

Discrete-to-continuum limit of magnetic forces

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Abstract

We derive a formula for the forces within a magnetized body, starting from a discrete configuration of magnetic dipoles on a Bravais lattice. The resulting force consists of the usual (nonlocal) volume term and an additional local surface term, whose coefficients involve a singular sum over the lattice. The force thus obtained is different from the usual continuum expression, reflecting the different character of the lattice regularization of the underlying hypersingular integral. *To cite this article: S. Müller, A. Schlömerkemper, C. R. Acad. Sci. Paris, Ser. I 335 (2002) 393–398.*

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Large limites de forces magnétiques du discret au continu

Résumé

Dans cette Note, nous dérivons une formule pour les forces dans un corps magnétisé rigide, prenant comme point de départ une configuration de dipôles magnétiques dans un réseau de Bravais et considérant la limite lorsque le paramètre de réseau tend vers zéro. Le terme volumique correspond à la formule pour les forces utilisée dans les théories de milieux continus. Le terme local de surface dans notre formule est, cependant, différent de celui de la théorie du continu. Mathématiquement ceci s'explique par le fait que l'approximation du réseau équivaut à une régularisation différente d'une intégrale hyper-singulière. *Pour citer cet article : S. Müller, A. Schlömerkemper, C. R. Acad. Sci. Paris, Ser. I 335 (2002) 393–398.*

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Dans cette Note, nous dérivons une formule pour les forces dans un corps magnétisé rigide, prenant comme point de départ une configuration de dipôles magnétiques dans un réseau de Bravais et considérant la limite lorsque le paramètre de réseau tend vers zéro. Nous considérons un réseau de Bravais d'atomes $\mathcal{L} = \{x \in \mathbb{R}^3 : x = \sum_{i=1}^3 \mu_i e_i, \mu_i \in \mathbb{Z}\}$, où (e_1, e_2, e_3) est une base de \mathbb{R}^3 . Nous supposons, pour simplifier, que la cellule unité $\mathcal{U} = \{\sum_{i=1}^3 \lambda_i e_i : 0 \leq \lambda_i < 1\}$ a un volume unité. Soit Ω un domaine borné de \mathbb{R}^3 et τ un sous-ensemble de Ω tel que $\partial\Omega \cap \partial\tau = \emptyset$. On note n la normale extérieure à $\partial\tau$. On se fixe une magnétisation ambiante $m : \Omega \rightarrow \mathbb{R}^3$. On associe à chaque point du réseau $\frac{1}{l}\mathcal{L}$, $l \in \mathbb{N}$, un moment dipolaire magnétique $m^{(l)}(x)$ donné par (5). Ce changement d'échelle assure que le moment magnétique totale par unité de volume est finie. Pour d'autres approches, nous nous référerons à [6].

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Le champ magnétique H_y généré par un dipôle $m^{(l)}(y)$ en y est donné par $(H_y)_i(x) = K_{ij}(x - y)m_j^{(l)}(y)$, où K est donné par (2). La force exercée par un dipôle en y sur un dipôle situé en x est donnée par $f_k = m_i^{(l)}(x)\partial_i(H_y)_k(x)$ (voir par exemple [2], p. 13). Puisque $\partial_i K_{kj} = \partial_i \partial_k \partial_j N$ est complètement symétrique en i, j, k , on a de manière équivalente $f_k = m_i^{(l)}(x)\partial_k(H_y)_i(x)$.

La force, $F_k^{(l)}$, exercée par les moments magnétiques dans $(\Omega \setminus \bar{\tau}) \cap \frac{1}{l}\mathcal{L}$ sur les moments magnétiques dans $\bar{\tau} \cap \frac{1}{l}\mathcal{L}$ est donnée par (6).

