varphi(z/\delta)$ , set

$$\begin{aligned} P_k^{(\delta)}(x-y) &:= \begin{cases} (\varphi^{(\delta)} \partial_k N)(x-y) & \text{for } d = 2, \\ \partial_k (\varphi^{(\delta)} N)(x-y) & \text{for } d \geq 3, \end{cases} \\ R_k^{(\delta)}(x-y) &:= \begin{cases} ((1 - \varphi^{(\delta)}) \partial_k N)(x-y) & \text{for } d = 2, \\ \partial_k ((1 - \varphi^{(\delta)}) N)(x-y) & \text{for } d \geq 3. \end{cases} \end{aligned} \quad (5)$$

Note that  $P_k^{(\delta)}$  is zero if  $|x-y|$  is greater than  $\delta$ , whereas  $R_k^{(\delta)}$  is zero if  $|x-y| < \delta/2$ . Since  $P_k^{(\delta)}(x-y) + R_k^{(\delta)}(x-y) = \partial_k N(x-y)$ , we can use these functions to split  $\mathbf{F}^{(\ell)}$  into a so-called long range part and a so-called short range part:

$$\begin{aligned} \mathbf{F}_k^{(\ell)}(A, B_\varepsilon) &= \gamma \sum_{x \in \bar{A} \cap \frac{1}{\ell} \mathcal{L}} \sum_{y \in B_\varepsilon \cap \frac{1}{\ell} \mathcal{L}} \partial_i \partial_j R_k^{(\delta)}(x-y) (\mathbf{m}_A^{(\ell)})_i(x) (\mathbf{m}_{B_\varepsilon}^{(\ell)})_j(y) \\ &\quad + \gamma \sum_{x \in \bar{A} \cap \frac{1}{\ell} \mathcal{L}} \sum_{y \in B_\varepsilon \cap \frac{1}{\ell} \mathcal{L}} \partial_i \partial_j P_k^{(\delta)}(x-y) (\mathbf{m}_A^{(\ell)})_i(x) (\mathbf{m}_{B_\varepsilon}^{(\ell)})_j(y) \\ &=: \mathbf{F}_k^{\text{long}(\ell, \delta)}(A, B_\varepsilon) + \mathbf{F}_k^{\text{short}(\ell, \delta)}(A, B_\varepsilon). \end{aligned} \quad (6)$$

This allows us to compute the continuum limit of  $\mathbf{F}^{(\ell)}$  as follows:

$$\begin{aligned} \mathbf{F}^{\text{lim}}(A, B, a) &:= \lim_{\ell \rightarrow \infty} \mathbf{F}^{(\ell)}(A, B_\varepsilon) \\ &= \lim_{\delta \rightarrow 0} \lim_{\ell \rightarrow \infty} \mathbf{F}^{\text{long}(\ell, \delta)}(A, B_\varepsilon) + \lim_{\delta \rightarrow 0} \lim_{\ell \rightarrow \infty} \mathbf{F}^{\text{short}(\ell, \delta)}(A, B_\varepsilon) \\ &=: \mathbf{F}^{\text{long}}(A, B, a) + \mathbf{F}^{\text{short}}(A, B, a), \end{aligned} \quad (7)$$

given that the limits of  $\mathbf{F}^{\text{long}(\ell,\delta)}(A, B_\varepsilon)$  and  $\mathbf{F}^{\text{short}(\ell,\delta)}(A, B_\varepsilon)$  exist, see below. Note  $\varepsilon \rightarrow 0$  in the continuum limit as  $\ell \rightarrow \infty$ . However, we expect/obtain that the continuum limit of the force depends on  $a$ .

For later reference we quote a formula for the magnetic field,  $\mathbf{H}_B$ . The magnetic field is a solution of the magnetostatic Maxwell equations  $\text{curl } \mathbf{H}_B = 0$  and  $\text{div } \mathbf{B}_B = 0$  with  $\mathbf{B}_B = \mathbf{H}_B + \gamma \mathbf{m}_B$ . By setting  $\mathbf{H}_B = -\nabla \phi_B$ ,  $\phi_B : \mathbb{R}^d \rightarrow \mathbb{R}$ , these equations can be written in form of a Poisson equation  $\text{div}(-\nabla \phi_B + \gamma \mathbf{m}_B) = 0$  with transition conditions  $[\nabla \phi_B \cdot \mathbf{n}_B] = -\gamma \mathbf{m}_B \cdot \mathbf{n}_B$  and  $[\phi_B] = 0$  on  $\partial B$ , where  $\mathbf{n}_B$  denotes the outer normal to  $\partial B$ . If  $x \notin \partial B$ , an integral representation of  $\mathbf{H}_B$  reads (cf. e.g. [ES98, p. 73])

$$\mathbf{H}_B(x) = -\gamma \int_B (-\nabla \cdot \mathbf{m}_B)(y) \nabla N(x-y) dy - \gamma \int_{\partial B} (\mathbf{m}_B \cdot \mathbf{n}_B)(y) \nabla N(x-y) ds_y, \quad (8)$$

where  $s_y$  denotes the  $d-1$  dimensional surface measure on  $\partial B$ . The magnetic field  $H_{A \cup B}$  generated by the magnetization in  $A$  and  $B$  is defined and can be represented similarly.

### 3 The discrete-to-continuum limit of the magnetic force

The following proposition on the long range part of the force is proven in [PPSa] in the case  $a = 0$ , to which the case  $a > 0$  can be reduced, cf. the proof below. The long range part of the magnetic interaction turns out to be independent of  $a$ .

**Proposition 3.1.** *Let Assumption  $\mathcal{A}$  hold. Then the limit  $\lim_{\delta \rightarrow 0} \lim_{\ell \rightarrow \infty} \mathbf{F}^{\text{long}(\ell,\delta)}(A, B_\varepsilon)$  exists, is independent of  $a$  and satisfies*

$$\mathbf{F}^{\text{long}}(A, B) = \int_A (\mathbf{m}_A \cdot \nabla) \mathbf{H}_{A \cup B} dx + \frac{\gamma}{2} \int_{\partial A} (\mathbf{m}_A \cdot \mathbf{n}_A) ((\mathbf{m}_A - \mathbf{m}_B) \cdot \mathbf{n}_A) \mathbf{n}_A ds_x. \quad (9)$$

Here,  $\mathbf{m}_B$  denotes the outer trace on  $\partial A$  with respect to  $A$ , i.e.,  $\mathbf{m}_B$  is equal to zero on  $\partial A \setminus (\partial A \cap \partial B)$  and equals the inner trace of  $\mathbf{m}_B$  on  $\partial A \cap \partial B$  with respect to  $B$ .



*Proof.* By definition (6) and (2),

$$\begin{aligned}
& \mathbf{F}^{\text{long}(\ell, \delta)}(A, B_\varepsilon) \\
&= \gamma \sum_{x \in \bar{A} \cap \frac{1}{\ell} \mathcal{L}} \sum_{y \in B_\varepsilon \cap \frac{1}{\ell} \mathcal{L}} \partial_i \partial_j R_k^{(\delta)}(x-y) (\mathbf{m}_A^{(\ell)})_i(x) (\mathbf{m}_{B_\varepsilon}^{(\ell)})_j(y) \\
&= \gamma \sum_{x \in \bar{A} \cap \frac{1}{\ell} \mathcal{L}} \sum_{y \in B_\varepsilon \cap \frac{1}{\ell} \mathcal{L}} \partial_i \partial_j R_k^{(\delta)}(x-y) (\mathbf{m}_A^{(\ell)})_i(x) \left( (\mathbf{m}_B^{(\ell)})_j(y - \varepsilon \nu) - (\mathbf{m}_B^{(\ell)})_j(y) \right) \\
&\quad + \gamma \sum_{x \in \bar{A} \cap \frac{1}{\ell} \mathcal{L}} \sum_{y \in B_\varepsilon \cap \frac{1}{\ell} \mathcal{L}} \partial_i \partial_j R_k^{(\delta)}(x-y) (\mathbf{m}_A^{(\ell)})_i(x) (\mathbf{m}_B^{(\ell)})_j(y).
\end{aligned} \tag{10}$$

Since  $\mathbf{m}$  is bounded and Lipschitz continuous on  $B$ , the first term on the right hand side can be estimated as follows:

$$\begin{aligned}
& \left| \sum_{x \in \bar{A} \cap \frac{1}{\ell} \mathcal{L}} \sum_{y \in B_\varepsilon \cap \frac{1}{\ell} \mathcal{L}} \partial_i \partial_j R_k^{(\delta)}(x-y) (\mathbf{m}_A^{(\ell)})_i(x) \left( (\mathbf{m}_B^{(\ell)})_j(y - \varepsilon \nu) - (\mathbf{m}_B^{(\ell)})_j(y) \right) \right| \\
&\leq C(\delta) \sum_{x \in \bar{A} \cap \frac{1}{\ell} \mathcal{L}} \ell^{-d} \sum_{y \in B_\varepsilon \cap \frac{1}{\ell} \mathcal{L}} \left| (\mathbf{m}_B^{(\ell)})_j(y - \varepsilon \nu) - (\mathbf{m}_B^{(\ell)})_j(y) \right| \\
&\leq C(\delta) \left( \sum_{y \in B_\varepsilon \cap B \cap \frac{1}{\ell} \mathcal{L}} \ell^{-d} \varepsilon + \sum_{y \in (B_\varepsilon \setminus B) \cap \frac{1}{\ell} \mathcal{L}} \ell^{-d} \right) \\
&\leq C(\delta) \left( \varepsilon + \ell^{-d} \# \left\{ (B_\varepsilon \setminus B) \cap \frac{1}{\ell} \mathcal{L} \right\} \right).
\end{aligned}$$

An application of the following Lemma 3.2 with  $z = \varepsilon \nu = \frac{\alpha}{\ell} \nu$  shows that this term converges to 0 as  $\ell \rightarrow \infty$ .

