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Bounds on the Geometric Complexity of Optimal Centroidal Voronoi Tesselations in 3D

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Abstract: Gersho's conjecture in 3D asserts the asymptotic periodicity and structure of the optimal centroidal Voronoi tessellation. This relatively simple crystallization problem remains to date open. We prove bounds on the geometric complexity of optimal centroidal Voronoi tessellations as the number of generators tends to infinity. Combined with an approach of Gruber in 2D, these bounds reduce the resolution of the 3D Gersho's conjecture to a finite, albeit very large, computation of an explicit convex problem in finitely many variables.

1. Introduction

A fundamental problem (cf. [6,7,17]) in both information theory and discrete geometry is known, respectively, as *optimal block quantization* or *optimal centroidal Voronoi tessellations* (CVT). To state the problem, consider a bounded domain in $\mathbb{R}^N$, say a cube $Q = [0, 1]^N$, and for a collection of points $y_k \in Y = \{y_1, \cdots, y_n\} \subseteq Q$, define the associated Voronoi regions (comprising a Voronoi tessellation of Q)

$$V_k = \{x \in Q \mid |x - y_k| \leq |x - y_i| \ \forall\ i \neq k\}.$$

A 2D illustration with $n = 6$ is presented on the left of Fig. 1. A centroidal Voronoi tessellation (cf. Fig. 1 right) amounts to finding a placement of the points y_k such that they are exactly the centroids of their associated Voronoi region V_k. A variational formulation is based upon minimization of the following nonlocal energy

$$E(Y) := \int_Q \mathrm{dist}^2(x, Y)\, \mathrm{d}x = \sum_{k=1}^{n} \int_{V_k} |x - y_k|^2\, \mathrm{d}x. \tag{1}$$

Criticality of E is exactly the condition that each y_k be the centroid of its Voronoi region V_k, that is

$$Y^* = \{y_i^*\} \quad \text{is a critical point of } E \qquad \text{iff} \qquad y_i^* = \int_{V_i} x\, dx, \quad \text{the centroid of } V_i.$$

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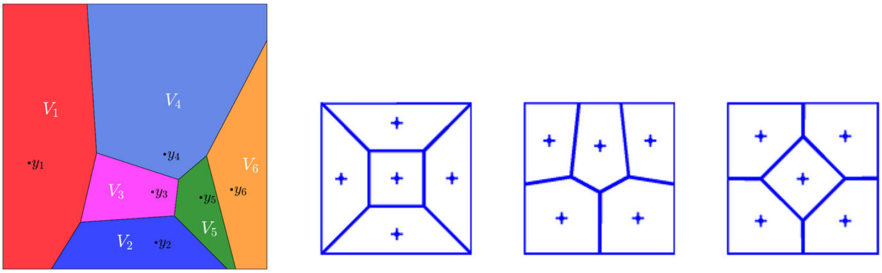

Fig. 1. Left: A Voronoi diagram (the Voronoi regions associated with six generators). Right: Three centroidal Voronoi tessellations with five generators

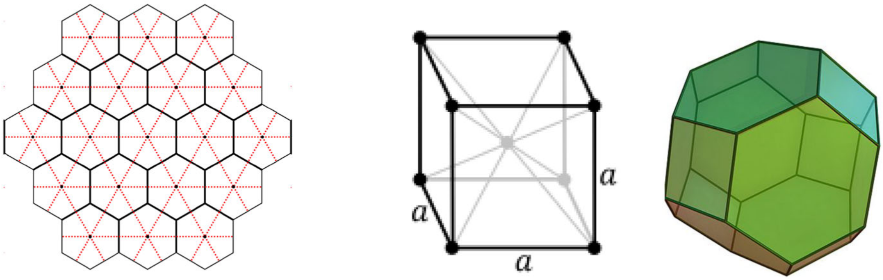

Fig. 2. Left: 2D Optimal placement of points on a triangular lattice with associated optimal Voronoi polytope a regular hexagon. Right: 3D Conjectured optimal placement of points on a BCC lattice and the associated optimal Voronoi polytope the truncated octahedron (Source: Wikipedia)

In the context of information theory, the set Y is viewed as a *quantizer* to quantize data which is distributed in Q according a continuous probability density, here taken to be uniformly distributed across Q. The *quantization error* is given by $E(Y)$. The *optimal quantizer* is the one with least error, alternatively *the CVT with lowest energy* (1).

A well-known conjecture attributed to Gersho [14] (cf. Conjecture (1.1) (a) below) addresses the periodic nature of the configuration with least error (alternatively, the CVT with lowest energy). This conjecture is completely solved in 2D but, to date, remains open in 3D. We present a precise statement of Gersho's conjecture (statement (a)) in its augmented form (statement (b)):

Conjecture 1.1. The Augmented Gersho's Conjecture

(a) *There exists a polytope V with $|V| = 1$ which tiles the space with congruent copies such that the following holds: let $(Y_n)_n$ be a sequence of minimizers, with $Y_n \in \operatorname{argmin}_{\sharp Y=n} E(Y)$, then all the Voronoi cells not intersecting the domain's boundary, the number of which is of order $n - o(n)$, are asymptotically congruent to $n^{-1/N} V$ as $n \to +\infty$.*

(b) *For dimension $N = 2$, the optimal polytope V is known to be a regular hexagon, corresponding to a optimal placement of points on a triangular lattice (cf. Fig. 2 left). For dimension $N = 3$, the optimal polytope V is the truncated octahedron, corresponding an optimal placement of points on a BCC (body centered cubic) lattice (cf. Fig. 2 right). While still unproven, this is supported by numerical simulations by Du and Wang [8].*

Conjecture 1.1 has been proven in 2D where hexagonal structures are pervasive[1] . The essential parts of the proof were first presented by Fejes Tóth [12] with later versions given, for example, by Newman [20]. However, as noted in [15], the first complete 2D proof of Gersho's conjecture was given by Gruber. To date, the conjecture remains open in 3D. In 3D, Barnes and Sloan [1] have proven the optimality of the BCC configuration amongst all lattice configurations, while Du and Wang [8] have presented numerical evidence supporting the conjecture. The nonlocal and nonconvex character of (1) insures a highly nontrivial energy landscape associated with a multitude of critical points with complex, albeit polygonal, Voronoi regions. Moreover, to divorce from boundary/size effects, one can only address the asymptotics as the number of generators n tends to infinity.