THÉORÈME 0.1. – *Supposons que τ est un domaine C^2 et que $\partial\tau$ satisfait la condition de non-dégénérescence (S) plus bas. Supposons que $m|_{\tau} \in W^{1,\infty}(\tau; \mathbb{R}^3)$ et que $m|_{\Omega \setminus \bar{\tau}} \in W^{1,\infty}(\Omega \setminus \bar{\tau}; \mathbb{R}^3)$. Alors, la limite $\lim_{l \rightarrow \infty} F^{(l)} = F^{(\text{lim})}$ existe et elle est donnée par (7), où H_Ω désigne le champ magnétique engendré par la magnétisation dans Ω (voir (1)) et m^+ et m^- désignent les traces extérieures et intérieures de m , respectivement.*

Ici, les S_{ijkp} ne dépendent que du réseau \mathcal{L} (et de γ) et sont donnés par la somme singulière, (8), où $\mathcal{L}^* = \mathcal{L} \setminus \{0\}$ et $K^{(\delta)}$ est un noyau régularisé (voir (10) plus bas).

On dit que $\partial\tau$ satisfait la condition de non-dégénérescence (S) si τ est un domaine de bord de régularité Lipschitz, que $\partial\tau$ peut être recouvert par l'adhérence d'un nombre fini de sous-variétés U_i de \mathbb{R}^3 de classe $C^{1,1}$ (telles que ∂U_i est une réunion finie de courbes rectifiables) et que le bord de l'ensemble $\partial^+\tau = \{x \in \partial\tau \cap (\bigcup_i U_i) : n(x) \cdot z > 0\}$ est une réunion finie de courbes rectifiables, où le nombre et la longueur des courbes doivent être bornés indépendamment de z . Cette condition est satisfaite, par exemple, par un polyèdre et par un ensemble uniformément convexe.

Un ingrédient crucial de la démonstration est une estimation de sommes de Riemann dans les domaines fins (voir Lemmes 5.1 et (13) plus bas). Le terme volumique dans $F^{(\text{lim})}$ correspond à la formule pour les forces (4) utilisée dans les théories de milieux continus (voir par exemple [2], p. 57; pour des expositions plus récentes de théories électrodynamiques du continu, voir [1,4]). Le terme local de surface dans notre formule est, cependant, différent de celui de la théorie du continu. Mathématiquement ceci s'explique par le fait que l'approximation du réseau équivaut à une régularisation différente d'une intégrale hyper-singulière.

Une motivation pour étudier les forces plutôt que l'énergie est la modélisation de nouveaux produits potentiels à base d'alliages à mémoire de formes ferro-magnétiques (voir [5]). Dans ce cadre, la compréhension de la dynamique de ces instruments requiert la compréhension de forces appropriées. Notre étude peut être vue comme un premier pas, modeste, dans cette direction : nous considérons un corps magnétisable rigide et étudions l'influence d'un réseau cristallin sous-jacent sur les forces magnétiques. Les résultats présentés ici constituent une partie de [7], à laquelle nous référons le lecteur pour plus de détails.

1. Introduction

In this note we derive a formula for the forces within a rigid magnetized body, starting from a configuration of magnetic dipoles on a Bravais lattice and considering the limit for vanishing lattice parameter (see Theorem 3.1 below). The limiting force consists of a nonlocal volume term and a local surface contribution. If the magnetization does not jump at the boundary of the subbody τ on which the force is exerted then the surface term is linear in the surface normal n and quadratic in the magnetization m . The coefficients depend only on the lattice \mathcal{L} .

The volume term agrees with the usual force formula (4) used in the continuum theory (see, e.g., [2], p. 57; for recent expositions of the electrodynamics of continua see [1,4]). The local surface term in our formula is, however, different from the one in the continuum theory. Mathematically this can be traced back to the fact that the lattice approximation amounts to a different regularization of a hypersingular integral. The same phenomenon occurs in the study of the limiting energy of a lattice of dipoles (see [6]). The study

of forces is more delicate since it involves hypersingular kernels (of order $|z|^{-4}$ in three dimensions) rather than singular kernels of order $|z|^{-3}$.

One motivation to study forces rather than energy is the modelling of potential new micro-devices based on ferromagnetic shape memory alloys (*see* [5]). To describe the dynamics of such devices one needs to understand the relevant forces. From the point of view of identifying materials which give particularly good performance one would like to obtain continuum models whose parameters are not only determined phenomenologically but can be related to known or computed atomistic properties.

Our study may be viewed as a modest first step in this direction. We consider a rigid magnetizable body and study the influence of an underlying lattice structure on the magnetic forces. The results reported here form part of [7], to which we refer for further details.