**Lemma 3.2.** *For  $z \in \mathbb{R}^d$  with  $|z| \geq \tilde{c} \ell^{-1}$  there is a constant  $C$  only depending on  $\tilde{c}$  and  $B$  such that*

$$\# \left\{ ((B+z) \Delta B) \cap \frac{1}{\ell} \mathcal{L} \right\} \leq C |z| \ell^d.$$

*Proof.* This is an immediate consequence of Assumption  $\mathcal{A}$  since all the elements of the set on the left hand side of the above inequality lie in a  $z$ -neighborhood of  $\partial B$ .  $\square$

Since replacing  $B_\varepsilon$  by  $B$  in the second term of the right hand side of (10) leads to an error term of order  $\ell^{-d} \# \{ (B \setminus B_\varepsilon) \cap \frac{1}{\ell} \mathcal{L} \}$  because  $\mathbf{m}_B^{(\ell)}$  vanishes on the

complement of  $B$ , another application of Lemma 3.2 with  $z = \varepsilon\nu = \frac{a}{\ell}\nu$  shows that in fact

$$\lim_{\ell \rightarrow \infty} \mathbf{F}^{\text{long}(\ell, \delta)}(A, B_\varepsilon) = \lim_{\ell \rightarrow \infty} \mathbf{F}^{\text{long}(\ell, \delta)}(A, B).$$

In particular this is independent of  $a$ . An application of Theorem 3.3 in [PPSa], which is based on [Scha, Theorem 13] hence yields the assertion.  $\square$

Contrary to the long range part, the short range contribution  $\mathbf{F}^{\text{short}}$  to the limit force does depend on  $a$ .

**Proposition 3.3.** *Let Assumption  $\mathcal{A}$  hold. Then the limit  $\mathbf{F}^{\text{short}}(A, B, a) := \lim_{\delta \rightarrow 0} \lim_{\ell \rightarrow \infty} \mathbf{F}^{\text{short}(\ell, \delta)}(A, B_\varepsilon)$  exists and is given by*

$$\begin{aligned} \mathbf{F}_k^{\text{short}}(A, B, a) &= \frac{1}{2} \sum_{i,j,p=1}^d S_{ijkp} \int_{\partial A \cap \partial B} (\mathbf{m}_A)_i(x) (\mathbf{m}_B)_j(x) (\mathbf{n}_A)_p(x) ds_x \\ &\quad - \gamma \int_{\partial A \cap \partial B} (\mathbf{m}_A)_i(x) (\mathbf{m}_B)_j(x) \times \\ &\quad \times \sum_{z \in \mathcal{L} \setminus \{0\}} \partial_i \partial_j \partial_k N(z) ((\mathbf{n}_A(x) \cdot (z - a\nu))_+ - (\mathbf{n}_A(x) \cdot z)_+) ds_x \end{aligned} \quad (11)$$

for  $k = 1, \dots, d$ , where  $\mathbf{m}_B$  is the outer trace of  $\mathbf{m}_B$  on  $\partial A$  with respect to  $A$  and

$$S_{ijkp} := -\gamma \lim_{\delta \rightarrow 0} \lim_{\ell \rightarrow \infty} \sum_{z \in B_\delta(0) \cap \frac{1}{\ell} \mathcal{L} \setminus \{0\}} (\partial_i \partial_j P_k^{(\delta)}(z)) z_p \frac{1}{\ell^d}. \quad (12)$$

The first term in (11) equals  $\mathbf{F}_k^{\text{short}}(A, B)$ , the short range formula that was obtained in [PPSa, Theorem 3.4] in the case of  $\varepsilon = 0$ , see also [Sch05, Theorem 2]. Numerical values of  $S_{ijkp}$  are given for the square/cubic lattice  $\mathcal{L} = \mathbb{Z}^d$  in  $d = 2$  [PPSa, Appendix A] and  $d = 3$  [Sch05, Section 6.1] dimensions. We denote the second, new term in (11), which is also a surface integral about the interface of  $A$  and  $B$ , by  $\mathbf{G}_k(a)$  and thus have

$$\mathbf{F}^{\text{short}}(A, B, a) = \mathbf{F}^{\text{short}}(A, B) + \mathbf{G}(a),$$

where  $\mathbf{G}(a) = (\mathbf{G}_1(a), \dots, \mathbf{G}_d(a))$ . Moreover, we observe that  $\mathbf{G}(0) = 0$ , i.e.,  $\mathbf{F}^{\text{short}}(A, B, 0) = \mathbf{F}^{\text{short}}(A, B)$ . For more properties of the additional term  $\mathbf{G}(a)$ , see Section 4.

Propositions 3.1 and 3.3 imply

**Theorem 3.4.** *Let Assumption  $\mathcal{A}$  hold. Then*

$$\mathbf{F}^{\text{lim}}(A, B, a) = \mathbf{F}^{\text{long}}(A, B) + \mathbf{F}^{\text{short}}(A, B) + \mathbf{G}(a).$$

*Proof of Proposition 3.3.* Recall the definition of  $\mathbf{F}_k^{\text{short}(\ell, \delta)}(A, B_\varepsilon)$  in (6). Similarly to [Sch05, p. 233], we reorganize the sums in order to get rid of the hyper-singular order of the kernel  $\partial_i \partial_j P_k^{(\delta)}(x - y)$ ; set  $z = y - x$  and note that  $z \in \frac{1}{\ell} \mathcal{L}$  by our assumptions,  $P_k^{(\delta)}(-z) = -P_k^{(\delta)}(z)$  and  $P_k^{(\delta)}(z)$  is supported on  $B_\delta(0)$ . We thus obtain

$$\begin{aligned} \mathbf{F}_k^{\text{short}(\ell, \delta)}(A, B_\varepsilon) &= \gamma \sum_{x \in \bar{A} \cap \frac{1}{\ell} \mathcal{L}} \sum_{y \in B_\varepsilon \cap \frac{1}{\ell} \mathcal{L}} \partial_i \partial_j P_k^{(\delta)}(x - y) (\mathbf{m}_A^{(\ell)})_i(x) (\mathbf{m}_{B_\varepsilon}^{(\ell)})_j(y) \\ &= \gamma \sum_{x \in \bar{A} \cap \frac{1}{\ell} \mathcal{L}} \sum_{\substack{z \in B_\delta(0) \cap \frac{1}{\ell} \mathcal{L} \setminus \{0\} \\ x+z \in B_\varepsilon}} \partial_i \partial_j P_k^{(\delta)}(-z) (\mathbf{m}_A^{(\ell)})_i(x) (\mathbf{m}_{B_\varepsilon}^{(\ell)})_j(x+z) \\ &= -\gamma \sum_{z \in B_\delta(0) \cap \frac{1}{\ell} \mathcal{L} \setminus \{0\}} \partial_i \partial_j P_k^{(\delta)}(z) \sum_{x \in A_z^\varepsilon \cap \frac{1}{\ell} \mathcal{L}} (\mathbf{m}_A^{(\ell)})_i(x) (\mathbf{m}_{B_\varepsilon}^{(\ell)})_j(x+z), \end{aligned} \quad (13)$$

where  $A_z^\varepsilon := \{x \in \bar{A} \mid x + z \in B_\varepsilon\}$ , which satisfies, by (1),

$$A_z^\varepsilon = \bar{A} \cap (B_\varepsilon - z) = \bar{A} \cap (B - (z - \varepsilon\nu)) =: A_{z - \varepsilon\nu}.$$

Since  $(\mathbf{m}_{B_\varepsilon}^{(\ell)})_j(x+z) = (\mathbf{m}_B^{(\ell)})_j(x+z - \varepsilon\nu)$ , cf. (2), we can apply a slightly varied version of Proposition 1 in [Schb], which is based on an idea of Cauchy [Cau90] developed for the discrete-to-continuum limit of elastic forces:

**Lemma 3.5.** *Let  $A$  and  $B$  satisfy Assumption  $\mathcal{A}$  and assume  $f : A_{z - \varepsilon\nu} \rightarrow \mathbb{R}$  to be Lipschitz continuous. Let  $0 < \delta \ll 1$  and  $z \in B_\delta(0) \cap \frac{1}{\ell} \mathcal{L} \setminus \{0\}$ . Then there exists an  $\ell_0 \in \mathbb{N}$  such that for all  $\ell \geq \ell_0$*

$$\left| \frac{1}{\ell^d} \sum_{x \in A_{z - \varepsilon\nu} \cap \frac{1}{\ell} \mathcal{L} \setminus \{0\}} f(x) - \int_{\partial A \cap \partial B} f(x) (\mathbf{n}_A(x) \cdot (z - \varepsilon\nu))_+ ds_x \right| \leq C|z|^{\frac{4}{3}}. \quad (14)$$

Here,  $(\cdot)_+ := \max\{0, \cdot\}$ , and the constants  $C$  and  $\ell_0$  only depend on  $\sup(f)$ , on the Lipschitz constant of  $f$ , on  $a$ , the dimension  $d$  and on the geometries of  $A$  and  $B$ .