The purpose of this paper is to present in 3D some quantitative bounds for the geometry of minimizing Voronoi regions (cf. Theorem 2.3). To our knowledge, these bounds are new. In particular, we prove an upper bound (independent of n) on the complexity (number of faces) of an optimal Voronoi cell. This is an important step: Indeed, to divorce from boundary/size effects, one can only address the asymptotics as the number of generators n tends to infinity. A priori, we cannot dismiss the possibility that the complexity of the Voronoi cells associated with a CVT is $O(n)$ as $n \to \infty$; what we can do is to prove that this is not the case for the *optimal* CVT. As we explain in Sect. 6, we can combine this bound with Gruber's two dimensional approach to reduce the 3D Gersho conjecture to a finite, albeit large, computation of an explicit convex problem in finitely many variables.

Remarkably, the proof of these bounds does not rely on any sophisticated mathematical machinery, rather solely on elementary estimates with distance functions. Our choice of domain (the unit square Q) is for convenience only: the analogous results hold for any finite domain or, for example, the flat torus.

Let us conclude the introduction by noting that Gersho's conjecture is related to a fundamental, largely open, question in condensed matter physics. The *Crystallization Conjecture* roughly states that within the confinements of some physical domain, n interacting particles arrange themselves into a periodic configuration. Precisely, let Ω be a domain in $\mathbb{R}^N$, $Y = \{y_1, \cdots, y_n\}$ a collection of n points in Ω, and define

$$F_{\mathcal{V}}(Y) := \sum_{i,j=1}^{n} \mathcal{V}(|y_i - y_j|), \tag{2}$$

where $\mathcal{V}$ is the interaction potential. Such $\mathcal{V}$ has to satisfy stringent technical assumptions, and it is often repulsive at short ranges, attractive at long ranges, with a very deep well around its minimum value. We refer the interested reader to [19,23] for examples of conditions imposed on $\mathcal{V}$. In this respect, the crystallization conjecture asserts that as $n \to \infty$, the minimizers of F_n over all possible points $y_1, \ldots, y_n \in \Omega$ arrange themselves in a periodic lattice. Typical physical interaction potentials, for example the Lennard-Jones potential, have the property that they are repulsive at short distances and attractive at large. To dispense with boundary effects, it is necessary to pose the problem as an asymptotic statement as the size of the domain get larger. Upon rescaling, this is equivalent to letting the number of particles $n \to \infty$. The crystallization conjecture remains one of the most fundamental and difficult problems in mathematical physics with rigorous results far and few (see, for example, [2,10,11,13,19,21,23]). It is clear from [19] that the crystallization conjecture is related to the sphere packing problems,

[1] For example, Hales' celebrated resolution of the Honeycomb Conjecture in [18].

since the proof of the main result in [19] directly relies on the fact that optimal sphere packing in 2D is achieved by placing centers along a triangular lattice. However, the sphere packing itself is a difficut problem and only solved in dimensions 2, 3, 8, and 24 (cf. [4,24]).

The relationship of our purely geometric variational problem (1) to the ubiquitous class (2) is not immediate; in the former, the points do interact with each other but implicitly, via the distance function (equivalently via the associated Voronoi regions). While there is no explicit effective interaction potential $\mathcal{V}$, one can reformulate the energy E in terms of the *Wasserstein-2 distance* W_2 (cf. [25]) between a weighed sum of delta functions and Lebesgue measure $\mathcal{L}_N$:

$$E(Y) = W_2\left(\sum_{i=1}^{n} |V_i|\delta_{y_i}\,,\, \mathcal{L}_N\right)^2,$$

where δ_{y_i} denotes the delta function with concentration at y_i. In other words, the quantization error is precisely the squared Wasserstein-2 distance distance between the weighted point quantities and the continuous probability density. Such *semi-discrete* optimal transportation problems have recently been studied in [3].

In our opinion, the optimal CVT problem is the simplest setting to prove 3D crystallization because:

- there is a simple and elegant characterization of criticality (critical points);
- working solely with distance functions facilitates the proof of estimates and quantitative bounds for optimal configurations entirely in terms of their convex polygonal Voronoi regions. In particular, the energy (1) has a pseudo-local character which means that one can readily estimate the total energy loss resulting from the addition of a new generator in a fixed Voronoi cell (cf. Lemma 3.1).

Our choice to work with a fixed domain $Q := [0, 1]^3$ is for convenience reasons, since doing so completely removes any issue that might arise from a moving domain.

