Continuum Surface Energy from a Lattice Model

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Abstract

We investigate some connections between the continuum and atomistic descriptions of deformable crystals, using some interesting results from number theory. The energy of a deformed crystal is calculated in the context of a lattice model with binary interactions in two dimensions. A new bond counting approach is used, which reduces the problem to the lattice point problem of number theory. When the crystal shape is a lattice polygon, we show that the energy equals the bulk elastic energy, plus the boundary integral of a surface energy density, plus the sum over the vertices of a corner energy function. This is an exact result when the interatomic potential has finite range; for infinite-range potentials it is asymptotically valid as the lattice parameter zero. The surface energy density is obtained explicitly as a function of the deformation gradient and boundary normal. The corner energy is found as an explicit function of the deformation gradient and the normals of the two facets meeting at the corner. For more general convex domains with possibly curved boundary, the surface energy density depends on the unit normal in a striking way. It is continuous at irrational directions, discontinuous at rational ones and nowhere differentiable. This pathology is alarming since it renders the surface energy minimization problem (under domain variations) ill-posed. An alternative approach of defining the continuum region is introduced, that restores continuity of the surface energy density function.

1 Introduction

This article is concerned with the derivation of continuum surface energy from a standard lattice model, by exploiting results related to certain lattice point problems of number theory, e.g. [BL, BR, Hu, IKM, Pi].

The problem of relating discrete energies of crystals to their continuum counterparts has a much simpler analogue: that of *mass*. Suppose the crystal is two-dimensional and consists of those atoms (points in the lattice $L = \mathbb{Z}^2$) that belong to a compact set Ω. Consider the problem of measuring the mass m of the crystal, given that each atom has unit mass. Then the exact mass is $m = \#(\Omega \cap L)$. Suppose further that the crystal is faceted; in particular, let Ω be a lattice polygon: one whose vertices

are lattice points. This implies that the facets, or sides of Ω are along crystallographic directions. One would be tempted to write the mass as $m = \int_\Omega 1dx = |\Omega|$ independently of Ω, but it turns out that this is not true in general, though it holds in the limit as the crystal becomes large. The exact mass can be found using a remarkable and quite old result, namely Pick's Theorem [Pi] (1899): *The area of a lattice polygon equals the number of atoms in the interior, plus half the number of atoms on the boundary, minus one*. This provides a *discrete* expression for the area—a "continuum" quantity—but it is equivalent to the following *continuum expression* (see Lemma 2.1 below) for the number of atoms (a "discrete" quantity) or the mass:

$$m = \#(\Omega \cap L) = \int_\Omega 1dx + \int_{\partial\Omega} \frac{1}{2|\bar{n}|} ds + \sum_{i=1}^{N} \frac{\theta_i}{2\pi}, \tag{1.1}$$

where $\bar{n}$ is an outward normal to $\partial\Omega$ whose components on each facet are irreducible integers, and θ_i are the dihedral angles of the N vertices of Ω. This is a continuum expression of the mass as a bulk integral of a (unit) mass density, plus the boundary integral of a *surface mass density*, plus contributions from the corners. In this paper we study the energy of a crystal due to pairwise atomic interactions, with emphasis on its dependence on the shape of the boundary. Some of our results express this energy of faceted crystals in a similar, continuum form, as bulk energy, plus the boundary integral of a surface energy density, plus a sum of corner energies. The surface and corner energies are found explicitly in terms of the interatomic potential, the deformation gradient, and the normal vectors. We also study the surface energy for smooth boundaries.

Perhaps the first rigorous derivation of continuum energy functions from atomistic models is due to Blanc, Le Bris and Lions [BBL], who study (among other problems) the energy of a crystal governed by an interatomic potential with binary central-force interactions, subject to a prescribed smooth deformation. An asymptotic form of the energy is obtained as the lattice parameter ε tends to zero. The dominant term is the usual elastic energy $\int_\Omega W(\nabla y(x))dx$, where Ω is the macroscopic reference domain occupied by the crystal, $y : \Omega \to \mathbb{R}^3$ is the prescribed smooth deformation, and the elastic stored energy function W is determined by the interatomic potential (cf. (3.3) below). The next term, of order ε in Theorem 3 of [BBL], is a surface integral over $\partial\Omega$ that involves values of the deformation gradient and unit normal. The form of this surface energy is not explicit and it is not clear to what extent it can be expressed as a function of those variables. Terms of order ε^2 include a volume integral of higher gradient energy, but also surface terms; the latter are left unspecified.

In studying the energy, one encounters sums of the form $\varepsilon^3 \sum_{x\in(\Omega\cap\varepsilon L)} f(x)$. Here εL is the rescaled lattice $L = \mathbb{Z}^3$ with lattice parameter ε. While these Riemann sums converge to $\int_\Omega f$ as

$\varepsilon \to 0$, there are higher order terms. Often, these are surface terms of order ε, the same order as the surface energy in [BBL]. The asymptotic behavior of Riemann sums, even in simple smooth domains, is not completely understood at present, unless strong specializing assumptions are made [BR]. This is true even when f is constant, and the problem reduces to the *lattice point problem*, well-known in number theory: find the asymptotics of the number of lattice points in Ω, namely $\#(\Omega \cap \varepsilon L)$ as $\varepsilon \to 0$, equivalently $\#(r\Omega \cap L)$ as $r \to \infty$ [BR, IKM, Ts]. Even in two dimensions, in the seemingly simple case where Ω is the unit disk, the problem—initially posed by Gauss—is not completely settled. Currently, the best available estimate seems to be due to Huxley [Hu]. Letting $R(r) = \#(r\Omega \cap L) - |r\Omega|$ be the *remainder*, then for the disk, or for sets with positive boundary curvature, $R(r) = O(r^a(\log r)^b)$, with $a = \frac{131}{208} \approx 0.63$ and $b = \frac{18627}{8230} \approx 2.25$ [Hu]. The remainder depends strongly on the shape of $\partial\Omega$; for Ω a lattice polygon (one whose vertices are lattice points), $R(r) = O(r)$. Letting $\varepsilon = 1/r$, the remainder would corresponds to a higher order term $Q(\varepsilon) = \varepsilon^2 R(1/\varepsilon)$ in the Riemann sum (of a constant function) $\varepsilon^2 \#(\Omega \cap \varepsilon L) = |\Omega| + Q(\varepsilon)$. For smooth, strictly convex domains, the order of $Q(\varepsilon)$ is between ε and ε^2 [IKM], that is, between the orders of the surface and the gradient energy of [BBL]. In addition, $Q(\varepsilon)$ is highly oscillatory and very difficult to characterize explicitly. In [BBL] it is assumed that there is a sequence $\varepsilon = \varepsilon_k \to 0$ as the integer $k \to \infty$, such that the number of lattice points in Ω is precisely $|\Omega|/\varepsilon_k^3$ (in three dimensions). This means that for some sequence $r_k \to \infty$, $\#(r_k\Omega \cap L) = |r_k\Omega|$. This is equivalent to $Q(\varepsilon_k) = 0$, thus it eliminates certain undesirable higher order terms from a Riemann sum of the elastic energy. Unfortunately however, it is not known for which choices of domain Ω such a sequence exists. As shown in one dimension by Mora-Corral [Mo], the higher order terms in the asymptotic expansion of the energy depend on the choice of the sequence ε_k.

For lattice polygons, $Q(\varepsilon) = O(\varepsilon)$ and it can be characterized explicitly in terms of geometrical quantities of Ω. The dominant term of $Q(\varepsilon)$ is a surface integral over $\partial\Omega$ (the second term in (1.1) after scaling); as such it furnishes an explicit contribution to surface energy that plays a rather subtle role, as we show in the present paper.

Crystals often occur in faceted form in their natural state. This means that they are polyhedral, and the facets inhabit crystallographic planes. This is because of surface energetics affecting crystal growth, but also because of cleavage fracture that creates new surfaces along special lattice planes. It turns out that considerable progress has been made in the lattice point problem for regions that are *lattice polytopes*, i.e., polyhedra whose vertices are lattice points [BP, BR, Re]. For lattice polygons in two dimensions the problem was solved by Pick [Pi], however, in three or more dimensions some issues remain open [BP, BR]. In Section 2 we assume that Ω is a lattice polytope. In order

to isolate the surface energy from other effects, such as higher gradient energy, we assume that the deformation is homogeneous (y is affine). To keep the geometry simple, we confine our analysis to two dimensions. Unlike [BBL, Mo], initially we do not employ a limit process, but rather a bond counting technique. For each lattice vector $w \in L$, we find the number of bonds between points in $\Omega \cap L$ that are w apart. This calculation reduces to a number of lattice point problems.

In Section 3 we compute the energy of polygonal (faceted) crystals. For an interatomic potential of finite, but otherwise arbitrary range, we compute the energy of essentially any convex lattice polygon exactly (Proposition 3.1). This result *is not asymptotic* and does not suffer from the sequential dependence issue explored in [Mo]. Let the deformation be $y(x) = Fx$, $x \in \Omega$. The energy equals the *exact* sum of the elastic energy $\int_\Omega W(F)dx$ plus the *surface energy* $\int_{\partial\Omega} \gamma_\diamond(F, \bar{n})dx$, plus the *corner energy* $\sum_{i=1}^{N} \tau(F, n_i, n_{i-1})$, summed over the N vertices of Ω. The surface energy density is explicitly obtained:

$$\gamma_\diamond(F, \bar{n}) = -\frac{1}{4} \sum_{w \in L \setminus \{0\}} \frac{1}{|\bar{n}|} \left(|w \cdot \bar{n}| - 1\right) \varphi(|Fw|), \tag{1.2}$$

where $\bar{n}$ is a normal to $\partial\Omega$ whose components on each facet are the Miller indices (irreducible integers) of the corresponding lattice plane, and φ is the interatomic potential. The corner energy $\tau(F, n_i, n_{i-1})$ is also explicit but more complicated; apart from F, it depends on the two unit normals of the facets meeting at the ith vertex.