*Proof.* Since  $|z| \geq \frac{\tilde{c}}{\ell}$  for some  $\tilde{c} > 0$  by assumption and  $|\varepsilon\nu| = \frac{a}{\ell}|\nu|$ , we have  $|z - \varepsilon\nu| \leq c|z|$ . Moreover, for  $\ell_0$  large enough we obtain  $z - \varepsilon\nu \in B_{2\delta}(0) \cap \frac{1}{\ell} \mathcal{L} \setminus \{0\}$ .

We can thus apply [Schb, Proposition 1] with  $z$  replaced with  $z - \varepsilon\nu$ , which yields

$$\left| \frac{1}{\ell^d} \sum_{x \in A_{z-\varepsilon\nu} \cap \frac{1}{\ell} \mathcal{L} \setminus \{0\}} f(x) - \int_{\partial A \cap \partial B} f(x) (\mathbf{n}_A(x) \cdot (z - \varepsilon\nu))_+ ds_x \right| \leq C |z - \varepsilon\nu|^{\frac{4}{3}}$$

and hence (14).  $\square$

With  $f(x) = (\mathbf{m}_A)_i(x) (\mathbf{m}_{B_\varepsilon})_j(x + z) = (\mathbf{m}_A)_i(x) (\mathbf{m}_B)_j(x + z - \varepsilon\nu)$ , which is Lipschitz continuous on  $A_{z-\varepsilon\nu}$  by assumption, we obtain

$$\begin{aligned} & \mathbf{F}_k^{\text{short}(\ell, \delta)}(A, B_\varepsilon) \\ &= -\gamma \sum_{z \in B_\delta(0) \cap \frac{1}{\ell} \mathcal{L} \setminus \{0\}} \partial_i \partial_j P_k^{(\delta)}(z) \frac{1}{\ell^d} \int_{\partial A \cap \partial B} (\mathbf{m}_A)_i(x) (\mathbf{m}_B)_j(x) (\mathbf{n}_A(x) \cdot (z - \varepsilon\nu))_+ ds_x \end{aligned} \quad (15)$$

up to terms of higher order. The terms of higher order converge to zero as  $\ell \rightarrow \infty$  and  $\delta \rightarrow 0$ , cf. e.g. [PPSa, Proof of Theorem 3.4].

Next we add and subtract  $(\mathbf{n}_A \cdot z)_+$  in (15). This yields another term discussed below

$$-\gamma \sum_{z \in B_\delta(0) \cap \frac{1}{\ell} \mathcal{L} \setminus \{0\}} \partial_i \partial_j P_k^{(\delta)}(z) \frac{1}{\ell^d} \int_{\partial A \cap \partial B} (\mathbf{m}_A)_i(x) (\mathbf{m}_B)_j(x) (\mathbf{n}_A(x) \cdot z)_+ ds_x,$$

which is the same as in [PPSa, (3.25)] and thus can be estimated accordingly. It converges to

$$\mathbf{F}^{\text{short}}(A, B) := \frac{1}{2} \sum_{i,j,p=1}^d (S_{ij1p}, \dots, S_{ijd p}) \int_{\partial A \cap \partial B} (\mathbf{m}_A)_i (\mathbf{m}_B)_j (\mathbf{n}_A)_p ds_x, \quad (16)$$

where  $S_{ijkp}$  is defined as in (12).

It remains to estimate

$$\begin{aligned} & -\gamma \sum_{z \in B_\delta(0) \cap \frac{1}{\ell} \mathcal{L} \setminus \{0\}} \partial_i \partial_j P_k^{(\delta)}(z) \frac{1}{\ell^d} \times \\ & \quad \times \int_{\partial A \cap \partial B} (\mathbf{m}_A)_i(x) (\mathbf{m}_B)_j(x) ((\mathbf{n}_A(x) \cdot (z - \varepsilon\nu))_+ - (\mathbf{n}_A(x) \cdot z)_+) ds_x \\ &= -\gamma \int_{\partial A \cap \partial B} (\mathbf{m}_A)_i(x) (\mathbf{m}_B)_j(x) \times \\ & \quad \times \sum_{z \in B_\delta(0) \cap \frac{1}{\ell} \mathcal{L} \setminus \{0\}} \partial_i \partial_j P_k^{(\delta)}(z) \frac{1}{\ell^d} ((\mathbf{n}_A(x) \cdot (z - \varepsilon\nu))_+ - (\mathbf{n}_A(x) \cdot z)_+) ds_x. \end{aligned} \quad (17)$$

Recalling that  $\varepsilon = \frac{a}{\ell}$ , we can write the sum in (17) as

$$\sum_{y \in \mathcal{L} \setminus \{0\}} \partial_i \partial_j P_k^{(\delta)}\left(\frac{y}{\ell}\right) \frac{1}{\ell^{d+1}} \left( (\mathbf{n}_A(x) \cdot (y - a\nu))_+ - (\mathbf{n}_A(x) \cdot y)_+ \right) \chi_{B_{\varepsilon\delta}(0)}(y). \quad (18)$$

Firstly we show that the terms in this sum are dominated by a function which is summable over  $B_\delta(0) \cap \frac{1}{\ell}\mathcal{L} \setminus \{0\}$ . Clearly

$$\begin{aligned} \left| (\mathbf{n}_A(x) \cdot (y - a\nu))_+ - (\mathbf{n}_A(x) \cdot y)_+ \right| &\leq \left| \mathbf{n}_A(x) \cdot (y - a\nu) - \mathbf{n}_A(x) \cdot y \right| \\ &= a\mathbf{n}_A(x) \cdot \nu \leq c, \end{aligned} \quad (19)$$

so an upper bound for the summands in (18) is given by  $c|y|^{-d-1}$ , which is summable over  $\mathcal{L} \setminus \{0\}$ . As an aside, note that the above  $c$  depends on  $a$  by the estimate in (19), i.e., we have only proved absolute convergence of the sum in (17) for fixed  $a \in \mathbb{R}$ .

Using the following identity, which can be immediately obtained with the chain rule, cf. [Schb, (27)],

$$\partial_i \partial_j P_k^{(\delta)}\left(\frac{y}{\ell}\right) \frac{1}{\ell^{d+1}} = \partial_i \partial_j P_k^{(\ell\delta)}(y), \quad (20)$$

we see next that the terms in (18) converge pointwise to  $\partial_i \partial_j \partial_k N(y) \left( (\mathbf{n}_A(x) \cdot (y - a\nu))_+ - (\mathbf{n}_A(x) \cdot y)_+ \right)$  as  $\ell \rightarrow \infty$ , because, if  $\ell \rightarrow \infty$ ,  $\varphi^{(\ell\delta)}(y)$  as well as  $\chi_{B_{\varepsilon\delta}(0)}(y)$  converge to 1 pointwise. Note that the limit does not depend on  $\delta$ . Thus we finally obtain by (5) and the theorem on dominated convergence that (17) converges to

$$\begin{aligned} & -\gamma \int_{\partial A \cap \partial B} (\mathbf{m}_A)_i(x) (\mathbf{m}_B)_j(x) \times \\ & \quad \times \sum_{y \in \mathcal{L} \setminus \{0\}} \partial_i \partial_j \partial_k N(y) \left( (\mathbf{n}_A(x) \cdot (y - a\nu))_+ - (\mathbf{n}_A(x) \cdot y)_+ \right) ds_x \end{aligned}$$

as  $\ell \rightarrow \infty$  (and  $\delta \rightarrow 0$ ), which finishes the proof of Proposition 3.3.  $\square$

Finally, we comment on how Assumption  $\mathcal{A}$  can be modified to include also more general domains  $A$  and  $B$ , cf. [PPSa, Remark 3.7].

**Remark 1.** Assumption  $\mathcal{A}$  is primarily supposed for an application of results in [Schb, Scha], cf. Proposition 3.1 and Lemma 3.5. However, in those articles, only weaker assumptions on  $A$  and  $B$  are imposed, which read:

$A$  and  $B$  are Lipschitz domains with piecewise  $C^{1,1}$  boundaries, see [Schb, Definition 2] for a precise definition. Furthermore, rather technical conditions are

assumed, which we outline only briefly (see [Schb] and [Scha] for details): (i)  $\overline{A} \cup \overline{B}$  satisfies an outer cone property [Schb, Assumption  $\mathcal{A}_1$ ]; (ii)  $\partial A$ ,  $\partial B$  and  $\partial A \cup \partial B$  satisfy a so-called non-degeneracy condition ( $S$ ) that controls the number of isolated points which have the same tangent vector, cf. [Schb, Definition 3]; (iii)  $\partial A \cap \partial B$  satisfies a so-called neighborhood estimate which allows one to bound volumes of tubes about relative boundaries of portions of  $\partial A \cap \partial B$ , see [Schb, Definition 4].

These weaker assumptions are for instance satisfied for the domains in Assumptions  $\mathcal{A}$ . We remark that all lemmas, propositions and theorems in this article also hold under the above weaker assumptions. (In particular, the non-degeneracy condition ( $S$ ) guarantees that  $\{x \in \partial A : \mathbf{n}_A \cdot \nu = 0\}$  has  $\mathcal{H}^{d-1}$ -measure zero. With this observation also the necessary modifications in the proof of Proposition 4.2 become straightforward.)