In the study of thermodynamic limits of many particle systems (cf. [22]), however, it is quite common to let the domain size diverge. In our case wherein the problem has an obvious scaling we can assume without loss of generality that the density of points is constantly equal to 1. Hence, our problem can be reformulated as follows: define the lowest energy of a domain Ω as

$$\mathcal{E}(\Omega) := \min_{\substack{Y\subseteq\Omega \\ \#Y=n=|\Omega|}} E_\Omega(Y) \tag{3}$$

where

$$\text{where} \quad E_\Omega(Y) := \int_\Omega \mathrm{dist}^2(x, Y)\,\mathrm{d}x = \sum_{i=1}^{n}\int_{V_i} |x - y_i|^2\,\mathrm{d}x \qquad Y = \{y_1, \cdots, y_n\}.$$

The goal is now to understand the structure of $\mathcal{E}$ when $\Omega \to \mathbb{R}^3$. It was shown in [27] that such energy $\mathcal{E}$ is *subadditive*, in the sense that if $\Omega = \Omega_1 \cup \Omega_2$, with $|\Omega_1|, |\Omega_2| \in \mathbb{N}$, then

$$\mathcal{E}(\Omega) \leq \mathcal{E}(\Omega_1) + \mathcal{E}(\Omega_2).$$

2. Optimal CVT and Gersho's Conjecture: Previous Results and the Statement of Our Main Theorem

2.1. Gruber's approach in two dimensions. In [15], Gruber presented an elementary proof in 2D of Gersho's conjecture based upon ideas of Fejes Tóth [12]. For convenience, he took the domain Ω to be a suitably-chosen regular polygon; however, one can work on an arbitrary domain at the expense of smaller-order boundary errors. His argument is as follows:

(i) First, it is shown that the functional

$$G(a,m) := \min_{\substack{A \text{ is an} \\ m\text{-gon with area } a}} \int_A |x-y|^2 \,\mathrm{d}x, \qquad y = \text{centroid of } A$$

is jointly convex. Here, one first shows that the minimum is attained on regular polygons. Then, via a direct Hessian computation, it is shown that there exists an extension of G, say $\tilde{G}$, whose second argument is defined over the positive real numbers, which is convex in both variables.

(ii) Second, it is shown that given a Voronoi tessellation $\{V_i\}_{i=1}^n$, the average number of sides is at most 6: let $E(F)$ be the number of sides of the face F, and by double counting (each side belongs to exactly 2 faces) we get $\sum_{\{F \text{ faces}\}} E(F) = 2e \leq 6n - 12$, where e is the total number of sides, and $2e \leq 6n - 12$ comes from Euler's formula for polytopes. Moreover, it is easy to check that

$$G(a,6) \leq \min\{G(a,3), G(a,4), G(a,5)\}$$

for all $a \geq 0$, by directly computing the values of $G(a,6)$, $G(a,3)$, $G(a,4)$, $G(a,5)$ on regular 3, 4, 5, 6-gons.

(iii) With these steps in hand, one proceeds as follows. Let $\{V_i\}_{i=1}^n$ be an arbitrary Voronoi tessellation and denote: by s_i the number of sides of V_i, by a_i its area, and

$$\bar{a} := \frac{1}{n}\sum_{i=1}^n a_i, \qquad \bar{s} := \frac{1}{n}\sum_{i=1}^n s_i.$$

The convexity of G then implies that

$$\begin{aligned}\sum_{i=1}^n \int_{V_i} |x-y_i|^2 \,\mathrm{d}x &\geq \sum_{i=1}^n G(a_i, s_i) \\ &\geq nG(\bar{a}, \bar{s}) + o(n) \\ &\geq nG(\bar{a}, 6) + o(n),\end{aligned}$$

where $o(n)$ is the contribution of the boundary terms, which vanish as $n \to +\infty$. The last inequality shows that the hexagonal partition is optimal.

The fundamental difficulty of applying Gruber's arguments in 3D case is establishing the convexity in m of

$$G(a,m) := \min_{\substack{V \text{ convex polytope, } |V|=a \\ V \text{ has at most } m \text{ faces}}} \int_V |x-y|^2 \,\mathrm{d}x, \qquad y = \text{ centroid of } V.$$

We do not have regular m-hedron in 3D, and computations are unfeasible. A priori, the maximum number of possible faces of the Voronoi polygons associated with a critical point can grow with n. One of the main results of this paper is to prove (cf. Theorem 2.3) upper bounds on the geometric complexity (including the number of faces) of such polygons which are independent of n. With such bounds in place, one could, in principle, have the computer verify the convexity of $G(a, m)$. As we explain in the last section (Sect. 6), this would then prove Gersho's conjecture in 3D.

Perhaps a deeper reason for the significantly increased difficulty in proving Gersho's in 3D, compared to 2D, is due to the fact that we do not expect the presence of a *universally optimal* configuration ([5, Definition 1.3]) in 3D. This is in stark contrast with the 2D case, where the triangular lattice is almost surely to be universally optimal (cf. [5]), although no rigorous proof is available. Gersho's conjecture would not be the first one in which such issue appears: it is well known that the solution to the optimal foam problem in 2D is given by the honeycomb structure, whose barycenters lie on the triangular lattice, while in 3D this is still open, and the long conjectured solution, i.e. the bitruncated cubic honeycomb, is surely not optimal, as it has higher energy than the Weaire-Phelan structure (cf. [26]).

Before presenting our results, let us document two known results in 3D.

2.2. *Two previous results in three dimensions.*

Theorem 2.1. (Gruber's Theorem 2 in *[16]*) *Let $(Y_n)_n$ be a sequence of minimizers, i.e. $(Y_n)_n$, with $Y_n \in \operatorname{argmin}_{\sharp Y=n} E(Y)$.*

(1) Then for some positive integer n_0, if $n > n_0$ there exists $\beta > 1$ such that Y_n is a $((1/\beta)n^{-1/3}, n^{-1/3})$-Delone set, i.e.,

$$n^{-1/3} \geq \min_{y, y' \in Y_n,\ y \neq y'} |y - y'| \geq (1/\beta)n^{-1/3}.$$

(2) Y_n is uniformly distributed in Q, i.e.

$$\sharp(K \cap Y_n) = |K|n + o(n) \qquad \text{as } n \to +\infty$$

for any Jordan measurable set $K \subseteq Q$.