For an infinite range potential this result retains only asymptotic validity for a lattice polygon $k\Omega$ as $k \to \infty$; the three energies just mentioned are the first three terms of the asymptotic expansion of the energy for large k (Proposition 3.3). The order of the remainder depends on the decay rate of the potential φ.

Because of its construction based on lattice polygons, the surface energy density (1.2) is only defined for "rational" directions of the surface normal ($n = (\nu_1, \nu_2) \in S^1$ is called *rational* if ν_2/ν_1 is a rational number or $\nu_1 = 0$, *irrational* otherwise). It is natural to ask how (1.2) can be extended to irrational normals. This is important because when Ω is strictly convex and $\partial\Omega$ is smooth for example, the normal to $\partial\Omega$ is irrational almost everywhere on $\partial\Omega$. We study this issue in Section 4. The main idea here is to approximate such a strictly convex, smooth Ω by a suitable lattice polygon. There is a natural way to do this: we consider the convex hull of all lattice points contained in Ω. This allows us to use number-theoretic results on the asymptotic properties of such sets due to Bárány and Larman [BL] and also Huxley [Hu]; see also the survey [IKM]. Perhaps surprisingly, the surface energy density we obtain for smooth strictly convex domains (Proposition 4.1) is *different*

from (1.2). It takes the form

$$\gamma_\circ(F,n) = -\frac{1}{4}\sum_{w\in L\setminus\{0\}} |w\cdot n|\varphi(|Fw|), \tag{1.3}$$

where n is now the *unit normal* to $\partial\Omega$ and can take on irrational values. This allows us to extend the definition of the surface energy density (1.2) to all values of the normal. We consider more general domains that are convex but whose boundary comprises flat facets as well as curves with positive curvature. In Proposition 4.3 we calculate the surface energy of such domains. It equals the boundary integral of an extended surface energy density function,

$$\hat\gamma(F,n) = \begin{cases} \gamma_\diamond(F,\bar n), & n \text{ rational } (\bar n/|\bar n| = n),\\ \gamma_\circ(F,n), & n \text{ irrational,}\end{cases} \tag{1.4}$$

with $\gamma_\diamond$ from (1.2) and $\gamma_\circ$ from (1.3). The dependence of the surface energy density on the surface normal is thus quite intricate. One can show that $\hat\gamma(F,\cdot)\colon S^1 \to \mathbb{R}$ is continuous at irrational n, discontinuous at rational n, and almost nowhere differentiable (Proposition 4.4). Because of the above pathological properties, the surface energy density does not satisfy the usual hypotheses of the Wulff theorem; see e.g. [Fo].

This difficulty is dealt with in Section 5. One observes that given a collection of lattice points within a convex domain, there is some freedom in choosing an alternative convex domain containing precisely the same lattice points. The choice of this domain plays a subtle but important role in the description of surface energy. Utilizing this, we are able to write the surface energy of the crystal in the form

$$\int_{\partial\Omega'} \gamma_\circ(F,n)ds,$$

where Ω' is a suitably conrtructed domain containing the same lattice points as Ω. The surface energy density $\gamma_\circ$, defined in (1.3), is actually Lipschitz continuous in the unit normal.

For finite range potentials, Herring [He] and Parry [Pa] give formulae for the surface energy of a planar surface that bear some similarity with $\gamma_\circ$ of (1.3).

A more realistic approach to surface energy would allow for local "relaxation" of atomic positions from the macroscopic deformation near the boundary. Such deviations would perhaps be determined by minimization of the atomistic energy. This seems to be a formidable problem in the setting considered here (more than one dimension, general boundary geometry, arbitrary interaction range, nonconvex potentials); there are very few explicit calculations of such a relaxed surface energy, even in substantially simplified settings. One of the first results in this direction is due to Braides and Cicalese [BC]; they obtain the relaxed surface energy of a one-dimensional atomic

chain using Γ-convergence. The result is not explicit and seems difficult to compare quantitatively with the explicit "constrained" energy of Mora-Corral [Mo]. In a two-dimensional setting, Theil [Th] calculates the relaxed surface energy of a crystal with quadratic short range potentials; the result is in the form of a perturbation of the constrained surface energy explored here.

In order to obtain some quantitative information on the difference between the relaxed and constrained surface energies, numerical optimization of the atomistic energy was recently performed for a completely unconstrained, Lennard-Jones two-dimensional crystal [Ro]. Atomic positions were allowed to relax from initial positions forming a lattice triange or hexagon with low Miller-index boundary. The constrained energy was obtained by minimizing over the deformation gradient matrix of a homogeneous deformation that the atoms are constrained to follow. It was found that the difference between the relaxed and constrained surface energies is typically less than three percent (after the appropriate scaling and bulk energy is accounted for). This suggests that there are some situations where the constrained surface energy is close to the unconstrained one. In analogous one-dimentional computations, the results agree qualitatively with the conclusions of [BC]; at the same time, the difference between relaxed and constrained surface energy is less than one percent.

Many of the results presented here, in particular expressions (1.2) through (1.4) for the surface enrgy density, are valid for three-dimensional crystals as well [Ro]. The three-dimensional version of Pick's Theorem that these results rely upon is not completely settled at this point [BP, BR].

2 The Bond Counting Approach

For subsets P, Q of $\mathbb{R}^n$, define the Minkowski sum $P \oplus Q = \{p+q : p \in P,\ q \in Q\}$ and write $p+Q = \{p\} \oplus Q$. The *lattice* is $L = \mathbb{Z}^2$ unless otherwise noted. This is not a restriction; the results can be adapted to any Bravais Lattice L^* by incorporating the linear mapping from L onto L^* into the deformation. For $x = (\alpha, \beta) \in \mathbb{Z}^2$ let

$$\gcd(x) = \gcd(|\alpha|, |\beta|), \quad \bar{x} = \frac{1}{\gcd(x)} x, \quad x^{\perp} = (\beta, -\alpha).$$

We assume that the reference region $\Omega \subset \mathbb{R}^2$ is a *convex body*, or a compact convex set with nonempty interior. One important case we will consider is when $\Omega \subset \mathbb{R}^2$ is a *convex lattice polygon*. In particular, $\Omega = \text{conv}\{v_1, \ldots, v_N\}$, the convex hull of its N *vertices* $v_i \in L$, $i \in \{1, \ldots, N\}$, which are lattice points. The boundary $\partial\Omega$ consists of N *facets* $S_i = \text{conv}\{v_i, v_{i+1}\}$, where $v_{N+1} = v_1$ and $S_{N+1} = S_1$. Letting $m_i = v_{i+1} - v_i$, $\bar{m}_i = m_i / \gcd(m_i)$, the *Miller normal* $\bar{n}_i$ to S_i is $\bar{n}_i = \bar{m}_i^{\perp}$, so that $\gcd(\bar{n}_i) = 1$. Fix $w \in L$, let $x \in L$ and define $b = b(x, w) = \{z \in \mathbb{R}^2 \colon z =$

$x + tw,\ 0 \le t \le 1\} = \text{conv}\{x, x + w\}$ as the *bond starting at* x *with bond vector* w . The set

$$B_w(\Omega) = \{b : b = b(x, w), x \in \Omega \cap L, x + w \in \Omega \cap L\} \tag{2.1}$$

is the set of all w-bonds of Ω (bonds with bond vector w). We will use the abbreviation

$$b_0 = b(0, w).$$

The energy of the homogeneous deformation $y(x) = Fx$ can be written as

$$E\{\Omega, y\} = \frac{1}{2} \sum_{x \in \Omega \cap L} \sum_{\substack{w \in L \setminus \{0\} \\ x+w \in \Omega \cap L}} \varphi(|Fw|). \tag{2.2}$$

The factor of $1/2$ occurs since $b(x, w) = b(x + w, -w)$ and the potential φ is even in w. Interchanging the order of summation above we obtain

$$E\{\Omega, y\} = \frac{1}{2} \sum_{w \in L \setminus \{0\}} \sum_{\substack{x \in \Omega \\ x+w \in \Omega \cap L}} \varphi(|Fw|) = \frac{1}{2} \sum_{w \in L \setminus \{0\}} \sum_{b \in B_w(\Omega)} \varphi(|Fw|) = \frac{1}{2} \sum_{w \in L \setminus \{0\}} \varphi(|Fw|) \sum_{b \in B_w(\Omega)} 1.$$

Evidently, in order to determine the energy, it suffices to calculate, for each $w \in L$, the w-*bond number of* Ω, i.e., $N_w(\Omega) = \#B_w(\Omega)$; see (2.1):

$$E\{\Omega, y\} = \frac{1}{2} \sum_{w \in L \setminus \{0\}} \varphi(|Fw|) N_w(\Omega). \tag{2.3}$$

Clearly the number of w-bonds "starting" in Ω equals the number of lattice points of Ω:

$$\#\{b = b(x, w) : x \in \Omega \cap L\} = \#(\Omega \cap L).$$

Some of these bonds are not contained in $B_w(\Omega)$:

$$N_w(\Omega) = \#(\Omega \cap L) - \#T_w(\Omega), \quad T_w(\Omega) = \{b = b(x, w) : x \in \Omega \cap L, x + w \notin \Omega \cap L\}. \tag{2.4}$$

Recall that $S = \partial\Omega$ consists of N facets S_i, $i = 1, \ldots, N$, each with unit normal n_i, outward with respect to Ω. Let

$$J(w) = \{i \in \mathbb{Z} : 1 \le i \le N, n_i \cdot w > 0\}, \quad S_w^+ = \bigcup_{i \in J(w)} S_i, \tag{2.5}$$

so that S_w^+ is the part of $\partial\Omega$ through which w points outwards. Denote by $T_w^\dagger(\Omega)$ the set of all w-bonds that intersect S_w^+ and terminate outside Ω.

$$T_w^\dagger(\Omega) = \{b : b = b(x, w) \in B_w(L), b \cap S_w^+ \neq \emptyset, x + w \notin \Omega\}. \tag{2.6}$$

Some of these bonds "straddle" Ω, that is, have both endpoints outside Ω but intersect $\partial\Omega$; specifically,

$$T_w^{\ddagger}(\Omega) = \{b(x,w) \in T_w^{\dagger}(\Omega) : x \notin \Omega, x+w \notin \Omega\}. \tag{2.7}$$

Then obviously in view of (2.4),

$$T_w(\Omega) = T_w^{\dagger}(\Omega) \setminus T_w^{\ddagger}(\Omega).$$

As a result,

$$N_w(\Omega) = \#(\Omega \cap L) - \#T_w^{\dagger}(\Omega) + \#T_w^{\ddagger}(\Omega). \tag{2.8}$$

Roughly speaking, the number of w-bonds in Ω equals the number of lattice points in it, minus the number of bonds that traverse the boundary at least once, plus the number of bonds that traverse the boundary twice. The reason for the splitting (2.8) is that each term can be evaluated using results from geometric number theory.

