WULFF-CRYSTALS IN FCC AND HCP LATTICES

MARCO CICALESE, LEONARD KREUTZ, AND GIAN PAOLO LEONARDI

Abstract. We consider a system of N hard spheres sitting on the nodes of a lattice and interacting via a sticky-disk potential. We obtain by Γ-convergence the variational coarse grained energy of the system as $N \to +\infty$ (continuum limit) and the interaction energy does not exceed the ground state energy more than $N^{2/3}$ (surface scaling). We prove that the limit energy is of perimeter type and we compute explicitly the Wulff shape of the continuum limit. Exploiting such a result, we prove that crystallization on the face-centered cubic lattice is preferred to crystallization on the hexagonal closed-packed lattice.

1. Introduction

A fundamental problem in crystallography is to understand why ensembles of large number of atoms arrange themselves into crystals at low temperatures. From the mathematical point of view, the challenge to prove that equilibrium configurations of certain phenomenological interaction energies exhibit these structures is referred to as the crystallization problem [6].

At zero temperature the internal energy of a configuration of atoms is expected to be solely governed by its geometric arrangement. Within the framework of molecular mechanics [1, 18, 24], one identifies each ensemble of atoms with its atomic positions $X = \{x_1, \dots, x_N\} \subset \mathbb{R}^3$ and associates to it a configurational energy of the form

$$\mathcal{E}(X) := \frac{1}{2} \sum_{i \neq j} V(|x_i - x_j|)\,, \tag{1}$$

where $V : \mathbb{R} \to \mathbb{R} \cup \{+\infty\}$ is an empirical pair interaction potential (the factor $\frac{1}{2}$ accounts for double counting). Such potentials are typically repulsive at short distances and attractive for large distances. The latter property favors the formation of clusters while the former prevents the atoms from getting too close to each other.

Notably, even under very simplifying assumptions on the interaction potentials, the mathematical literature on rigorous crystallization results is scarce. In fact, for finite N finite, only results in one and two space dimensions are available. In particular, for Lennard–Jones type potentials, that share the same characteristics as V above in one space dimension crystallization has been proved in [19]. In higher space dimensions only partial results are available. Most importantly, in [12, 14, 28] it has been proven that crystalline structures have optimal bulk energy scaling. In two dimensions, only results for (some variants of) the sticky disc potential (see Fig. 1)

$$V(r) := \begin{cases} +\infty & \text{if } r < 1\,, \\ -1 & \text{if } r = 1\,, \\ 0 & \text{otherwise} \end{cases} \tag{2}$$

Key words and phrases. Wulff shape, isoperimetric inequality, crystallization.

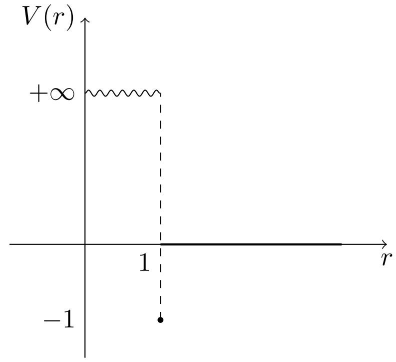

FIGURE 1. The sticky disc interaction potential V.

are available [11, 21, 23, 26]. More recently, crystallization results have been proved for ionic compounds [15, 16] and carbon structures in [25]. The potential given in (2) models the atoms as hard spheres that interact exactly when two are tangent. In $\mathbb{R}^d$ the kissing number $k(d)$ is the highest number of d-dimensional spheres of radius $\frac{1}{2}$ to a given sphere of the same size. It is well known that $k(2) = 6$ and $k(3) = 12$, see [27]. For a given configurations of non-overlapping equal balls centered at $X = \{x_1, \ldots, x_N\} \subset \mathbb{R}^d$, $N \in \mathbb{N} \cup \{+\infty\}$ the coordination number of $x \in X$ is the number of those spheres tangent to the one centered at x. In two dimension there is a unique (up to a rigid motion) configuration such that all atoms have as coordination number the kissing number. In this case the set X is the triangular lattice with lattice spacing one. In three dimensions the problem is much more intricate. In fact, there exist infinitely many configurations with constant coordination number equal to $k(3)$. An infinite class of configurations can be obtained by stacking in opportune way layers of triangular lattices. A remarkable result by Hales [20] shows that such structures solve Kepler's conjecture in that they have the maximal packing density in $\mathbb{R}^3$. Two notable cases of the aforementioned structures are the face-centered cubic lattice $\mathcal{L}_{\mathrm{FCC}}$ and the hexagonal closed-packed lattice $\mathcal{L}_{\mathrm{HCP}}$ (see (8)–(10) for their precise definition) which are the most prevalent among the crystalline arrangements in the periodic table of elements.

In this paper we want to investigate already crystallized configurations, i.e. configurations $X \subset \mathcal{L}$ where $\mathcal{L} = \mathcal{L}_{\mathrm{FCC}}$ or $\mathcal{L} = \mathcal{L}_{\mathrm{HCP}}$. For such $X = \{x_1, \ldots, x_N\} \subset \mathcal{L}$, fixing the lattice spacing to be 1, we have

$$\mathcal{E}(X) = \frac{1}{2}\sum_{i \neq j} V(|x_i - x_j|) = -\sum_{i=1}^{n} \#(\mathcal{N}(x_i) \cap X)\,, \text{ where } \mathcal{N}(x) = \{y \in \mathcal{L} \colon |x - y| = 1\}\,.$$

As described above the minimal energy per atom is $-k(3) = -12$. Further information on $\mathcal{E}$ as N grows can be obtained by referring it to the minimal energy per atom and calculating the excess energy $E_N(X)$. More precisely, in Theorem 2.2, we carry out a rigorous variational asymptotic expansion (see [8]) of $\mathcal{E}(X)$, by considering

$$E_N(X) = N^{-2/3}\left(\mathcal{E}(X) + 12N\right) = N^{-2/3}\sum_{i=1}^{N}(12 - \#(\mathcal{N}(x) \cap X)) \tag{3}$$

and calculating its Γ-limit [7, 10] as N tends to infinity. This analysis has been done out in two dimensions for configurations confined to the triangular lattice [5] as well as without any confinement assumptions [17]. Note that, the scaling factor $N^{-2/3}$ is used in order to keep the energy bounded as the number of atoms grows. In fact, by the isoperimetric inequality, given N atoms, the number of those contributing to the energy has the perimeter scaling $N^{2/3}$. By associating to each configuration its rescaled emprical measures

$$\mu_N(X) := \frac{1}{N}\sum_{i=1}^{N} \delta_{N^{-1/3}x_i}\,, \tag{4}$$

we show in Theorem 2.2 i) that the sequence of rescaled energies (3) is equi-coercive with respect to the weak star convergence of the associated empirical measures. In Theorem 2.2 ii), iii) we exploit integral representation theorems [2, 4] to show that the limit energy is finite on the set of measures $\mu = \sqrt{2}\mathcal{L}^3 \llcorner E$, where $E \subset \mathbb{R}^3$ is a set of finite perimeter, on which it takes the form

$$E_{\mathcal{L}}(\mu) := \int_{\partial^* E} \varphi_{\mathcal{L}}(\nu)\,\mathrm{d}\mathcal{H}^2\,. \tag{5}$$

Here, $\partial^* E$ denotes the measure reduced boundary of the set E, $\nu(x)$ denotes its unit outer normal at the point $x \in \partial^* E$ and $\varphi_{\mathcal{L}}$ is an anisotropic surface energy density depending on the underlying lattice $\mathcal{L}$. The main body of this work lies in the characterization of the surface energy density $\varphi_{\mathcal{L}} \colon \mathbb{R}^3 \to [0, +\infty)$. Here, we exploit a recent finite cell formula [9], to be able to explicitly calculate the density for both the FCC and the HCP lattice. Finally, for each lattice, we solve the associated isoperimetric problem [13]

$$m_{\mathcal{L}} := \min\left\{\int_{\partial^* E} \varphi_{\mathcal{L}}(\nu)\,\mathrm{d}\mathcal{H}^2 \colon |E| = 1\right\} \tag{6}$$

by calculating the (up to translation unique) set minimizing (6), also known as Wulff crystal [29]. We show that $m_{\mathrm{FCC}} < m_{\mathrm{HCP}}$ which also implies (since Γ-convergence and coercivity implies the convergence of minimum values) that, for large number of atoms, crystallization on the face-centered cubic lattice is preferred to that on the hexagonal-closed packed lattice.

The article is structured as follows. In Section 2, we introduce the necessary mathematical preliminaries, the model, and the main results. In section 3 we prove Proposition 2.3 and 2.4, by calculating the surface energy density as well as the Wulff crystal associated to each lattice. The content of Section 4 is the proof of Theorem 2.2.

2. Setting and Notation

Given a set of vectors $V \subset \mathbb{R}^3$ we denote by $\mathrm{span}_{\mathbb{Z}} V$ the set of finite linear combinations of elements of V with coefficients in $\mathbb{Z}$. We denote by $\mathfrak{M}$ the collection of all Lebesgue measurable subsets of $\mathbb{R}^3$. Given $E \in \mathfrak{M}$ we denote by $|E|$ its 3-dimensional Lebesgue measure and $\mathcal{H}^2$ its 2-dimensional Hausdorff measure. Given X a countable set, we denote by $\#X$ the cardinality of X. Given $a, b \in \mathbb{R}^3$ we denote by $\langle a, b\rangle$ their scalar product. We denote by $\mathbb{S}^2$ the set of unitary vectors in $\mathbb{R}^3$. For any $\nu \in \mathbb{S}^2$ let $\{\nu_1, \nu_2, \nu\}$ be an orthonormal basis of $\mathbb{R}^3$, and let $Q := \{x \in \mathbb{R}^3 \colon |\langle x, \nu_i\rangle| < 1/2,\, |\langle x, \nu\rangle| < 1/2,\, i = 1, 2\}$ be a unit cube centered at the origin with two of its faces orthogonal to the direction ν. For $T > 0$ and $x \in \mathbb{R}^3$ we set $Q^\nu_T(x) = x + TQ^\nu$ and we write $Q^\nu_T = Q^\nu_T(0)$. We define the set of positive Radon measures by $\mathcal{M}_+(\mathbb{R}^3)$. We say that $\{\mu_n\}_n \subset \mathcal{M}_+(\mathbb{R}^3)$ converges to $\mu \in \mathcal{M}_+(\mathbb{R}^3)$ with respect to the weak star topology and we write $\mu_n \overset{*}{\rightharpoonup} \mu$ if

$$\lim_{n\to\infty} \int_{\mathbb{R}^3} \varphi\,\mathrm{d}\mu_n = \int_{\mathbb{R}^3} \varphi\,\mathrm{d}\mu \text{ for all } \varphi \in C_c(\mathbb{R}^3)\,.$$

Given $\Omega \subset \mathbb{R}^3$ open we denote by $BV(\Omega)$ the space of functions of bounded variation in Ω and we denote by $BV_{\mathrm{loc}}(\Omega) = \{u \colon u \in BV(K) \text{ for all } K \subset\subset \Omega, K \text{ open}\}$.

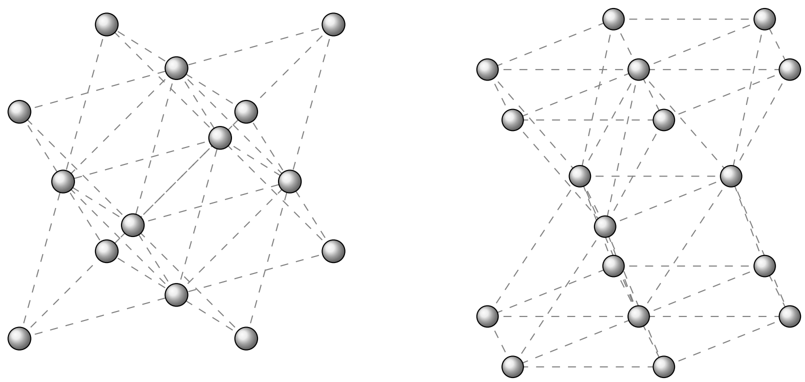

FIGURE 2. On the left: The FCC-lattice. On the right: The HCP-lattice. Pairs of points at distance one are connected via the dashed lines.

Definition of HCP and FCC lattices. In the following we define the *face-centered cubic lattice* (short FCC-lattice) and the *hexagonal closed-packed lattice* (short HCP-lattice). To this end, we introduce the verctors

$$b_1 := \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\\0\end{pmatrix}\,, \quad b_2 := \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\1\end{pmatrix}\,, \quad b_3 := \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\1\end{pmatrix} \tag{7}$$

and

$$e_1 := \begin{pmatrix}1\\0\\0\end{pmatrix}\,, \quad e_2 := \frac{1}{2}\begin{pmatrix}1\\\sqrt{3}\\0\end{pmatrix}\,, \quad e_3 := \frac{2}{3}\sqrt{6}\begin{pmatrix}0\\0\\1\end{pmatrix}\,, \quad v_1 := \frac{1}{3}(e_1+e_2)+\frac{1}{2}e_3\,. \tag{8}$$

We define the FCC-lattice as

$$\mathcal{L}_{\mathrm{FCC}} := \mathrm{span}_{\mathbb{Z}}\{b_1, b_2, b_3\} \tag{9}$$

and the HCP-lattice by

$$\mathcal{L}_{\mathrm{HCP}} := \mathrm{span}_{\mathbb{Z}}\{e_1, e_2, e_3\} \cup (\mathrm{span}_{\mathbb{Z}}\{e_1, e_2, e_3\} + v_1)\,. \tag{10}$$

The two lattices are illustrated in Figure 2. We shall write $\mathcal{L}$ to generically denote one of the two lattices defined above. We define the *neighborhood* of a point $x \in \mathcal{L}_{\mathrm{FCC}}$ as the set

$$\mathcal{N}_{\mathrm{FCC}}(x) := \{\pm b_1, \pm b_2, \pm b_3, \pm(b_1-b_2), \pm(b_1-b_3), \pm(b_2-b_3)\} + x\,. \tag{11}$$

Similarly, for a point $x \in \mathcal{L}_{\mathrm{HCP}}$ we define its *neighborhood* as follows: if $x \in \mathrm{span}_{\mathbb{Z}}\{e_1, e_2, e_3\}$ then

$$\mathcal{N}_{\mathrm{HCP}}(x) := \{\pm e_1, \pm e_2, \pm(e_1-e_2), v_1, v_1-e_1, v_1-e_2, v_1-e_3, v_1-e_1-e_3, v_1-e_2-e_3\} + x\,, \tag{12}$$

while if $x \in \mathrm{span}_{\mathbb{Z}}\{e_1, e_2, e_3\} + v_1$ then

$$\mathcal{N}_{\mathrm{HCP}}(x) := \{\pm e_1, \pm e_2, \pm(e_1-e_2), -v_1, e_1-v_1, e_2-v_1, e_3-v_1, e_1+e_3-v_1, e_2+e_3-v_1\} + x\,. \tag{13}$$

Note that $\mathcal{N}_{\mathrm{FCC}}(x) = \mathcal{N}_{\mathrm{FCC}}(0)+x$ for all $x \in \mathcal{L}_{\mathrm{FCC}}$, while this is no more the case for $x \in \mathcal{L}_{\mathrm{HCP}}$. Also for $\mathcal{N}$ we omit the subscript if we do not need to distinguish between FCC and HCP. It is straightforward to check that for all $x, y \in \mathcal{L}$,

$$x \in \mathcal{N}(y) \iff |x - y| = 1\,.$$

Given $\mathcal{L}$ we define the *Voronoi cell* of $x \in \mathcal{L}$ (with respect to $\mathcal{L}$) by

$$\mathcal{V}_{\mathcal{L}}(x) := \{y \in \mathbb{R}^3 \colon |y - x| \leq |y - z| \text{ for all } z \in \mathcal{L}\}\,. \tag{14}$$

Accordingly, given $\varepsilon > 0$ we write $\mathcal{V}_{\varepsilon\mathcal{L}}(x)$ for the Voronoi cell centered at $x \in \varepsilon\mathcal{L}$ with respect to the scaled lattice $\varepsilon\mathcal{L}$. Given $X \subset \varepsilon\mathcal{L}$ we say that $y \in \mathcal{N}_\varepsilon(x)$ if and only if $\varepsilon^{-1}y \in \mathcal{N}(\varepsilon^{-1}x)$.