Theorem 2.2. (Zador's uniform energy formula in *[27]*, 3D case) *There exists some constant $\tau > 0$ such that given any sequence $Y_n \in \operatorname{argmin}_{\sharp Y=n} E(Y)$, we have*

$$n^{2/3} E(Y_n) \ \to\ \tau.$$

Zador's result has been extended by Gruber in the general setting of manifolds [16]. However, to our knowledge, no further description of the geometry of Voronoi cells has been proven, nor any explicit lower bounds on τ. We remark that in terms of the reformulation $\mathcal{E}(\Omega)$ defined in (3), we have

$$\tau \ =\ \lim_{n\to\infty} \frac{\mathcal{E}(\Omega_n)}{|\Omega_n|} \quad \text{as} \quad \Omega_n \to \mathbb{R}^3,$$

the *thermodynamic limit* of the system.

2.3. The statement of our results. For the remainder of this article we assume the space dimension $N = 3$.

Theorem 2.3. *Let $n \in \mathbb{N}$ and Y_n be a minimizer of (1). Then for any $y \in Y_n$, with V denoting its Voronoi cell, we have:*
(i) There exists constants $\Gamma_1, \ldots, \Gamma_5$ (independent of n) such that

$$\mathrm{diam}(V) \geq \Gamma_3 n^{-1/3}, \tag{4}$$

$$|V| \geq \omega_3 \Gamma_5^3 n^{-1}, \tag{5}$$

$$\mathrm{diam}(V) \leq \Gamma_4 (n-2)^{-1/3}, \tag{6}$$

$$V \text{ has at most } N_* := 2(3\Gamma_4/\Gamma_5)^3 \text{ faces}, \tag{7}$$

where $\omega_3 := 4\pi/3$, and

$$\Gamma_1 := (2/5)^{2/3}/40 \approx 0.013572,$$
$$\Gamma_3 := \omega_3^{-1/5}\Gamma_1^{1/5} \approx 0.317769,$$
$$\Gamma_5 := \frac{1}{4}\left(\sqrt{1 + \frac{2^4 \cdot 3^3}{5^2 \cdot 10^3}} - 1\right)\Gamma_3 \approx 0.000451,$$
$$\Gamma_4 := \frac{2 \cdot 12^{1/4}(16)^{1/3}}{\pi^{1/4}\omega_3^{1/12}}\left(\sqrt{1 + \frac{2^4 \cdot 3^3}{5^2 \cdot 10^3}} - 1\right)^{-1/2}\left(\frac{5^2 \cdot 10^3}{2^2 \cdot 3^3}\right)^{1/4} \approx 333.18$$
$$N_* \approx 2.94 \times 10^{20}.$$

(ii) Let τ be the constant in Zador's asymptotic estimate (cf. Theorem 2.2), that is,

$$n^{2/3} E(Y_n) \to \tau.$$

Then we have

$$n^{2/3} E(Y_n) \geq \tau \qquad \forall n \gg 1 \tag{8}$$

with

$$\tau \geq \frac{2\pi}{5}\omega_3^{-5/3} \approx 0.11545. \tag{9}$$

The lower bound on τ given in (9) is approximately half the energy density of the BCC lattice (≈ 0.23562), the conjectured asymptotically optimal configuration. Although this lower bound is surely non optimal (cf. [15, Table 1]), its proof will be rather simple. The proofs of the statements comprising Theorem 2.3 are presented in Sect. 3-5.
Remark: While we state and prove Theorem 2.3 in three dimensions, our proofs work in *any* space dimension, with appropriate adjustments for the constants.

We expect the upper bound N_* to be significantly suboptimal, as it is significantly larger than the average number of faces in a Voronoi tessellation, which was shown in [9] to be at most 14. Moreover, it is currently computationally unfeasible to perform simulations with such a large N_*. We do not expect such N^* to depend significantly on the shape of the domain.

3. The Proof of Theorem 2.3*(i)*

In this section we prove the statements (4)–(7) of Theorem 2.3, in the exact same order they are stated. Their proofs will rely on the following two lemmas whose proofs are presented later in Sect. 5.

Lemma 3.1. *Given a compact, convex set $V \subseteq \mathbb{R}^3$, a point y in the interior of V, then there exists $y' \in V$ such that*

$$\int_V [|x-y|^2 - d^2(x,\{y,y'\})]\,\mathrm{d}x \geq \max\left\{\frac{2^2\cdot 3^3}{5^2\cdot 10^3} r^2|V|, \Gamma_1|V|^{5/3}\right\}, \tag{10}$$

where $r := \max_{z'\in\partial V}|z'-y|$, $\Gamma_1 = (2/5)^{2/3}/40$.

Lemma 3.2 (Lower bound on the distance to a closest neighbor). *Given n, let Y_n be a minimizer. Then for any $y \in Y_n$ with V denoting its Voronoi cell, we have*

$$\min_{z\in Y_n\setminus\{y\}}|y-z| \geq r\left(\sqrt{1+\frac{2^4\cdot 3^3}{5^2\cdot 10^3}}-1\right) \geq \Gamma_2|V|^{1/3},$$

where

$$\Gamma_2 := \left(\sqrt{1+\frac{2^4\cdot 3^3}{5^2\cdot 10^3}}-1\right)\omega_3^{-1/3} \quad \text{and} \quad r := \max_{z'\in\partial V}|z'-y|.$$

3.1. Lower bound on the diameter: proof of statement (4). To proof of statement (4) of Theorem 2.3 will only require Lemma 3.1.