## 4 Properties of the additional, $a$ -dependent contribution to the limit force

Here we study properties of the term

$$\begin{aligned} \mathbf{G}_k(a) = & -\gamma \int_{\partial A \cap \partial B} (\mathbf{m}_A)_i(x) (\mathbf{m}_B)_j(x) \times \\ & \times \sum_{z \in \mathcal{L} \setminus \{0\}} \partial_i \partial_j \partial_k N(z) \left( (\mathbf{n}_A(x) \cdot (z - a\nu))_+ - (\mathbf{n}_A(x) \cdot z)_+ \right) ds_x. \end{aligned} \quad (21)$$

Recall that  $\mathbf{n}_A(x) \cdot \nu > 0$  for all  $x \in \partial A \cap \partial B$  by Assumption  $\mathcal{A}$ . See Figure 2 for sketches of the sets defined in the following lemma.

**Lemma 4.1.** *Let  $x \in \partial A \cap \partial B$ .*

(i) *On  $\mathcal{C}_{a,x} := \{z \in \mathbb{R}^d \setminus \{0\} \mid (\mathbf{n}_A(x) \cdot z) \geq a(\mathbf{n}_A(x) \cdot \nu)\}$  we have*

$$(\mathbf{n}_A(x) \cdot (z - a\nu))_+ - (\mathbf{n}_A(x) \cdot z)_+ = -a\mathbf{n}_A(x) \cdot \nu.$$

(ii) *On  $\mathcal{D}_{a,x} := \{z \in \mathbb{R}^d \setminus \{0\} \mid 0 \leq (\mathbf{n}_A(x) \cdot z) < a(\mathbf{n}_A(x) \cdot \nu)\}$  we have*

$$(\mathbf{n}_A(x) \cdot (z - a\nu))_+ - (\mathbf{n}_A(x) \cdot z)_+ = -\mathbf{n}_A(x) \cdot z.$$

(iii) *On  $\mathbb{R}^d \setminus (\mathcal{C}_{a,x} \cup \mathcal{D}_{a,x})$  we have*

$$(\mathbf{n}_A(x) \cdot (z - a\nu))_+ - (\mathbf{n}_A(x) \cdot z)_+ = 0.$$

□

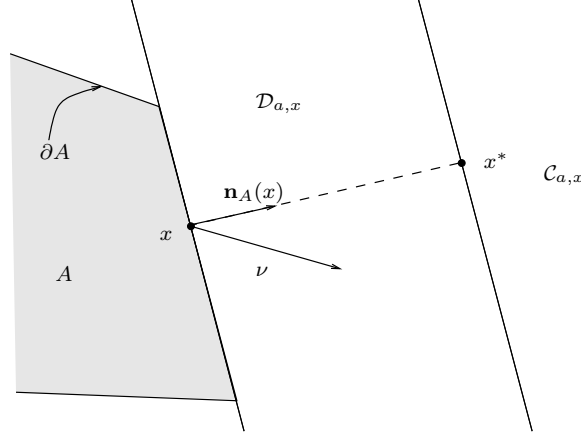


Figure 2: Sketch of the sets  $\mathcal{C}_{a,x}$  and  $\mathcal{D}_{a,x}$  with  $a = 2$ .

In the spirit of Lemma 4.1 we rewrite the additional term  $\mathbf{G}(a)$  as

$$\mathbf{G}_k(a) = a \gamma \int_{\partial A \cap \partial B} (\mathbf{m}_A)_i(x) (\mathbf{m}_B)_j(x) (\mathbf{n}_A(x) \cdot \nu) \sum_{z \in \mathcal{C}_{a,x} \cap \mathcal{L}} \partial_i \partial_j \partial_k N(z) ds_x \quad (22)$$

$$+ \gamma \int_{\partial A \cap \partial B} (\mathbf{m}_A)_i(x) (\mathbf{m}_B)_j(x) \sum_{z \in \mathcal{D}_{a,x} \cap \mathcal{L}} \partial_i \partial_j \partial_k N(z) (\mathbf{n}_A(x) \cdot z) ds_x. \quad (23)$$

Next we study the limit of  $\mathbf{G}(a)$  as  $a$  tends to  $\infty$ , which corresponds to two bodies which are infinitely far apart on the lattice scale ( $\lim_{\ell \rightarrow \infty} \lim_{a \rightarrow \infty} \varepsilon = \infty$ ), but are in contact on the continuum scale ( $\lim_{a \rightarrow \infty} \lim_{\ell \rightarrow \infty} \varepsilon = 0$ ).

**Proposition 4.2.** *Let Assumption  $\mathcal{A}$  be satisfied. Then*

$$\lim_{a \rightarrow \infty} \mathbf{G}_k(a) = -\mathbf{F}_k^{\text{short}}(A, B) + \frac{\gamma}{2} \int_{\partial A \cap \partial B} (\mathbf{m}_A \cdot \mathbf{n}_A)(x) (\mathbf{m}_B \cdot \mathbf{n}_A)(x) (\mathbf{n}_A)_k(x) ds_x.$$

Brown's formula [Bro66, p. 57], see also [PPSa, Section 3.1], is given by

$$\mathbf{F}^{\text{Br}}(A, B) = \int_A (\mathbf{m}_A \cdot \nabla) \mathbf{H}_{A \cup B} dx + \frac{\gamma}{2} \int_{\partial A} (\mathbf{m}_A \cdot \mathbf{n}_A)^2 \mathbf{n}_A ds_x. \quad (24)$$

By Propositions 3.1 and 4.2 and Theorem 3.4 we thus obtain

**Theorem 4.3.** *Let Assumption  $\mathcal{A}$  be satisfied. Then*

$$\lim_{a \rightarrow \infty} \mathbf{F}^{\text{lim}}(A, B, a) = \mathbf{F}^{\text{Br}}(A, B).$$

This proves a claim of Brown [Bro66, p. 53], who expected additional contributions to the magnetic force from dipole-dipole interactions close to the (macroscopic) interface between  $A$  and  $B$  to be of short range character, i.e., he expected those contributions to converge to zero as the (microscopic) distance becomes large.

*Proof of Proposition 4.2.* We will in fact prove that the integrands in (22) and (23) converge uniformly in  $x$ . So without loss of generality we may assume that  $x$  is fixed with  $\mathbf{n}_A(x) = \mathbf{e}_1$ , see Step 6 for a verification.

*Step 1.* We consider the term on the right hand side in (22) as  $a \rightarrow \infty$  and show that it converges to zero. For this we replace the sum with a Riemann integral. Set  $z = \frac{y}{a}$  and apply an analog of (20). Then

$$a \sum_{z \in \mathcal{C}_{a,x} \cap \mathcal{L}} \partial_i \partial_j \partial_k N(z) = \sum_{y \in \mathcal{C}_{1,x} \cap \frac{1}{a} \mathcal{L}} \partial_i \partial_j \partial_k N(y) a^{-d},$$

which converges to  $\int_{\mathcal{C}_{1,x}} \partial_i \partial_j \partial_k N(y) dy$  as  $a \rightarrow \infty$  since  $|\partial_i \partial_j \partial_k N(y)| \leq c|y|^{-d-1}$  implies that both

$$\sum_{y \in (\mathcal{C}_{1,x} \setminus B_R(0)) \cap \frac{1}{a} \mathcal{L}} |\partial_i \partial_j \partial_k N(y)| a^{-d} \quad \text{and} \quad \int_{\mathcal{C}_{1,x} \setminus B_R(0)} |\partial_i \partial_j \partial_k N(y)| dy$$

are bounded by  $cR^{-1}$  for arbitrary  $R > 0$ . The claim then follows by choosing  $R$  large and applying a Riemann sum argument for the domain  $\mathcal{C}_{1,x} \cap B_R(0)$ .

Now, let  $x^*$  be the projection of 0 on  $\partial \mathcal{C}_{1,x}$ , cf. Figure 2. Since  $|\partial_j \partial_k N(y)| \leq c(R - |x^*|)^{-d}$  for all  $y \in \mathcal{C}_{1,x} \cap \partial B_R(x^*)$ , an integration by parts yields

$$\int_{\mathcal{C}_{1,x}} \partial_i \partial_j \partial_k N(y) dy = \lim_{R \rightarrow \infty} \int_{\partial \mathcal{C}_{1,x} \cap B_R(x^*)} -(\mathbf{n}_A)_i(x) \partial_j \partial_k N(y) ds_y,$$

which is zero for  $i \neq 1$  as  $\mathbf{n}_A = \mathbf{e}_1$  by assumption. If  $j \neq 1$  we can integrate by parts once more and obtain

$$\lim_{R \rightarrow \infty} (\mathbf{n}_A)_i(x) \int_{\partial \mathcal{C}_{1,x} \cap \partial B_R(x^*)} \frac{y'_j}{|y'|} \partial_k N(y) dl_y,$$

where  $l_y$  denotes the  $d - 2$  dimensional surface measure on  $\partial \mathcal{C}_{1,x} \cap B_R(x^*)$  and  $y' := (y_2, \dots, y_d)$ , i.e.,  $\frac{y'_j}{|y'|}$  is the outward normal to  $\partial \mathcal{C}_{1,x} \cap \partial B_R(x^*)$  within the hyperplane  $\partial \mathcal{C}_{1,x}$ . The integral is now easily seen to be bounded by  $cR^{-d+1}R^{d-2}$ . This is still true if both  $i$  and  $j$  are equal to 1 because of  $\Delta N = 0$ , i.e.,  $\partial_1^2 N =$



$-(\partial_2^2 N + \dots + \partial_d^2 N)$ , and  $\int_{C_{1,x}} \partial_i^2 \partial_k N(y) dy = 0$  for  $i \neq 1$ . Sending  $R$  to infinity shows that  $\int_{C_{1,x}} \partial_i \partial_j \partial_k N(y) dy = 0$  for all  $i, j, k = 1, \dots, d$ .