Definition of the Energy. Given $X \subset \mathcal{L}$ and $A \subset \mathbb{R}^3$ we define the configurational energy of X localized to the set A as

$$E_{\mathcal{L}}(X, A) := \sum_{x \in X \cap A} (12 - \#(\mathcal{N}(x) \cap X))\,. \tag{15}$$

In the formula above we can interpret the set X as the occupancy of the crystal $\mathcal{L}$, i.e., the set of those nodes of $\mathcal{L}$ occupied by atoms. The quantity $12 - \#(\mathcal{N}_{\mathcal{L}}(x) \cap X)$ is also known as the valence of the point x with respect to X, i.e., the number of neighbours missing in X in order to have a neighbourhood of maximal cardinality (the number 12 in the formula). Note that we can also rewrite the energy as

$$E_{\mathcal{L}}(X, A) = \frac{1}{2} \sum_{x \in \mathcal{L} \cap A} \sum_{y \in \mathcal{L}} c(x, y) |\chi_X(y) - \chi_X(x)|\,,$$

where

$$c(x, y) = \begin{cases} 1 & \text{if } y \in \mathcal{N}(x)\,, \\ 0 & \text{otherwise.} \end{cases} \tag{16}$$

Periodicity of the interaction coefficients. By definition

$$\mathcal{L}_{\text{FCC}} = \mathcal{L}_{\text{FCC}} + b_1 = \mathcal{L}_{\text{FCC}} + b_2 = \mathcal{L}_{\text{FCC}} + b_3.$$

As a consequence of that, for any $x, y \in \mathcal{L}_{\text{FCC}}$ it holds that

$$c(x + b_1, y + b_1) = c(x + b_2, y + b_2) = c(x + b_3, y + b_3) = c(x, y)\,.$$

According to the last two equalities, we say that the lattice $\mathcal{L}_{\text{FCC}}$ as well as the interaction coefficients of its configurational energy are periodic with periodicity cell

$$T_{\text{FCC}} = \{\lambda_1 b_1 + \lambda_2 b_2 + \lambda_3 b_3 \colon \lambda_i \in [0, 1)\}\,, \tag{17}$$

or simply that they are T_{FCC}-periodic. Similarly, we observe that $\mathcal{L}_{\text{HCP}}$ and its interaction coefficients are T_{HCP}-periodic, where the periodicity cell is defined as

$$T_{\text{HCP}} = \{\lambda_1 e_1 + \lambda_2 e_2 + \lambda_3 e_3 \colon \lambda_i \in [0, 1)\}\,. \tag{18}$$

Surface scaling of the configurational energy. For $\varepsilon > 0$ such that $\varepsilon^3 \# X \to 1$ as $\varepsilon \to 0$ we consider the following family of scaled energies

$$G_{\mathcal{L},\varepsilon}(X) := \varepsilon^2 \sum_{x \in X} (12 - \#(\mathcal{N}_\varepsilon(x) \cap X))\,. \tag{19}$$

Note that, modeling the points in $X \subset \varepsilon\mathcal{L}$ as hard-spheres of ε diameter, the quantity $\varepsilon^3 \# X$ is of order one (according to the scaling assumption above) and proportional to the volume of the union of the spheres in X. Hence, the scaling factor ε^2 in the energy functional turns out to be a surface scaling. We also define the rescaled empirical measures associated to the configuration X as

$$\mu_\varepsilon := \varepsilon^3 \sum_{x\in X} \delta_x \,. \tag{20}$$

Upon identifying $X \subset \varepsilon\mathcal{L}$ with its empirical measure μ_ε, we can regard these energies to be defined on $\mathcal{M}_+(\mathbb{R}^3)$ by setting

$$E_{\mathcal{L},\varepsilon}(\mu) := \begin{cases} G_{\mathcal{L},\varepsilon}(X) & \text{if } \mu := \varepsilon^3 \sum_{x\in X}\delta_x \text{ for some } X \subset \varepsilon\mathcal{L}\,,\\ +\infty & \text{otherwise.}\end{cases} \tag{21}$$

The coarse grained continuum energy. For $\mathcal{L}$ we define the *homogenized surface energy density* $\varphi_\mathcal{L}\colon \mathbb{R}^3 \to [0,+\infty]$ as the convex positively homogeneous function of degree one such that for all $\nu \in \mathbb{S}^2$ we have

$$\varphi_\mathcal{L}(\nu) := \lim_{T\to+\infty} \frac{1}{T^2} \inf\left\{E_\mathcal{L}(X, Q_T^\nu) : X \subset \mathcal{L}, \chi_X(i) = u_\nu(i) \text{ for } i \in \mathcal{L}\setminus Q^\nu_{T-3}\right\}\,, \tag{22}$$

where

$$u_\nu(x) = \begin{cases} 1 & \text{if } \langle x,\nu\rangle \geq 0\,,\\ 0 & \text{otherwise.}\end{cases}$$

In order to be able to apply [9, Proposition 2.6] to obtain an alternative representation of $\varphi_\mathcal{L}$ (Up to a coordinate transformation and reparametrization of the interaction coefficients), we define for $u\colon \mathcal{L}\to\mathbb{R}$, $A \subset \mathbb{R}^3$ the energy

$$F_\mathcal{L}(u,A) := \frac{1}{2}\sum_{x\in\mathcal{L}\cap A}\sum_{y\in\mathcal{L}} c(x,y)|u(y)-u(x)|\,.$$

We are now in position to state [9, Proposition 2.6].

Proposition 2.1. *Let $c(x,y)$ be as in* (16)*. Then*

$$\varphi_\mathcal{L}(\nu) = \frac{1}{|T_\mathcal{L}|}\inf\left\{F_\mathcal{L}(u,T_\mathcal{L}) : u\colon \mathcal{L}\to\mathbb{R}, u(\cdot) - \langle \nu,\cdot\rangle \text{ is } T_\mathcal{L}\text{-periodic}\right\}\,. \tag{23}$$

With the definition of surface energy density at hand we can define the *coarse-grained continuum energy* $E_\mathcal{L}\colon \mathcal{M}_+(\mathbb{R}^3)\to[0,+\infty]$ as

$$E_\mathcal{L}(\mu) := \begin{cases} \int_{\partial^* E}\varphi_\mathcal{L}(\nu)\,\mathrm{d}\mathcal{H}^2 & \text{if } \mu = \sqrt{2}\mathcal{L}^3\llcorner E, \chi_E \in BV_{\mathrm{loc}}(\mathbb{R}^3)\,,\\ +\infty & \text{otherwise.}\end{cases} \tag{24}$$

with $\varphi_\mathcal{L}$ given by (22). Here, $\partial^* E$ denotes the reduced boundary of the set E and $\mathcal{H}^2$, as noted at the beginning of this section, stands for the 2-dimensional Hausdorff measure in $\mathbb{R}^3$ (cf. [3], Chapters 2.8 and 3.5).

In what follows we say that F_ε Γ-converges to F if for all sequences $\{\varepsilon_j\}_j$ converging to 0 we have Γ-$\lim_j F_{\varepsilon_j} = F$.

The following variational coarse-graining result is proved in Section 4.

Theorem 2.2. *Let $\varepsilon \to 0$, and let $E_{\mathcal{L},\varepsilon}$ and $E_\mathcal{L}$ be the energy functionals defined in* (21) *and* (24)*, respectively.*

i) *(Compactness) Let* $\{\mu_\varepsilon\}_\varepsilon \subset \mathcal{M}_+(\mathbb{R}^3)$ *be such that*

$$\sup_{\varepsilon>0} E_{\mathcal{L},\varepsilon}(\mu_\varepsilon) < +\infty\,.$$

Then there exists $E \subset \mathbb{R}^2$ *such that* $\chi_E \in BV_{\mathrm{loc}}(\mathbb{R}^3)$, $\mu = \sqrt{2}\mathcal{L}^3 \llcorner E, \mu \in \mathcal{M}_+(\mathbb{R}^3)$, *and a subsequence (not relabeled) such that* $\mu_\varepsilon \overset{*}{\rightharpoonup} \mu$.

ii) *(Liminf inequality) Let* $\mu \in \mathcal{M}_+(\mathbb{R}^3)$ *be such that* $\mu_\varepsilon \overset{*}{\rightharpoonup} \mu$. *Then*

$$E_{\mathcal{L}}(\mu) \le \liminf_{\varepsilon\to 0} E_{\mathcal{L},\varepsilon}(\mu_\varepsilon)\,.$$

iii) *(Limsup inequality) Let* $\mu \in \mathcal{M}_+(\mathbb{R}^3)$. *Then there exists* $\{\mu_\varepsilon\}_\varepsilon \subset \mathcal{M}_+(\mathbb{R}^3)$ *such that* $\mu_\varepsilon \overset{*}{\rightharpoonup} \mu$ *and*

$$E_{\mathcal{L}}(\mu) \ge \liminf_{\varepsilon\to 0} E_{\mathcal{L},\varepsilon}(\mu_\varepsilon)\,.$$

The Wulff Crystal. In this section we calculate the Wulff crystals of the coarse grained FCC and HCP lattices. To the best of our knowledge, this is the first time that such a calculation has been carried out in a rigorous analytical way.

Given $\varphi\colon \mathbb{R}^3 \to [0,+\infty)$ convex, non-degenerate, (i.e. there exist $0 < c < C$ such that $c \le \varphi(\nu) \le C$ for all $\nu \in \mathbb{S}^2$) positively homogeneous of degree one, we define the Wulff set of φ by

$$W_\varphi := \{\zeta \in \mathbb{R}^3 : \langle \zeta, \nu\rangle \le \varphi(\nu) \text{ for all } \nu \in \mathbb{S}^2\}\,.$$

Thanks to the anistropic isoperimetric inequality (cf. [13]), we have that W_φ is the unique (up to rigid motions) minimizer of

$$\min\left\{\int_{\partial^* E} \varphi(\nu)\,\mathrm{d}\mathcal{H}^2 \colon |E| = |W_\varphi|\right\}\,.$$

We recall here that, defining $\varphi^\circ\colon \mathbb{R}^3 \to [0,+\infty)$ by

$$\varphi^\circ(\xi) = \sup_{\nu\in\mathbb{S}^2} \frac{\langle \nu, \xi\rangle}{\varphi(\nu)}\,, \tag{25}$$

it holds that $W_\varphi = \{\varphi^\circ \le 1\}$.

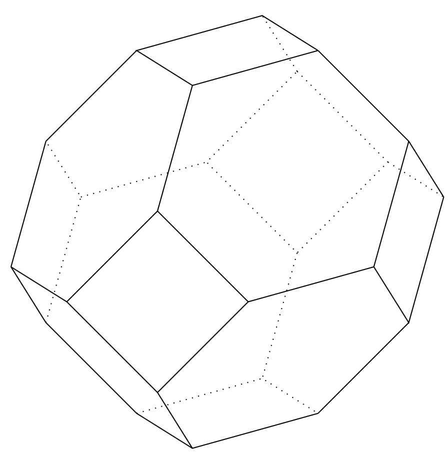

FIGURE 3. The Wulff Crystal of the FCC-lattice

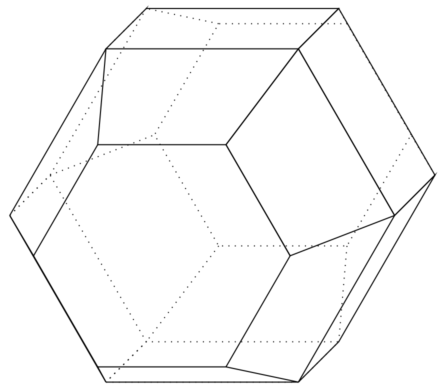

FIGURE 4. The Wulff Crystal of the HCP-lattice

Explicit formula of the surface energy densities. Taking advantage of the representation formula (23) stated in Proposition (2.1), we provide the explicit formulas of the surface energy density $\varphi_{\mathcal{L}_{\rm FCC}}$ and $\varphi_{\mathcal{L}_{\rm HCP}}$. With the two explicit formulas at hand we can calculate the polars of both densities, the associated Wulff shapes and the surface energy per unit volume of both the FCC and HCP crystals. In order not to overburden the reader with notation, we write $\varphi_{\rm FCC}$ and $\varphi_{\rm HCP}$ for $\varphi_{\mathcal{L}_{\rm FCC}}$ and $\varphi_{\mathcal{L}_{\rm HCP}}$ as well as $W_{\rm FCC}$ and $W_{\rm HCP}$ instead of $W_{\varphi_{\mathcal{L}_{\rm FCC}}}$ and $W_{\varphi_{\mathcal{L}_{\rm HCP}}}$.

Proposition 2.3. *The following formulas hold true.*

$$\varphi_{\rm FCC}(\nu) = |\nu_1+\nu_2| + |\nu_1+\nu_3| + |\nu_2+\nu_3| + |\nu_1-\nu_2| + |\nu_1-\nu_3| + |\nu_2-\nu_3|\,, \tag{26}$$

and

$$\varphi^\circ_{\rm FCC}(\zeta) = \max\left\{\frac{1}{4}\|\zeta\|_\infty, \frac{1}{6}\|\zeta\|_1\right\}. \tag{27}$$

In particular, $W_{\rm FCC}$ *is a truncated octahedron and its surface energy per unit volume is*

$$|W_{\rm FCC}|^{-2/3}\int_{\partial^* W_{\rm FCC}} \varphi_{\rm FCC}(\nu)\,\mathrm{d}\mathcal{H}^2 = 3\cdot 2^2\cdot 2^{2/3}\,. \tag{28}$$

Proposition 2.4. *The following formulas hold true.*

$$\begin{aligned}\varphi_{\rm HCP}(\nu) = \sqrt{2}\,(|\langle e_1,\nu\rangle| + |\langle e_2,\nu\rangle| + |\langle e_1-e_2,\nu\rangle|) + \frac{1}{\sqrt{2}}|\langle e_3,\nu\rangle| \\ + \sqrt{2}\max\{|\langle e_1,\nu\rangle|, |\langle e_2,\nu\rangle|, |\langle e_3,\nu\rangle|, |\langle e_1-e_2,\nu\rangle|\}\,,\end{aligned} \tag{29}$$

and

$$\begin{aligned}\varphi^\circ_{\rm HCP}(\zeta) = \max\Big\{ &\frac{2}{7\sqrt{2}}\left(|\zeta_1| + \frac{1}{\sqrt{3}}|\zeta_2| + \frac{3}{2\sqrt{6}}|\zeta_3|\right), \frac{1}{2\sqrt{3}}|\zeta_3|, \\ &\frac{2}{3\sqrt{6}}|\zeta_2|, \frac{4}{7\sqrt{6}}|\zeta_2| + \frac{3}{14\sqrt{3}}|\zeta_3|, \frac{1}{3\sqrt{2}}\left(|\zeta_1| + \frac{1}{\sqrt{3}}|\zeta_2|\right)\Big\}.\end{aligned} \tag{30}$$

In particular, $W_{\rm HCP}$ *is a truncated elongated hexagonal bipyramid and and its surface energy per unit volume is*

$$|W_{\rm HCP}|^{-2/3}\int_{\partial^* W_{\rm HCP}} \varphi_{\rm HCP}(\nu)\,\mathrm{d}\mathcal{H}^2 = 3\cdot 2^{2/3}\cdot 65^{1/3}\,. \tag{31}$$

3. Proof of Proposition 2.3 and Proposition 2.4

In this section we prove Proposition 2.3 and Proposition 2.4. To this end, we use Proposition 2.1 to note that $\varphi_{\mathcal{L}}$ is given by (23).

Proof of Proposition 2.3. We divide the proof into several steps. First, we calculate φ_{FCC}. Then, we calculate $\varphi^\circ_{\mathrm{FCC}}$. Lastly, we calculate (28).
Step 1.(Calculation of φ_{FCC})We make use of Proposition 2.1 in order to calculate φ_{FCC}. First of all, owing to (17), we note that

$$|T_{\mathrm{FCC}}| = \frac{1}{3}\sqrt{6}\cdot\frac{1}{2}\sqrt{3} = \frac{1}{2}\sqrt{2}\,. \tag{32}$$

Given $u\colon \mathcal{L}_{\mathrm{FCC}} \to \mathbb{R}$ such that $u(\cdot)-\langle \nu,\cdot\rangle$ is T_{FCC}-periodic we have that $u(x+b_i) = u(x)+\langle b_i,\nu\rangle$ for all $i = 1,2,3$. Therefore, u is an affine function of the form $u(x) = \langle x,\nu\rangle + c\,, x \in \mathcal{L}_{\mathrm{FCC}}$ for some $c \in \mathbb{R}$. Lastly, note that $\mathcal{L}_{\mathrm{FCC}} \cap T_{\mathrm{FCC}} = \{0\}$. Using (23) and (32), we obtain

$$\varphi_{\mathrm{FCC}}(\nu) = \frac{1}{2}\sqrt{2}\sum_{\xi\in\mathcal{N}_{\mathrm{FCC}}} |u(\xi)-u(0)| = \frac{1}{2}\sqrt{2}\sum_{\xi\in\mathcal{N}_{\mathrm{FCC}}} |\langle \xi,\nu\rangle|\,.$$