Proof. **(of statement (4))** Let $s := \mathrm{diam}(V)$. We claim:

$$\text{there exists } y' \in Y_n\setminus\{y\} \text{ such that } |y'-y| \leq 2s. \tag{11}$$

The proof is by contradiction: assume the opposite, i.e. there are no other points of $Y_n\setminus\{y\}$ in the ball $B(y, 2(s+\varepsilon))$ for some $\varepsilon > 0$. Then let z be an arbitrary point with $|z-y| = s+\varepsilon/2$: clearly $z \in V$, as the opposite would give the existence of $y' \in Y_n$ with $|z-y'| \leq |z-y| = s+\varepsilon/2$, hence

$$2(s+\varepsilon) \leq |y'-y| \leq |z-y'| + |z-y| \leq 2s+\varepsilon,$$

which is a contradiction. Thus any such z satisfying $|z-y| = s+\varepsilon/2$ belongs to V, hence $B(y, s+\varepsilon/2) \subseteq V$, contradicting $\mathrm{diam}(V) = s$, and (11) is proven.

Let $y' \in Y_n\setminus\{y\}$ be a point satisfying $|y'-y| \leq 2s$. If we remove y, then all points of V can still project on y', in the sense that for any $x \in V$ we have

$$\begin{aligned}|x-y'|^2 - |x-y|^2 &= (|x-y'| - |x-y|)(|x-y'| + |x-y|)\\ &\leq |y-y'|(2s + |y-y'|) \leq 8s^2.\end{aligned}$$

Integrating over V yields

$$\int_V [|x-y'|^2 - |x-y|^2]\,\mathrm{d}x \leq 8s^2|V|.$$

Since $\mathrm{diam}(V) = s$, it follows that V is contained in a ball of diameter s, hence

$$\int_V [|x-y'|^2 - |x-y|^2]\,\mathrm{d}x \le 8s^2|V| \le \omega_3 s^5.$$

Thus by removing y, the energy increases by at most $\omega_3 s^5$. The average volume of all Voronoi cells is n^{-1}, thus there exists y' whose Voronoi cell V' has volume at least n^{-1}. Lemma 3.1 gives that it is possible to add $\tilde{y}'$ in V', and the energy is decreased by at least $\Gamma_1 n^{-5/3}$. By the minimality of Y_n we get

$$\omega_3 s^5 \ge \Gamma_1 n^{-5/3} \Longrightarrow s \ge \Gamma_3 n^{-1/3}, \qquad \Gamma_3 = \omega_3^{-1/5}\Gamma_1^{1/5},$$

concluding the proof. □

3.2. Lower bound on the volume: proof of statement (5). The proof of (5) only requires Lemma 3.2.

Proof. **(of statement (5))** Consider an arbitrary $y \in Y_n$, and denote by V its Voronoi cell. Set $r := \max_{z' \in \partial V} |z' - y|$, and for any pair $z_1, z_2 \in V$ such that $|z_1 - z_2| = \mathrm{diam}(V)$, we have

$$\mathrm{diam}(V) = |z_1 - z_2| \le |z_1 - y| + |y - z_2| \le 2r \Longrightarrow r \ge \mathrm{diam}(V)/2. \tag{12}$$

Choose $y' \in Y_n \backslash \{y\}$ such that $|y - y'| = \min_{z \in Y_n \backslash \{y\}} |y - z|$, and by Lemma 3.2, (12) and (4) we have

$$\begin{aligned} |y-y'| &\overset{\text{Lemma 3.2}}{\ge} r\left(\sqrt{1+\frac{2^4\cdot 3^3}{5^2\cdot 10^3}}-1\right) \\ &\overset{(12)}{\ge} \frac{1}{2}\left(\sqrt{1+\frac{2^4\cdot 3^3}{5^2\cdot 10^3}}-1\right)\mathrm{diam}(V) \\ &\overset{(4)}{\ge} \frac{1}{2}\left(\sqrt{1+\frac{2^4\cdot 3^3}{5^2\cdot 10^3}}-1\right)\Gamma_3 n^{-1/3} \end{aligned} \tag{13}$$

and hence

$$B(y, \Gamma_5 n^{-1/3}) \subseteq V \qquad \text{where} \qquad \Gamma_5 = \frac{1}{4}\left(\sqrt{1+\frac{2^4\cdot 3^3}{5^2\cdot 10^3}}-1\right)\Gamma_3. \tag{14}$$

Thus (14) is proven, which in turn gives

$$\omega_3 \Gamma_5^3 n^{-1} = |B(y, \Gamma_5 n^{-1/3})| \le |V|,$$

hence (5). □

3.3. Upper bound on the diameter: proof of statement (6). The proof of (6) requires both Lemma 3.1 and Lemma 3.2.

Proof. **(of statement (6))** Upon renaming, let y_1 be such that its Voronoi cell V_1 has maximum diameter. Let $r_1 := \max_{z' \in \partial V_1} |z' - y_1|$, and note that denoting by $w, u \in V_1$ two points realizing the diameter, we have

$$|w - u| = \operatorname{diam}(V_1) \leq |w - y_1| + |u - y_1| \leq 2r_1.$$

Next we prove the existence of a cell V_2, with generator y_2, such that

$$|V_2| \leq \frac{2}{(n-2)} \quad \text{and} \quad \sigma(y_2)^3 \leq \frac{16}{\omega_3(n-2)} \quad \text{where} \quad \sigma(y_2) := \min_{z \in Y_n \setminus \{y_2\}} |y_2 - z|. \tag{15}$$

To this end, we note the following.