In the remaining steps of the proof we will show that the term in (23) converges to

$$-\mathbf{F}_k^{\text{short}}(A, B) + \frac{\gamma}{2} \int_{\partial A \cap \partial B} (\mathbf{m}_A \cdot \mathbf{n}_A)(x) (\mathbf{m}_B \cdot \mathbf{n}_A)(x) \mathbf{n}_A(x) ds_x$$

as  $a \rightarrow \infty$ . To this end we prove in Steps 2 to 4 that

$$\begin{aligned} & \sum_{z \in \mathcal{D}_{a,x} \cap \mathcal{L}} \partial_i \partial_j \partial_k N(z) z_1 \\ & \longrightarrow \delta_{i1} \delta_{j1} \int_{\partial C_{1,x}} \partial_j \partial_k N(y) y_1 ds_y - \delta_{i1} \delta_{j1} \int_{\partial C_{1,x}} \partial_k N(y) ds_y - \frac{1}{2\gamma} S_{ijk1} \end{aligned} \quad (25)$$

as  $a \rightarrow \infty$ .

*Step 2.* Again we replace  $z$  with  $\frac{y}{a}$  and obtain for the sum in (23)

$$\begin{aligned} \sum_{z \in \mathcal{D}_{a,x} \cap \mathcal{L}} \partial_i \partial_j \partial_k N(z) (\mathbf{n}_A(x) \cdot z) &= \sum_{y \in \mathcal{D}_{1,x} \cap \frac{1}{a} \mathcal{L}} \partial_i \partial_j \partial_k N(y) (\mathbf{n}_A(x) \cdot y) a^{-d} \\ &= \sum_{y \in \mathcal{D}_{1,x} \cap \frac{1}{a} \mathcal{L}} \partial_i \partial_j \partial_k N(y) y_1 a^{-d}. \end{aligned} \quad (26)$$

Note that the terms in the sum are symmetric in  $y$  with respect to the origin. Thus

$$\sum_{y \in \mathcal{D}_{1,x} \cap \frac{1}{a} \mathcal{L}} \partial_i \partial_j \partial_k N(y) y_1 a^{-d} = \frac{1}{2} \sum_{y \in \tilde{\mathcal{D}}_{1,x} \cap \frac{1}{a} \mathcal{L}} \partial_i \partial_j \partial_k N(y) y_1 a^{-d},$$

where  $\tilde{\mathcal{D}}_{a,x} := \{z \in \mathbb{R}^d \setminus \{0\} \mid -a\nu_1 < z_1 < a\nu_1\}$ , which is invariant under the transformation  $z \mapsto -z$ . Set  $r = \nu_1$ . It will turn out to be useful to split the above sum as follows:

$$\begin{aligned} & \frac{1}{2} \sum_{y \in \tilde{\mathcal{D}}_{1,x} \cap \frac{1}{a} \mathcal{L}} \partial_i \partial_j \partial_k N(y) y_1 a^{-d} \\ &= \frac{1}{2} \sum_{y \in \tilde{\mathcal{D}}_{1,x} \cap \frac{1}{a} \mathcal{L} \cap B_r(0)} \partial_i \partial_j \partial_k N(y) y_1 a^{-d} + \frac{1}{2} \sum_{y \in (\tilde{\mathcal{D}}_{1,x} \cap \frac{1}{a} \mathcal{L}) \setminus B_r(0)} \partial_i \partial_j \partial_k N(y) y_1 a^{-d}. \end{aligned} \quad (27)$$

We consider the first term in (27) further below (see Step 4). The second term in (27) converges to the Riemann integral  $\frac{1}{2} \int_{\tilde{\mathcal{D}}_{1,x} \setminus B_r(0)} \partial_i \partial_j \partial_k N(y) y_1 dy$  as  $a \rightarrow \infty$  by

a Riemann sum argument. To prove this, we split the sum into one part where  $|y| \leq R$  and another part where  $|y| > R$  for some  $R > r$ . The first part is a bounded Riemann sum on a bounded domain. The error terms, i.e., the sum, resp., integral, over  $y$  with  $|y| \geq R$  are seen to converge to 0 as  $R \rightarrow \infty$  similarly as in Step 1, since  $|y_1|$  is bounded on  $\tilde{\mathcal{D}}_{1,x}$ .

*Step 3.* Integrations by parts of  $\frac{1}{2} \int_{\tilde{\mathcal{D}}_{1,x} \setminus B_r(0)} \partial_i \partial_j \partial_k N(y) y_1 dy$  yield

$$\begin{aligned} & \frac{1}{2} \int_{\partial B_r(0)} -\frac{y_i}{|y|} \partial_j \partial_k N(y) y_1 ds_y + \frac{1}{2} \int_{\partial \tilde{\mathcal{D}}_{1,x}} \mu_i \partial_j \partial_k N(y) y_1 ds_y \\ & + \frac{1}{2} \delta_{i1} \int_{\partial B_r(0)} \frac{y_j}{|y|} \partial_k N(y) ds_y - \frac{1}{2} \delta_{i1} \int_{\partial \tilde{\mathcal{D}}_{1,x}} \mu_j \partial_k N(y) ds_y, \end{aligned} \quad (28)$$

where  $\mu$  denotes the outer normal to  $\partial \tilde{\mathcal{D}}_{1,x}$ . (Note that the fourth integral does not converge absolutely. This integral is understood in the principal value sense  $\lim_{R \rightarrow \infty} \int_{\partial \tilde{\mathcal{D}}_{1,x} \cap \partial B_R(0)} (\dots) ds_y$ . The aforementioned integrations by parts are justified since the surface measure of  $\tilde{\mathcal{D}}_{1,x} \cap \partial B_R(0)$  is bounded by  $cR^{d-2}$  while  $|\partial_j \partial_k N(y) y_1|$  and  $|\partial_k N(y)|$  are bounded by  $cR^{-d+1}$  and the corresponding integrals thus tend to zero.)

By construction,  $\mu$  equals the constant vectors  $\mathbf{n}_A(x) = \mathbf{e}_1$  and  $-\mathbf{n}_A(x) = -\mathbf{e}_1$ , respectively. By antisymmetry of  $\partial_j \partial_k N(y) y_1$ , the second term in (28) is equal to  $\delta_{i1} \int_{\partial \mathcal{C}_{1,x}} \partial_j \partial_k N(y) y_1 ds_y$ . Similarly, the fourth term in (28) becomes  $-\delta_{i1} \delta_{j1} \int_{\partial \mathcal{C}_{1,x}} \partial_k N(y) ds_y$ .

Hence, if  $j \neq 1$ , the fourth term in (28) vanishes and the second term can be integrated by parts once more and becomes  $\lim_{R \rightarrow \infty} \delta_{i1} \int_{\partial \mathcal{C}_{1,x} \cap \partial B_R(x^*)} \frac{y'_j}{|y'|} \partial_k N(y) y_1 dl_y$ , which is zero. Indeed,

$$\begin{aligned} & \int_{\partial \mathcal{C}_{1,x} \cap \partial B_R(x^*)} \frac{y'_j}{|y'|} \partial_k N(y) y_1 dl_y \\ & = \int_{R^{-1}(\partial \mathcal{C}_{1,x} \cap \partial B_R(x^*))} \frac{(Ry')_j}{|Ry'|} \partial_k N(Ry) Ry_1 R^{d-2} dl_y \\ & = \int_{\{y_1 = R^{-1} \nu_1, |y'|^2 = 1\}} \frac{y'_j}{|y'|} \partial_k N(y) y_1 dl_y \\ & = \int_{\{y_1 = 0, |y'|^2\}} \frac{y'_j}{|y'|} \partial_k N(y) y_1 dl_y + \mathcal{O}(R^{-1}), \end{aligned}$$

since  $\partial_k N(y) y_1$  is uniformly Lipschitz continuous in  $y_1$  on  $\{y \in \mathbb{R}^d \mid |y'|^2 = 1\}$ .

By antisymmetry of the integrand, the last integral vanishes. Hence we obtain indeed that  $\int_{\partial\mathcal{C}_{1,x} \cap \partial B_R(x^*)} \frac{y'_i}{|y|} \partial_k N(y) y_1 dl_y \rightarrow 0$  as  $R \rightarrow \infty$ . We study the remaining terms in (28) and the case  $j = 1$  further below.