Employing now (11), we obtain (26).
Step 2.(Calculation of $\varphi^\circ_{\mathrm{FCC}}$) Let G be the isometry group on $\mathbb{R}^3$ whose elements $g \in G$ are the linear isometries $g\colon \mathbb{R}^3 \to \mathbb{R}^3$ defined by $g(\nu_1,\nu_2,\nu_3) = (b_1\nu_{\pi_1}, b_2\nu_{\pi_2}, b_3\nu_{\pi_3})$ where π is a permutation on $\{1,2,3\}$ and $b_i \in \{-1,1\}$. Since $\varphi_{\mathrm{FCC}}(g(\nu)) = \varphi_{\mathrm{FCC}}(\nu)$ for all $g \in G$, $\nu \in \mathbb{R}^3$, we infer that

$$\varphi^\circ_{\mathrm{FCC}}(\zeta) := \max_{\substack{\nu\in\mathbb{R}^3\\ \varphi_{\mathrm{FCC}}(\nu)\leq 1}} \langle \zeta,\nu\rangle = \max_{\substack{\nu\in\mathbb{R}^3\\ \varphi_{\mathrm{FCC}}(g^{-1}(\nu))\leq 1}} \langle \zeta, g^{-1}(\nu)\rangle = \max_{\substack{\nu\in\mathbb{R}^3\\ \varphi_{\mathrm{FCC}}(\nu)\leq 1}} \langle g(\zeta),\nu\rangle = \varphi^\circ_{\mathrm{FCC}}(g(\zeta))\,,$$

also relying on the property $g^T = g^{-1}$. Therefore, we can assume that $0 \leq \zeta_1 \leq \zeta_2 \leq \zeta_3$. Thus, if we want to maximize $\langle \zeta,\nu\rangle$ under the condition $\varphi_{\mathrm{FCC}}(\nu) \leq 1$, we can as well assume that $0 \leq \nu_1 \leq \nu_2 \leq \nu_3$, so that condition $\varphi_{\mathrm{FCC}}(\nu) \leq 1$ becomes equivalent to

$$4\nu_3 + 2\nu_2 \leq 1\,.$$

Therefore, noting that any linear function attains its maximum at the extreme points of a convex set and consulting Figure 5, we obtain

$$\begin{aligned}\max_{\substack{0\leq\nu_1\leq\nu_2\leq\nu_3\\ 4\nu_3+2\nu_2\leq 1}} \zeta_1\nu_1+\zeta_2\nu_2+\zeta_3\nu_3 = \max_{\substack{0\leq\nu_2\leq\nu_3\\ 4\nu_3+2\nu_2\leq 1}} (\zeta_1+\zeta_2)\nu_2+\zeta_3\nu_3 &= \max\left\{\frac{1}{4}\zeta_3, \frac{1}{6}(\zeta_1+\zeta_2+\zeta_3)\right\}\\ &= \max\left\{\frac{1}{4}\|\zeta\|_\infty, \frac{1}{6}\|\zeta\|_1\right\}\,.\end{aligned}$$

This is the desired formula and concludes Step 2.
Step 3.(Calculation of (28)) Note that the set $W_{\varphi_{\mathrm{FCC}}}$ is the intersection of a cube $\|\zeta\|_\infty \leq 4$ with an octahedron $\|\zeta\|_1 \leq 6$, see Fig. 3. Its boundary has 6 square faces, where $\nu = \pm(1,0,0)$ (resp. $\pm(0,1,0)$ or $\pm(0,0,1)$) and 8 hexagonal faces, where $\nu = \frac{1}{\sqrt{3}}(\pm1\pm1\pm1)$. First, we consider the set where $\nu = (1,0,0)$, the other cases where $\varphi^\circ_{\mathrm{FCC}}(\zeta) = \frac{1}{4}\|\zeta\|_\infty = 1$ contributing with the same value. The square is given by

$$S_1^+ = \{(4,\zeta_2,\zeta_3)\colon |\zeta_2|+|\zeta_3| \leq 2\} = \left\{\frac{1}{4}\|\zeta\|_\infty = \frac{1}{4}\zeta_1 = 1\right\} \cap \left\{\frac{1}{6}\|\zeta\|_1 \leq 1\right\}\,.$$

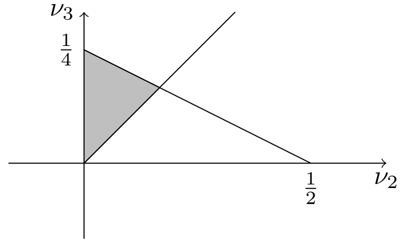

FIGURE 5. The set $\{0 \le \nu_2 \le \nu_3\} \cap \{4\nu_3 + 2\nu_1 \le 1\}$ depicted in gray.

Therefore, $\mathcal{H}^2(S_1^+) = 8$ and $\varphi_{\mathrm{FCC}}((1,0,0)) = 4$. Similarly, we obtain the same measure and value of φ_{FCC} for the other squares S_1^-, $S_2^\pm$,$S_3^\pm$, where ν is (up to sign) one of the coordinate unit vectors. Hence,

$$\sum_{i=1}^{3} \int_{S_i^+} \varphi_{\mathrm{FCC}}(\nu)\,\mathrm{d}\mathcal{H}^2 + \sum_{i=1}^{3} \int_{S_i^-} \varphi_{\mathrm{FCC}}(\nu)\,\mathrm{d}\mathcal{H}^2 = 6 \cdot 8 \cdot 4 = 3 \cdot 2^6 \,. \tag{33}$$

Next, we consider the contribution of a hexagon. We consider the hexagon contained in the set $\zeta_i \ge 0$ for all i. Here, we have $\nu = \frac{1}{\sqrt{3}}(1,1,1)$ and $\varphi_{\mathrm{FCC}}(\nu) = 2\sqrt{3}$. The 6 sides of the hexagon have all side-length $2\sqrt{2}$. To see this, there are sides of the form $(4, 2-t, t), t \in [0,2]$ or $(4-t, 0, 2+t), t \in [0,2]$ and their permutations (up to identifying t with $2-t$ in the first case and $4-t$ and $2+t$ in the second case). An equilateral hexagon H of side-length $2\sqrt{2}$ satisfies $\mathcal{H}^2(H) = 12\sqrt{3}$. Labeling the hexagons by H_i, $i = 0, \dots, 7$, we obtain

$$\sum_{i=0}^{7} \int_{H_i} \varphi_{\mathrm{FCC}}(\nu)\,\mathrm{d}\mathcal{H}^2 = 8 \cdot \mathcal{H}^2(H_i) \cdot \varphi_{\mathrm{FCC}}\left(\frac{1}{\sqrt{3}}(\pm 1, \pm 1, \pm 1)\right) = 8 \cdot 12\sqrt{3} \cdot 2\sqrt{3} = 3^2 \cdot 2^6 \,. \tag{34}$$

Using (33) and (34), we obtain

$$\int_{\partial W_{\mathrm{FCC}}} \varphi_{\mathrm{FCC}}(\nu)\,\mathrm{d}\mathcal{H}^2 = 3 \cdot 2^6 + 3^2 \cdot 2^6 = 3 \cdot 2^8 \,. \tag{35}$$

Let $C := \{\zeta \in \mathbb{R}^3 \colon \zeta_i \ge 0 \text{ for all } i = 1,2,3 \text{ and } \frac{1}{4}\|\zeta\|_\infty \ge \frac{1}{6}\|\zeta\|_1\}$ and $C^c := \{\zeta \in \mathbb{R}^3 \colon \zeta_i \ge 0 \text{ for all } i = 1,2,3 \text{ and } \frac{1}{4}\|\zeta\|_\infty < \frac{1}{6}\|\zeta\|_1\}$. We split the calculation of the volume $W \cap \{\zeta \in \mathbb{R}^3 \colon \zeta_i \ge 0 \text{ for all i}\}$ into the set $C \cap W_{\mathrm{FCC}}$ and $C^c \cap W_{\mathrm{FCC}}$. Noting that on this set $|\nabla \varphi^\circ_{\mathrm{FCC}}(\zeta)| = \frac{1}{4}\ \mathcal{L}^3$-a.e. on C, due to the coarea-formula, we have

$$\begin{aligned} |\{C \cap W_{\mathrm{FCC}}\}| &= 4 \int_{C \cap W_{\mathrm{FCC}}} |\nabla \varphi^\circ_{\mathrm{FCC}}(\zeta)|\,\mathrm{d}\zeta = 4 \int_0^1 \mathcal{H}^2(C \cap \{\varphi^\circ_{\mathrm{FCC}}(\zeta) = s\})\,\mathrm{d}s \\ &= \int_0^1 4 \cdot s^2 \cdot 6\,\mathrm{d}s = 8 \,. \end{aligned}$$

Here we used that, $C \cap \{\varphi^\circ_{\mathrm{FCC}}(\zeta) = s\} = s(S_1^+ \cup S_2^+ \cup S_3^+) \cap \{\zeta_i \ge 0\}$ and the scaling properties of the 2-dimensional Hausdorff-measure. On the other hand, using that $|\nabla \varphi^\circ_{\mathrm{FCC}}(\zeta)| = \frac{\sqrt{3}}{6}\ \mathcal{L}^3$-a.e. on C^c, we have

$$\begin{aligned} |\{C^c \cap W_{\mathrm{FCC}}\}| &= 2\sqrt{3} \int_{C^c \cap W_{\mathrm{FCC}}} |\nabla \varphi^\circ_{\mathrm{FCC}}(\zeta)|\,\mathrm{d}\zeta = 2\sqrt{3} \int_0^1 \mathcal{H}^2(C^c \cap \{\varphi^\circ_{\mathrm{FCC}}(\zeta) = s\})\,\mathrm{d}s \\ &= 2\sqrt{3} \int_0^1 s^2 \cdot 12\sqrt{3}\,\mathrm{d}s = 3 \cdot 2^3 \,. \end{aligned}$$

Taking into account also the sets $\{\pm\zeta_i \geq 0\}$, we obtain

$$|W_{\mathrm{FCC}}| = 8(8 + 3 \cdot 2^3) = 2^8\,.$$

Now, this together with (35) yields (28). □

Proof of Proposition 2.4. We divide the proof into several steps. First, we calculate φ_{HCP}. Then, we calculate $\varphi^\circ_{\mathrm{HCP}}$. Lastly, we calculate (31).

Step 1.(Calculation of φ_{HCP}) We make use of Proposition 2.1 in order to calculate φ_{HCP}. First of all, due to (18), note that

$$|T_{\mathrm{HCP}}| = \frac{2}{3}\sqrt{6}\cdot\frac{1}{2}\sqrt{3} = \sqrt{2}\,. \tag{36}$$

Given $u\colon \mathcal{L}_{\mathrm{FCC}} \to \mathbb{R}$ such that $u(\cdot) - \langle \nu, \cdot\rangle$ we have that $u(x+\xi) = u(x) + \langle \xi, \nu\rangle$ for all $\xi \in \{e_1, e_2, e_3\}$ and $\mathcal{L}_{\mathrm{HCP}} \cap T_{\mathrm{HCP}} = \{0, v_1\}$. Hence, there exist $c_1, c_2 \in \mathbb{R}$ such that

$$u(x) = \begin{cases} \langle x, \nu\rangle + c_1 & x \in \mathrm{span}_{\mathbb{Z}}\{e_1, e_2, e_3\}\ ; \\ \langle x_0, \nu\rangle + c_2 & x = x_0 + v_1,\ \text{with } x_0 \in \mathrm{span}_{\mathbb{Z}}\{e_1, e_2, e_3\}\ . \end{cases}$$

Setting $c_2 - c_1 = t$, we therefore obtain

$$\begin{aligned} F_{\mathcal{L}_{\mathrm{HCP}}}(u, T_{\mathrm{HCP}}) = {} & 2\left(|\langle e_1,\nu\rangle| + |\langle e_2,\nu\rangle| + |\langle e_1 - e_2,\nu\rangle|\right) + |t| + |t - \langle e_1,\nu\rangle| + |t - \langle e_2,\nu\rangle| \\ & + |t - \langle e_3,\nu\rangle| + |t - \langle e_3 + e_1,\nu\rangle| + |t - \langle e_3 + e_2\rangle|\,. \end{aligned}$$

Employing Proposition 2.1 and (36), we have

$$\varphi_{\mathrm{HCP}}(\nu) = \sqrt{2}\left(|\langle e_1,\nu\rangle| + |\langle e_2,\nu\rangle| + |\langle e_1 - e_2,\nu\rangle|\right) + \frac{1}{\sqrt{2}}\min_{t\in\mathbb{R}} g_\nu(t)\,, \tag{37}$$

where

$$g_\nu(t) := |t| + |t - \langle e_1,\nu\rangle| + |t - \langle e_2,\nu\rangle| + |t - \langle e_3,\nu\rangle| + |t - \langle e_3 + e_1,\nu\rangle| + |t - \langle e_3 + e_2\rangle|\,.$$

Next, we show that

$$\min_{t\in\mathbb{R}} g_\nu(t) = |\langle e_3,\nu\rangle| + 2\max\{|\langle e_1,\nu\rangle|,\ |\langle e_2,\nu\rangle|,\ |\langle e_1 - e_2,\nu\rangle|,\ |\langle e_3,\nu\rangle|\}\,. \tag{38}$$

Note that if (38) is shown, (29) is proven and Step 1 is concluded. In order to prove (38), we first note that $g_\nu(t)$ is a piecewise affine function such that $g_\nu(t) \to +\infty$ as $|t| \to +\infty$. Hence, it attains its minimum at a point of non-differentiability. The function g_ν is not differentiable for $t \in \{0, \langle e_1,\nu\rangle, \langle e_2,\nu\rangle, \langle e_3,\nu\rangle, \langle e_3 + e_1,\nu\rangle, \langle e_3 + e_2,\nu\rangle\}$ and therefore

$$\min_{t\in\mathbb{R}} g_\nu(t) = |\langle e_3,\nu\rangle| + \min\{f_k(\nu)\colon k \in \{0,\dots,5\}\}\,,$$

where

$$\begin{aligned} f_0(\nu) &= |\langle e_1,\nu\rangle| + |\langle e_2,\nu\rangle| + |\langle e_3 + e_1,\nu\rangle| + |\langle e_3 + e_2,\nu\rangle|\,, \\ f_1(\nu) &= |\langle e_1,\nu\rangle| + |\langle e_1 - e_2,\nu\rangle| + |\langle e_3 - e_1,\nu\rangle| + |\langle e_3 + e_2 - e_1,\nu\rangle|\,, \\ f_2(\nu) &= |\langle e_2,\nu\rangle| + |\langle e_1 - e_2,\nu\rangle| + |\langle e_3 - e_2,\nu\rangle| + |\langle e_3 + e_1 - e_2,\nu\rangle|\,, \\ f_3(\nu) &= |\langle e_1,\nu\rangle| + |\langle e_2,\nu\rangle| + |\langle e_3 - e_1,\nu\rangle| + |\langle e_3 - e_2,\nu\rangle|\,, \\ f_4(\nu) &= |\langle e_1,\nu\rangle| + |\langle e_1 - e_2,\nu\rangle| + |\langle e_3 + e_1,\nu\rangle| + |\langle e_3 + e_1 - e_2,\nu\rangle|\,, \\ f_5(\nu) &= |\langle e_2,\nu\rangle| + |\langle e_1 - e_2,\nu\rangle| + |\langle e_3 + e_2,\nu\rangle| + |\langle e_3 + e_2 - e_1,\nu\rangle|\,. \end{aligned}$$

It is easy to see that

$$\min_{t\in\mathbb{R}} g_\nu(t) = |\langle e_3,\nu\rangle| + \min\big\{|\langle e_1,R_k\nu\rangle| + |\langle e_2,R_k\nu\rangle| + |\langle e_3+e_1,R_k\nu\rangle| \\ + |\langle e_3+e_2,R_k\nu\rangle|\colon k\in\{0,\dots,5\}\big\}\,,$$

where R_k is the rotation of angle $k\pi/3$ around the x_3-axis. Noting also that $\min_{t\in\mathbb{R}} g_\nu(t) = \min_{t\in\mathbb{R}} g_{-\nu}(t)$, it is not restrictive to assume that $\langle e_1,\nu\rangle\geq 0, \langle e_2,\nu\rangle \geq 0, \langle e_3,\nu\rangle\geq 0$. We only consider the case, where $\langle e_1,\nu\rangle \geq \langle e_2,\nu\rangle \geq \langle e_3,\nu\rangle \geq 0$, the other being dealt with in a similar fashion. In this case we have $f_0(\nu)\geq f_3(\nu)$, $f_4(\nu)\geq f_5(\nu)$, and

$$\begin{aligned} f_1(\nu) &= \langle e_1,\nu\rangle + \langle e_1-e_2,\nu\rangle + \langle e_1-e_3,\nu\rangle + |\langle e_3+e_2-e_1,\nu\rangle| \\ &= 2\langle e_1,\nu\rangle + \langle e_1-e_2-e_3,\nu\rangle + |\langle e_3+e_2-e_1,\nu\rangle| \geq 2\langle e_1,\nu\rangle\,; \\ f_2(\nu) &= \langle e_2,\nu\rangle + \langle e_1-e_2,\nu\rangle + \langle e_2-e_3,\nu\rangle + \langle e_3+e_1-e_2,\nu\rangle = 2\langle e_1,\nu\rangle\,; \\ f_3(\nu) &= \langle e_1,\nu\rangle + \langle e_2,\nu\rangle + \langle e_1-e_3,\nu\rangle + \langle e_2-e_3,\nu\rangle = 2\langle e_1,\nu\rangle + 2\langle e_2,\nu\rangle - 2\langle e_3,\nu\rangle \geq 2\langle e_1,\nu\rangle\,; \\ f_5(\nu) &= \langle e_2,\nu\rangle + \langle e_1-e_2,\nu\rangle + \langle e_3+e_2,\nu\rangle + |\langle e_3+e_2-e_1,\nu\rangle| \\ &= 2\langle e_1,\nu\rangle + \langle e_3+e_2-e_1,\nu\rangle + |\langle e_3+e_2-e_1,\nu\rangle| \geq 2\langle e_1,\nu\rangle\,. \end{aligned}$$

Hence, we see that (38) holds true. This together with (37) establishes (29) and concludes Step 1.