(a) Denoting by

$$\mathcal{V}_n := \{y \in Y_n : \text{ the Voronoi cell } V_y \text{ of } y \text{ satisfies } |V_y| \geq 2/(n-2)\},$$

we claim $\sharp \mathcal{V}_n \leq \lceil n/2 \rceil$. This is because the total number of cells is n, and if the opposite holds, i.e. if there exists at least $n - \lceil n/2 \rceil \geq (n-1)/2$ cells with volume greater than $2/(n-2)$, we conclude that

$$1 = |Q| \geq \sum_{y \notin \mathcal{V}_n} |V_y| \geq (n - \lceil n/2 \rceil) \frac{2}{n-2} \geq \frac{n-1}{2} \frac{2}{n-2} > 1.$$

(b) Similarly if we denote by

$$\mathcal{S}_n := \left\{ y \in Y_n : \sigma(y)^3 \leq \frac{16}{\omega_3(n-2)} \right\}, \qquad \sigma(y) := \min_{z \in Y_n \setminus \{y\}} |y - z|,$$

we claim $\sharp \mathcal{S}_n \geq \lceil n/2 \rceil + 1$. To this end, for any y we have $B(y, \sigma(y)/2) \subseteq V_y$, and hence $|V_y| \geq \omega_3 \sigma(y)^3/8$. If by contraction we had $\sharp \mathcal{S}_n \leq \lceil n/2 \rceil$, i.e. there exist at least $n - \lceil n/2 \rceil$ generators y with $\sigma(y)^3 \geq \frac{16}{\omega_3(n-2)}$, we would conclude that

$$1 = |Q| \geq \sum_{y \notin \mathcal{S}_n} |V_y| \geq \frac{\omega_3}{8} \sum_{y \notin \mathcal{S}_n} \sigma(y)^3 \geq \frac{\omega_3}{8} \frac{n-1}{2} \frac{16}{\omega_3(n-2)} > 1.$$

Combining (a) and (b) above yields the existence of a cell V_2 with generator y_2 satisfying (15).

Next, we estimate how much the total energy increases if we remove y_2. Let y_3 be such that $|y_2 - y_3| = \sigma(y_2)$. Then for any $x \in V_2$, we have

$$|x - y_3|^2 - |x - y_2|^2 \leq |y_2 - y_3|(|x - y_3| + |x - y_2|) \leq \sigma(y_2)(2|x - y_2| + \sigma(y_2)).$$

Noting that the midpoint $\bar{y} := (y_2 + y_3)/2 \in \partial V_2$, we have

$$\sigma(y_2) = 2|y_2 - \bar{y}| \leq 2 \operatorname{diam}(V_2) \leq 2 \operatorname{diam}(V_1).$$

Thus we have

$$|x - y_3|^2 - |x - y_2|^2 \leq 4 \operatorname{diam}(V_1) \sigma(y_2)$$

which implies

$$\begin{aligned}\int_{V_2}(|x-y_3|^2-|x-y_2|^2)\,\mathrm{d}x &\le 4\,\mathrm{diam}(V_1)\sigma(y_2)|V_2| \\ &\overset{(15)}{\le} \frac{8\cdot(16)^{1/3}\,\mathrm{diam}(V_1)}{\omega_3^{1/3}(n-2)^{4/3}} \\ &\le \frac{(16)^{4/3}r_1}{\omega_3^{1/3}(n-2)^{4/3}}. \end{aligned} \tag{16}$$

By Lemma 3.1, we can always add a point in V_1 and the energy is decreased by at least $\frac{2^2\cdot 3^3}{5^2\cdot 10^3}r_1^2|V_1|$. Hence we need to bound $|V_1|$ from below. To this end, choose an arbitrary z_1 such that $|z_1-y_1|=r_1$, and let ℓ be the line through y_1 and z_1, and let Π be the plane through y_1 and orthogonal to ℓ. By Lemma 3.2, we have

$$\sigma(y_1):=\min_{z\in Y_n\setminus\{y_1\}}|y_1-z|\ge r_1\left(\sqrt{1+\frac{2^4\cdot 3^3}{5^2\cdot 10^3}}-1\right),$$

and hence $B(y_1,\sigma(y_1)/2)\subseteq V_1$. In particular, by convexity of V_1, the disk $\Pi\cap B(y_1,\sigma(y_1)/2)\subseteq V_1$, and the cone with base $\Pi\cap B(y_1,\sigma(y_1)/2)$ and height $\{(1-s)y_1+sz_1 : s\in[0,1]\}$ is again contained in V_1. It follows that

$$|V_1|\ge r_1\frac{\pi\sigma(y_1)^2}{12}\ge r_1^3\frac{\pi}{12}\left(\sqrt{1+\frac{2^4\cdot 3^3}{5^2\cdot 10^3}}-1\right)^2.$$

Consequently, there exists $y'\in V_1$ such that

$$\begin{aligned}\int_{V_1}(|x-y_1|^2-d^2(x,\{y_1,y'\}))\,\mathrm{d}x &\overset{\text{Lemma 3.1}}{\ge} \frac{2^2\cdot 3^3}{5^2\cdot 10^3}r_1^2|V_1| \\ &\ge \frac{\pi}{12}\left(\sqrt{1+\frac{2^4\cdot 3^3}{5^2\cdot 10^3}}-1\right)^2\frac{2^2\cdot 3^3}{5^2\cdot 10^3}r_1^5.\end{aligned}$$