The number of lattice points in Ω, $\#(\Omega \cap L)$, is addressed by Pick's Theorem, [Pi, Re], a variant of which is the following

Lemma 2.1. *Let Ω be a simple closed lattice polygon with facets S_i and outward Miller normal $\bar{n} = \bar{n}_i$ on S_i. Then*

$$\#(\Omega \cap L) = |\Omega| + \frac{1}{2}\sum_{i=1}^{N} \frac{|S_i|}{|\bar{n}_i|} + 1. \tag{2.9}$$

Equivalently, letting θ_i be the (dihedral) angle between normals of facets meeting at the ith vertex,

$$\#(\Omega \cap L) = \int_{\Omega} 1 dx + \int_{\partial\Omega} \frac{1}{2|\bar{n}|} ds + \sum_{i=1}^{N} \frac{\theta_i}{2\pi}. \tag{2.10}$$

Proof. Pick's Theorem [Pi, Re] states that

$$|\Omega| = \#(\mathring{\Omega} \cap L) + \frac{1}{2}\#(\partial\Omega \cap L) - 1 = \#(\Omega \cap L) - \frac{1}{2}\#(\partial\Omega \cap L) - 1 \tag{2.11}$$

(since Ω is closed). If two neighboring lattice points in a facet S_i differ by $\bar{m}_i \in L$ (with relatively prime components), then $\#(S_i \cap L) = |S_i|/|\bar{m}_i| + 1$ while $\#(\partial\Omega \cap L) = \sum_{i=1}^{N}[\#(S_i \cap L) - 1] = \sum_{i=1}^{N} |S_i|/|\bar{m}_i|$ since each S_i contains both its endpoints. Now the Miller normal $\bar{n}_i = \bar{m}_i^{\perp}$, so that $|\bar{n}_i| = |\bar{m}_i|$ and (2.9) follows. Also, (2.10) is a trivial consequence of (2.9), given that the sum in (2.10) equals 1. □

Eq. (2.10) has an interesting interpretation. It exactly equates a discrete quantity (number of atoms in Ω) with a continuum expression: the "volume" integral of a bulk density, plus the "surface"

integral of a surface density, plus contributions of corners. We will show in the sequel that both the w-bond number $N_w(\Omega)$ and the energy admit analogous representations.

The first term in (2.8) is given by (2.9). Turning to the second term, let $P_i(w)$ be the parallelogram $b_0 \oplus S_i$ with two parallel sides S_i and $w + S_i$ if $w \cdot n_i > 0$, $P_i(w) = \emptyset$ otherwise. Then it is easy to see that $b(x, w) \in T_w^\dagger(\Omega)$ if and only if $x + w \in P_i(w) \setminus S_i$ for some $i \in J(w)$; see (2.5). Thus

$$T_w^\dagger(\Omega) = \{b(x, w) : x + w \in P(w) \cap L\}, \quad P(w) = \bigcup_{i \in J(w)} P_i(w) \setminus S_i = (b_0 \oplus S_w^+) \setminus S_w^+. \tag{2.12}$$

It follows that

$$\#T_w^\dagger(\Omega) = \#(P(w) \cap L). \tag{2.13}$$

In general, $P(w)$ is not convex. However, if one defines

$$\Omega_w = b_0 \oplus \Omega = \bigcup_{t \in [0,1]} (tw + \Omega), \tag{2.14}$$

then Ω_w is a convex lattice polygon, being the Minkowski sum of two such sets. In fact,

$$\Omega_w = \mathrm{conv}\{\Omega, w + \Omega\}. \tag{2.15}$$

Also $P(w) = \Omega_w \setminus \Omega$, while $\Omega \subset \Omega_w$. This and (2.13) imply

$$\#T_w^\dagger(\Omega) = \#(\Omega_w \cap L) - \#(\Omega \cap L). \tag{2.16}$$

The right hand side can be evaluated using Lemma 2.1 for each term. Note that $\partial\Omega_w$ comprises $\partial\Omega \setminus S_w^+$, $w + S_w^+$ and two w-bonds joining these two pieces. The result is

$$\#T_w^\dagger(\Omega) = \sum_{i \in J(w)} |S_i| w \cdot n_i + |b|/|\bar{w}| = \sum_{i=1}^N |S_i| \langle w \cdot n_i \rangle + \gcd(w), \tag{2.17}$$

where $\langle x \rangle = (x + |x|)/2$ for $x \in \mathbb{R}$ and $n = n_i$ on S_i is the unit outward normal to $\partial\Omega$. Here $|b|/|\bar{w}| = \gcd(w)$.

It remains to evaluate $T_w^\ddagger(\Omega)$. If a bond $b = b(x, w)$ terminates in $w + \Omega$, or $x + w \in w + \Omega$, then $x \in \Omega$. This together with (2.7) and (2.12) immediately shows that $b \in T_w^\ddagger(\Omega)$ if and only if $x + w \in P(w) \setminus w + \Omega$. Since $P(w) = \Omega_w \setminus \Omega$,

$$\#T_w^\ddagger(\Omega) = \#(Q(w) \cap L), \quad Q(w) = \Omega_w \setminus (\Omega \cup (w + \Omega)). \tag{2.18}$$

We will show next that for $|w|$ small enough compared to the facets of Ω, $Q(w)$ consists of one or two triangles, each having a vertex at one of the two ends of the simple polygonal line S_w^+. For

example, if $\Omega = [0,3]^2$ and $w = (1,1)$, $Q(w)$ consists of the triangle with vertices $(0,3)$, $(1,4)$ and $(1,3)$ and its image under reflection about the $(1,1)$-axis. Any $b \in T_w^\ddagger(\Omega)$ intersects two different facets of $\partial\Omega$ by (2.7). Let

$$\delta = \delta(\Omega) = \min_{\substack{1\le i,j\le N \\ v_i \notin S_j}} \text{dist}(v_i, S_j) \tag{2.19}$$

where $v_i \in \mathbb{Z}^2$ are the vertices of Ω. The shortest line segment with endpoints on non-adjacent facets has length δ. If $|w| < \delta$, $b \in T_w^\ddagger(\Omega)$ necessarily intersects two *adjacent* facets, say S_i and S_{i-1} meeting at some vertex v_i, with outward normals n_i, n_{i-1} (where $n_0 = n_N$). Since both endpoints of b are outside Ω, $w\cdot n_i$ and $w\cdot n_{i-1}$ must have opposite signs. Then in case $w\cdot n_i > 0$ and $w\cdot n_{i-1} < 0$, $x + w$ is in the triangle with vertices v_i, $v_i + w$ and the intersection of S_i and $w + S_{i-1}$, which is therefore is part of $Q(w)$. If the reverse inequality holds, the triangle with vertices $v_i, v_i + w$ and the intersection of $w + S_i$ and S_{i-1} is part of $Q(w)$. Regarding lattice point count, both cases reduce to the triangle with base b_0 and sides normal to n_i and n_{i-1}:

$$T(w, n_i, n_{i-1}) = \text{conv}\{0, w, q\}, \quad q\cdot n_i = 0, \quad (q-w)\cdot n_{i-1} = 0, \quad (w\cdot n_i)(w\cdot n_{i-1}) < 0. \tag{2.20}$$

In addition, the relative interior of the base $b(v_i, w)$ of the triangle with endpoints $v_i, v_i + w$ is also part of $Q(w)$ and contains $\gcd(w) - 1$ lattice points. Consequently, if $|w| < \delta$,

$$\#T_w^\ddagger(\Omega) = \sum_{\substack{1\le i\le N \\ (w\cdot n_i)(w\cdot n_{i-1})<0}} [\gcd(w) - 1 + \#T(w, n_i, n_{i-1})]. \tag{2.21}$$

Unfortunately, $T(w, n_i, n_{i-1})$ is not a lattice polygon in general, since q need not have integer coordinates and Lemma 2.1 does not apply. Instead, we count the lattice points inside the triangle more directly:

Lemma 2.2. Suppose $(w\cdot n_i)(w\cdot n_{i-1}) < 0$ and let $T = T(w, n_i, n_{i-1}) \subset \mathbb{R}^2$ be the triangle of (2.20). Let $u \in \mathbb{Z}^2$ be such that $\{u, \bar{w}\}$ is a lattice basis for $\mathbb{Z}^2$. Then

$$\#(\mathring{T} \cap L) = N_T(w, n_i, n_{i-1}),$$

where for $w \in \mathbb{Z}^2$ and unit $n, m \in \mathbb{R}^2$ with $(w\cdot n)(w\cdot m) < 0$,

$$N_T(w, n, m) = s\left(q\cdot\bar{w}^\perp, q\cdot u^\perp, \gcd(w)\right), \quad q = \frac{m\cdot w}{m\cdot n^\perp} n^\perp \tag{2.22}$$

and $s : \mathbb{R}\times\mathbb{R}\times\mathbb{Z} \to \mathbb{R}$ is given by

$$s(\alpha, \beta, k) = (1 - \lceil\, |\alpha| \,\rceil)(k-1) + \sum_{j=1}^{\lceil |\alpha| \rceil - 1} \left(\left\lceil \frac{\beta - k}{|\alpha|} j \right\rceil - \left\lfloor \frac{\beta}{|\alpha|} j \right\rfloor \right) \tag{2.23}$$

with $s(0, \beta, k) = 0$.