Step 2.(Calculation of $\varphi^\circ_{\mathrm{HCP}}$) In order to calculate $\varphi^\circ_{\mathrm{HCP}}$, we exploit the symmetries of $\varphi^\circ_{\mathrm{HCP}}$. Note that

$$\varphi_{\mathrm{HCP}}\left(-\begin{pmatrix}\nu_1\\\nu_2\\\nu_3\end{pmatrix}\right) = \varphi_{\mathrm{HCP}}\left(\begin{pmatrix}\nu_1\\\nu_2\\-\nu_3\end{pmatrix}\right) = \varphi_{\mathrm{HCP}}\left(\begin{pmatrix}-\nu_1\\\nu_2\\\nu_3\end{pmatrix}\right) = \varphi_{\mathrm{HCP}}\left(\begin{pmatrix}\nu_1\\\nu_2\\\nu_3\end{pmatrix}\right)\,. \tag{39}$$

Given $\zeta\in\mathbb{R}^3$ we can find $R = T_1^{\alpha_1}\circ T_2^{\alpha_2}\circ T_3^{\alpha_3}$, $\alpha_i\in\{0,1\}$ such that $(R\zeta)_i\geq 0$ for all i. Thus,

$$\begin{aligned} \varphi^\circ_{\mathrm{HCP}}(\zeta) &= \max_{\varphi_{\mathrm{HCP}}(\nu)\leq 1}\langle\nu,\zeta\rangle = \max_{\varphi_{\mathrm{HCP}}(\nu)\leq 1}\langle R\nu,R\zeta\rangle \\ &= \max_{\varphi_{\mathrm{HCP}}(R^{-1}\nu)\leq 1}\langle\nu,R\zeta\rangle = \max_{\varphi_{\mathrm{HCP}}(\nu)\leq 1}\langle\nu,R\zeta\rangle = \varphi^\circ_{\mathrm{HCP}}(R\zeta)\,. \end{aligned} \tag{40}$$

It therefore suffices to calculate $\varphi^\circ_{\mathrm{HCP}}$ for $\zeta\in\mathbb{R}^3$ such that $\zeta_i\geq 0$. This together with (39) implies that if $\nu=(\nu_1,\nu_2,\nu_3)$ is such that $\varphi_{\mathrm{HCP}}(\nu)\leq 1$ and

$$\langle\nu,\zeta\rangle = \max_{\varphi_{\mathrm{HCP}}(\nu)\leq 1}\langle\nu,\zeta\rangle\,,$$

then $\nu_i\geq 0$ for all i. Additionally, a maximizer ν can be chosen such that φ_{HCP} is not differentiable at ν. Therefore, there are the following cases to consider:

(a) $\langle e_1-e_2,\nu\rangle = 0$;
(b) $\langle e_1-e_3,\nu\rangle = 0, \langle e_1-e_2,\nu\rangle\geq 0$;
(c) $\langle e_2-e_3,\nu\rangle = 0, \langle e_3-e_1,\nu\rangle\geq 0$;
(d) $\langle e_3,\nu\rangle = 0$;
(e) $\langle e_1,\nu\rangle = 0$.

Here, we point out that the points on the boundary $\nu_2=0$ are excluded as possible maximum points by arguing in the following way: If there were a point ν such that $\nu_2=0$, then $\varphi_{\mathrm{HCP}}(\nu)$ would either be differentiable and thus ν would not be a maximum point or ν would satisfy one of the cases (a)-(e).

Maximum of case (a). Since $\langle e_1-e_2,\nu\rangle = 0$, we have $\nu_1=\sqrt{3}\nu_2$. Hence, $\nu = (t,\frac{1}{\sqrt{3}}t,s)$ for some $t, s \geq 0$. Now, using (29), we have

$$\varphi_{\mathrm{HCP}}(\nu) = \sqrt{2}\left(2\nu_1 + \frac{1}{3}\sqrt{6}\nu_3 + \max\{\nu_1, \frac{2}{3}\sqrt{6}\nu_3\}\right).$$

(a.1) $t \geq \frac{2}{3}\sqrt{6}s$: Since the maximum is attained for $\varphi_{\mathrm{HCP}}(\nu) = 1$, we have $t = \frac{1}{3\sqrt{2}} - \frac{1}{9}\sqrt{6}s$. Now, $t \geq 0$ together with $t \geq \frac{2}{3}\sqrt{6}s$ implies $0 \leq s \leq \frac{3}{14\sqrt{3}}$. Noting that

$$\langle \nu, \zeta\rangle = t\left(\zeta_1 + \frac{1}{\sqrt{3}}\zeta_2\right) + s\zeta_3 = \left(\frac{1}{3\sqrt{2}} - \frac{1}{9}\sqrt{6}s\right)\left(\zeta_1 + \frac{1}{\sqrt{3}}\zeta_2\right) + s\zeta_3\,,$$

we obtain

$$\max_{\nu \text{ sat. (a.1)}} \langle \nu, \zeta\rangle = \max\left\{\frac{2}{7\sqrt{2}}\left(\zeta_1 + \frac{1}{\sqrt{3}}\zeta_2 + \frac{3}{2\sqrt{6}}\zeta_3\right), \frac{1}{3\sqrt{2}}\left(\zeta_1 + \frac{1}{\sqrt{3}}\zeta_2\right)\right\}. \tag{41}$$

(a.2) $t \leq \frac{2}{3}\sqrt{6}s$: Using $\varphi_{\mathrm{HCP}}(\nu) = 1$, we obtain $t = \frac{1}{2\sqrt{2}} - \frac{\sqrt{6}}{2}s$. Now, $t \geq 0$ together with $t \leq \frac{2}{3}\sqrt{6}s$ implies $\frac{3}{14\sqrt{3}} \leq s \leq \frac{1}{2\sqrt{3}}$. Noting that

$$\langle \nu, \zeta\rangle = t\left(\zeta_1 + \frac{1}{\sqrt{3}}\zeta_2\right) + s\zeta_3 = \left(\frac{1}{3\sqrt{2}} - \frac{1}{9}\sqrt{6}s\right)\left(\zeta_1 + \frac{1}{\sqrt{3}}\zeta_2\right) + s\zeta_3\,,$$

we obtain

$$\max_{\nu \text{ sat. } (a.2)} \langle \nu, \zeta\rangle = \max\left\{\frac{2}{7\sqrt{2}}\left(\zeta_1 + \frac{1}{\sqrt{3}}\zeta_2 + \frac{3}{2\sqrt{6}}\zeta_3\right), \frac{1}{2\sqrt{3}}\zeta_3\right\}. \tag{42}$$

Maximum of case (b). Since $\langle e_1 - e_3, \nu\rangle = 0$, we have $\nu_1 = \frac{2}{3}\sqrt{6}\nu_3$. Hence, $\nu = (t, s, \frac{3}{2\sqrt{6}}t)$ for some $t, s \geq 0$. Now using (29), we have

$$\varphi_{\mathrm{HCP}}(\nu) = \frac{7}{2}\sqrt{2}\nu_1\,.$$

Hence, since the maximum is attained for $\varphi_{\mathrm{HCP}}(\nu) = 1$, we have $\nu_1 = \frac{2}{7\sqrt{2}}$. Additionally, since $\langle e_1 - e_2, \nu\rangle \geq 0$, we have $\nu_2 \leq \frac{2}{7\sqrt{6}}$, and due to the form of ν, we have $\nu_3 = \frac{3}{14\sqrt{3}}$. This implies

$$\max_{\nu \text{ sat. (b)}} \langle \nu, \zeta\rangle = \frac{2}{7\sqrt{2}}\left(\zeta_1 + \frac{1}{\sqrt{3}}\zeta_2 + \frac{3}{2\sqrt{6}}\zeta_3\right). \tag{43}$$

Maximum of case (c). Since $\langle e_2 - e_3, \nu\rangle = 0$, we have $\frac{1}{2}\nu_1 + \frac{1}{2}\sqrt{3}\nu_2 = \frac{2}{3}\sqrt{6}\nu_3$. Now using (29), we have

$$\varphi_{\mathrm{HCP}}(\nu) = \frac{7}{2}\sqrt{2}\langle e_3, \nu\rangle = \frac{14}{3}\sqrt{3}\nu_3\,.$$

Hence, since the maximum is attained for $\varphi_{\mathrm{HCP}}(\nu) = 1$, we have $\nu_3 = \frac{3}{14\sqrt{3}}$. Additionally, since $\langle e_3 - e_1, \nu\rangle \geq 0$, we have $\nu_1 \leq \frac{2}{7\sqrt{2}}$. Due to the form of $\langle e_2 - e_3, \nu\rangle = 0$, we have $\nu_2 = \frac{4}{7\sqrt{6}} - \frac{1}{\sqrt{3}}\nu_1$. Note that $\nu_2 \geq 0$ for all $0 \leq \nu_1 \leq \frac{2}{7\sqrt{2}}$. Therefore

$$\langle \nu, \zeta\rangle = \nu_1\zeta_1 + \left(\frac{4}{7\sqrt{6}} - \frac{1}{\sqrt{3}}\nu_1\right)\zeta_2 + \frac{3}{14\sqrt{3}}\zeta_3\,.$$

This implies

$$\max_{\nu \text{ sat. (c)}} \langle \nu, \zeta\rangle = \max\left\{\frac{4}{7\sqrt{6}}\zeta_2 + \frac{3}{14\sqrt{3}}\zeta_3, \frac{2}{7\sqrt{2}}\left(\zeta_1 + \frac{1}{\sqrt{3}}\zeta_2 + \frac{3}{2\sqrt{6}}\zeta_3\right)\right\}. \tag{44}$$

Maximum of case (d). We have $\nu_3 = 0$ and therefore

$$\varphi_{\mathrm{HCP}}(\nu) = \sqrt{2}\left(\langle e_1, \nu\rangle + \langle e_2, \nu\rangle + |\langle e_1 - e_2, \nu\rangle| + \max\{\langle e_1, \nu\rangle, \langle e_2, \nu\rangle\}\right)$$

We distinguish to cases

(d.1) $\langle e_1 - e_2, \nu\rangle \geq 0$;
(d.2) $\langle e_1 - e_2, \nu\rangle \leq 0$.

Maximum of case (d.1). In the case $\langle e_1 - e_2, \nu\rangle \geq 0$ we have $\varphi_{\mathrm{HCP}}(\nu) = 3\sqrt{2}\nu_1$ and therefore, since $\varphi_{\mathrm{HCP}}(\nu) = 1$, $\nu_1 = \frac{1}{3\sqrt{2}}$. The inequality $\langle e_1 - e_2, \nu\rangle \geq 0$ implies that $0 \leq \nu_2 \leq \frac{1}{\sqrt{3}}\nu_1 = \frac{1}{3\sqrt{6}}$. Hence,

$$\max_{\nu \text{ sat. (d.1)}} \langle \nu, \zeta\rangle = \frac{1}{3\sqrt{2}}\left(\zeta_1 + \frac{1}{\sqrt{3}}\zeta_2\right) . \tag{45}$$

Maximum of case (d.2). In the case $\langle e_1 - e_2, \nu\rangle \leq 0$ we have

$$\varphi_{\mathrm{HCP}}(\nu) = 3\sqrt{2}\langle e_2, \nu\rangle = \sqrt{2}\left(\frac{3}{2}\nu_1 + \frac{3}{2}\sqrt{3}\nu_2\right) .$$

This, together with $\varphi_{\mathrm{HCP}}(\nu) = 1$, implies, $\nu_1 = \frac{2}{3\sqrt{2}} - \sqrt{3}\nu_2$ and therefore $\nu_2 \leq \frac{2}{3\sqrt{6}}$. Additionally, since $\langle e_1 - e_2\rangle \leq 0$, we have $\frac{1}{3\sqrt{6}} \leq \nu_2$. Therefore,

$$\langle \nu, \zeta\rangle = \nu_1\zeta_1 + \nu_2\zeta_2 = \left(\frac{3}{2\sqrt{2}} - \sqrt{3}\nu_2\right)\zeta_1 + \nu_2\zeta_2 \,.$$

This implies

$$\max_{\nu \text{ sat. (d.2)}} \langle \nu, \zeta\rangle = \max\left\{\frac{2}{3\sqrt{6}}\zeta_2, \frac{1}{3\sqrt{2}}\left(\zeta_1 + \frac{1}{\sqrt{3}}\zeta_2\right)\right\} . \tag{46}$$

Maximum of case (e). In the case $\nu_1 = 0$ we have

$$\varphi_{\mathrm{HCP}}(\nu) = \sqrt{2}\left(\sqrt{3}\nu_2 + \frac{1}{3}\sqrt{6}\nu_3 + \max\left\{\frac{\sqrt{3}}{2}\nu_2, \frac{2}{3}\sqrt{6}\nu_3\right\}\right) .$$

We distinguish between two cases:

(e.1) $\langle e_2, \nu\rangle \geq \langle e_3, \nu\rangle$;
(e.2) $\langle e_2, \nu\rangle \leq \langle e_3, \nu\rangle$.

Maximum of case (e.1). In this case, we have

$$\varphi_{\mathrm{HCP}}(\nu) = \sqrt{2}\left(\frac{3}{2}\sqrt{3}\nu_2 + \frac{1}{3}\sqrt{6}\nu_3\right) .$$

Therefore, since $\varphi_{\mathrm{HCP}}(\nu) = 1$, we have $\nu_2 = \frac{2}{3\sqrt{6}} - \frac{2}{9}\sqrt{2}\nu_3$. Hence, $\nu_3 \leq \frac{3}{2\sqrt{3}}$. Additionally, since $\langle e_2 - e_3, \nu\rangle \geq 0$, we have $\nu_3 \leq \frac{3}{14\sqrt{3}}$. Therefore,

$$\langle \nu, \zeta\rangle = \nu_2\zeta_2 + \nu_3\zeta_3 = \left(\frac{2}{3\sqrt{6}} - \frac{2}{9}\sqrt{2}\nu_3\right)\zeta_2 + \nu_3\zeta_3 \,.$$

Hence,

$$\max_{\nu \text{ sat. (e.1)}} \langle \nu, \zeta\rangle = \max\left\{\frac{2}{3\sqrt{6}}\zeta_2, \frac{4}{7\sqrt{6}}\zeta_2 + \frac{3}{14\sqrt{3}}\zeta_3\right\} . \tag{47}$$

Maximum of case (e.2). In this case, we have

$$\varphi_{\mathrm{HCP}}(\nu) = \sqrt{2}\left(\sqrt{3}\nu_2 + \sqrt{6}\nu_3\right) .$$

Therefore, since $\varphi_{\rm HCP}(\nu)=1$, we have $\nu_2=\frac{1}{\sqrt{6}}-\sqrt{2}\nu_3$. Hence, $\nu_3\leq\frac{1}{2\sqrt{3}}$. Additionally, since $\langle e_2-e_3,\nu\rangle\leq 0$, we have $\nu_3\geq\frac{3}{14\sqrt{3}}$. Therefore,

$$\langle\nu,\zeta\rangle=\nu_2\zeta_2+\nu_3\zeta_3=\left(\frac{1}{3\sqrt{6}}-\sqrt{2}\nu_3\right)\zeta_2+\nu_3\zeta_3\,.$$

Hence,

$$\max_{\nu \text{ sat. (e.1)}}\langle\nu,\zeta\rangle=\max\left\{\frac{1}{2\sqrt{3}}\zeta_3,\frac{4}{7\sqrt{6}}\zeta_2+\frac{3}{14\sqrt{3}}\zeta_3\right\}\,. \tag{48}$$

Exploiting (41)–(48), and (40), we obtain (30). This concludes Step 2.

Step 3.(Calculation of (31)) In order to calculate (31), we split the calculation of $\partial^*W_{\rm HCP}=\{\varphi^\circ_{\rm HCP}(\zeta)=1\}$ into different sets, where the maximum of $\varphi^\circ_{\rm HCP}$ is attained. We consider the following cases

(a) $A_a:=\{\zeta\in\mathbb{R}^3\colon\varphi^\circ_{\rm HCP}(\zeta)=\frac{1}{2\sqrt{3}}|\zeta_3|=1\}$;
(b) $A_b:=\{\zeta\in\mathbb{R}^3\colon\varphi^\circ_{\rm HCP}(\zeta)=\frac{2}{3\sqrt{6}}|\zeta_2|=1\}$;
(c) $A_c:=\{\zeta\in\mathbb{R}^3\colon\varphi^\circ_{\rm HCP}(\zeta)=\frac{4}{7\sqrt{6}}|\zeta_2|+\frac{3}{14\sqrt{3}}|\zeta_3|=1\}$;
(d) $A_d:=\{\zeta\in\mathbb{R}^3\colon\varphi^\circ_{\rm HCP}(\zeta)=\frac{1}{3\sqrt{2}}(|\zeta_1|+\frac{1}{\sqrt{3}}|\zeta_2|)=1\}$;
(e) $A_e:=\{\zeta\in\mathbb{R}^3\colon\varphi^\circ_{\rm HCP}(\zeta)=\frac{2}{7\sqrt{2}}(|\zeta_1|+\frac{1}{\sqrt{3}}|\zeta_2|+\frac{3}{2\sqrt{6}}|\zeta_3|)=1\}$.