Combining with (16) and using the minimality of Y_n, we infer

$$\begin{aligned}&\frac{(16)^{4/3}r_1}{\omega_3^{1/3}(n-2)^{4/3}} \\ &\quad\ge \frac{\pi}{12}\left(\sqrt{1+\frac{2^4\cdot 3^3}{5^2\cdot 10^3}}-1\right)^2\frac{2^2\cdot 3^3}{5^2\cdot 10^3}r_1^5 \\ &\quad\Longrightarrow r_1^4\le\frac{12(16)^{4/3}}{\pi\omega_3^{1/3}(n-2)^{4/3}}\left(\sqrt{1+\frac{2^4\cdot 3^3}{5^2\cdot 10^3}}-1\right)^{-2}\frac{5^2\cdot 10^3}{2^2\cdot 3^3} \\ &\quad\Longrightarrow \mathrm{diam}(V_1)\le 2r_1\le\frac{2\cdot 12^{1/4}(16)^{1/3}}{\pi^{1/4}\omega_3^{1/12}(n-2)^{1/3}}\left(\sqrt{1+\frac{2^4\cdot 3^3}{5^2\cdot 10^3}}-1\right)^{-1/2}\left(\frac{5^2\cdot 10^3}{2^2\cdot 3^3}\right)^{1/4},\end{aligned}$$

concluding the proof. □

3.4. Upper bound on the number of faces: proof of statement (7). The bounds on the diameter (statement (6)) and volume (statement (5)) of Voronoi cells allow us to bound their geometric complexity (i.e. the maximum number of faces).

Proof. **(of statement (7))** Consider an arbitrary $y \in V$. By construction, its Voronoi cell V is the bounded convex region delimited by the axial planes (i.e. the plane orthogonal to the line segment and passing through its midpoint) of the line segments connecting y and some other generator $y' \in Y_n$.

Statement (6) implies that any Voronoi cell has diameter not exceeding $\Gamma_4(n-2)^{-1/3}$. Thus if two generators $y', y'' \in Y_n$ satisfy $|y'-y''| > 2\Gamma_4(n-2)^{-1/3}$, then their Voronoi cells do not share boundaries. Thus only the generators $y' \in B(y, 2\Gamma_4(n-2)^{-1/3})$ can have their Voronoi region share a boundary with V. Again, the upper bound on the diameter given by estimate (6) gives that any Voronoi cell (of any generator $y' \in B(y, 2\Gamma_4(n-2)^{-1/3})$) is entirely contained in $B(y, 3\Gamma_4(n-2)^{-1/3})$.

Statement (5) implies that each Voronoi cell has volume at least $\omega_3\Gamma_5^3 n^{-1}$, so the ball

$$B(y, 3\Gamma_4(n-2)^{-1/3})$$

can contain only

$$\frac{\omega_3(3\Gamma_4(n-2)^{-1/3})^3}{\omega_3\Gamma_5^3 n^{-1}} = (3\Gamma_4/\Gamma_5)^3\frac{n}{n-2} \leq 2(3\Gamma_4/\Gamma_5)^3 =: N_*$$

whole Voronoi cells. The last factor 2 comes from the fact that any polyhedron has at least 4 faces, and $n/(n-2) \leq 2$ for all $n \geq 4$. Thus V can share boundary with at most N_* other Voronoi cells. □

4. Energy Estimates: Proof of Theorem 2.3*(ii)*

4.1. Proof of (8). As is common in statistical mechanics (cf. [22]), the proof of the lower bound on the thermodynamic limit follows quite straightforwardly from the subadditivity property of the energy $\mathcal{E}$, defined in (3). Thus in this proof it is convenient to use the equivalent formulation (3) with the fixed average density of points which, without loss of generality, is set to 1. Proving (8) is equivalent to proving

$$\lim_{\Omega_n \to \mathbb{R}^3} \frac{\mathcal{E}(\Omega_n)}{|\Omega_n|} \geq \tau. \tag{17}$$

Proof. **(of estimate (17))** We first consider the case where Ω is a cube with volume $n = 8^k$. We partition Ω into 8 cubes of volume 8^{k-1} and use the subadditivity of to yield

$$\frac{\mathcal{E}(8^k)}{8^k} \leq \frac{\mathcal{E}(8^{k-1})}{8^{k-1}},$$

where for simplicity we denote by $\mathcal{E}(n)$ $(n \in \mathbb{N})$ the energy of the cube with volume n. Hence the limit as $k \to +\infty$ exists. Similarly, the same arguments show that for any n of the form $n = 8^k n_0$ $(n_0 \in \mathbb{N})$, such a limit, which we denote by $\tau(n_0)$, also exists.

By the subadditivity of $\mathcal{E}$, we have $\mathcal{E}(8^k n_0) \leq n_0\mathcal{E}(8^k)$, hence $\tau(n_0) \leq \tau(1)$.

Next we show that τ is actually independent of n_0. To this end, write $8^k = p8^\ell n_0 + q$, with $q = o(8^k)$. Pack the cube of volume 8^k with p cubes of volume $8^\ell n_0$, and denote by Ω_q the remaining part. Note that Ω_q is the difference between a larger cube (of volume 8^k), and p smaller cubes (of volume $8^\ell n_0$), so it might not be a cube itself. The subadditivity of $\mathcal{E}$ gives

$$\mathcal{E}(8^k) \leq p\mathcal{E}(8^k n_0) + \mathcal{E}(\Omega_q).$$

Place q points inside Ω_q on a cubic lattice to obtain $\mathcal{E}(q) \leq Cq = o(8^k)$. Therefore,

$$\frac{\mathcal{E}(8^k)}{8^k} \leq \frac{\mathcal{E}(8^\ell n_0)}{8^\ell n_0} + o(1).$$

Passing to the limit $k \to +\infty$ and $\ell \to +\infty$ gives $\tau(n_0) \geq \tau(1)$, and hence $\tau(n_0) = \tau(1) =: \tau$ for all n_0.