Proof. Let $n = n_i$, $m = n_{i-1}$. Since in (2.20) $q \cdot n = 0$, $q = \lambda n^\perp$ for some $\lambda \in \mathbb{R}$. Then solving $(q - w) \cdot m = 0$ for λ gives q as in the second of (2.22). Let $\bar{w} = w/\gcd(w) = (\bar{w}_1, \bar{w}_2)$ and suppose $u = (u_1, u_2) \in \mathbb{Z}^2$ solves $u \cdot \bar{w}^\perp = 1$, or $\bar{w}_2 u_1 - \bar{w}_2 u_2 = 1$. This is solvable by Bezout's Lemma since $\gcd(\bar{w}_1, \bar{w}_2) = 1$. Then the matrix $A = \mathrm{col}(u, \bar{w})$ has unit determinant $u \cdot \bar{w}^\perp = 1$ and integer entries, hence so does $A^{-1} = \mathrm{row}(\bar{w}^\perp, u^\perp)$. As a result $\{u, \bar{w}\}$ is a lattice basis for $\mathbb{Z}^2$, while the linear transformation with matrix A^{-1} is lattice invariant . Now $T' = A^{-1}T$ has vertices $0, (0, k) \in \mathbb{Z}^2$ and $p = (\alpha, \beta)$, where

$$k = \gcd(w), \quad (\alpha, \beta) = (q \cdot \bar{w}^\perp, q \cdot u^\perp); \tag{2.24}$$

in general p is not a lattice point. Suppose for the moment that $\alpha > 0$. Then

$$\mathring{T}' \cap L = \left\{ (x_1, x_2) \in \mathbb{Z}^2 : 0 < x_1 < \alpha, \quad \frac{\beta}{\alpha} x_1 < x_2 < k + \frac{\beta - k}{\alpha} x_1 \right\}.$$

For $x \in \mathbb{R}$ let $\lfloor x \rfloor'$ be the greatest integer *strictly less* than x and $\lceil x \rceil'$ the least integer *strictly greater* than x. Then the number of lattice points on a segment $\{(x_1, x_2) : x_1 = j, \ \mu < x_2 < \nu\}$, where $j \in \mathbb{Z}$ and $\mu < \nu \in \mathbb{R}$ equals $\lfloor \nu \rfloor' - \lceil \mu \rceil' + 1$. Hence,

$$\#(\mathring{T}' \cap L) = \sum_{j=1}^{\lfloor \alpha \rfloor'} \left(\left\lfloor k + \frac{\beta - k}{\alpha} j \right\rfloor' - \left\lceil \frac{\beta}{\alpha} j \right\rceil' + 1 \right).$$

Since $\lfloor x \rfloor' = \lceil x \rceil - 1$ and $\lceil x \rceil' = \lfloor x \rfloor + 1$, the above reduces to $s(\alpha, \beta, k)$ in (2.23). It then follows from (2.24) and (2.22) that $\#(\mathring{T}' \cap L) = N_T(w, n, m)$. The linear transformation with matrix A is lattice invariant and thus $\#(A\mathring{T}' \cap L) = \#(\mathring{T}' \cap L)$ [BP], while $AT' = T$. In case $\alpha < 0$, reflect T' by replacing α by $|\alpha|$. If $\alpha = 0$ then $\mathring{T}' = \emptyset$. □

This together with (2.21) gives

$$\#T_w^\ddagger(\Omega) = \sum_{\substack{1 \le i \le N \\ (w \cdot n_i)(w \cdot n_{i-1}) < 0}} [\gcd(w) - 1 + N_T(w, n_i, n_{i-1})]. \tag{2.25}$$

To obtain an expression for the w-bond number of Ω, merely substitute (2.9), (2.17) and (2.25) into (2.8) and rearrange. Observe that for a given bond vector w, $N_w(\Omega)$ is completely determined by the area $|\Omega|$, the lengths $|S_i|$ of the facets, and their orientations through the Miller normals $\bar{n}_i$:

Lemma 2.3. Suppose $|w| < \delta$, cf. (2.19). Then the w-bond number of Ω is given by

$$N_w(\Omega) = |\Omega| + \frac{1}{2} \sum_{i=1}^{N} \frac{|S_i|}{|\bar{n}_i|} (1 - 2\langle w \cdot \bar{n}_i \rangle) + 1 - \gcd(w) + \sum_{\substack{1 \le i \le N \\ (w \cdot n_i)(w \cdot n_{i-1}) < 0}} [\gcd(w) - 1 + N_T(w, n_i, n_{i-1})]. \tag{2.26}$$

The above can readily be written in a form similar to (2.10):

$$N_w(\Omega) = \int_\Omega 1dx + \int_{\partial\Omega} g(w, \bar{n})ds + \sum_{i=1}^{N} h(w, n_i, n_{i-1}), \quad w \in L,$$

as a bulk integral, plus a "surface" integral, plus corner contributions, for suitable normal-dependent densities g and h.

The present approach of counting bonds has certain similarities with the bond density lemma of Shapeev [Sh].

3 Surface Energy of Lattice Polygons

We are now in a position to compute the energy. Consider first a *finite-range potential* that only involves bonds within a bounded set. Let *the bond range* $R \subset L \setminus \{0\}$ be symmetric, so that $w \in R \implies -w \in R$. Allow the interatomic potential $\varphi_w(\cdot)$ to depend explicitly on w, require

$$\varphi_w(\cdot) = \varphi_{-w}(\cdot)\ \forall w \in L, \quad \varphi_w(\cdot) \equiv 0\ \forall w \in L \setminus R, \tag{3.1}$$

and define the energy of the homogeneous deformation $y(x) = Fx, x \in \Omega$,

$$E\{\Omega, y\} = \frac{1}{2} \sum_{x \in \Omega \cap L} \sum_{\substack{w \in R \\ x+w \in \Omega \cap L}} \varphi_w(|Fw|), \tag{3.2}$$

where $\varphi_w : (0, \infty) \to \mathbb{R}$ is not restricted to be regular in any way.

Proposition 3.1. *For $F \in M^{2\times 2}_+$, $\bar{m} \in \mathbb{Z}^2$ and unit $n, m \in \mathbb{R}^2$ define the* stored energy function

$$W(F) = \frac{1}{2} \sum_{w \in R} \varphi_w(|Fw|), \tag{3.3}$$

the surface energy density function

$$\gamma_\diamond(F, \bar{m}) = -\frac{1}{4} \sum_{w \in R} \frac{1}{|\bar{m}|} \left(|w \cdot \bar{m}| - 1\right) \varphi_w(|Fw|) \tag{3.4}$$

and the vertex energy function

$$\tau(F, n, m) = \frac{1}{2} \sum_{w \in R} \left\{ \left[H_{n,m}(w) - \frac{1}{2\pi}\theta(n, m) \right] (\gcd(w) - 1) + H_{n,m}(w) N_T(w, n, m) \right\} \varphi_w(|Fw|), \tag{3.5}$$

where the sector step function

$$H_{n,m}(w) = \begin{cases} 1 & \text{if } (w \cdot n)(w \cdot m) < 0, \\ 0 & \text{if } (w \cdot n)(w \cdot m) \geq 0, \end{cases}$$

and $\theta(n,m)$ is the angle between n and m, while N_T is defined in Lemma 2.2. Suppose the bond range R is bounded with $\max_{w\in R}|w|<\delta$, cf. (2.19). *Let $\bar n=\bar n_i$ on S_i. Then the following expression is exact:*

$$E\{\Omega,y\}=\int_\Omega W(F)dx+\int_{\partial\Omega}\gamma_\diamond(F,\bar n)ds+\sum_{i=1}^N\tau(F,n_i,n_{i-1}). \tag{3.6}$$

Proof. As in the argument leading to (2.3), one can write (3.2) as

$$E\{\Omega,y\}=\frac12\sum_{w\in R}N_w(\Omega)\varphi_w(|Fw|).$$

By the hypothesis on R, Lemma 2.3 holds for all $w\in R$. Multiply (2.26) by $\varphi_w(|Fw|)$ and sum the result over $w\in R$. Interchange the order of summations, noting that

$$\sum_{w\in R}\langle w\cdot\bar n_i\rangle\varphi_w(|Fw|)=\frac12\sum_{w\in R}|w\cdot\bar n_i|\varphi_w(|Fw|)$$

by the symmetry of R and the first of (3.1), also that the sum of the (dihedral) angles between normals of facets meeting at vertices $\sum_{i=1}^N\theta(n_i,n_{i-1})=1$, and finally that summation over w in the sector of R where $(w\cdot n)(w\cdot m)<0$ can be replaced by summation over R provided the summand is multiplied by $H_{n,m}(w)$. □

Next we consider *infinite-range potentials*, where $R=L\setminus\{0\}$. We seek the energy of the kth dilation $k\Omega$ of the domain, $k\in\mathbb{Z}_+$. Here we have no choice but to let k k be an integer; otherwise $k\Omega$ is not a lattice polygon in general. The following will be useful.

Lemma 3.2. Let M be a positive integer. For $\rho>0$ sufficiently large and $p>0$,

$$\sum_{w\in\mathbb{Z}^M,\,|w|>\rho}|w|^{-(M+p)}<C\rho^{-p}$$

(where $C>0$ is independent of ρ and p).