*Step 4.* Next we consider the first term in (27) and show that

$$\begin{aligned} & \sum_{y \in \tilde{\mathcal{D}}_{1,x} \cap \frac{1}{a} \mathcal{L} \cap B_r(0)} \partial_i \partial_j \partial_k N(y) y_1 a^{-d} + \int_{\partial B_r(0)} \left( -\frac{y_i}{|y|} \partial_j \partial_k N(y) y_1 + \delta_{i1} \frac{y_j}{|y|} \partial_k N(y) \right) ds_y \\ & \longrightarrow -\frac{1}{\gamma} S_{ijk1} \quad \text{as } a \rightarrow \infty, \end{aligned} \tag{29}$$

which implies (25). To prove (29), recall [Schb, Theorem 13] and observe that

$$\begin{aligned} -\frac{1}{\gamma} S_{ijk1} &= \lim_{\delta \rightarrow 0} \lim_{\ell \rightarrow \infty} \sum_{z \in B_\delta(0) \cap \frac{1}{\ell} \mathcal{L} \setminus \{0\}} \partial_i \partial_j P_k^{(\delta)}(z) z_1 \frac{1}{\ell^d} \\ &= \lim_{n \rightarrow \infty} \sum_{z \in B_n(0) \cap \mathcal{L} \setminus \{0\}} \partial_i \partial_j P_k^{(n)}(z) z_1 \\ &= \lim_{a \rightarrow \infty} \sum_{z \in B_{2ar}(0) \cap \mathcal{L} \setminus \{0\}} \partial_i \partial_j P_k^{(2ar)}(z) z_1 \end{aligned}$$

for some  $r = \nu_1 > 0$  as above. We split the latter sum into a sum over  $B_{ar}(0)$  and a sum over  $B_{2ar}(0) \setminus B_{ar}(0)$ . Since  $B_{ar}(0) \cap \mathcal{L} \setminus \{0\} = a\tilde{\mathcal{D}}_{1,x} \cap \mathcal{L} \cap B_{ar}(0)$  and  $P_k^{(2ar)}(z) = \partial_k N(z)$  on  $B_{ar}(0)$  by definition, we have

$$\sum_{z \in B_{ar}(0) \cap \mathcal{L} \setminus \{0\}} \partial_i \partial_j P_k^{(2ar)}(z) z_1 = \sum_{y \in \tilde{\mathcal{D}}_{1,x} \cap \frac{1}{a} \mathcal{L} \cap B_r(0)} \partial_i \partial_j \partial_k N(y) y_1 a^{-d}. \tag{30}$$

Hence it remains to study the sum over  $B_{2ar}(0) \setminus B_{ar}(0)$ . A scaling of the lattice with  $\frac{1}{a}$  yields

$$\sum_{y \in (B_{2r}(0) \setminus B_r(0)) \cap \frac{1}{a} \mathcal{L} \setminus \{0\}} \partial_i \partial_j P_k^{(2r)}(y) y_1 a^{-d} \longrightarrow \int_{B_{2r}(0) \setminus B_r(0)} \partial_i \partial_j P_k^{(2r)}(y) y_1 dy$$

as  $a \rightarrow \infty$ . Finally, by the definition of  $P_k^{(2r)}$  in (5) and integrations by parts we obtain

$$\begin{aligned} & \int_{B_{2r}(0) \setminus B_r(0)} \partial_i \partial_j P_k^{(2r)}(y) y_1 dy \\ &= \int_{\partial B_r(0)} -\frac{y_i}{|y|} \partial_j \partial_k N(y) y_1 ds_y + \delta_{ip} \int_{\partial B_r(0)} \frac{y_j}{|y|} \partial_k N(y) ds_y \end{aligned}$$

and thus (29).

*Step 5.* Collecting all terms, we have shown that

$$a\nu_1 \sum_{z \in \mathcal{C}_{a,x} \cap \mathcal{L}} \partial_i \partial_j \partial_k N(z) + \sum_{z \in \mathcal{D}_{a,x} \cap \mathcal{L}} \partial_i \partial_j \partial_k N(z) z_1 + \frac{1}{2\gamma} S_{ijk1} \quad (31)$$

converges to 0 as  $a \rightarrow \infty$  for  $j \neq 1$ . Indeed, the first term converges to zero by Step 1 and the convergence of the second term follows by (25). By symmetry in  $i$  and  $j$ , this is also true for  $j = 1$ ,  $i \neq 1$ . For  $i = j = 1$ , (31) converges to

$$\int_{\partial \mathcal{C}_{1,x}} \partial_1 \partial_k N(y) y_1 ds_y - \int_{\partial \mathcal{C}_{1,x}} \partial_k N(y) ds_y = \delta_{1k} \int_{\partial \mathcal{C}_{1,x}} \partial_1^2 N(y) y_1 - \partial_1 N(y) ds_y \quad (32)$$

as  $a \rightarrow \infty$  by a symmetry argument. Now using that

$$\partial_1 N(y) = -\frac{\Gamma(\frac{d}{2})}{2\pi^{d/2}} \frac{y_1}{|y|^d} \quad \text{and} \quad \partial_1^2 N(y) = \frac{\Gamma(\frac{d}{2})}{2\pi^{d/2}} \left( \frac{dy_1^2}{|y|^{d+2}} - \frac{1}{|y|^d} \right)$$

we find that

$$\partial_1^2 N(y) y_1 - \partial_1 N(y) = \frac{\Gamma(\frac{d}{2})}{2\pi^{d/2}} \frac{dy_1^3}{|y|^{d+2}},$$

and (32) becomes

$$\begin{aligned} & \delta_{1k} \frac{d\Gamma(\frac{d}{2})}{2\pi^{d/2}} \int_{\partial \mathcal{C}_{1,y}} \frac{y_1^3}{|y|^{d+2}} ds_y \\ &= \delta_{1k} \frac{d\Gamma(\frac{d}{2})}{2\pi^{d/2}} \int_{\mathbb{R}^{d-1}} \frac{\nu_1^3}{(\nu_1^2 + y_2^2 + \dots + y_d^2)^{d/2+1}} dy_2 \dots dy_d \\ &= \delta_{1k} \frac{d\Gamma(\frac{d}{2})}{2\pi^{d/2}} |\partial B_1^{(d-1)}(0)| \nu_1^3 \int_0^\infty \frac{r^{d-2}}{(\nu_1^2 + r^2)^{d/2+1}} dr \\ &= \delta_{1k} \frac{d\Gamma(\frac{d}{2})}{2\pi^{d/2}} \frac{2\pi^{(d-1)/2}}{\Gamma(\frac{d-1}{2})} \nu_1^3 \int_0^\infty \frac{r^{d-2}}{(\nu_1^2 + r^2)^{d/2+1}} dr \\ &= \delta_{1k} \frac{d\Gamma(\frac{d}{2})}{\pi^{1/2} \Gamma(\frac{d-1}{2})} \int_0^\infty \frac{r^{d-2}}{(1+r^2)^{d/2+1}} dr. \end{aligned} \quad (33)$$

To calculate the latter integral, we change variables via  $r \mapsto (\frac{1}{1-t} - 1)^{\frac{1}{2}}$  and obtain

$$\int_0^\infty \frac{r^{d-2}}{(1+r^2)^{d/2+1}} dr = \frac{1}{2} \int_0^1 t^{\frac{d-3}{2}} (1-t)^{\frac{1}{2}} dt.$$

This can be written in terms of the Euler beta function  $B(a, b) := \int_0^1 t^{a-1}(1-t)^{b-1} dt = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)}$ :

$$\frac{1}{2} \int_0^1 t^{\frac{d-3}{2}} (1-t)^{\frac{1}{2}} dt = \frac{1}{2} B\left(\frac{d-1}{2}, \frac{3}{2}\right) = \frac{1}{2} \frac{\Gamma(\frac{d-1}{2})\Gamma(\frac{3}{2})}{\Gamma(\frac{d}{2}+1)}.$$

With  $\frac{d}{2}\Gamma(\frac{d}{2}) = \Gamma(\frac{d}{2}+1)$  and  $\Gamma(\frac{3}{2}) = \frac{1}{2}\pi^{\frac{1}{2}}$  we obtain that (33) and hence (32) is equal to  $\frac{1}{2}\delta_{1k}$ .

Hence, by (31), (32) and the definition of  $\mathbf{G}_k(a)$  in (22) and (23), we finally obtain that

$$\begin{aligned} & a\nu_1 \sum_{z \in \mathcal{C}_{a,x} \cap \mathcal{L}} \partial_i \partial_j \partial_k N(z) + \sum_{z \in \mathcal{D}_{a,x} \cap \mathcal{L}} \partial_i \partial_j \partial_k N(z) z_1 \\ & \longrightarrow -\frac{1}{2\gamma} S_{ijk1} + \begin{cases} \delta_{1k} \frac{1}{2} & \text{if } i = j = 1 \\ 0 & \text{else} \end{cases} \quad \text{as } a \rightarrow \infty. \end{aligned} \quad (34)$$

*Step 6.* Recall that we have assumed  $\mathbf{n}_A(x) = \mathbf{e}_1$  so far. The general case is obtained as follows. Let  $Q = (q_{ij}) = Q(x)$  be some orthogonal matrix mapping  $\mathbf{n}_A(x)$  to  $\mathbf{e}_1$  and transform coordinates according to  $Qz = \tilde{z}$ . Then

$$a(\mathbf{n}_A(x) \cdot \nu) \sum_{z \in \mathcal{C}_{a,x} \cap \mathcal{L}} \partial_i \partial_j \partial_k N(z) = a(\mathbf{e}_1 \cdot Q\nu) \sum_{\tilde{z} \in Q\mathcal{C}_{a,x} \cap Q\mathcal{L}} q_{ri} \partial_{\tilde{z}_r} q_{sj} \partial_{\tilde{z}_s} q_{tk} \partial_{\tilde{z}_t} N(\tilde{z}),$$

where  $Q\mathcal{C}_{a,x} = \{\tilde{z} \mid \tilde{z}_1 \geq a(Q\nu)_1\}$ . Similarly, for the sum in (23) we obtain

$$\sum_{z \in \mathcal{D}_{a,x} \cap \mathcal{L}} \partial_i \partial_j \partial_k N(z) (\mathbf{n}_A(x) \cdot z) = \sum_{\tilde{z} \in Q\mathcal{D}_{a,x} \cap Q\mathcal{L}} q_{ri} \partial_{\tilde{z}_r} q_{sj} \partial_{\tilde{z}_s} q_{tk} \partial_{\tilde{z}_t} N(\tilde{z}) (\mathbf{e}_1 \cdot \tilde{z})$$

with  $Q\mathcal{D}_{a,x} = \{\tilde{z} \mid 0 \leq \tilde{z}_1 < a(Q\nu)_1\}$ . The sum of these two terms converges to

$$q_{ri} q_{sj} q_{tk} \left( -\frac{1}{2\gamma} S_{rstu}^Q \delta_{1u} + \frac{1}{2} \delta_{1r} \delta_{1s} \delta_{1t} \right)$$

as  $a \rightarrow \infty$  by (34). Here,  $S^Q$  denotes the tensor that arises when replacing the lattice  $\mathcal{L}$  by  $Q\mathcal{L}$ .