2. Continuous setting

A magnetizable rigid body is identified with a bounded domain $\Omega \subset \mathbb{R}^3$ and $m : \Omega \rightarrow \mathbb{R}^3$ denotes its magnetization (in the following we extend m by zero to \mathbb{R}^3). The magnetic field H generated by m is the unique L^2 solution of Maxwell's equations $\operatorname{curl} H = 0$, $\operatorname{div}(\gamma m + H) = 0$, where γ is a constant which depends on the system of physical units used. For $m \in L^2(\Omega)$ the field H is (up to a factor $-\gamma$) the L^2 projection onto gradient fields and its i -th component is given by the singular integral

$$H_i(x) = \int K_{ij}(x - y)m_j(y) dy, \quad (1)$$

$$K_{ij}(z) = \partial_i \partial_j N(z) = -\frac{\gamma}{4\pi |z|^3} \left(\mathbb{1} - 3 \frac{z}{|z|} \otimes \frac{z}{|z|} \right)_{ij}, \quad N(z) = \frac{\gamma}{4\pi} \frac{1}{|z|}. \quad (2)$$

If A and B are two bodies with positive distance and m_A and m_B are their magnetizations then the force exerted by A and B is given by (*see*, e.g., [2], p. 55)

$$F_{AB} = \int_A (m_A \cdot \nabla) H_B dx. \quad (3)$$

We are interested in the force exerted on a subbody $\tau \subset \Omega$ by its complement $\Omega \setminus \bar{\tau}$ (for simplicity we will always assume that $\partial\tau \cap \partial\Omega = \emptyset$). This is more delicate because τ and $\Omega \setminus \bar{\tau}$ are not separated. Indeed, a formal application of the force formula (3) leads to a hypersingular integral. Nonetheless one can show that the integral exists, e.g., if $\partial\tau$ is C^2 and if $m|_\tau$ and $m|_{\Omega \setminus \bar{\tau}}$ belong to $W^{1,2}$ (see [7]). If one writes $H_\Omega = H_\tau + H_{\Omega \setminus \bar{\tau}}$, where H_τ is the field induced by $m|_\tau$, and performs a careful integration by parts, one obtains Brown's force formula

$$F^{(Br)} = \int_\tau (m \cdot \nabla) H_\Omega dx + \frac{\gamma}{2} \int_{\partial\tau} (m^- \cdot n)^2 n d\mathcal{H}^2, \quad (4)$$

where n is the outer normal of $\partial\tau$ and m^- is the inner trace of m ; later m^+ denotes the outer trace. Interestingly the surface term is not linear in the normal n , i.e. it is different from a usual surface force term in continuum mechanics, which in view of Cauchy's theorem should be linear in n . Brown argues that formula (4) in fact only gives the long range contribution and that there will be other local forces (which are included in a phenomenological continuum model anyhow) which restore the validity of Cauchy's theorem (*see* [2], Section 5). Brown suggests ([2], p. 52) to determine such local corrections from an atomistic approach. One such approach, starting from a lattice of dipoles, is carried out in the next section. DeSimone and Podio-Guidugli [3] have shown in a careful analysis that (4) is consistent with the usual setting of continuum mechanics if one takes the relevant self-forces properly into account.

3. Discrete setting and continuum limit

We consider a Bravais lattice $\mathcal{L} = \{x \in \mathbb{R}^3 : x = \sum_{i=1}^3 \mu_i e_i, \mu_i \in \mathbb{Z}\}$ of atoms, where (e_1, e_2, e_3) is a basis of \mathbb{R}^3 . For convenience we assume that the unit cell $\mathcal{U} = \{\sum_{i=1}^3 \lambda_i e_i : 0 \leq \lambda_i < 1\}$ has unit volume.

Let Ω be a bounded domain in \mathbb{R}^3 and let τ be a subset of Ω such that $\partial\Omega \cap \partial\tau = \emptyset$. We fix a background magnetization $m : \Omega \rightarrow \mathbb{R}^3$. To each point in the scaled lattice $\frac{1}{l}\mathcal{L}$, $l \in \mathbb{N}$, we assign a magnetic dipole moment

$$m^{(l)}(x) = \frac{1}{l^3}m(x), \quad \text{for } x \in \frac{1}{l}\mathcal{L}. \quad (5)$$

This scaling ensures that we obtain a finite total magnetic moment per unit volume. For other ways to relate the dipole moments on different lattices and to define a limiting continuous magnetization see [6].