In each of the cases, one can determine the area, shape and normal of the set, by invoking the condition that the maximum is attained $\varphi^\circ_{\rm HCP}$ for the respective function and therefore all the other functions f in the definition of $\varphi^\circ_{\rm HCP}$ satisfy $f\leq 1$. In the following, we only collect the results, since the calculations are elementary (but very long).

Calculations for case (a). In this case, we see that $\nu=(0,0,\pm1)$ $\mathcal{H}^2$-a.e., since this set is contained in the level set of the function $|\zeta_3|=c$ for some $c>0$. Additionally, we see that the set is a union of two hexagons of side length $2\sqrt{2}$. Therefore, for each of the two hexagons H_i we have $\mathcal{H}^2(H_i)=12\sqrt{3}$. Furthermore, $\varphi_{\rm HCP}(\nu)=2\sqrt{3}$. Hence

$$\int_{A_a}\varphi_{\rm HCP}(\nu)\,\mathrm{d}\mathcal{H}^2=2\cdot 12\sqrt{3}\cdot 2\sqrt{3}=2^4\cdot 3^2\,. \tag{49}$$

Calculations for case (b). In this case, we see that $\nu=(0,\pm1,0)$ $\mathcal{H}^2$-a.e., since this set is contained in the level set of the function $|\zeta_2|=c$ for some $c>0$. Additionally, we see that the set is a union of two rectangles with side lengths $3\sqrt{2}$ and $\frac{4}{3}\sqrt{3}$. Therefore, for each of the two rectangles S_i we have $\mathcal{H}^2(S_i)=4\sqrt{6}$. Furthermore, $\varphi_{\rm HCP}(\nu)=\frac{3}{2}\sqrt{6}$. Hence

$$\int_{A_b}\varphi_{\rm HCP}(\nu)\,\mathrm{d}\mathcal{H}^2=2\cdot 4\sqrt{6}\cdot\frac{3}{2}\sqrt{6}=2^3\cdot 3^2\,. \tag{50}$$

Calculations for case (c). In this case, we see that $\nu=(3/41)^{1/2}(0,\pm 8/\sqrt{6},\pm\sqrt{3})$ $\mathcal{H}^2$-a.e., since this set is contained in the level set of the function $\frac{4}{7\sqrt{6}}|\zeta_2|+\frac{3}{14\sqrt{3}}|\zeta_3|=c$ for some $c>0$. Additionally, we see that the set is a union of four trapezoids with height $(41/6)^{1/2}$ and two parallel sides o lengths $3\sqrt{2}$ and $2\sqrt{2}$. Therefore, for each of the four trapezoids T_i we have $\mathcal{H}^2(T_i)=\frac{5}{2}(\frac{41}{3})^{1/2}$. Furthermore, $\varphi_{\rm HCP}(\nu)=14(\frac{3}{41})^{1/2}$. Hence

$$\int_{A_c}\varphi_{\rm HCP}(\nu)\,\mathrm{d}\mathcal{H}^2=4\cdot\frac{5}{2}\left(\frac{41}{3}\right)^{1/2}\cdot 14\left(\frac{3}{41}\right)^{1/2}=2^2\cdot 5\cdot 7\,. \tag{51}$$

Calculations for case (d). In this case, we see that $\nu = \frac{1}{2}(\pm\sqrt{3}, \pm 1, 0)$ $\mathcal{H}^2$-a.e., since this set is contained in the level set of the function $|\zeta_1| + \frac{1}{\sqrt{3}}|\zeta_2| = c$ for some $c > 0$. Additionally, we see that the set is a union of four rectangles with side length $3\sqrt{2}$ and $\frac{4}{3}\sqrt{3}$. Therefore, for each of the four rectangles R_i we have $\mathcal{H}^2(R_i) = 4\sqrt{6}$. Furthermore, $\varphi_{\mathrm{HCP}}(\nu) = \frac{3}{2}\sqrt{6}$. Hence

$$\int_{A_d} \varphi_{\mathrm{HCP}}(\nu)\,\mathrm{d}\mathcal{H}^2 = 4 \cdot 4\sqrt{6} \cdot \frac{3}{2}\sqrt{6} = 2^4 \cdot 3^2\,. \tag{52}$$

Calculations for case (e). In this case, we see that $\nu = 2(6/41)^{1/2}(\pm 1, \pm\frac{1}{\sqrt{3}}, \frac{3}{2\sqrt{6}})$ $\mathcal{H}^2$-a.e., since this set is contained in the level set of the function $|\zeta_1| + \frac{1}{\sqrt{3}}|\zeta_2| + \frac{3}{2\sqrt{6}}|\zeta_3| = c$ for some $c > 0$. Additionally, we see that the set is a union of eight trapezoids with height $(41/6)^{1/2}$ and two parallel sides o lengths $3\sqrt{2}$ and $2\sqrt{2}$. Therefore, for each of the eight trapezoids Z_i we have $\mathcal{H}^2(Z_i) = \frac{5}{2}(\frac{41}{3})^{1/2}$. Furthermore, $\varphi_{\mathrm{HCP}}(\nu) = 14(\frac{3}{41})^{1/2}$. Hence

$$\int_{A_e} \varphi_{\mathrm{HCP}}(\nu)\,\mathrm{d}\mathcal{H}^2 = 8 \cdot \frac{5}{2}\left(\frac{41}{3}\right)^{1/2} \cdot 14\left(\frac{3}{41}\right)^{1/2} = 2^3 \cdot 5 \cdot 7\,. \tag{53}$$

Taking into account (49)–(53), we obtain

$$\int_{\partial^* W_{\mathrm{HCP}}} \varphi_{\mathrm{HCP}}(\nu)\,\mathrm{d}\mathcal{H}^2 = 2^5 \cdot 3^2 + 2^3 \cdot 3^2 + 2^2 \cdot 5 \cdot 7 + 2^4 \cdot 3^2 + 2^3 \cdot 5 \cdot 7 = 780\,. \tag{54}$$

Next, we need to calculate $|W_{\mathrm{HCP}}|$, since $W_{\mathrm{HCP}} = \{\varphi^\circ_{\mathrm{HCP}} \le 1\} \cap (C_a \cup C_b \cup C_c \cup C_d \cup C_e)$, where

$$\begin{aligned}
C_a &= \{\zeta \in \mathbb{R}^3 \colon \varphi^\circ_{\mathrm{HCP}}(\zeta) = \frac{1}{2\sqrt{3}}|\zeta_3|\}\,,\\
C_b &:= \{\zeta \in \mathbb{R}^3 \colon \varphi^\circ_{\mathrm{HCP}}(\zeta) = \frac{2}{3\sqrt{6}}|\zeta_2|\}\,,\\
C_c &:= \{\zeta \in \mathbb{R}^3 \colon \varphi^\circ_{\mathrm{HCP}}(\zeta) = \frac{4}{7\sqrt{6}}|\zeta_2| + \frac{3}{14\sqrt{3}}|\zeta_3|\}\,,\\
C_d &:= \{\zeta \in \mathbb{R}^3 \colon \varphi^\circ_{\mathrm{HCP}}(\zeta) = \frac{1}{3\sqrt{2}}(|\zeta_1| + \frac{1}{\sqrt{3}}|\zeta_2|)\}\,,\\
C_e &:= \{\zeta \in \mathbb{R}^3 \colon \varphi^\circ_{\mathrm{HCP}}(\zeta) = \frac{2}{7\sqrt{2}}(|\zeta_1| + \frac{1}{\sqrt{3}}|\zeta_2| + \frac{3}{2\sqrt{6}}|\zeta_3|)\}\,.
\end{aligned}$$

Note that $\mathcal{H}^2(C_\alpha \cap \{\varphi^\circ_{\mathrm{HCP}}(\zeta) = s\}) = s^2\mathcal{H}^2(A_\alpha)$ for all $\alpha \in \{a,b,c,d,e\}$. In the set C_a we have that $|\nabla\varphi^\circ_{\mathrm{HCP}}(\zeta)| = \frac{1}{2\sqrt{3}}$ $\mathcal{L}^3$-a.e.. Due to the coarea formula, we have

$$\begin{aligned}
|C_a \cap W_{\mathrm{HCP}}| &= 2\sqrt{3}\int_{C_a \cap W_{\mathrm{HCP}}} |\nabla\varphi^\circ_{\mathrm{HCP}}(\zeta)|\,\mathrm{d}\zeta\\
&= 2\sqrt{3}\int_0^1 \mathcal{H}^2(C_a \cap \{\varphi^\circ_{\mathrm{HCP}}(\zeta) = s\})\,\mathrm{d}s = \frac{2}{3}\sqrt{3}\mathcal{H}^2(A_a) = 2^4 \cdot 3\,.
\end{aligned} \tag{55}$$

In the set C_b, we have that $|\nabla\varphi^\circ_{\mathrm{HCP}}(\zeta)| = \frac{2}{3\sqrt{6}}$ $\mathcal{L}^3$-a.e.. Due to the coarea formula, we have

$$\begin{aligned}
|C_b \cap W_{\mathrm{HCP}}| &= \frac{3}{2}\sqrt{6}\int_{C_b \cap W_{\mathrm{HCP}}} |\nabla\varphi^\circ_{\mathrm{HCP}}(\zeta)|\,\mathrm{d}\zeta\\
&= \frac{3}{2}\sqrt{6}\int_0^1 \mathcal{H}^2(C_b \cap \{\varphi^\circ_{\mathrm{HCP}}(\zeta) = s\})\,\mathrm{d}s = \frac{1}{2}\sqrt{6}\mathcal{H}^2(A_b) = 2^3 \cdot 3\,.
\end{aligned} \tag{56}$$

In the set C_c, we have that $|\nabla\varphi^\circ_{\mathrm{HCP}}(\zeta)| = \frac{1}{14}(41/3)^{1/2}$ $\mathcal{L}^3$-a.e.. Due to the coarea formula, we have

$$
\begin{aligned}
|C_c \cap W_{\mathrm{HCP}}| &= 14\left(\frac{3}{41}\right)^{1/2}\int_{C_c\cap W_{\mathrm{HCP}}} |\nabla\varphi^\circ_{\mathrm{HCP}}(\zeta)|\,\mathrm{d}\zeta \\
&= 14\left(\frac{3}{41}\right)^{1/2}\int_0^1 \mathcal{H}^2(C_c \cap \{\varphi^\circ_{\mathrm{HCP}}(\zeta) = s\})\,\mathrm{d}s \\
&= \frac{1}{3}14\left(\frac{3}{41}\right)^{1/2}\mathcal{H}^2(A_c) = \frac{2^2\cdot 5\cdot 7}{3}\,.
\end{aligned}
\tag{57}
$$

In the set C_d, we have that $|\nabla\varphi^\circ_{\mathrm{HCP}}(\zeta)| = \frac{2}{3\sqrt{6}}$ $\mathcal{L}^3$-a.e.. Due to the coarea formula, we have

$$
\begin{aligned}
|C_d \cap W_{\mathrm{HCP}}| &= \frac{3}{2}\sqrt{6}\int_{C_d\cap W_{\mathrm{HCP}}} |\nabla\varphi^\circ_{\mathrm{HCP}}(\zeta)|\,\mathrm{d}\zeta \\
&= \frac{3}{2}\sqrt{6}\int_0^1 \mathcal{H}^2(C_d \cap \{\varphi^\circ_{\mathrm{HCP}}(\zeta) = s\})\,\mathrm{d}s \\
&= \frac{1}{2}\sqrt{6}\mathcal{H}^2(A_d) = 2^4\cdot 3\,.
\end{aligned}
\tag{58}
$$

In the set C_e, we have that $|\nabla\varphi^\circ_{\mathrm{HCP}}(\zeta)| = \frac{1}{14}(41/3)^{1/2}$ $\mathcal{L}^3$-a.e.. Due to the coarea formula, we have

$$
\begin{aligned}
|C_e \cap W_{\mathrm{HCP}}| &= 14\left(\frac{3}{41}\right)^{1/2}\int_{C_e\cap W_{\mathrm{HCP}}} |\nabla\varphi^\circ_{\mathrm{HCP}}(\zeta)|\,\mathrm{d}\zeta \\
&= 14\left(\frac{3}{41}\right)^{1/2}\int_0^1 \mathcal{H}^2(C_e \cap \{\varphi^\circ_{\mathrm{HCP}}(\zeta) = s\})\,\mathrm{d}s \\
&= \frac{1}{3}14\left(\frac{3}{41}\right)^{1/2}\mathcal{H}^2(A_e) = \frac{2^3\cdot 5\cdot 7}{3}\,.
\end{aligned}
\tag{59}
$$

Using (55)–(59), we obtain $|W_{\mathrm{HCP}}| = 260$. This together with (54) yields (31). □

4. Γ-convergence

In this section we prove Theorem 2.2. In order to prove the compactness statement, we provide some preliminary lemmata about the shape of the Voronoi cells of the FCC-lattice as well as the HCP-lattice (see Figure 6). In what follows we use the notation $\mathcal{N}_{\mathrm{FCC}} = \mathcal{N}_{\mathcal{L}_{\mathrm{FCC}}}(0)$, $\mathcal{N}_{\mathrm{HCP}} = \mathcal{N}_{\mathcal{L}_{\mathrm{HCP}}}(0)$.

Lemma 4.1. *(Voronoi cell in the* FCC*-lattice) Let $x \in \mathcal{L}_{\mathrm{FCC}}$. Then*

$$
\mathcal{V}_{\mathcal{L}_{\mathrm{FCC}}}(x) = x + V_{\mathrm{FCC}}\,, \qquad \text{where } V_{\mathrm{FCC}} := \left\{y \in \mathbb{R}^3\colon \max_{b\in\mathcal{N}_{\mathrm{FCC}}} \langle b, y\rangle \le \frac{1}{2}\right\}. \tag{60}
$$

Given $b_0 \in \mathcal{N}_{\mathrm{FCC}}$ the face

$$
S_{b_0} := \left\{y \in \mathbb{R}^3\colon \max_{b\in\mathcal{N}_{\mathrm{FCC}}} \langle b, y\rangle = \langle b_0, y\rangle = \frac{1}{2}\right\} \tag{61}
$$

is a rhombus with $\mathcal{H}^2(S_{b_0}) = \frac{1}{4}\sqrt{2}$. Moreover, for each $b_0 \in \mathcal{N}_{\mathrm{FCC}}$ the face S_{b_0} of $\mathcal{V}_{\mathrm{FCC}}(0)$ is shared with the Voronoi cell $\mathcal{V}_{\mathrm{FCC}}(b_0)$. Lastly, we have $|\mathcal{V}_{\mathrm{FCC}}(x)| = \frac{1}{2}\sqrt{2}$ for all $x \in \mathcal{L}_{\mathrm{FCC}}$.

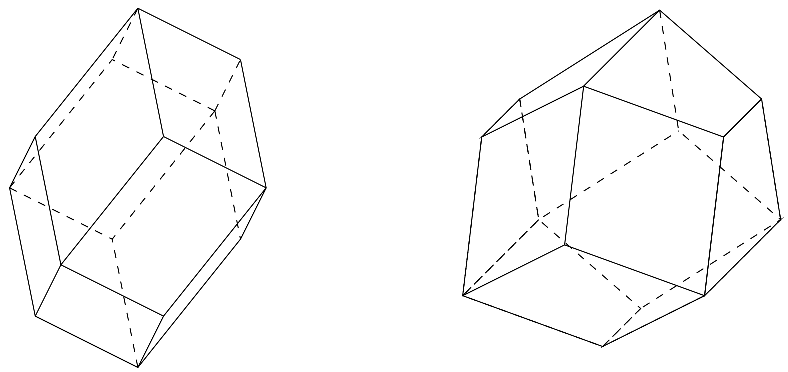

FIGURE 6. Left: the Voronoi cell V_{FCC} of the FCC lattice. Right: the Voronoi cell V_{HCP} of the HCP lattice.

Lemma 4.2. *(Voronoi cell in the* HCP*-lattice) Let* $x \in \mathcal{L}_{\mathrm{HCP}}$*. Then*

$$\mathcal{V}_{\mathcal{L}_{\mathrm{HCP}}}(x) = \begin{cases} x + V_{\mathrm{HCP}} & \text{if } x \in \mathrm{span}_{\mathbb{Z}}\{e_1, e_2, e_3\}\,, \\ x - V_{\mathrm{HCP}} & \text{if } x \in (v_1 + \mathrm{span}_{\mathbb{Z}}\{e_1, e_2, e_3\})\,, \end{cases} \tag{62}$$

where

$$V_{\mathrm{HCP}} := \left\{ y \in \mathbb{R}^3 \colon \max_{b \in \mathcal{N}_{\mathrm{HCP}}} \langle b, y \rangle \leq \frac{1}{2} \right\}.$$

For $b_0 \in \mathcal{N}_{\mathrm{HCP}}$ *we set*

$$S_{b_0} := \left\{ y \in \mathbb{R}^3 \colon \max_{b \in \mathcal{N}_{\mathrm{HCP}}} \langle b, y \rangle = \langle b_0, y \rangle = \frac{1}{2} \right\}. \tag{63}$$

If $b_0 \in \{\pm e_1, \pm e_2, \pm(e_1 - e_2)\}$ *the face* S_{b_0} *is a trapezoid of area* $\frac{1}{4}\sqrt{2}$*. If* $b_0 \in \{v_1, v_1 - e_1, v_1 - e_2, v_1 - e_3, v_1 - e_1 - e_3, v_1 - e_2 - e_3\}$ *the face* S_{b_0} *is a rhombus of area* $\frac{1}{8}\sqrt{6}$*. Moreover, for each* $b_0 \in \mathcal{N}_{\mathrm{HCP}}$ *the face* S_{b_0} *is shared with the Voronoi cell* $\mathcal{V}_{\mathcal{L}_{\mathrm{HCP}}}(b_0)$*. Lastly, we have* $|\mathcal{V}_{\mathcal{L}_{\mathrm{HCP}}}(x)| = \frac{1}{2}\sqrt{2}$ *for all* $x \in \mathcal{L}_{\mathrm{HCP}}$*.*

Proof of Lemma 4.1. We split the proof of the lemma into four steps. First, we prove (60). In the second step, we show that each face is a rhombus and calculate its area. Lastly, we show that each neighboring Voronoi cell $V_{\mathrm{FCC}}(b)$, $b \in \mathcal{N}_{\mathrm{FCC}}$ shares one face with the Voronoi cell $V_{\mathrm{FCC}}(0)$.