Proof. Let $\hat x:\mathbb{R}^M\to\mathbb{Z}^M$ be the map $\hat x(\sum_{i=1}^M x_ie_i)=\sum_{i=1}^M\lfloor x_i\rfloor e_i$, $x_i\in\mathbb{R}$, with e_i standard basis vectors for $\mathbb{R}^M$. Thus $|x-\hat x(x)|\le D$, the unit cell diameter. Write $\hat x(x)=x+(\hat x(x)-x)$ and invoke the triangle inequality to conclude $|x|-D\le|\hat x(x)|\le|x|+D$. Then also $|\hat x(x)|\ge\rho$ implies $|x|>\rho-D$, while $|\hat x(x)|^{-(3+p)}\le||x|-D|^{-(3+p)}$. Thus $A_\rho=\{x\in\mathbb{R}^M:|\hat x(x)|\ge\rho\}\subset\mathbb{R}^M\setminus B_{\rho-D}(0)$.

$$\begin{aligned}0<\sum_{w\in\mathbb{R}^M\setminus B_\rho(0)}|w|^{-(M+p)}&=\int_{A_\rho}|\hat x(x)|^{-(M+p)}dx\le C\int_{\rho-D}^\infty(r-D)^{-(M+p)}r^{M-1}dr\\&\le C\int_{\alpha\rho}^\infty(\alpha r)^{-(M+p)}r^{M-1}dr=C\int_\rho^\infty r^{-(1+p)}dr=C\rho^{-p},\end{aligned}$$

where $\alpha \in (0,1)$ is such that $\alpha\rho = \rho - D$, so that $\alpha \in (1/2, 1)$ for $\rho > 2D$ and C takes possibly different values on different sides of an equation. □

For convenience we suppose that the interatomic potential $\varphi_w(\cdot) = \varphi(\cdot)$ (does not explicitly depend on w), although this is not essential.

Proposition 3.3. *Suppose the interatomic potential $\varphi : (0,\infty) \to \mathbb{R}$ satisfies the following: for each $r_0 > 0$ and for some constants $C = C(r_0)$ and $d > 2$,*

$$|\varphi(r)| < Cr^{-(2+d)} \quad \textit{for } r \in [r_0, \infty). \tag{3.7}$$

Let the bond range $R = L \setminus \{0\}$ in (3.2) *and in the definitions* (3.3) *of W,* (3.4) *of $\gamma_\diamond$ and* (3.5) *of τ. Then as $k \to \infty$, $k \in \mathbb{Z}_+$,*

$$E\{k\Omega, y\} = k^2 \int_\Omega W(F)dx + k \int_{\partial\Omega} \gamma_\diamond(F, \bar{n})ds + \sum_{i=1}^{N} \tau(F, n_i, n_{i-1}) + O(k^{2-d}). \tag{3.8}$$

Proof. Note that $\delta(k\Omega) = k\delta(\Omega) = k\delta$ in (2.19), so that Lemma 2.3 for $k\Omega$ holds provided

$$w \in R_k = (L \setminus \{0\}) \cap B_{k\delta}(0) = (L \cap B_{k\delta}(0)) \setminus \{0\}. \tag{3.9}$$

Split the energy as follows:

$$E\{k\Omega, y\} = \frac{1}{2} \sum_{w \in R_k} N_w(k\Omega)\varphi(|Fw|) + \frac{1}{2} \sum_{w \in L \setminus R_k} N_w(k\Omega)\varphi(|Fw|). \tag{3.10}$$

Now it is clear that for any $w \in L$ and $k \in \mathbb{Z}_+$,

$$0 \le N_w(k\Omega) \le \#(k\Omega \cap L) < Ck^2$$

for some constant $C > 0$, since all bonds within $k\Omega$ start in $k\Omega$ and by Lemma 2.1 applied to $k\Omega$ (the dominant term in (2.9) would be $|k\Omega| = k^2\Omega$). This provides a bound for the second term in (3.10):

$$\left| \sum_{w \in L \setminus R_k} N_w(k\Omega)\varphi(|Fw|) \right| < Ck^2 \sum_{w \in L \setminus R_k} |\varphi(|Fw|)| < Ck^2 \sum_{w \in \mathbb{Z}^2,\, |w| > k\delta} |\alpha w|^{-(2+d)} < Ck^{2-d}, \tag{3.11}$$

where we invoked (3.7), $\alpha > 0$ is such that $|Fz| > \alpha|z|$ for all $z \in \mathbb{R}^2$ and we used Lemma 3.2 with $\rho = k\delta$ and $p = d$; C is a generic constant with different values on either side of an (in)equality.

The first term in (3.10) is covered by Proposition 3.1 applied to $k\Omega$, since $w \in R_k$ means $|w| < k\delta = \delta(k\Omega)$. Noting that $|k\Omega| = k^2|\Omega|$, $|kS_i| = k|S_i|$, Proposition 3.1 implies

$$\frac{1}{2}\sum_{w\in R_k} N_w(k\Omega)\varphi(|Fw|) = k^2|\Omega|W_k(F) + k\sum_{i=1}^{N}|S_i|\gamma_k(F,\bar{n}_i) + \sum_{i=1}^{N}\tau_k(F,n_i,n_{i-1}), \tag{3.12}$$

where W_k, γ_k and τ_k are given by (3.3), (3.4) and (3.5) with R_k in place of R; see (3.9). Recalling that W, $\gamma_\diamond$ and τ are defined by the same equations with $R = L \setminus \{0\}$, using Lemma 3.2 with $M = 2$, we may estimate (omitting arguments)

$$|W - W_k| < Ck^{-d}, \quad |\gamma - \gamma_k| < Ck^{1-d}, \quad |\tau - \tau_k| < Ck^{2-d}. \tag{3.13}$$

We only demonstrate the third of these, the others being easier. Recall that in (3.5), N_T is the number of lattice points in the interior of a certain triangle T whose area is bounded above by $C|w|^2$, cf. Lemma 2.2. By Pick's Theorem (2.11) (applied to the lattice parallelogram of smallest area A containing T, and having the same base) the area A exceeds N_T hence $N_T < C|w|^2$. Also $\gcd(w) \le |w|$, $|H_{n,m}| \le 1$, hence we have from (3.5),

$$|\tau - \tau_k| < \sum_{w\in\mathbb{Z}^2,\,|w|>k\delta} C|w|^2|\varphi(|Fw|)| < C\sum_{w\in\mathbb{Z}^2,\,|w|>k\delta}|w|^{-d} < Ck^{2-d}$$

proceeding as in (3.11). By (3.13), replacing W, $\gamma_\diamond$ and τ by W_k, γ_k and τ_k in (3.12) produces an error of $O(k^{2-d})$. Combine this with (3.11) and (3.10) to obtain (3.8). □

4 Surface Energy for More General Boundaries

We examine the surface energy density function $\gamma_\diamond$ in (3.4) more closely, paying attention to its dependence on the surface normal. Due to its construction, $\gamma_\diamond(F,\cdot)\colon \bar{M} \to \mathbb{R}$ is defined only for "rational directions", that is, on the set of Miller normals

$$\bar{M} = \{\bar{n} : \bar{n} = (\nu_1,\nu_2) \in \mathbb{Z}^2,\ \gcd(\nu_1,\nu_2) = 1\}. \tag{4.1}$$

Using (3.3), we rewrite $\gamma_\diamond$ in (3.4) as

$$\gamma_\diamond(F,\bar{n}) = -\frac{1}{4}\sum_{w\in R}|w\cdot n|\,\varphi(|Fw|) + \frac{1}{2|\bar{n}|}W(F), \quad n = \bar{n}/|\bar{n}|, \quad \bar{n}\in\bar{M}. \tag{4.2}$$

The first term (involving the sum) reduces to a function of the unit normal n, and trivially admits a unique continuous extension onto the whole of the unit circle S^1. There is no such extension for the second term. Define the *rational* and *irrational direction sets* as

$$S^1_R = \{n : n\in S^1,\ n = \bar{n}/|\bar{n}|,\ \bar{n}\in\bar{M}\}, \quad S^1_I = S^1 \setminus S^1_R, \tag{4.3}$$

respectively, where $\bar{M}$ is defined in (4.1). Thus a vector is rational (irrational) if the tangent of the angle it makes with the usual basis vectors is rational (irrational). Since facets of lattice polygons have rational normals, the surface energy density $\gamma_\diamond$ is defined only for such directions. Note that for each $n \in S^1_R$ there is a unique $\bar{n} = \bar{n}(n) \in \bar{M}$ with $\bar{n}/|\bar{n}| = n$. The question arises as to how one can extend the definition of $\tilde{\gamma}_\diamond(F, n) = \gamma_\diamond(F, |\bar{n}(n)|n)$, $n \in S^1_R$, to the whole of S^1. This is related to another question: what is the surface energy when $\partial\Omega$ is *smooth*, for example $\partial\Omega = S^1$? It turns out that this question can be answered, at least partially, using the present approach. The basic idea is that even if $\partial\Omega$ is not polygonal, but smooth, the convex hull of all lattice points inside Ω is a convex lattice polygon.

Proposition 4.1. *Let $\Omega \subset \mathbb{R}^2$ be strictly convex and $\partial\Omega$ be C^2 with positive curvature. Suppose φ is as in Proposition 3.3, but with $d > 3$. Define the reduced surface energy density $\gamma_\circ : M^{2\times 2}_+ \times S^1 \to \mathbb{R}$ by*

$$\gamma_\circ(F, m) = -\frac{1}{4} \sum_{w \in L\setminus\{0\}} |w \cdot m|\, \varphi(|Fw|), \quad F \in M^{2\times 2}_+, \quad m \in S^1. \tag{4.4}$$

Then for any sequence $r = r_k \to \infty$ as $k \to \infty$ ($r_k \in \mathbb{R}_+$, $k \in \mathbb{Z}_+$),

$$E\{r\Omega, y\} = r^2 \int_\Omega W(F)dx + r \int_{\partial\Omega} \gamma_\circ(F, n)ds + O(r^{2/3}), \tag{4.5}$$

where $n : \partial\Omega \to S^1$ is the unit outward normal to $\partial\Omega$.