The magnetic field H_y generated by a dipole $m^{(l)}(y)$ at y is given by $(H_y)_i(x) = K_{ij}(x - y)m_j^{(l)}(y)$, where K is given by (2). The force exerted by a dipole at y on a dipole at x is given by $f_k = m_i^{(l)}(x)\partial_i(H_y)_k(x)$ (see, e.g., [2], p. 13). Since $\partial_i K_{kj} = \partial_i \partial_k \partial_j N$ is totally symmetric in i, j, k , we have equivalently $f_k = m_i^{(l)}(x)\partial_k(H_y)_i(x)$.

The force which magnetic moments in $(\Omega \setminus \bar{\tau}) \cap \frac{1}{l}\mathcal{L}$ exert on magnetic moments in $\bar{\tau} \cap \frac{1}{l}\mathcal{L}$ is given by

$$F_k^{(l)} = \sum_{x \in \bar{\tau} \cap \frac{1}{l}\mathcal{L}} \sum_{y \in (\Omega \setminus \bar{\tau}) \cap \frac{1}{l}\mathcal{L}} \partial_k K_{ij}(x - y)m_i^{(l)}(x)m_j^{(l)}(y). \quad (6)$$

THEOREM 3.1. – Suppose that τ is a C^2 domain and $\partial\tau$ satisfies the non-degeneracy condition (S) below. Suppose that $m|_\tau \in W^{1,\infty}(\tau; \mathbb{R}^3)$ and $m|_{\Omega \setminus \bar{\tau}} \in W^{1,\infty}(\Omega \setminus \bar{\tau}; \mathbb{R}^3)$. Then the limit $\lim_{l \rightarrow \infty} F^{(l)} = F^{(\lim)}$ exists and

$$\begin{aligned} F_k^{(\lim)} &= \int_\tau (m(x) \cdot \nabla)(H_\Omega)_k(x) dx + \frac{\gamma}{2} \int_{\partial\tau} (m^- \cdot n)(x) ((m^- - m^+) \cdot n)(x) n_k(x) d\mathcal{H}^2(x) \\ &\quad + \frac{1}{2} \int_{\partial\tau} m_i^-(x) m_j^+(x) S_{ijkp} n_p(x) d\mathcal{H}^2(x). \end{aligned} \quad (7)$$

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

$$S_{ijkp} := -\lim_{\delta \rightarrow 0} \lim_{l \rightarrow \infty} \sum_{z \in B_\delta \cap \frac{1}{l}\mathcal{L}^*} \partial_k (K - K^{(\delta)})_{ij}(z) z_p \frac{1}{l^3}, \quad (8)$$

where $\mathcal{L}^* = \mathcal{L} \setminus \{0\}$ and where $K^{(\delta)}$ is the regularized kernel defined in (10) below. For the cubic unit lattice \mathbb{Z}^3 all entries of S vanish except

$$S_{iikk} = -\frac{1}{2}\mathcal{S} + \frac{\gamma}{5}, \quad \text{for } i \neq k, \quad S_{kkkk} = \mathcal{S} + \frac{3\gamma}{5},$$

where $\mathcal{S} \approx \frac{\gamma}{4\pi} 9.33 \dots$

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

$$\partial^+ \tau = \left\{ x \in \partial\tau \cap \left(\bigcup_i U_i \right) : n(x) \cdot z > 0 \right\} \quad (9)$$

is a finite union of rectifiable curves, where the number and the length of the curves are bounded independently of z . This condition is for example satisfied by polyhedra or by uniformly convex sets.