Step 1.(Proof of (60)) To check (60), since $\mathcal{L}_{\mathrm{FCC}}$ is a Bravais-lattice, it suffices to consider the case $x = 0$. Let $\mathcal{V}_{\mathcal{L}_{\mathrm{FCC}}}(0)$ denote the Voronoi cell of $\mathcal{L}_{\mathrm{FCC}}$ at $x = 0$ defined according to (14).

Step 1.1.($\mathcal{V}_{\mathcal{L}_{\mathrm{FCC}}}(0) \subset V_{\mathrm{FCC}}$) Let $y \in \mathcal{V}_{\mathcal{L}_{\mathrm{FCC}}}(0)$. By the very definition of Voronoi cell we have that for all $b \in \mathcal{N}_{\mathrm{FCC}}$ it holds $|y| \leq |y - b|$. Noting that $|b| = 1$ for all $b \in \mathcal{N}_{\mathrm{FCC}} \subset \mathcal{L}_{\mathrm{FCC}}$, we have

$$|y| \leq |y - b| \iff |y|^2 \leq |y - b|^2 = |y|^2 - 2\langle b, y \rangle + |b|^2 \iff \langle b, y \rangle \leq \frac{1}{2},$$

that is the inclusion $\mathcal{V}_{\mathcal{L}_{\mathrm{FCC}}}(0) \subset V_{\mathrm{FCC}}$.

Step 1.2.($V_{\mathrm{FCC}} \subset \mathcal{V}_{\mathcal{L}_{\mathrm{FCC}}}(0)$) We show that for $y \in V_{\mathrm{FCC}}$ we have $|y| \leq |y - z|$ for all $z \in \mathcal{L}_{\mathrm{FCC}}$. This is equivalent to

$$y \in V_{\mathrm{FCC}} \implies \langle y, z \rangle \leq \tfrac{1}{2}|z|^2 \quad \text{for all } z \in \mathcal{L}_{\mathrm{FCC}}\,. \tag{64}$$

We first observe that if $z \in \mathcal{N}_{\mathrm{FCC}}$, (64) is trivial since $|z| = 1$. Next, we prove (64) for all $z \in \mathcal{L}_{\mathrm{FCC}} \setminus \mathcal{N}_{\mathrm{FCC}}$. We distinguish two cases:

(a) $z = \lambda_1 b_j + \lambda_2 b_k$ $\lambda_1, \lambda_2 \in \mathbb{Z}$, $j, k \in \{1,2,3\}, j \neq k$;
(b) $z = \lambda_1 b_1 + \lambda_2 b_2 + \lambda_3 b_3$ $\lambda_1, \lambda_2, \lambda_3 \in \mathbb{Z}$.

Proof in case (a). We only show the statement for $z = \lambda_1 b_1 + \lambda_2 b_2$ for $\lambda_1, \lambda_2 \in \mathbb{Z}$, the cases with any other combination of two vectors being analogous. If $\lambda_1\lambda_2 \geq 0$, since $\langle b_1, b_2\rangle \geq 0$, we have

$$\begin{aligned}\langle y, z\rangle &= \langle y, \lambda_1 b_1 + \lambda_2 b_2\rangle \leq \frac{1}{2}|\lambda_1 b_1|^2 + \frac{1}{2}|\lambda_2 b_2|^2 \\ &= \frac{1}{2}|\lambda_1 b_1 + \lambda_2 b_2|^2 - \lambda_1\lambda_2\langle b_1, b_2\rangle \leq \frac{1}{2}|\lambda_1 b_1 + \lambda_2 b_2|^2 = \frac{1}{2}|z|^2\,.\end{aligned}$$

On the other hand, if $\lambda_1\lambda_2 \leq 0$ and without loss of generality $|\lambda_1| \leq |\lambda_2|$, noting that $b_1 - b_2 \in \mathcal{N}_{\mathrm{FCC}}$, we have

$$\begin{aligned}\langle y, z\rangle &= \langle y, \lambda_1 b_1 + \lambda_2 b_2\rangle = \langle y, (\lambda_2+\lambda_1) b_2 + \lambda_1(b_1 - b_2)\rangle \leq \frac{1}{2}|(\lambda_2+\lambda_1) b_2|^2 + \frac{1}{2}|\lambda_1(b_1-b_2)|^2 \\ &= \frac{1}{2}|\lambda_1 b_1 + \lambda_2 b_2|^2 - \lambda_1(\lambda_2+\lambda_1)\langle (b_1-b_2), b_2\rangle \leq \frac{1}{2}|\lambda_1 b_1 + \lambda_2 b_2|^2\,.\end{aligned}$$

Here, the last inequality follows, since $|b_1| = |b_2|$ and therefore $\lambda_1(\lambda_2+\lambda_1)\langle (b_1-b_2), b_2\rangle \geq 0$. This concludes case (a).
Proof in case (b). We now show that (60) holds true in the case of $b = \lambda_1 b_1 + \lambda_2 b_2 + \lambda_3 b_3$ with $\lambda_i \in \mathbb{Z}$. We restrict to the case $\lambda_1 \geq 0, \lambda_2 \geq 0$ and $\lambda_3 \leq 0$, since if all λ_i are of the same sign, (60) can be deduced from the fact that it holds true for $b \in \mathcal{N}_{\mathrm{FCC}}$ and the fact that $\langle b_j, b_k\rangle \geq 0$. Without loss of generality, we assume $|\lambda_2| \leq |\lambda_3|$. Hence, observing that $b_2 - b_3 \in \mathcal{N}_{\mathrm{FCC}}$, we have

$$\begin{aligned}\langle y, z\rangle &= \langle y, \lambda_1 b_1 + \lambda_2 b_2 + \lambda_3 b_3\rangle = \langle y, \lambda_1 b_1 + (\lambda_3+\lambda_2) b_3 + \lambda_2(b_2 - b_3)\rangle \\ &\leq \frac{1}{2}|\lambda_1 b_1 + (\lambda_3+\lambda_2) b_3|^2 + \frac{1}{2}|\lambda_2(b_2-b_3)|^2 \\ &= \frac{1}{2}|\lambda_1 b_1 + \lambda_2 b_2 + \lambda_3 b_3|^2 - \langle (\lambda_1 b_1 + (\lambda_3+\lambda_2) b_3), \lambda_2(b_2-b_3)\rangle \\ &= \frac{1}{2}|\lambda_1 b_1 + \lambda_2 b_2 + \lambda_3 b_3|^2 - (\lambda_3+\lambda_2)\lambda_2\langle b_2 - b_3, b_3\rangle \leq \frac{1}{2}|\lambda_1 b_1 + \lambda_2 b_2 + \lambda_3 b_3|^2\,.\end{aligned}$$

Here, the last inequality follows from $|b_2| = |b_3|$ and $\lambda_3 + \lambda_2 \leq 0$ whereas the equality in the last line is due to $\langle b_1, b_2\rangle = \langle b_1, b_3\rangle = \langle b_2, b_3\rangle$. This concludes case (b) and with that Step 1.2.
Step 2.(The faces of the Voronoi cell) To show that each face of the Voronoi cell V_{FCC} is a rhombus with area $\frac{1}{4}\sqrt{2}$ we first exploit its symmetries. Let $i \in \{1,2,3\}$ and let $T_i\colon \mathbb{R}^3 \to \mathbb{R}^3$ be the linear mapping that flips the i-th entry, i.e.

$$(T_i x)_j = \begin{cases} -x_i & \text{if } i = j\,, \\ x_j & \text{otherwise.}\end{cases}$$

We observe that

$$T_i\mathcal{N}_{\mathrm{FCC}} = \{T_i b \colon b \in \mathcal{N}_{\mathrm{FCC}}\} = \mathcal{N}_{\mathrm{FCC}}\,, \text{ for all } i \in \{1,2,3\}.$$

Moreover, given a permutation $\pi \in S_3$ we have that

$$\pi\mathcal{N}_{\mathrm{FCC}} = \{\pi b \colon b \in \mathcal{N}_{\mathrm{FCC}}\} = \mathcal{N}_{\mathrm{FCC}}\,.$$

It therefore suffices to restrict only to the case in which the vector b_0 agrees with the vector $b_1 \in \mathcal{N}_{\mathrm{FCC}}$. We claim that this face has corners given by

$$c_1 = \left(\frac{1}{2}\sqrt{2}, 0, 0\right), c_2 = \left(0, \frac{1}{2}\sqrt{2}, 0\right), c_3 = \frac{1}{4}\left(\sqrt{2}, \sqrt{2}, \sqrt{2}\right), c_4 = \frac{1}{4}\left(\sqrt{2}, \sqrt{2}, -\sqrt{2}\right). \quad (65)$$

Note that, if this were true then it is easy to see that S_{b_0} is a rhombus and $\mathcal{H}^2(S_{b_0}) = \frac{1}{4}\sqrt{2}$. It remains to prove (65). Let us denote by y a corner of S_{b_0}. We can assume that $y_1, y_2 \geq 0$. Were this not the case, then there could be $b' \in \mathcal{N}_{\mathrm{FCC}}$ such that $\langle b', y\rangle > \langle b, y\rangle$, thus contradicting the definition of S_{b_0} in (61). If $y_1 = 0$ (or $y_2 = 0$), then $y_2 = \frac{1}{2}\sqrt{2}$ (resp. $y_1 = \frac{1}{2}\sqrt{2}$) and since, $\langle b', y\rangle \leq \frac{1}{2}$ for all $b' \in \mathcal{N}_{\mathrm{FCC}}$ we have $y_3 = 0$. Hence, we find the two corners with coordinates $(\frac{1}{2}\sqrt{2}, 0, 0)$ and $(0, \frac{1}{2}\sqrt{2}, 0)$. Now, if $y_1 > 0$ and $y_2 > 0$, then assuming that $y_3 \geq 0$ we have that the corner is equal to $\langle b_1, y\rangle = \langle b_2, y\rangle = \langle b_3, y\rangle = \frac{1}{2}\sqrt{2}$. Thus, necessarily $y_1 = y_2 = y_3 = \frac{1}{4}\sqrt{2}$. If instead $y_3 < 0$, then the corner is equal to $\langle b_1, y\rangle = \langle b_2, y\rangle = \langle b_1 - b_3, y\rangle = \frac{1}{2}\sqrt{2}$ which implies $y_1 = y_2 = -y_3 = \frac{1}{4}\sqrt{2}$. Hence (65) holds true and this concludes Step 2.
Step 3.(Neighbors share faces) We want to show that for each $b_0 \in \mathcal{N}_{\mathrm{FCC}}$ we have that the face S_{b_0} of $V_{\mathrm{FCC}}(0)$ is shared with the Voronoi cell $V_{\mathrm{FCC}}(b_0)$. By the symmetries shown in Step 2 it suffices to prove this statement only for $b_0 = b_1$. Using (65) we see that the corners of the face S_{b_0} of the Voronoi cell $V_{\mathrm{FCC}}(0)$ coincide with the corners of the face $S_{-b_0} + b_0$ of the Voronoi cell $V_{\mathrm{FCC}}(b_0)$.
Step 4.(Volume of the Voronoi cell) In order to calculate the volume of the Voronoi cell we note that $\mathcal{L}_{\mathrm{FCC}}$ is a Bravais-lattice with spanning vectors b_1, b_2, b_3. Since, the Voronoi cells of all the points are the same, it suffices to calculate the fraction of points per unit volume. This, then gives also the volume per point. Since, the Voronoi cells are space filling the volume per point is equal to the volume of each Voronoi cell. Due to (17) we have that

$$|T_{\mathrm{FCC}}| = \frac{1}{2}\sqrt{2}.$$

Furthermore, we have that

$$\bigcup_{x \in \mathcal{L}_{\mathrm{FCC}}} (x + T_{\mathrm{FCC}}) = \mathbb{R}^3, \text{ and } \mathcal{L}_{\mathrm{FCC}} \cap T_{\mathrm{FCC}} = \{0\}.$$

Hence, each points of the lattice occupies a volume $|T_{\mathrm{FCC}}| = \frac{1}{2}\sqrt{2}$ and the volume of the Voronoi cell must be the same. This concludes Step 3 and thus the proof of the lemma. □

Proof of Lemma 4.2. We split the proof of the lemma into four steps. First, we prove (62). In the second step, we show that 6 of the faces are rhombi, the 6 other faces are trapezoids, and we calculate the area of each face. Lastly, given $x \in \mathcal{L}_{\mathrm{HCP}}$, we show that each neighboring Voronoi cell $\mathcal{V}_{\mathcal{L}_{\mathrm{HCP}}}(y), y \in \mathcal{N}_{\mathrm{HCP}}(x)$ shares a face with the Voronoi cell $V_{\mathrm{HCP}}(x)$.
Step 1.(Shape of the Voronoi cell) The purpose of this step is to prove (62). Here, we only show this equality in the case that $x = 0$, the case $x \neq 0$ being treated in a similar fashion.
Step 1.1.($\mathcal{V}_{\mathcal{L}_{\mathrm{HCP}}}(0) \subset V_{\mathrm{HCP}}$) Given $y \in \mathcal{V}_{\mathcal{L}_{\mathrm{HCP}}}(0)$ we have that $|y| \leq |y - b|$. Now, noting that $|b| = 1$ for all $b \in \mathcal{N}_{\mathrm{HCP}} \subset \mathcal{L}_{\mathrm{HCP}}$, we have

$$|y|^2 \leq |y - b|^2 = |y|^2 - 2\langle y, b\rangle + |b|^2 \iff \langle b, y\rangle \leq \frac{1}{2}.$$

This concludes Step 1.1.
Step 1.2.($V_{\mathrm{HCP}} \subset \mathcal{V}_{\mathcal{L}_{\mathrm{HCP}}}(0)$) We show that for $y \in V_{\mathrm{HCP}}$ we have $|y| \leq |y - z|$, for all $z \in \mathcal{L}_{\mathrm{HCP}}$. This is equivalent to

$$y \in V_{\mathrm{HCP}} \implies \langle y, z\rangle \leq \tfrac{1}{2}|z|^2 \quad \text{for all } z \in \mathcal{L}_{\mathrm{HCP}}. \quad (66)$$

Since, $|b| = 1$ for all $b \in \mathcal{N}_{\mathrm{HCP}}$ (66) is true for all $b \in \mathcal{N}_{\mathrm{HCP}}$. Next, we prove (66) for all $z \in \mathcal{L}_{\mathrm{HCP}} \setminus \mathcal{N}_{\mathrm{HCP}}$. We distinguish several cases:

(a) $z = \lambda_1 e_1 + \lambda_2 e_2, \lambda_1, \lambda_2 \in \mathbb{Z}\,;$
(b) $z = \lambda_1 e_1 + \lambda_2 e_2 + \lambda_3 e_3, \lambda_1, \lambda_2, \lambda_3 \in \mathbb{Z}\,;$
(c) $z = v_1 + \lambda_1 e_1 + \lambda_2 e_2, \lambda_1, \lambda_2 \in \mathbb{Z}\,;$
(d) $z = v_1 + \lambda_1 e_1 + \lambda_2 e_2 + \lambda_3 e_3, \lambda_1, \lambda_2, \lambda_3 \in \mathbb{Z}\,;$

Proof in case (a). If $\lambda_1, \lambda_2 \geq 0$, using that $\langle e_1, e_2 \rangle \geq 0$, we have

$$\begin{aligned}\langle y, z \rangle &= \langle y, \lambda_1 e_1 + \lambda_2 e_2 \rangle \leq \frac{1}{2}|\lambda_1 e_1|^2 + \frac{1}{2}|\lambda_2 e_2|^2 \\ &= \frac{1}{2}|\lambda_1 e_1 + \lambda_2 e_2|^2 - \lambda_1 \lambda_2 \langle e_1, e_2 \rangle \leq \frac{1}{2}|\lambda_1 e_1 + \lambda_2 e_2|^2 = \frac{1}{2}|z|^2\,.\end{aligned}$$