Proof. For each $r > 0$, let $\Omega_r = \mathrm{conv}(r\Omega \cap L)$. Then $\Omega_r \subset r\Omega$ is a convex lattice polygon, while $r\Omega \cap L = \Omega_r \cap L$. Hence, in view of (2.2),

$$E\{r\Omega, y\} = E\{\Omega_r, y\}, \tag{4.6}$$

where $y(x) = Fx$ for $x \in r\Omega$. The calculation of $E\{\Omega_r, y\}$ proceeds as above with one exception. For any $w \in L$, the condition $|w| < \delta(\Omega_r)$ (see (2.19)) may be violated for large enough r, since facets may become as small as the shortest lattice bonds. This affects $N_w(\Omega_r)$, but only the part regarding $\#T^\ddagger_w(\Omega_r)$—see (2.8), (2.18)—which we merely need to estimate. Given any convex body $D \subset \mathbb{R}^2$, let

$$\hat{Q}_w(D) = (b_0 \oplus D) \setminus [D \cup (w + D)], \quad Q_w(D) = \hat{Q}_w(D) \cap L,$$

where $b_0 = \mathrm{conv}\{0, w\}$. Then by (2.18) and (2.15), $\#T^\ddagger_w(\Omega_r) = \#Q(\Omega_r)$. Since $\Omega_r \subset r\Omega$, and $r\Omega \setminus \Omega_r$ contains no lattice points, (2.18) and (2.15) imply

$$Q_w(\Omega_r) \subset Q_w(r\Omega). \tag{4.7}$$

Let q, $q' \subset \partial(r\Omega)$ be the two points of $\partial(r\Omega)$ where the tangent vector is w, and $B_{r\rho} \subset r\Omega$ be a disk with $\partial B_{r\rho}$ tangent to $\partial(r\Omega)$ at q, where ρ is the smallest radius of curvature of $\partial\Omega$. Also let $B'_{r\rho} \subset r\Omega$ be a similar disk tangent to $\partial(r\Omega)$ at q'. Then for r large enough it is easy to see that

$$Q_w(r\Omega) \subset Q_w(B_{r\rho}) \cup Q_w(B'_{r\rho}). \tag{4.8}$$

The connected component of $\hat{Q}_w(B_{r\rho})$ containing q is contained inside an isosceles triangle with base a w-bond (with length $|w|$), and height the distance from the base middle to the intersection of the two circles $\partial B_{r\rho}$ and $w + \partial B_{r\rho}$; these are tangent to the base at its endpoints. The triangle height is thus bounded by $C(r)|w|$, where $C(r)$ approaches zero for large r. A crude but sufficient upper bound of the lattice point count of this set, hence also of the right hand of (4.8), is $C|w|^2$, with C independent of r. In view of of (4.7), $\#T^{\ddagger}_w(\Omega_r)$ is also bounded by $C|w|^2$. This estimate replaces the sum over vertices (second sum) in (2.26). Since $\sum_{w\in L\setminus\{0\}} |w|^p \varphi(|Fw|)$ are absolutely convergent for $p = 0, 1, 2$ as one infers from Lemma 3.2, it follows that

$$\begin{aligned} E\{\Omega_r, y\} =& |\Omega_r| W(F) + \int_{\partial\Omega_r} \gamma_\diamond(F, \bar{n}) ds + O(1) \\ =& \left[|\Omega_r| + \int_{\partial\Omega_r} \frac{1}{2|\bar{n}|} ds \right] W(F) + \int_{\partial\Omega_r} \gamma_\circ(F, n) ds + O(1) \\ =& \#\left(r\Omega \cap L\right) W(F) + \int_{\partial\Omega_r} \gamma_\circ(F, n) ds + O(1). \end{aligned} \tag{4.9}$$

Here we have used (4.2) and (4.4), then (2.10), in which the last term (sum) equals 1, together with the fact $r\Omega \cap L = \Omega_r \cap L$. We turn to $\int_{\partial\Omega_r} \gamma_\circ(F, n) ds$. Recalling (4.4), a typical term involves

$$\int_{\partial\Omega_r} |w \cdot n| ds = 2|\mathrm{Proj}_{w^\perp} \partial\Omega_r||w|, \tag{4.10}$$

$|\mathrm{Proj}_{w^\perp} \partial\Omega_r|$ being the length of the projection of $\partial\Omega_r$ onto a line perpendicular to w. This follows after splitting $\partial\Omega_r$ into two pieces, over which $w \cdot n$ is ≥ 0 and ≤ 0, and using the Divergence Theorem on each. Next, we show that

$$0 < |\mathrm{Proj}_{w^\perp} \partial(r\Omega)| - |\mathrm{Proj}_{w^\perp} \partial\Omega_r| < C|w|^2, \tag{4.11}$$

where the constant C is independent of $r > 1$ and w. There are lattice points z^- and $z^+ \in \partial\Omega_r \cap L$, such that Ω_r lies entirely between lattice lines l^-, l^+ with normal $w^\perp$ and containing z^-, z^+, respectively. Consider the part of $\partial(r\Omega)$ that lies outside the strip bounded by l^+ and l^-. It consists of two disjoint arcs, one to the "right" of l^+ and the other to the "left" of l^-. The length of the projections of these two arcs onto the $w^\perp$ axis equals the difference in (4.11). Let c^+ be the arc to

the right of l^+ (with endpoints in l^+). Let s be the region bounded by c^+ and l^+. The only lattice points it contains are in l^+. This is true since $r\Omega \setminus \Omega_r$ is free of lattice points. By the strict convexity of $r\Omega$, there is a unique $q \in c^+$ where the normal to c^+ is $w^\perp$. Consider the osculating circle of c^+ at q. Let $s' \subset s$ be the portion of the osculating disc contained in s; it is a circular segment whose height (in the direction $w^\perp$) equals the thickness of s (the length of its projection onto a line along $w^\perp$). The radius of the circle is $r\rho$ for some $\rho > 0$. There are two possibilities. Either s' lies between l^+ and the next lattice line l' with normal w to the right of l^+, or it extends beyond l' to the right. In the first case the height of the segment s' is $1/|\bar{w}|$, the distance between adjacent lattice lines with normal $w^\perp$. In the second case, let s'' be the portion of s' to the right of l'. Then s'' is also a circular segment and free of lattice points. Suppose its chord length is c and height is h. Since the radius of the circular arc is $r\rho$ we have $h^2 - 2r\rho h + c^2/4 = 0$. Solving this for $h/(r\rho)$ and using the inequality $1 - \sqrt{1-x} < x$ for $0 < x < 1$ yields $h < c^2/(4r\rho)$. Now since the circular segment s'' is free of lattice points and its chord is in l', the chord length $c < |\bar{w}| \leq |w|$ (since the distance between adjacent lattice points in l' is $|\bar{w}|$.) Hence $h < |w|^2/(4r\rho)$. The total height of the larger circular segment s' is $h + 1/|\bar{w}|$ which is thus bounded by $C|w|^2$ for $r \geq 1$. The thickness of s in the direction normal to w is the same as this height. This shows (4.11).

Combining (4.11) with (4.10) shows

$$\left| \int_{\partial(r\Omega)} |w \cdot n| ds - \int_{\partial\Omega_r} |w \cdot n| ds \right| < C|w|^3. \tag{4.12}$$

In view of (4.4) and since the sum $\sum_{w \in L \setminus \{0\}} |w|^3 \varphi(|Fw|)$ converges absolutely by hypothesis, one deduces

$$\int_{\partial\Omega_r} \gamma_\circ(F, n) ds = \int_{\partial(r\Omega)} \gamma_\circ(F, n) ds + O(1) = r \int_{\partial\Omega} \gamma_\circ(F, n) ds + O(1). \tag{4.13}$$

Our hypotheses on $\partial\Omega$ ensure that $\#(r\Omega \cap L) = r^2|\Omega| + O(r^{2/3})$, e.g. [Hu, IKM]. This together with (4.13) in (4.9) and (4.6) proves (4.5). □

According to Proposition 4.1, when $\partial\Omega$ is smooth and strictly convex, so that the normal vector is *irrational* almost everywhere on $\partial\Omega$, the surface energy density is given by (4.4); in contrast, for lattice polygons (with rational normal a.e. on $\partial\Omega$), the surface energy density is given by (4.2). This suggests that we combine the two expressions in defining a surface energy density for all values of the unit normal. That will allow us to treat the general case when Ω is a (not necessarily strictly) convex body. We do place some restrictions on $\partial\Omega$: flat parts of $\partial\Omega$ must be lattice segments (with rational normals). Corners have to be lattice points.

We will need the following auxiliary result:

Lemma 4.2. Let $D \subset \mathbb{R}^2$ be a strictly convex body and ∂D be C^2 with positive curvature. For $r > 0$ define the convex lattice polygon $D_r = \text{conv}(rD \cap L)$ with Miller normal $\bar{n} : \partial D_r \to \bar{M}$. Then as $r \to \infty$,

$$\int_{\partial D_r} \frac{1}{|\bar{n}|} ds = O(r^{2/3}).$$

Proof. By Pick's Theorem (Lemma 2.1), and since $\#(D_r \cap L) = \#(rD \cap L)$,

$$\int_{\partial D_r} \frac{1}{2|\bar{n}|} ds = \#(D_r \cap L) - |D_r| - 1 = \#(rD \cap L) - |rD| + |rD| - |D_r| - 1.$$

Now $\#(rD \cap L) - |rD| = o(r^{2/3})$ by [Hu]. In view of Theorem 4 and Remark 2 of [BL], and since $D_r \subset rD$,

$$0 < |rD| - |D_r| < Cr^{2/3} \tag{4.14}$$

for some constant C. The result follows. □

We now state the main result of this section:

Proposition 4.3. *Assume that Ω is a convex body with $\partial\Omega$ Lipschitz, and that there is a finite set of lattice points $\{v_1, \dots, v_N\} \subset \partial\Omega \cap L$, that partitions $\partial\Omega$ into N curves S_i, $\partial\Omega = \bigcup_{i=1}^N S_i$, each with endpoints v_i and v_{i+1} ($v_{N+1} = v_1$), such that $S_i \cap S_{i+1} = v_{i+1}$, S_i is a C^2 curve and one of the following two alternatives holds:*
(i) For $i \in J_c \subset \{1, \dots, N\}$, $S_i \subset \Gamma_i$, where Γ_i is a simple closed C^2 curve with positive curvature, or
(ii) For $i \in J_f = \{1, \dots, N\} \setminus J_c$, S_i is a straight segment.
Suppose φ is as in Proposition 3.3, but with $d > 3$. Define the extended surface energy density *$\hat{\gamma}(F, \cdot) \colon S^1 \to \mathbb{R}$ as follows:*

$$\hat{\gamma}(F, n) = \begin{cases} -\dfrac{1}{4} \displaystyle\sum_{w \in L \setminus \{0\}} |w \cdot n| \, \varphi(|Fw|) + \frac{1}{2|\bar{n}|} W(F), & n \in S_R^1 \ \ (\bar{n} \in \bar{M},\ \bar{n}/|\bar{n}| = n), \\ \\ -\dfrac{1}{4} \displaystyle\sum_{w \in L \setminus \{0\}} |w \cdot n| \, \varphi(|Fw|) = \gamma_\circ(F, n), & n \in S_I^1, \end{cases} \tag{4.15}$$

with $\gamma_\circ$ defined in (4.4) *and S_R^1, S_I^1 defined in* (4.3)*. Then as $k \to \infty$, $k \in \mathbb{Z}_+$,*

$$E\{k\Omega, y\} = k^2 \int_\Omega W(F) dx + k \int_{\partial\Omega} \hat{\gamma}(F, n) ds + O(k^{2/3}), \tag{4.16}$$

where $n : \partial\Omega \to S^1$ is the unit outward normal to $\partial\Omega$.

Proof. We now choose $r = k \in \mathbb{Z}_+$ and let $\Omega_k = \text{conv}(k\Omega \cap L)$. The part of the proof of Proposition 4.1 prior to (4.9) is easily adapted to the present setting, so that once again, as $k \to \infty$, with $\gamma_\diamond$ as in (4.2),

$$E\{\Omega_k, y\} = |\Omega_k| W(F) + \int_{\partial\Omega_k} \gamma_\diamond(F, \bar{n}) ds + O(1). \tag{4.17}$$

Let $\partial\Omega_f$ be the union of those S_i that are straight segments and $\partial\Omega_c$ the union of the S_i with positive curvature, so that $\partial\Omega = \partial\Omega_f \cap \partial\Omega_c$. By hypothesis, for $k \in \mathbb{Z}_+$ we have $kv_i \in \partial(k\Omega) \cap L$, hence also $kv_i \in \partial(\Omega_k) \cap L$. Then $k\partial\Omega_f \subset \partial\Omega_k = \partial(\Omega_k)$. Let $\partial\Omega_k^c = \partial\Omega_k \setminus k\partial\Omega_f$. Then

$$E\{\Omega_k, y\} = |\Omega_k| W(F) + \int_{\partial\Omega_k^c} \gamma_\diamond(F, \bar{n}) ds + \int_{k\partial\Omega_f} \gamma_\diamond(F, \bar{n}) ds + O(1).$$

Our hypotheses regarding $\partial\Omega_c$, specifically alternative (i), ensure that $n \in S_I^1$ a.e. on $k\partial\Omega_c$, while (ii) implies that $n \in S_I^1$ a.e. on $k\partial\Omega_f$. Using (4.15), rewrite the above as

$$E\{\Omega_k, y\} = |k\Omega| W(F) + \int_{k\partial\Omega_c} \gamma_\circ(F, n) ds + \int_{k\partial\Omega_f} \hat{\gamma}(F, n) ds + R(k), \tag{4.18}$$

where

$$R(k) = \left[|\Omega_k| - |k\Omega| + \int_{\partial\Omega_k^c} \frac{1}{2|\bar{n}|} ds \right] W(F) + \int_{\partial\Omega_k^c} \gamma_\circ(F, n) ds - \int_{k\partial\Omega_c} \gamma_\circ(F, n) ds + O(1). \tag{4.19}$$

It remains to show that $R(k) = O(k^{2/3})$ as $k \to \infty$, $k \in \mathbb{Z}_+$. Let $i \in J_c$, so that S_i satisfies alternative (i) in the statement of Proposition 4.3. Let S_k^i be the portion of $\partial\Omega_k^c$ between kv_i and kv_{i+1}, i.e., terminating at these two points and containing no other kv_j. Let the strictly convex body D^i be such that $\partial D^i = \Gamma_i$. Let G_k^i be the bounded region whose boundary is $kS_i \cup S_k^i$; this is well defined since both curves terminate at kv_i and kv_{i+1}. Then $G_k^i \subset kD^i \setminus D_k^i$, where $D_k^i = \text{conv}(kD_i \cap L)$, and

$$|k\Omega \setminus \Omega_k| = \sum_{i \in J_c} |G_k^i| \leq \sum_{i \in J_c} |kD^i \setminus D_k^i| < Ck^{2/3} \tag{4.20}$$

in view of (4.14) applied to D^i for $r = k \in \mathbb{Z}_+$.

Next, note that $S_k^i \subset \partial D_k^i$. As a result,

$$0 < \int_{\partial\Omega_k^c} \frac{1}{2|\bar{n}|} ds = \sum_{i \in J_c} \int_{S_k^i} \frac{1}{2|\bar{n}|} ds \leq \sum_{i \in J_c} \int_{\partial D_k^i} \frac{1}{2|\bar{n}|} ds < Ck^{2/3} \tag{4.21}$$

by Lemma 4.2 with $D = D^i$.

Next, we turn to the difference of the last two integrals in (4.19). Recalling (4.4), we write this as follows:

$$\sum_{i\in J_c}\sum_{w\in L\setminus\{0\}}\varphi(Fw)I_k^i(w),\qquad I_k^i(w)=\int_{kS_i}|w\cdot n|ds-\int_{S_k^i}|w\cdot n|ds=\int_{\partial G_k^i}|w\cdot\tilde{n}|ds,$$

where n is the outward unit normal to $k\partial\Omega$ and $\partial\Omega_k$ in the first two integrals, while $\tilde{n}$ is outward unit normal to ∂G_k^i. Hence $I_k^i(w)>0$, and since $G_k^i\subset kD^i\setminus D_k^i$,

$$0<I_k^i(w)\le\int_{\partial(kD^i)}|w\cdot n|ds-\int_{\partial D_k^i}|w\cdot n|ds<C|w|^3,$$

where the estimate follows from (4.12) by replacing Ω of Proposition 4.1 by D^i; the constant C is independent of k. Since the sum $\sum_{w\in L\setminus\{0\}}|w|^3\varphi(|Fw|)$ converges absolutely by hypothesis, so does the double sum in the previous equation; therefore

$$\int_{\partial\Omega_k^c}\gamma_\circ(F,n)ds-\int_{k\partial\Omega_c}\gamma_\circ(F,n)ds=O(1).$$

This together with (4.20) and (4.21) shows that $R(k)=O(k^{2/3})$. The normal is irrational a.e. on $\partial\Omega_c$. Consequently $\int_{k\partial\Omega_c}\gamma_\circ ds=\int_{k\partial\Omega_c}\hat{\gamma}ds=k\int_{\partial\Omega_c}\hat{\gamma}ds$, and (4.16) follows from (4.18), since (4.6) holds. □

Proofs of the Wulff theorem associated with surface energy minimization [Fo] over domains with given measure typically rely on continuity of the surface energy density with respect to the unit normal. Perhaps surprisingly, the extended surface energy density $\hat{\gamma}(F,\cdot)\colon S^1\to\mathbb{R}$ exhibits a dense set of discontinuities as we show next.

Proposition 4.4. *Suppose φ is as in Proposition 3.3 and fix $F\in M^{2\times2}_+$. Then*

(i) $\gamma_\circ(F,\cdot)\colon S^1\to\mathbb{R}$ in (4.4) *is Lipschitz continuous on S^1.*

(ii) $\hat{\gamma}(F,\cdot)\colon S^1\to\mathbb{R}$ defined in (4.15) *is continuous at $n\in S_I^1$, discontinuous at $n\in S_R^1$ and differentiable at most on a subset of S_I^1 of measure zero.*

Proof. Arrange the elements of $L\setminus\{0\}$ in a sequence: $\{w_j\}$, $j=1,2,\dots$, such that $|w_{j+1}|\ge|w_j|$, and define $g_j(n)=(-1/4)\varphi(|Fw_j|)|w_j\cdot n|$ for $n\in S^1$. Then clearly $g_j\colon S^1\to\mathbb{R}$ is Lipschitz on S^1 and (formally for the moment) $\gamma_\circ(F,n)=\sum_{j=1}^\infty g_j(n)$. Now since $|g_j|\le M_j=|\varphi(|Fw_j|)|\ |w_j|$ on S^1 and the series $\sum_{j=1}^\infty M_j=\sum_{w\in L\setminus\{0\}}|\varphi(|Fw|)|\ |w|$ converges in view of Lemma 3.2, then $G_k(n)=\sum_{j=1}^k g_j(n)$ converge uniformly as $k\to\infty$ to $\gamma_\circ(F,n)$ on S^1 by the Weierstrass M test.

Since $n \mapsto |w \cdot n|$, $n \in S^1$ is Lipschitz with constant $|w|$, the Lipschitz constant of G_k is bounded above by

$$\sum_{j=1}^{k} |\varphi(|Fw_j|)| \, |w_j| < \sum_{w \in L \setminus \{0\}} |\varphi(|Fw|)| \, |w| < \infty.$$

The uniform convergence of the G_k together with the uniform bound on their Lipschitz constants guarantee that the limit function $\gamma_\circ(F, \cdot)$ is also Lipschitz on S^1 and (i) holds.