4. Sketch of proof: Long range term

We first split the kernel K into a long range smooth part and a short range part. Let $\varphi \in C_0^\infty(\mathbb{R}^3)$ with $0 \leq \varphi \leq 1$, $\varphi(z) = 1$ if $|z| \leq \frac{1}{2}$, $\varphi(z) = 0$ if $|z| \geq 1$. Set $\varphi^{(\delta)}(z) = \varphi(z/\delta)$,

$$K_{ij}^{(\delta)}(z) = \partial_i \partial_j ((1 - \varphi^{(\delta)}(z)) N(z)), \quad (10)$$

and define the long range and the short range part of the force by

$$F_k^{(l,\delta)} = \sum_{x \in \bar{\tau} \cap \frac{1}{l}\mathcal{L}} \sum_{y \in (\Omega \setminus \bar{\tau}) \cap \frac{1}{l}\mathcal{L}} \partial_k K_{ij}^{(\delta)}(x-y) m_i^{(l)}(x) m_j^{(l)}(y), \quad (11)$$

$$\mathcal{F}_k^{(l,\delta)} = \sum_{x \in \bar{\tau} \cap \frac{1}{l}\mathcal{L}} \sum_{y \in (\Omega \setminus \bar{\tau}) \cap \frac{1}{l}\mathcal{L}} \partial_k (K - K^{(\delta)})_{ij}(x-y) m_i^{(l)}(x) m_j^{(l)}(y). \quad (12)$$

We first take the limit $l \rightarrow \infty$ and then $\delta \rightarrow 0$. Since $K^{(\delta)}$ is regular, the limit $\lim_{l \rightarrow \infty} F_k^{(l,\delta)}$ just amounts to the replacement of a Riemann sum by an integral. The subsequent limit $\delta \rightarrow 0$ can be handled by a careful analysis of the relevant singular integrals (see [7]) and we get

$$\lim_{\delta \rightarrow 0} \lim_{l \rightarrow \infty} F_k^{(l,\delta)} = \int_{\tau} (m(x) \cdot \nabla) (H_{\Omega})_k(x) dx + \frac{\gamma}{2} \int_{\partial\tau} (m^- \cdot n)(x) ((m^- - m^+) \cdot n)(x) n_k(x) d\mathcal{H}^2(x).$$

5. Sketch of proof: Short range term

This term is more delicate since the sum in (12) is hypersingular, the kernel $\partial_k (K - K^{(\delta)})(z)$ grows like $|z|^{-4}$. We first use an argument by Cauchy to reorganize the sum; this can be also seen as clever summation by parts. After this we are still left with Riemann sums whose discretization is of the same order as one dimension of the summation domain. These will be treated by a careful exploitation of the lattice structure and an application of the coarea formula.

Let B_{δ} be an open ball with radius δ and for $z \in B_{\delta}$ consider the set

$$\tau_z = \{x \in \bar{\tau} : x + z \in \Omega \setminus \bar{\tau}\}. \quad (13)$$

Using the change of variables $y = x + z$ and the definition of $m^{(l)}$ we can rewrite the expression (12) for the short range term as

$$F_k^{(l,\delta)} = - \sum_{z \in B_{\delta} \cap \frac{1}{l}\mathcal{L}^*} \partial_k (K - K^{(\delta)})_{ij}(z) l^{-6} \sum_{x \in \tau_z \cap \frac{1}{l}\mathcal{L}} m_i(x) m_j(x+z). \quad (14)$$

Suppose for a moment that m was constant in a neighbourhood of $\partial\tau$. Then we had to evaluate the sum

$$l^{-3} \sum_{z \in B_{\delta} \cap \frac{1}{l}\mathcal{L}^*} \partial_k (K - K^{(\delta)})_{ij}(z) l^{-3} \# \left(\tau_z \cap \frac{1}{l}\mathcal{L} \right),$$

where $\#A$ denotes the number of points in a set A . One can show (e.g. using the coarea formula) that the volume of the set τ_z is given by $\int_{\partial\tau} (z \cdot n)_+ d\mathcal{H}^2 + \mathcal{O}(|z|^{1+\beta})$, with $\beta > 0$. Once we have the same expression for $l^{-3} \#(\tau_z \cap \frac{1}{l}\mathcal{L})$, we can conclude easily since $\partial_k (K - K^{(\delta)})_{ij}(z)$ is antisymmetric in z and the sum over the error term can be bounded by $C \int_{B_{\delta}} |z|^{\beta-3} \leq C \delta^{\beta}$ and vanishes as $\delta \rightarrow 0$. For z of the order of $\frac{1}{l}$ one might expect, however, that the relative error between $\#(\tau_z \cap \frac{1}{l}\mathcal{L})$ and the volume is of order 1, since the discretization is comparable to the width of τ_z . Due to the $|z|^{-4}$ singularity of $\partial_k K_{ij}$ this would lead to an error of order 1 in the sum. A more careful analysis shows that for $z \in \frac{1}{l}\mathcal{L}$ this difficulty can be overcome.