On the other hand, if $\lambda_1 \lambda_2 \leq 0$ and without loss of generality $\lambda_1 \geq |\lambda_2| \geq 0$, noting that $e_2 - e_1 \in \mathcal{N}_{\mathrm{HCP}}$, we have

$$\begin{aligned}\langle y, z \rangle = \langle y, \lambda_1 e_1 + \lambda_2 e_2 \rangle &= \langle y, \lambda_2(e_2 - e_1) + (\lambda_1 + \lambda_2) e_1 \rangle \leq \frac{1}{2}|\lambda_2(e_2 - e_1)|^2 + \frac{1}{2}|(\lambda_2 + \lambda_1) e_1|^2 \\ &= \frac{1}{2}|\lambda_1 e_1 + \lambda_2 e_2|^2 - \lambda_2(\lambda_1 + \lambda_2)\langle e_2 - e_1, e_1 \rangle \leq \frac{1}{2}|\lambda_1 e_1 + \lambda_2 e_2|^2 = \frac{1}{2}|z|^2\,.\end{aligned}$$

Here, the last inequality follows, since $\lambda_2 \leq 0 \leq \lambda_1 + \lambda_2$ and $\langle e_2 - e_1, e_1 \rangle \leq 0$. This concludes case (a).
Proof in case (b). We first show that $\langle y, e_3 \rangle \leq \frac{1}{2}|e_3|^2$. Using that $v_1, v_1 - e_1, v_1 - e_2 \in \mathcal{N}_{\mathrm{HCP}}$, that $3v_1 - e_1 - e_2 = \frac{3}{2} e_3$ we have

$$\begin{aligned}\langle y, e_3 \rangle &= \frac{2}{3}\langle y, v_1 + v_1 - e_1 + v_1 - e_2 \rangle \\ &\leq \frac{1}{3}\left(\left|\frac{1}{3}(e_1 + e_2)\right|^2 + \left|\frac{1}{3}(e_2 - 2e_1)\right|^2 + \left|\frac{1}{3}(e_1 - 2e_2)\right|^2\right) + \left|\frac{1}{2}e_3\right|^2 \leq \frac{1}{2}|e_3|^2\,.\end{aligned}$$

Here, the last inequality follows by calculating the norms of $e_1 + e_2, e_1 - 2e_2, e_2 - 2e_1$ and e_3 by using (8). Note that now, the case of $z = \lambda_1 e_1 + \lambda_2 e_2 + \lambda_3 e_3$ follows from case (a) using that $\langle e_3, e_1 \rangle = \langle e_3, e_2 \rangle = 0$.
Proof of case (c). Let $z = v_1 + \lambda_1 e_1 + \lambda_2 e_2$. If $\lambda_1, \lambda_2 \geq 0$ we have

$$\begin{aligned}\langle y, z \rangle = \langle y, v_1 + \lambda_1 e_1 + \lambda_2 e_2, \rangle &\leq \frac{1}{2}|v_1|^2 + \frac{1}{2}|\lambda_1 e_1|^2 + \frac{1}{2}|\lambda_2 e_2|^2 \leq \frac{1}{2}|v_1|^2 + \frac{1}{2}|\lambda_1 e_1 + \lambda_2 e_2|^2 \\ &= \frac{1}{2}|v_1 + \lambda_1 e_1 + \lambda_2 e_2|^2 - \langle v_1, \lambda_1 e_1 + \lambda_2 e_2 \rangle \leq \frac{1}{2}|v_1 + \lambda_1 e_1 + \lambda_2 e_2|^2\,.\end{aligned}$$

The second inequality uses that $\langle e_1, e_2 \rangle \geq 0$ and the last inequality uses that $\langle v_1, e_1 \rangle, \langle v_1, e_2 \rangle \geq 0$. Now assume that $\lambda_1 \geq 0, \lambda_2 < 0$. Then, since $\langle (v_1 - e_2), e_1 \rangle = 0$ and $\langle v_1 - e_2, e_2 \rangle \leq 0$, again exploiting that $v_1 - e_2 \in \mathcal{N}_{\mathrm{HCP}}$ it holds that

$$\begin{aligned}\langle y, z \rangle &= \langle y, (v_1 - e_2) + \lambda_1 e_1 + (\lambda_2 + 1) e_2 \rangle \leq \frac{1}{2}|v_1 - e_2|^2 + \frac{1}{2}|\lambda_1 e_1 + (\lambda_2 + 1) e_2|^2 \\ &= \frac{1}{2}|v_1 + \lambda_1 e_1 + \lambda_2 e_2|^2 - \langle v_1 - e_2, \lambda_1 e_1 + (\lambda_2 + 1) e_2 \rangle \leq \frac{1}{2}|v_1 + \lambda_1 e_1 + \lambda_2 e_2|^2 = \frac{1}{2}|z|^2\,.\end{aligned}$$

The case where $\lambda_1 < 0, \lambda_2 \geq 0$ (resp. $\lambda_1, \lambda_2 < 0$) is being treated in a similar fashion by replacing $v_1 - e_2$ with $v_1 - e_1$ (resp. $v_1 - e_1 - e_2$). *Proof in case* (d). Here, we only treat the case of

$z = v_1 + \lambda_1 e_1 + \lambda_2 e_2 + \lambda_3 e_3$, $\lambda_3 \geq 0$. Since $\langle v_1 + \lambda_1 e_1 + \lambda_2 e_2, e_3\rangle \geq 0$, we have

$$\begin{aligned}\langle y, z\rangle &= \langle y, v_1 + \lambda_1 e_1 + \lambda_2 e_2 + \lambda_3 e_3\rangle \leq \frac{1}{2}|v_1 + \lambda_1 e_1 + \lambda_2 e_2|^2 + \frac{1}{2}|\lambda_3 e_3|^2 \\ &= \frac{1}{2}|v_1 + \lambda_1 e_1 + \lambda_2 e_2 + \lambda_3 e_3|^2 - \langle v_1 + \lambda_1 e_1 + \lambda_2 e_2, e_3\rangle \leq \frac{1}{2}|v_1 + \lambda_1 e_1 + \lambda_2 e_2 + \lambda_3 e_3|^2 = \frac{1}{2}|z|^2 .\end{aligned}$$

The case of $\lambda_3 < 0$ follows by replacing v_1 with $v_1 - e_3$ in the last two cases (c) and (d). This concludes Step 1.2 and, together with Step 1.1, shows (62).

Step 2.(The faces of the Voronoi cell) In order to calculate the faces of V_{HCP} we use (62) and exploit its symmetries. We note that if $R \in SO(3)$ is any rotation of integer multiples of $2\pi/3$ around the x_3-axis we have that

$$R\mathcal{N}_{\mathrm{HCP}} = \{Rb \colon b \in \mathcal{N}_{\mathrm{HCP}}\} = \mathcal{N}_{\mathrm{HCP}} . \tag{67}$$

Moreover, if $T_3 \colon \mathbb{R}^3 \to \mathbb{R}^3$ is the reflection with respect to the (x_1, x_2)-plane, i.e.

$$(T_3 x)_j := \begin{cases} x_j & j = 1, 2 , \\ -x_3 & j = 3 , \end{cases} \tag{68}$$

we have that

$$T_3\mathcal{N}_{\mathrm{HCP}} = \{T_3 b \colon b \in \mathcal{N}_{\mathrm{HCP}}\} = \mathcal{N}_{\mathrm{HCP}} . \tag{69}$$

Exploiting (67) and (69), it suffices to find the corners of S_{b_0} in (63) for

$$\text{(a)} \quad b_0 = e_1 , \quad \text{(b)} \quad b_0 = -e_1 , \quad \text{(c)} \quad b_0 = v_1 .$$

Corners in case (a). We claim that in the case of $b_0 = e_1$ that the corners of S_{b_0} are given by the points

$$\begin{aligned} c_1 &= \left(\frac{1}{2}, \frac{1}{6}\sqrt{3}, \frac{1}{12}\sqrt{6}\right) , c_2 = \left(\frac{1}{2}, \frac{1}{6}\sqrt{3}, -\frac{1}{12}\sqrt{6}\right) , \\ c_3 &= \left(\frac{1}{2}, -\frac{1}{6}\sqrt{3}, \frac{1}{6}\sqrt{6}\right) , c_4 = \left(\frac{1}{2}, -\frac{1}{6}\sqrt{3}, -\frac{1}{6}\sqrt{6}\right) . \end{aligned} \tag{70}$$

In particular, the face S_{b_0} is a trapezoid with two bases of length $\frac{1}{6}\sqrt{6}$, $\frac{1}{3}\sqrt{6}$ and height $\frac{1}{3}\sqrt{3}$. Hence, $\mathcal{H}^2(S_{b_0}) = \frac{1}{4}\sqrt{2}$. It remains to prove (70). Let $y \in S_{b_0}$ be a corner. Due to (69), we can assume that $y_3 \geq 0$, since the other corners are just found by applying the mapping T_3 (see (68)) to the corners with positive coordinates. By the definition of S_{b_0} we have that $\langle y, e_1\rangle \geq \langle y, e_1 - e_2\rangle$ which is equivalent to $\langle y, e_2\rangle \geq 0$. Now, if $\langle y, e_2\rangle > 0$, then y is given by $\langle y, e_1\rangle = \langle y, e_2\rangle = \langle y, v_1\rangle = \frac{1}{2}$. This linear system has a unique solution given by $c_1 = \left(\frac{1}{2}, \frac{1}{6}\sqrt{3}, \frac{1}{12}\sqrt{6}\right)$. On the other hand, if $\langle y, e_2\rangle = 0$, then y is given by $\langle y, e_2\rangle = 0, \langle y, e_1\rangle = \langle y, v_1\rangle = \frac{1}{2}$. The unique solution of this linear system is given by $c_3 = \left(\frac{1}{2}, -\frac{1}{6}\sqrt{3}, \frac{1}{6}\sqrt{6}\right)$. This shows (70) and concludes case (a).

Corners in case (b). We claim that in the case of $b_0 = -e_1$ that the corners of S_{b_0} are given by the points

$$\begin{aligned} c_1 &= \left(-\frac{1}{2}, \frac{1}{6}\sqrt{3}, \frac{1}{12}\sqrt{6}\right) , c_2 = \left(-\frac{1}{2}, \frac{1}{6}\sqrt{3}, -\frac{1}{12}\sqrt{6}\right) , \\ c_3 &= \left(-\frac{1}{2}, -\frac{1}{6}\sqrt{3}, \frac{1}{6}\sqrt{6}\right) , c_4 = \left(-\frac{1}{2}, -\frac{1}{6}\sqrt{3}, -\frac{1}{6}\sqrt{6}\right) . \end{aligned} \tag{71}$$

In particular, the face S_{b_0} is a trapezoid with two bases of length $\frac{1}{6}\sqrt{6}$, $\frac{1}{3}\sqrt{6}$ and height $\frac{1}{3}\sqrt{3}$. Hence, $\mathcal{H}^2(S_{b_0}) = \frac{1}{4}\sqrt{2}$. It remains to prove (71). Let $y \in S_{b_0}$ be a corner. Due to (69), as in case (a), we can assume that $y_3 \geq 0$. By the definition of S_{b_0} we have that $\langle y, -e_1\rangle \geq$

$\langle y, e_2 - e_1\rangle$ which is equivalent to $\langle y, e_2\rangle \le 0$. Now, if $\langle y, e_2\rangle = 0$, then y is given by $\langle y, e_2\rangle = 0, \langle y, v_1 - e_1\rangle = \langle y, -e_1\rangle = \frac{1}{2}$. We see that the unique solution of this linear system is given by $c_1 = \left(-\frac{1}{2}, \frac{1}{6}\sqrt{3}, \frac{1}{12}\sqrt{6}\right)$. On the other hand, if $\langle y, e_2\rangle < 0$, then y is given by $\langle y, v_1\rangle = 0, \langle y, -e_1\rangle = \langle y, -e_2\rangle = \frac{1}{2}$. The unique solution is now given by $c_3 = \left(-\frac{1}{2}, -\frac{1}{6}\sqrt{3}, \frac{1}{6}\sqrt{6}\right)$. This shows (71) and concludes case (b).
Corners in case (c). We claim that in the case of $b_0 = v_1$ that the corners of S_{b_0} are given by the points

$$\begin{aligned} c_1 &= \left(\frac{1}{2}, \frac{1}{6}\sqrt{3}, \frac{1}{12}\sqrt{6}\right), c_2 = \left(0, 0, \frac{1}{4}\sqrt{6}\right), \\ c_3 &= \left(0, \frac{1}{3}\sqrt{3}, \frac{1}{6}\sqrt{6}\right), c_4 = \left(\frac{1}{2}, -\frac{1}{6}\sqrt{3}, \frac{1}{6}\sqrt{6}\right). \end{aligned} \tag{72}$$

In particular, the face S_{b_0} is a rhombus. Hence, $\mathcal{H}^2(S_{b_0}) = \frac{1}{8}\sqrt{6}$. It remains to prove (70). Let $y \in S_{b_0}$ be a corner. By the definition of S_{b_0} we have that $\langle y, v_1\rangle \ge \langle y, v_1 - e_1\rangle, \langle y, v_1 - e_2\rangle$ which is equivalent to $\langle y, e_1\rangle, \langle y, e_2\rangle \ge 0$. Now if, $\langle y, e_2\rangle > 0$ then the corner solves the linear system $\langle y, e_1\rangle = \langle y, e_2\rangle = \langle y, v_1\rangle = \frac{1}{2}$. Its unique solution is $c_1 = (\frac{1}{2}, \frac{1}{6}\sqrt{3}, \frac{1}{12}\sqrt{6})$. On the other hand if $\langle y, e_2\rangle = 0$, then the corners are given by those y such that $\langle y, e_2\rangle = 0, \langle y, e_1\rangle = \langle y, v_1\rangle = \frac{1}{2}$ or $\langle y, e_1\rangle = \langle y, e_2\rangle = 0, \langle y, v_1\rangle = \frac{1}{2}$. These points have coordinates $c_2 = (\frac{1}{2}, -\frac{1}{6}\sqrt{3}, \frac{1}{6}\sqrt{6})$ and $c_3 = (0, 0, \frac{1}{4}\sqrt{6})$. Finally, if $\langle y, e_1\rangle = 0$ and $\langle y, e_2\rangle > 0$, then y is obtained by solving $\langle y, e_1\rangle = 0, \langle y, e_2\rangle = \langle y, v_1\rangle = \frac{1}{2}$. Hence it has coordinates $c_4 = (0, \frac{\sqrt{3}}{3}, \frac{\sqrt{6}}{6})$. This proves (72) and concludes Step 2.
Step 3.(Neighbors share faces) We want to show that for each $b_0 \in \mathcal{N}_{\mathrm{HCP}}$ we have that the face S_{b_0} of $\mathcal{V}_{\mathcal{L}_{\mathrm{HCP}}}(0)$ is shared with the Voronoi cell $\mathcal{V}_{\mathcal{L}_{\mathrm{HCP}}}(b_0)$. By Step 1 we have that $\mathcal{V}_{\mathcal{L}_{\mathrm{HCP}}}(0) = V_{\mathrm{HCP}}$ and $\mathcal{V}_{\mathcal{L}_{\mathrm{HCP}}}(b_0) = b_0 - V_{\mathrm{HCP}}$. Hence, they share the side $\langle y, b_0\rangle = \frac{1}{2} = \langle b_0 - y, b_0\rangle$.

Step 4.(Volume of the Voronoi cell) In order to calculate the volume of the Voronoi cell we note that $\mathcal{L}_{\mathrm{HCP}}$ is periodic with respect to the vectors e_1, e_2, e_3. Since the Voronoi cells of all the points occupy the same volume, it suffices to calculate the fraction of points per unit volume. The inverse of this number is the volume per point. Since the Voronoi cells are space filling the volume per point is equal to the volume of each Voronoi cell. Due to (18) we have that

$$|T_{\mathrm{HCP}}| = \sqrt{2}\,.$$

Furthermore, we have that

$$\bigcup_{x \in \mathrm{span}_{\mathbb{Z}}\{e_1,e_2,e_3\}} (x + T_{\mathrm{HCP}}) = \mathbb{R}^3\,, \text{ and } \mathcal{L}_{\mathrm{HCP}} \cap T_{\mathrm{HCP}} = \{0, v_1\}\,.$$

Hence, the volume per point is $\frac{1}{2}|T_{\mathrm{HCP}}| = \frac{1}{2}\sqrt{2}$ and it agrees with the volume of the Voronoi cell. This concludes Step 4 and thus the proof of the lemma. □

Let $X \subset \varepsilon\mathcal{L}$. We define the union of the Voronoi cells $\mathcal{V}_{\varepsilon\mathcal{L}}$ of the $\varepsilon\mathcal{L}$ lattice as

$$E_\varepsilon := \bigcup_{x \in X} \mathcal{V}_{\varepsilon\mathcal{L}}(x)\,. \tag{73}$$

This first proposition is the content of Theorem 2.2 i).

Proposition 4.3. *(Compactness of the piecewise-constant interpolants) Let $\mathcal{L}$ be either the* FCC*-lattice or the* HCP*-lattice and recall* (19) *and* (73)*. Let $\{X_\varepsilon\}_\varepsilon \subset \varepsilon\mathcal{L}$ be such that*

$$\sup_{\varepsilon > 0} E_{\mathcal{L},\varepsilon}(X_\varepsilon) < +\infty\,.$$

Then there exists a set of finite perimeter $E \subset \mathbb{R}^3$ and a subsequence (not relabeled) such that $\chi_{E_\varepsilon} \to \chi_E$ with respect to the strong $L^1_{\mathrm{loc}}(\mathbb{R}^3)$-topology.