Now note that  $S_{rstu}^Q = q_{ri} q_{sj} q_{tk} q_{up} S_{ijkp}$ , which follows from (12) and the definition of  $P_k^{(\delta)}$  similarly as the previous transformation rules. Since  $\sum_r q_{ri}^2 = \sum_s q_{sj}^2 = \sum_t q_{tk}^2 = 1$  and  $Q^T \mathbf{e}_1 = \mathbf{n}_A(x)$ , the above expression equals

$$\begin{aligned} & -\frac{1}{2\gamma} q_{up} \delta_{1u} S_{ijkp} + \frac{1}{2} q_{ri} \delta_{1r} q_{sj} \delta_{1s} q_{tk} \delta_{1t} \\ & = -\frac{1}{2\gamma} (\mathbf{n}_A)_p(x) S_{ijkp} + \frac{1}{2} (\mathbf{n}_A)_i(x) (\mathbf{n}_A)_j(x) (\mathbf{n}_A)_k(x). \end{aligned}$$

Summarizing, we obtain

$$\begin{aligned} \lim_{a \rightarrow \infty} \mathbf{G}_k(a) &= -\frac{1}{2} \sum_{i,j,p=1}^d S_{ijkp} \int_{\partial A \cap \partial B} (\mathbf{m}_A)_i(x) (\mathbf{m}_B)_j(x) (\mathbf{n}_A)_p(x) ds_x \\ &\quad + \frac{\gamma}{2} \int_{\partial A \cap \partial B} (\mathbf{m}_A \cdot \mathbf{n}_A)(x) (\mathbf{m}_B \cdot \mathbf{n}_A)(x) (\mathbf{n}_A)_k(x) ds_x. \end{aligned}$$

□

In order to calculate  $\mathbf{G}(a)$  for finite values of  $a$ , we write  $\mathbf{G}(a)$  as

$$\mathbf{G}_k(a) = -\gamma \int_{\partial A \cap \partial B} (\mathbf{m}_A)_i(x) (\mathbf{m}_B)_j(x) H_{ijk}(a, x) ds_x \quad (35)$$

with

$$H_{ijk}(a, x) = \sum_{z \in \mathcal{L} \setminus \{0\}} \partial_i \partial_j \partial_k N(z) \left( (\mathbf{n}_A(x) \cdot (z - a\nu))_+ - (\mathbf{n}_A(x) \cdot z)_+ \right).$$

**Example 4.4.** Suppose that  $\gamma = 1$ ,  $\mathbf{n}_A \equiv \mathbf{e}_1 \in \mathbb{R}^d$  on  $\partial A \cap \partial B$  and that the underlying lattice is the cubic lattice  $\mathcal{L} = \mathbb{Z}^d$ . If  $\nu = \mathbf{e}_1$ , then, for all  $x \in \partial A \cap \partial B$ ,

$$H_{ijk}(a, x) = \sum_{z_1=1}^{\infty} \left( (z_1 - a)_+ - (z_1)_+ \right) \sum_{z_2, \dots, z_d \in \mathbb{Z}} \partial_i \partial_j \partial_k N(z).$$

Due to the symmetry of  $N$ , the inner sum is zero unless two of the indices  $i, j, k$  are equal and the third one equals 1. Moreover, if the two like indices are different from one, then  $H_{ijk}(a) = -\frac{1}{d-1} H_{111}(a)$  since  $\Delta N = 0$  on  $\mathbb{R}^d \setminus \{0\}$ . Observe that the Fourier transform of  $\partial_1^3 N(z)$  with respect to  $(z_2, \dots, z_d) \in \mathbb{R}^{d-1}$  is given by

$$\int_{\mathbb{R}^{d-1}} \partial_1^3 N(z_1, \dots, z_d) e^{-i(z_2 \zeta_2 + \dots + z_d \zeta_d)} dz_2 \dots dz_d = -\frac{1}{2} (\zeta_2^2 + \dots + \zeta_d^2) e^{-z_1 \sqrt{\zeta_2^2 + \dots + \zeta_d^2}}$$

for  $z_1 > 0$ . (This can be seen, e.g., by noting that the full  $d$ -dimensional Fourier transform of  $N$  is  $-(\zeta_1^2 + \dots + \zeta_d^2)^{-1}$ . An inverse Fourier transform of this expression with respect to  $\zeta_1$  and a subsequent calculation of the three partial derivatives with respect to  $z_1$  yields the asserted formula.) So we obtain by Poisson

summation that

$$\begin{aligned}
H_{111}(a) &= 2\pi^2 \sum_{z_1=1}^{\infty} ((z_1)_+ - (z_1 - a)_+) \sum_{\zeta_2, \dots, \zeta_d \in \mathbb{Z}} (\zeta_2^2 + \dots + \zeta_d^2) e^{-2\pi z_1 \sqrt{\zeta_2^2 + \dots + \zeta_d^2}} \\
&= 2\pi^2 \sum_{\zeta_2, \dots, \zeta_d \in \mathbb{Z}} (\zeta_2^2 + \dots + \zeta_d^2) \left( \sum_{z_1=1}^{a-1} z_1 e^{-2\pi z_1 \sqrt{\zeta_2^2 + \dots + \zeta_d^2}} + \sum_{z_1=a}^{\infty} a e^{-2\pi z_1 \sqrt{\zeta_2^2 + \dots + \zeta_d^2}} \right) \\
&= 2\pi^2 \sum_{\zeta \in \mathbb{Z}^{d-1} \setminus \{0\}} |\zeta|^2 \frac{e^{-2\pi|\zeta|} (1 - e^{-2\pi a|\zeta|})}{(1 - e^{-2\pi|\zeta|})^2}.
\end{aligned}$$

That is,  $H_{111}(a)$  turns out to be monotonically increasing and converges to its limit value for  $a \rightarrow \infty$  exponentially fast. But then, by (35), also  $\mathbf{G}(a)$  converges exponentially fast as  $a \rightarrow \infty$ .

For the physically interesting cases  $d = 2$  and  $3$  a numerical evaluation of  $H_{111}$  yields:

$a$	$H_{111}(a) - H_{111}(a-1)$ for $d = 2$	$H_{111}(a) - H_{111}(a-1)$ for $d = 3$
$a = 1$	0.07441...	0.1713...
$a = 2$	$1.379 \dots \cdot 10^{-4}$	$2.788 \dots \cdot 10^{-4}$
$a = 3$	$2.575 \dots \cdot 10^{-7}$	$5.155 \dots \cdot 10^{-7}$
$a = 4$	$4.810 \dots \cdot 10^{-10}$	$9.620 \dots \cdot 10^{-10}$

If for example  $\mathbf{m}_A = \mathbf{m}_B = \mathbf{e}_1$ , by (35) we can write the limiting force in Theorem 3.4 as

$$\begin{aligned}
\mathbf{F}^{\text{lim}}(A, B, a) &= \mathbf{F}^{\text{long}}(A, B) + \mathbf{F}^{\text{short}}(A, B) + \mathbf{G}(a-1) - (H_{111}(a) - H_{111}(a-1)) |\partial A \cap \partial B| \mathbf{e}_1.
\end{aligned}$$

Let  $A$  and  $B$  be for instance two cuboids of width 1, depth 8 and height 8 such that  $|\partial A \cap \partial B| = 64$  and such that  $A$  and  $B$  are two lattice spacings apart (which corresponds to  $a = 1$ ). As was computed in [PPSb, Exp. 3<sub>3D</sub>],  $\mathbf{F}^{\text{lim}}(A, B, 0) = \mathbf{F}^{\text{lim}}(A, B) = 17.414$ . Hence we obtain  $\mathbf{F}^{\text{lim}}(A, B, 1) = 6.451$ . For a comparison we note that  $\mathbf{F}^{\text{lim}}(A, B, \infty) = \mathbf{F}^{\text{Br}}(A, B) = 6.431$  [PPSb, Exp. 3<sub>3D</sub>], which demonstrates the exponential decay of  $\mathbf{G}(a)$  with  $a$  strikingly.

## 5 Further distance regimes

In this section we investigate the limiting force for spatially separated bodies and for  $a$  scaling with  $\ell$ . We first consider the case that  $A$  and  $B$  are separated by a macroscopic distance greater than 0.

### 5.1 $A$ and $B$ macroscopically separated

In the discrete-to-continuum setting, this case corresponds to  $a \sim \ell$ , i.e.,  $\varepsilon = \frac{a}{\ell} = \text{const.} > 0$ .