To show (ii), consider the function

$$h(n) = \begin{cases} \frac{1}{|\bar{n}|}, & n \in S^1_R \ \ (\bar{n} \in \bar{M}, \ \bar{n}/|\bar{n}| = n), \\ \\ 0, & n \in S^1_I. \end{cases}$$

In other words, letting $n = (\nu_1, \nu_2) \in S^1$,

$$h(\nu_1, \nu_2) = \begin{cases} \frac{1}{\sqrt{p^2+q^2}}, & \nu_2/\nu_1 = p/q, \ \ (p,q) \in \mathbb{Z}^2, \ \ \gcd(p,q) = 1, \\ 0, & \nu_1 = 0, \\ 0, & \text{otherwise.} \end{cases} \tag{4.22}$$

Then one has

$$\hat{\gamma}(F, n) = \gamma_\circ(F, n) + \frac{1}{2} W(F) h(n) \quad \forall n \in S^1. \tag{4.23}$$

By (i), it suffices to prove that h is continuous at irrational n and discontinuous at rational n to show the continuity part of (ii). In fact, h is very similar to the Thomae function $T(x) = 1/q$ for $x = p/q$, p, q coprime integers (x rational), and zero for x irrational; see e.g. Proposition 4.1 in [Sa]. Adapting these results to the h is trivial in view of (4.22). Thus h is continuous at irrational n and discontinuous at rational n and so is $\hat{\gamma}(F, \cdot)$. Also h is nowhere differentiable by a simple adaptation of Proposition 6.1, [Sa]. Since by part (i) $\gamma_\circ$ is Lipschitz, it is differentiable a.e. on S^1 by the Rademacher theorem. Then $\hat{\gamma}(F, \cdot)$ fails a.e. to be differentiable by (4.23). Also it is not differentiable at rational n as it is not continuous there. □

5 A Continuous Surface Energy Density

The difficulty caused by the lack of continuity of $\hat{\gamma}$ is in to some extent artificial and can be overcome, as we explain next. The previous result suggests that the problem of minimising the integral $\int_{\partial\Omega} \hat{\gamma}(F, n) ds$ (for fixed F) over a suitable class of domains Ω with $|\Omega|$ fixed may be ill posed, in view of [Fo] (due to lack of continuity of $\hat{\gamma}(F, \cdot)$). However, this is not a physically appropriate problem, since by Pick's Theorem, fixing $|\Omega|$ is not equivalent to fixing the total mass, or the number

of lattice points of Ω. If the minimization were over the class of lattice polygons with fixed lattice point number, the appropriate constraint would fix $|\Omega| + \int_{\partial\Omega} 1/(2|\bar{n}|)ds$ instead of $|\Omega|$. Interestingly enough, the term $1/|\bar{n}|$ in the last integral is the one responsible for the lack of continuity of $\hat{\gamma}$. At the same time, given a collection of atoms within a convex domain Ω, there is some freedom in choosing an alternative convex domain Ω' containing precisely the same atoms. By choosing Ω' in a specific way, we can rewrite the surface energy as the integral of a continuous surface density. The shortest distance between parallel lattice lines with Miller normal $\bar{n}$ is $1/|\bar{n}|$ (also equal to the interpalanar distance in 3D). If Ω is a lattice polygon, construct Ω' by moving each side with Miller normal $\bar{n}_i$ of $\partial\Omega$ outward by $1/(2|\bar{n}_i|)$, half the inteplanar distance. Then Ω' is also a polygon (not a lattice polygon) that contains the same atoms as Ω and has the same normal fan, although it is not a dilation of Ω. Performing the same operation on $k\Omega$ and writing the energy in terms of the modified domain, one arrives at the following representation of the energy:

Proposition 5.1. *Let φ be as in Proposition 3.3, with $d > 3$. Suppose $\Omega \subset \mathbb{R}^2$ is (a) a lattice polygon, or (b) a smooth domain as in Proposition 4.1, or (c) the piecewise smooth domain of Proposition 4.3. In case (c) assume further that straight and curved sides of $\partial\Omega$ are not tangent at their common points. Then for $k \in \mathbb{Z}_+$, there exists a convex $\Omega(k) \subset \mathbb{R}^2$ containing the same lattice points as $k\Omega$ and whose measure equals the lattice point number of $k\Omega$ to order $O(k)$ as $k \to \infty$:*

$$\Omega(k)\cap L = k\Omega\cap L, \qquad |\Omega(k)| = \#(k\Omega\cap L)+o(k) = |k\Omega|+O(k), \qquad |\partial\Omega(k)| = |k\partial\Omega|+O(1), \tag{5.1}$$

such that

$$E\{k\Omega, y\} = \int_{\Omega(k)} W(F)dx + \int_{\partial\Omega(k)} \gamma_\circ(F, n)ds + o(k). \tag{5.2}$$

Moreover, in case (a) the $o(k)$ terms above are $O(1)$, while in cases (b), (c), they are $O(k^{2/3})$. Finally, in case (b), (5.2) *holds for all $k \in \mathbb{R}_+$ and not merely integers.*

Proof. Case (a): Suppose Ω is a lattice polygon. Then $k\Omega = \{x \in \mathbb{R}^2 \colon x \cdot \bar{n}_i \le kd_i,\ i = 1, \dots, N\}$, is the intersection of N half-planes of the form $x \cdot \bar{n}_i \le kd_i$, where $\bar{n}_i \in \bar{M}$ is the Miller normal of the ith side and d_i are integers independent of k. Let $\Omega(k) = \{x \in \mathbb{R}^2 \colon x \cdot \bar{n}_i \le kd_i + 1/2,\ i = 1, \dots, N\}$. Thus to construct $\Omega(k)$, each straight line containing a side of Ω with Miller normal $\bar{n}_i$ is translated outward (in the direction $\bar{n}_i$) by a k-independent distance $1/(2|\bar{n}_i|)$. The intersection of the half-planes of the translated lines is $\Omega(k)$ This adds to Ω a layer whose thickness equals $1/(2|\bar{n}_i|)$ on the ith side, hence

$$|\Omega(k)| = |k\Omega| + k\int_{\partial\Omega} \frac{1}{2|\bar{n}|}ds + O(1) = \#(k\Omega \cap L) + O(1). \tag{5.3}$$

The $O(1)$ term is a correction due to intersection, in the neighborhood of corners, of layers corresponding to adjacent sides, since directions and thicknesses of layers are k-independent. The second equality above follows from (2.10) of Lemma 2.1. The $O(1)$ terms in (5.3) are actually constant (depend only on Ω and not on k) as is easily shown. This establishes the middle assertion in (5.1). Since the distance of adjacent lattice lines with normal $\bar{n}_i$ is $1/|\bar{n}_i|$, the added layers (whose thickness is half that distance) contain no new lattice points; thus the first assertion of (5.1) holds true, while the last is trivial. Now (5.2) follows immediately from Proposition 3.3, (5.3) and the definitions (3.4) and (4.4).

Case (b): Suppose Ω is a smooth domain as in Proposition 4.1. Then choose $\Omega(k) = \Omega$, to that (5.1) follows from [Hu] and note that (5.2) is the same as (4.5) with $k = r \in \mathbb{R}_+$.

Case (c): Let Ω comply with Proposition 4.3 . For each k let $\Omega(k)$ be the set obtained by moving only the flat sides $kS_i \subset \partial\Omega_f$, $i \in J_f$ of $k\Omega$ outwards by $1/(2|\bar{n}_i|)$ (and discarding portions of the added layers that lie outside the curves Γ_j near the endpoints where S_i join curved sides of $\partial\Omega$). Thus

$$|\Omega(k)| = |k\Omega| + k\int_{\partial\Omega_f} \frac{1}{2|\bar{n}|} ds + O(1) = \#(k\Omega \cap L) + O(k^{2/3}) \tag{5.4}$$

The second equality follows from (4.20) and (4.21). Hence (5.1) holds (the last assertion is easy). One again, (5.2) follows easily from (4.17) and (5.4). □

The second relation in (5.1) means that the measure of $\Omega(k)$ is chosen to equal the number of lattice points of Ω up to the order of the surface energy. This reminds us of the condition in Theorem 3 of [BBL] that—in present notation—supposes the existence of a sequence $r_k \to \infty$ such that $\#(r_k\Omega \cap L) = |r_k\Omega|$. Provided that such a sequence of dilation factors r_k exists, then it is possible to modify the results of the previous section to show that for the types of domains considered here,

$$E\{r_k\Omega, y\} = r_k^2 \int_\Omega W(F)dx + r_k \int_{\partial\Omega} \gamma_\circ(F, n)ds + O(1),$$

thus the non-explicit surface energy density of Theorem 3 in [BBL] is now determined to be $\gamma_\circ$ defined in (4.4). Apparently, it does not seem to be known for which domains Ω such a sequence of dilation factors r_k exists. We are thus led to the construction of the domains $\Omega(k)$ of Proposition 5.1, which are not dilations of Ω of the form $r\Omega$, since they involve different translations of different facets.

Proposition 5.1 indicates that the appropriate surface energy shape optimization problem of Wulff type involves minimizing $\int_{\partial\Omega'} \gamma_\circ(F, n)ds$ over a suitable class of domains Ω' with $|\Omega'|$ fixed.

This entails fixing the mass of the crystal. The integrand $\gamma_\circ$ is now Lipschitz continuous in the unit normal as guarranteed by Proposition 4.4.

We must remark, however, that while (5.2) has the aforementioned advantages as regards surface energy minimization, it is not appropriate as an asymptotic series in k, since the domains of integration depend on the latter variable. The appropriate asymptotic series remains (4.16).

It is interesting that in cases where the normal is rational on a subset of $\partial\Omega$ of positive measure, the dilation factors are restricted to be integers. In one dimension it is has been shown [Mo] that the coefficients in the asymptotic expansion of the energy depend on the sequence of dilation factors. It should be kept in mind that there is no counterpart in one dimension of an irrational surface, which is purely a higher-dimensional occurence. Accordingly, the result of Proposition 4.1 (the case of smooth, strictly convex domains with irrational normal almost everywhere on $\partial\Omega$) is sequence independent.

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