LEMMA 5.1. – 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

$$\left| \frac{1}{l^3} \sum_{x \in \tau_z \cap \frac{1}{l}\mathcal{L}} f(x) - \int_{\partial\tau} f(\xi) (n(\xi) \cdot z)_+ d\mathcal{H}^2(\xi) \right| \leq C |z|^{4/3}. \quad (15)$$

The constant C depends only on $\sup |f|$, the Lipschitz constant of f and on τ .

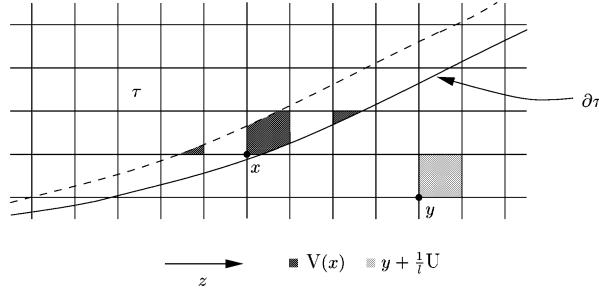


Figure 1. – A modified unit cell.

Figure 1. – Une maille élémentaire modifiée.

Since $x \mapsto m^-(x)m^+(x+z)$ is Lipschitz on τ_z , the lemma yields the convergence of the short range term and hence Theorem 3.1 (to show the convergence of the singular sum (8) one approximates the sum in the far field by an integral and uses suitable integration by parts).

Proof of Lemma 5.1 (sketch). – Let $\Gamma = \partial(\partial^+\tau) \cup \bigcup_i \partial U_i$ where $\partial^+\tau$ is given by (9). For $x \in \tau_z$ let $r_z(x) \in \partial\tau$ denote the first intersection point of the half-line $x + tz$, $t \geq 0$, with $\partial\tau$. By definition of τ_z this intersection point corresponds to a value $t \in [0, 1]$. We first consider the two bad sets $\mathcal{B}_I = \{x \in \frac{1}{l}\mathcal{L} : \text{dist}(x, \Gamma) < 8\varrho\}$, where $\varrho = C_0(|z| + l^{-\beta})$, $\beta \in (\frac{1}{2}, 1)$, and $\mathcal{B}_{II} = \{x \in (r_z \cap \frac{1}{l}\mathcal{L}) \setminus \mathcal{B}_I : n(r_z(x)) \cdot z \leq C_1(l^{\beta-1} + \varrho)|z|\}$, and we estimate $\#\mathcal{B}_I \leq Cl^3|z|^{2\beta}$, $\#\mathcal{B}_{II} \leq Cl^3|z|^{2-\beta}$ and finally set $\beta = \frac{2}{3}$. The first estimate follows by covering Γ with suitable balls which contain for each point in \mathcal{B}_I also a full unit cell in $\frac{1}{l}\mathcal{L}$. The second estimate is more delicate. Since z is nearly tangential to $\partial\tau$, a unit cell around $x \in \mathcal{B}_{II}$ is projected by r_z to a large set on $\partial\tau$. These projections are essentially disjoint and this yields an estimate for $\#\mathcal{B}_{II}$.

Finally consider x in the good set $G = (\tau_z \cap \frac{1}{l}\mathcal{L}) \setminus (\mathcal{B}_I \cup \mathcal{B}_{II})$. The unit cell $x + \frac{1}{l}\mathcal{U}$ may not be contained in τ_z (see Fig. 1) and this is the reason why one cannot naively compare the number of points in τ_z with the volume of τ_z . Thus we define a modified unit cell $\mathcal{V}(x) = \bigcup_{k=-K}^K (x + kz + \frac{1}{l}\mathcal{U}) \cap \tau_z$, where $K = [\varrho/|z|]$. Then we can show that $\mathcal{V}(x)$ has volume l^{-3} and that the volume of the difference between τ_z and $\bigcup_{x \in G} \mathcal{V}(x)$ is of lower order. The proof is finished by an application of the coarea formula.

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