Proof. In the following fix $\mathcal{L}$ to be either the FCC or the HCP lattice and let $\{X_\varepsilon\}_\varepsilon \subset \varepsilon\mathcal{L}$ be such that

$$\sup_{\varepsilon>0} E_{\mathcal{L},\varepsilon}(X_\varepsilon) < +\infty\,. \tag{74}$$

Using Lemma 4.1 and Lemma 4.2, we observe that for every $x \in X_\varepsilon$ and $y \in \mathcal{N}_\varepsilon(x)$ we have that the face $\varepsilon S_{\frac{y-x}{\varepsilon}} + x \subset \partial\mathcal{V}_{\varepsilon\mathcal{L}}(x)$ contributes to the perimeter of E_ε only if $y \notin X_\varepsilon$. Using (73), we have that

$$\mathcal{H}^2(\partial E_\varepsilon) = \sum_{x\in X_\varepsilon}\sum_{y\in\mathcal{N}_\varepsilon(x)\setminus X_\varepsilon} \varepsilon^2\mathcal{H}^2(S_{\frac{y-x}{\varepsilon}}) \le C\sum_{x\in X_\varepsilon}\varepsilon^2(12-\#(\mathcal{N}_\varepsilon(x)\cap X_\varepsilon)) = CE_{\mathcal{L},\varepsilon}(X_\varepsilon)\,.$$

Given $R>0$, we therefore have that there exists $C>0$ such that

$$\|\chi_{E_\varepsilon}\|_{L^1(B_R)} + |D\chi_{E_\varepsilon}|(B_R) \le C(R^3+\mathcal{H}^2(\partial E_\varepsilon)) \le C(R^3+E_{\mathcal{L},\varepsilon}(X_\varepsilon)) \le C(R^3+\sup_{\varepsilon>0}E_{\mathcal{L},\varepsilon}(X_\varepsilon))\,.$$

By (74) and [[3], Theorem 3.39], we obtain the desired result. □

Lemma 4.4. *(Piecewise-constant interpolants) Let $\mathcal{L}$ be either the* FCC*-lattice or the* HCP*-lattice and recall* (19)–(20)*, and* (73)*. Let $E \subset \mathbb{R}^3$ be a set of finite perimeter and let $\{X_\varepsilon\}_\varepsilon \subset \varepsilon\mathcal{L}$ for each $\varepsilon > 0$ and be such that*

$$\sup_{\varepsilon>0} E_{\mathcal{L},\varepsilon}(X_\varepsilon) < +\infty\,.$$

The following two are equivalent:

(i) $\mu_\varepsilon \overset{*}{\rightharpoonup} \mu$ *with respect to the weak star topology of measures and* $\mu = \sqrt{2}\mathcal{L}^3\llcorner E$.
(ii) $\chi_{E_\varepsilon} \to \chi_E$ *with respect to the strong* $L^1_{\mathrm{loc}}(\mathbb{R}^3)$*-topology.*

Proof. We show the two implications separately.
Step 1.((ii) $\implies$ (i)) We show that if there exists $E \subset \mathbb{R}^3$ such that $\chi_{E_\varepsilon} \to \chi_E$ with respect to the strong $L^1_{\mathrm{loc}}(\mathbb{R}^3)$ convergence, then $\mu_\varepsilon \overset{*}{\rightharpoonup} \sqrt{2}\mathcal{L}^3\llcorner E$ with respect to the weak star convergence of measures. To this end, let $v \in C_c(\mathbb{R}^3)$. There exists $R>0$ such that $\operatorname{supp} v \subset B_R$. Therefore, we have that

$$\left|\int_{\mathbb{R}^3}(\chi_{E_\varepsilon}-\chi_E)v\,\mathrm{d}y\right| \le \|v\|_{L^\infty(\mathbb{R}^3)}\|\chi_{E_\varepsilon}-\chi_E\|_{L^1(B_R)} \to 0\,.$$

Observe that $|\mathcal{V}_\varepsilon(x)| = \varepsilon^3\frac{1}{2}\sqrt{2}$ for all $x \in \varepsilon\mathcal{L}$ and therefore

$$\begin{aligned}\int_{\mathbb{R}^3} v\,\mathrm{d}\mu_\varepsilon = \sum_{x\in X_\varepsilon}\varepsilon^3 v(x) = \sqrt{2}&\sum_{x\in X_\varepsilon}\mathcal{V}_\varepsilon(x)v(x)\\ = \sqrt{2}&\sum_{x\in X_\varepsilon\cap B_R}\int_{\mathcal{V}_\varepsilon(x)} v(y)\,\mathrm{d}y + \sqrt{2}\sum_{x\in X_\varepsilon\cap B_R}\int_{\mathcal{V}_\varepsilon(x)}(v(x)-v(y))\,\mathrm{d}y\\ = \sqrt{2}&\int_{\mathbb{R}^3}\chi_{E_\varepsilon}v\,\mathrm{d}y + \sqrt{2}\sum_{x\in X_\varepsilon\cap B_R}\int_{V_\varepsilon(x)}(v(x)-v(y))\,\mathrm{d}y\,.\end{aligned}$$

In order to obtain the statement it remains to prove that as $\varepsilon \to 0$ we have

$$\sum_{x\in X_\varepsilon\cap B_R}\int_{V_\varepsilon(x)}(v(x)-v(y))\,\mathrm{d}y \to 0\,. \tag{75}$$

To this end it is enough to observe that, having compact support, v is uniformly continuous. Denoting by $\omega\colon [0,+\infty) \to [0,+\infty)$ such that $\omega(r) \to 0$ as $r \to 0$ its modulus of continuity and noting that $\mathrm{diam}\mathcal{V}_\varepsilon \le C\varepsilon$ for some fixed constant $C > 0$, we obtain

$$\left|\sum_{x \in X_\varepsilon \cap B_R} \int_{\mathcal{V}_\varepsilon(x)} (v(x) - v(y))\,\mathrm{d}y\right| \le \sum_{x \in \mathcal{L} \cap B_R} |\mathcal{V}_\varepsilon(x)| \sup_{|x-y| \le C\varepsilon} |v(x) - v(y)| \le |B_{2R}|\,\omega(C\varepsilon)\,.$$

for $\varepsilon > 0$ small enough. This shows (75) and concludes Step 1.

Step 2.((i) $\implies$ (ii)) Let $E \subset \mathbb{R}^3$ be a set of finite perimeter and assume that $\mu_\varepsilon \overset{*}{\rightharpoonup} \mu$ and $\mu = \sqrt{2}\mathcal{L}^3 \llcorner E$. Take an arbitrary subsequence (not relabbeled) of $\{X_\varepsilon\}_\varepsilon$. We show that there exists a further subsequence (again not relabbeled) such that $\chi_{E_\varepsilon} \to \chi_E$ with respect to the strong $L^1_{\mathrm{loc}}(\mathbb{R}^3)$-topology. Since $L^1_{\mathrm{loc}}(\mathbb{R}^3)$-topology satisfies the Uryson property this implies the claim. By proposition 4.3 we have that there exists a set of finite perimeter $E' \subset \mathbb{R}^3$ and a further subsequence $\{X_{\varepsilon_k}\}_k \subset \{X_\varepsilon\}_\varepsilon$ such that $\chi_{E_\varepsilon} \to \chi_{E'}$ with respect to the strong $L^1_{\mathrm{loc}}(\mathbb{R}^3)$-topology. By the first step we necessarily must have $E = E'$ which implies the claim and concludes the proof of the lemma. □

In order to prove Theorem 2.2 we make use of [2, Theorem 5.5]. We state a simplified and sufficient version of it below (up to changing the set $\{\pm 1\}$ to the set $\{0,1\}$). Let $(\Omega, \mathbb{P}, \mathcal{F})$ be a probability space and recall [2, Definition 5.1 and Definition 5.4].

Theorem 4.5. *Let $\mathcal{L}$ be a stationary and ergodic stochastic lattice and let $c(x,y) = c(x-y)$ satisfy* [2, Hypothesis 1]. *For $\mathbb{P}$-almost every ω the functionals $F_\varepsilon(\omega)$ Γ-converge with respect to the strong $L^1(D)$-topology to the functional $F_{\mathrm{hom}}\colon L^1(D) \to [0,+\infty]$ defined by*

$$F_{\mathrm{hom}}(u) := \begin{cases} \int_{S(u)} \varphi_{\mathrm{hom}}(\nu_u)\,\mathrm{d}\mathcal{H}^2 & \text{if } u \in BV(D;\{0,1\}),\\ +\infty & \text{otherwise.}\end{cases}$$

The function $\varphi_{\mathrm{hom}}\colon \mathbb{R}^3 \to [0,+\infty]$ is given by

$$\varphi_{\mathrm{hom}}(\nu) = \lim_{T\to+\infty} \frac{1}{T^2}\int_\Omega \inf\left\{F(u, Q_T^\nu)\colon u\colon \mathcal{L}(\omega) \to \{0,1\}, u(i) = u_\nu(i) \text{ for } i \in \mathcal{L}(\omega) \setminus Q^\nu_{T-3}\right\} \mathrm{d}\mathbb{P}(\omega)\,.$$

Proof of Theorem 2.2. We first prove i) and then prove ii) and iii) at the same time.

Step 1.(Proof of i)) Statement i) of Theorem 2.2 follows directly by recalling (21), noting that

$$E_{\mathcal{L},\varepsilon}(\mu_\varepsilon) < +\infty \implies \mu_\varepsilon = \varepsilon^3 \sum_{x \in X_\varepsilon} \delta_x \text{ for some } X_\varepsilon \subset \varepsilon\mathcal{L}\,,$$

applying Proposition 4.3, and Lemma 4.4.

Step 2.(Proof of ii) and iii)] We exploit the integral representation result Theorem 5.5 in [2] to obtain the specific form of the Γ-limit. First of all note that, due to Step 1 and Lemma 4.4 the Γ-convergence in the variable of the empirical measures with the energies defined on $\mathcal{M}_+(\mathbb{R}^3)$ is equivalent to the Γ-convergence of the energies defined for the piecewise-constant interpolants given in (73) and the energies defined in $L^1_{\mathrm{loc}}(\mathbb{R}^3)$. Now, we fix $(\Omega, \mathcal{F}, \mathbb{P}) = (\{0\}, \{\{0\}, \emptyset\}, \delta_0)$ to be a probability space and an additive and ergodic group action (see Definition 5.1 in [2]) $\tau_z\colon \{0\} \to \{0\}, z \in \mathbb{Z}^3$ by setting $\tau_z(0) = 0$. We now set $\mathcal{L}(0) = \mathcal{L}_{\mathrm{FCC}}$ or $\mathcal{L}(0) = \mathcal{L}_{\mathrm{HCP}}$ to be an admissible stochastic lattice according to Definition 5.4 in [2]. Furthermore, since

$$\mathcal{L}_{\mathrm{FCC}} = \mathcal{L}_{\mathrm{FCC}} + b_k\,, k = 1,2,3, \text{ and } \mathcal{L}_{\mathrm{HCP}} = \mathcal{L}_{\mathrm{HCP}} + e_k\,, k = 1,2,3,$$

we see that with this choice both $\mathcal{L}_{\rm FCC}$ and $\mathcal{L}_{\rm HCP}$ are stationary and ergodic through the group action

$$\mathcal{L}(0) = \mathcal{L}_{\rm FCC}\,, \mathcal{L}(\tau_z(0)) = \mathcal{L}_{\rm FCC} + \sum_{k=1}^{3} z_k b_k \text{ or } \mathcal{L}(0) = \mathcal{L}_{\rm HCP}\,, \mathcal{L}(\tau_z(0)) = \mathcal{L}_{\rm HCP} + \sum_{k=1}^{3} z_k e_k\,.$$

Therefore, all conditions of 4.5 are satisfied. This yields the desired integral representation and concludes the proof. □

Acknowledgements

This work was supported by the DFG project FR 4083/1-1 and by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Germany's Excellence Strategy EXC 2044 -390685587, Mathematics Münster: Dynamics–Geometry–Structure. The work of M. Cicalese was supported by the DFG Collaborative Research Center TRR 109, "Discretization in Geometry and Dynamics".

References

[1] N.L. Allinger. *Molecular structure: understanding steric and electronic effects from molecular mechanics.* John Wiley & Sons (2010).

[2] R. Alicandro, M. Cicalese, M. Ruf. Domain formation in magnetic polymer composites: an approach via stochastic homogenization. *Arch. Ration. Mech. Anal.* **218** (2015), 945–984.

[3] L. Ambrosio, N. Fusco, D. Pallara. *Functions of bounded variation and free discontinuity problems.* Oxford Mathematical Monographs, The Clarendon Press, Oxford University Press, New York, 2000.

[4] R. Alicandro, M.S. Gelli. *Local and non local continuum limits of Ising-type energies for spin systems.* SIAM J. Math. Anal. **48** (2016), 895–931.

[5] Y. Au Yeung, G. Friesecke, B. Schmidt. *Minimizing atomic configurations of short range pair potentials in two dimensions: crystallization in the Wulff shape.* Calc. Var. Partial Differential Equations **44** (2012) 81–100.

[6] X. Blanc, M. Lewin. *The crystallization conjecture: a review.* EMS Surv. Math. Sci. **2** (2015), 255–306.

[7] A. Braides. *Γ-convergence for Beginners.* Oxford University Press, Oxford 2002.

[8] A. Braides, L. Truskinovsky. *Asymptotic expansions by Γ-convergence.* Contin. Mech. Thermodyn. **20** (2008) 21–62.

[9] A. Chambolle, L. Kreutz. *Cristallinity of the homogenized surface energy density of periodic lattice systems.* Preprint (2021) ArXiv:2106.08111.

[10] G. Dal Maso. *An introduction to Γ-convergence.* Springer Science & Business Media, **8** (2012).

[11] L. De Luca, G. Friesecke. *Crystallization in two dimensions and a discrete GaussBonnet Theorem.* J. Nonlinear Sci. **28** (2017), 69–90.

[12] W. E, D. Li. *On the crystallization of 2D hexagonal lattices.* Comm. Math. Phys. **286** (2009), 1099–1140.

[13] I. Fonseca, S. Müller. *A uniqueness proof for the Wulff theorem.* Proc. Roy. Soc. Edinburgh Sect. **119** (1991) 125–136.

[14] L. C. Flatley, F. Theil. *Face-centered cubic crystallization of atomistic configurations.* Arch. Ration. Mech. Anal. **218** (2015), 363–416.

[15] M. Friedrich, L. Kreutz. *Finite crystallization and Wulff shape emergence for ionic compounds in the square lattice.* Nonlinearity **33** (2020), 1240–1296.

[16] M. Friedrich, L. Kreutz. *Crystallization in the hexagonal lattice for ionic dimers.* Math. Models Methods Appl. Sci. **29** (2019), 1853–1900.

[17] M. Friedrich, L. Kreutz, B. Schmidt. *Emergence of rigid Polycrystals from atomistic Systems with Heitmann-Radin sticky disk energy.* Arch. Ration. Mech. Anal. **240** (2021), 627–698.

[18] G. Friesecke, F. Theil. *Molecular geometry optimization, models.* In the Encyclopedia of Applied and Computational Mathematics, B. Engquist (Ed.), Springer, 2015.

[19] C. S. Gardner, C. Radin. *The infinite-volume ground state of the Lennard-Jones potential.* J. Stat. Phys. **20** (1979), 719–724.

[20] T.C. Hales. *A proof of the Kepler conjecture.* Ann. Math. **162** (2005), 1065–1185.

[21] H. Harborth. *Lösung zu Problem 664 a.* Elem. Math. **29** (1974), 14–15.

[22] L.H. Harper. *Global methods for combinatorial isoperimetric problems.* Cambridge University Press **90** (2004).
[23] R. Heitmann, C. Radin. *The ground state for sticky disks.* J. Stat. Phys. **22** (1980) 281–287.
[24] E. G. Lewars. *Computational Chemistry.* 2nd edition, Springer, 2011.
[25] E. Mainini, U. Stefanelli. *Crystallization in carbon nanostructures.* Comm. Math. Phys. **328** (2014), 545–571.
[26] C. Radin. *The ground state for soft disks.* J. Stat. Phys. **26** (1981), 365–373.
[27] K. Schütte, B.L. van der Waerden. *Das Problem der dreizehn Kugeln.* Math. Ann. **125** (1952), 324–334.
[28] F. Theil. *A proof of crystallization in two dimensions.* Comm. Math. Phys. **262** (2006), 209–236.
[29] G. Wulff. *Zur Frage der Geschwindigkeit des Wachstums und der Auflösung der Kristallflächen.* Z. Krist. **34** (1901), 449–530.

(Marco Cicalese) TU München, Germany

E-mail address: cicalese@ma.tum.de

(Leonard Kreutz) WWU Münster, Germany

E-mail address: lkreutz@uni-muenster.de

(Gian Paolo Leonardi) Università di Trento, Italy

E-mail address: gianpaolo.leonardi@unitn.it