**Proposition 5.1.** *Suppose  $A$  and  $B$  are not in contact, i.e.,  $\bar{A} \cap \bar{B} = \emptyset$ , but still satisfy the remaining conditions of Assumption  $\mathcal{A}$ . Then the discrete-to-continuum limit  $\mathbf{F}_{\text{sep}}^{\text{lim}}(A, B)$  exists and satisfies*

$$\mathbf{F}_{\text{sep}}^{\text{lim}}(A, B) = \int_A (\mathbf{m}_A(x) \cdot \nabla) \mathbf{H}_B(x) dx. \quad (36)$$

*Proof.* As in Section 3, we split the discrete sum into long and short range contributions, cf. (6). It is easily seen that  $\mathbf{F}^{\text{short}}(A, B) = 0$ . Indeed, since  $P_k^{(\delta)}(x - y) = 0$  for  $|x - y| \geq \delta$ , we have  $\mathbf{F}^{\text{short}(\ell, \delta)}(A, B) = 0$  if  $\delta \leq \text{dist}(A, B)$ .

The limit  $\ell \rightarrow \infty$  of the long range part can be identified by a Riemann sum argument as

$$\lim_{\ell \rightarrow \infty} \mathbf{F}_k^{\text{long}(\ell, \delta)}(A, B) = \gamma \int_A \int_B \partial_i \partial_j R_k^{(\delta)}(x - y) (\mathbf{m}_A)_i(x) (\mathbf{m}_B)_j(y) dy dx.$$

Since this expression is in fact independent of  $\delta$  for  $\delta \leq \text{dist}(A, B)$ , it follows that

$$\begin{aligned} \mathbf{F}_k^{\text{long}}(A, B) &= \gamma \int_A \int_B \partial_i \partial_j \partial_k N(x - y) (\mathbf{m}_A)_i(x) (\mathbf{m}_B)_j(y) dy dx \\ &= \gamma \int_A (\mathbf{m}_A)_i(x) \partial_i \int_B \partial_j \partial_k N(x - y) (\mathbf{m}_B)_j(y) dy dx \\ &= \gamma \int_A (\mathbf{m}_A)_i(x) \partial_i \left( \int_B \partial_j (\mathbf{m}_B)_j(y) \partial_k N(x - y) dy \right. \\ &\quad \left. - \int_{\partial B} (\mathbf{m}_B)_j(y) (\mathbf{n}_B)_j(y) \partial_k N(x - y) ds_y \right) dx \end{aligned}$$

and hence  $\mathbf{F}^{\text{long}}(A, B) = \int_A (\mathbf{m}_A(x) \cdot \nabla) \mathbf{H}_B(x) dx$  by (8).  $\square$



**Remark 2.** The formula for  $\mathbf{F}_{\text{sep}}^{\text{lim}}(A, B)$  is equal to the well-known formula for the magnetic force,  $\mathbf{F}(A, B)$ , between two bodies being a macroscopic distance apart, see e.g. [Bro66]. As proven in [PPSa],  $\mathbf{F}$  converges to  $\mathbf{F}^{\text{Br}}$  as  $\text{dist}(A, B) \rightarrow 0$ . Furthermore, by Theorem 3.1 in [PPSa], a formal application of the formulae for  $\mathbf{F}^{\text{lim}}$  and  $\mathbf{F}^{\text{Br}}$  to the case of separated bodies yields (36) since then the trace of  $\mathbf{m}_B$  on  $\partial A$  is zero, i.e., formally, all forces coincide in this case.

## 5.2 $\ell$ -dependent $a$ .

In order to complete the picture of limiting forces in dependence of the distance of two bodies, we finally analyze the regime in which  $\varepsilon = a/\ell$ , where  $a = a(\ell) \rightarrow \infty$  such that  $a/\ell \rightarrow 0$  as  $\ell \rightarrow \infty$ . That is, we consider two bodies which are in contact on the macroscale whose microscopic distance tends to infinity with the lattice constant  $\ell^{-1}$  converging to 0. By Theorem 4.3 and Remark 2 we expect to recover Brown's formula. In fact, this turns out to be true:

**Theorem 5.2.** *Let  $\varepsilon(\ell) := a(\ell)/\ell$ ,  $a(\ell) \in \mathbb{N}$ , such that  $\varepsilon(\ell) \rightarrow 0$  and  $a(\ell) \rightarrow \infty$  as  $\ell \rightarrow \infty$  and let Assumption  $\mathcal{A}$  hold. Then*

$$\lim_{\ell \rightarrow \infty} \mathbf{F}_k^{(\ell)}(A, B) = \mathbf{F}^{\text{Br}}(A, B),$$

where  $\mathbf{F}_k^{(\ell)}(A, B)$  is as in (4) with  $\varepsilon = \varepsilon(\ell)$ .

*Proof.* We split into long and short range parts as before. Literally the same argument as for fixed  $a$  (Proposition 3.1) shows that again

$$\mathbf{F}^{\text{long}}(A, B) = \int_A (\mathbf{m}_A \cdot \nabla) \mathbf{H}_{A \cup B} dx + \frac{\gamma}{2} \int_{\partial A} (\mathbf{m}_A \cdot \mathbf{n}_A) ((\mathbf{m}_A - \mathbf{m}_B) \cdot \mathbf{n}_A) \mathbf{n}_A ds_x. \quad (37)$$

The short range term is more subtle. Note that Lemma 3.5 also holds if  $a$  depends on  $\ell$  such that  $a(\ell)/\ell \rightarrow 0$ . To prove this, note that the left-hand side in (14) vanishes unless  $|z| \geq c\varepsilon$ . Hence we obtain equation (15) and it remains to estimate

$$\begin{aligned} & -\gamma \int_{\partial A \cap \partial B} (\mathbf{m}_A)_i(x) (\mathbf{m}_B)_j(x) \times \\ & \quad \times \sum_{z \in \frac{1}{\ell} \mathcal{L} \setminus \{0\}} \partial_i \partial_j P_k^{(\delta)}(z) \frac{1}{\ell^d} ((\mathbf{n}_A(x) \cdot (z - \varepsilon(\ell)\nu))_+ - (\mathbf{n}_A(x) \cdot z)_+) ds_x. \end{aligned} \quad (38)$$

Observe that  $|(\mathbf{n}_A(x) \cdot (z - \varepsilon(\ell)\nu))_+ - (\mathbf{n}_A(x) \cdot z)_+| \leq c\varepsilon(\ell)$ . Moreover, since  $|P_k^{(\delta)}(z) - \partial_i \partial_j \partial_k N(z)|$  can be estimated by a constant  $c(\delta)$  for  $|z| \leq \delta$  and by  $c|z|^{-d-1}$  for  $|z| \geq \delta$ , replacing the term  $\partial_i \partial_j P_k^{(\delta)}(z)$  in the sum in (38) by  $\partial_i \partial_j \partial_k N(z)$  leads to an error term which is bounded by

$$\begin{aligned} \sum_{z \in \frac{1}{\ell}\mathcal{L}, |z| \leq \delta} c(\delta) \frac{\varepsilon(\ell)}{\ell^d} + \sum_{z \in \frac{1}{\ell}\mathcal{L}, |z| \geq \delta} c|z|^{-d-1} \frac{\varepsilon(\ell)}{\ell^d} &\leq c(\delta) |B_\delta(0)| \ell^d \frac{\varepsilon}{\ell^d} + c\varepsilon \int_\delta^\infty r^{-d-1} r^{d-1} dr \\ &= c(\delta)\varepsilon(\ell) \rightarrow 0 \end{aligned}$$

as  $\ell \rightarrow \infty$ . So (38) equals  $\mathbf{G}_k(a)$  in (21) up to negligible errors. Now Theorem 5.2 follows by Proposition 4.2.  $\square$

## 6 Conclusions

We have derived limiting force formulae for two magnetic bodies in dependence on their mutual distance starting from atomistic dipole-dipole interactions. Brown's classical formula has been justified in the regime where the two bodies are far apart from each other on a microscopical scale, i.e., their distance is large compared to the lattice spacing  $\ell^{-1}$ . For distances of only few atomic lattice spacings, however, our results show that the limiting forces have to be augmented by an additional, distance-dependent term that reflects the discrete nature of the underlying atomic lattice. In particular, for bodies in contact on the microscale we recover the results of [Sch05, PPSa]. The following table summarizes the regimes that we have investigated and the corresponding limit forces:

$\varepsilon$	micro distance	macro distance	force
$\varepsilon = 0$	$a = 0$	0	$\mathbf{F}^{\text{lim}} = \mathbf{F}^{\text{long}} + \mathbf{F}^{\text{short}}$
$\varepsilon = \frac{a}{\ell}, a \in \mathbb{N}$ const	$a$ finite	0	$\mathbf{F}^{\text{lim}}(a) = \mathbf{F}^{\text{lim}} + \mathbf{G}(a)$
	$a \rightarrow \infty$	0	$\lim_{a \rightarrow \infty} \mathbf{F}^{\text{lim}}(a) = \mathbf{F}^{\text{Br}}$
$\varepsilon = \frac{a(\ell)}{\ell}, a(\ell) \rightarrow \infty$ such that $\varepsilon \rightarrow 0$ as $\ell \rightarrow \infty$	$a(\ell) \rightarrow \infty$	0	$\mathbf{F}^{\text{lim}} = \mathbf{F}^{\text{Br}}$
$\varepsilon > 0$ const	$\infty$	$> 0$	$\mathbf{F}_{\text{sep}}^{\text{lim}} = \mathbf{F}$

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