Finally, to obtain the limit for all n, we write $n = p8^\ell n_0 + q$ and repeat the above arguments. Similarly, it can be shown that, for any reasonably regular sequence Ω_n which tends to $\mathbb{R}^3$, that does not create too much surface tension, we also have $\mathcal{E}(\Omega_n)/|\Omega_n| \to \tau$. □

4.2. Proof of (9). We will use the following result, easily derived from simple rearrangement inequalites.

Lemma 4.1. *Among all convex sets with fixed volume and centroid at the origin, the sphere has the lowest energy in the sense that*

$$\int_V |x|^2\,\mathrm{d}x \geq \int_B |x|^2\,\mathrm{d}x, \qquad B := \textit{ball of volume } |V|.$$

Proof. **(of statement (9))** Consider a sequence of minimizers $(Y_n)_n$, and choose an arbitrary element Y_m. Note that the union $\bigcup_{y\in Y_m} V_y$ has volume 1, where V_y denotes the Voronoi cell of y. Lemma 4.1 gives that among all convex sets of unit volume, the sphere has the lowest energy, which is equal to

$$\frac{2\pi}{5}\left(\frac{3}{4\pi}\right)^{5/3}.$$

Scaling arguments give that as the volume scales by a factor of s, the energy scales by a factor of $s^{5/3}$, hence the energy of a Voronoi cell with volume $|V|$ is at least

$$\frac{2\pi}{5}\left(\frac{3}{4\pi}\right)^{5/3}|V|^{5/3}.$$

Therefore,

$$E(Y_m) = \sum_{y\in Y_m}\int_{V_y}|x-y|^2\,\mathrm{d}x \geq \frac{2\pi}{5}\left(\frac{3}{4\pi}\right)^{5/3}\sum_{y\in Y_n}|V_y|^{5/3}.$$

Using the convexity of $f(t) = t^{5/3}$ and the fact that the average volume is $1/m$, we infer

$$E(Y_m) \geq \frac{2\pi}{5}\left(\frac{3}{4\pi}\right)^{5/3}\sum_{y\in Y_n}|V_y|^{5/3} \geq \frac{2\pi}{5}\left(\frac{3}{4\pi}\right)^{5/3} m^{-2/3},$$

hence

$$\frac{2\pi}{5}\left(\frac{3}{4\pi}\right)^{5/3} \leq m^{2/3}E(Y_m) \to \tau,$$

and the proof is complete. □

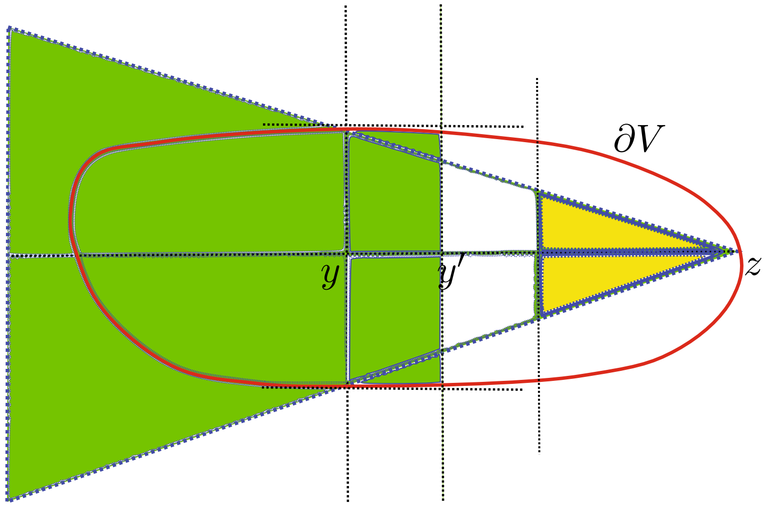

Fig. 3. Simplified 2D representation of the construction. The extra point we added is y', and the entire yellow region, whose volume is a significant fraction of $|V|$, contributes to decrease the energy

5. Proofs of Lemmas 3.1 and 3.2

Proof. **(of Lemma** 3.1**)** We first prove

$$\int_V [|x-y|^2 - d^2(x, \{y, y'\})]\,\mathrm{d}x \geq \frac{2^2 \cdot 3^3}{5^2 \cdot 10^3} r^2 |V|. \tag{18}$$

Let $z \in \partial V$ be a point satisfying

$$|z-y| = \max_{z' \in V} |z'-y| = \max_{z' \in \partial V} |z'-y|,$$

and let $r := |z-y|$. Endow $\mathbb{R}^3$ with the cartesian system (x_1, x_2, x_3) with

$$y = (0,0,0), \qquad z = (r,0,0),$$

and we add a point $y' = (x, 0, 0) \in V$, with fixed $x \in (0, r)$ to be determined shortly. We provide a schematic of the following steps in Fig. 3.

Define the planes $\Pi_x := \{x_1 = x\}$. Since V is convex, the intersection $\Pi_x \cap V$ is also convex for all x, and the boundary $\partial V \cap \Pi_x$ is a convex Jordan curve. Let $\gamma : [0,1] \longrightarrow \partial V \cap \Pi_x$ be an arbitrary parameterization, and for any $t \in [0,1]$, let ℓ_t be the half-line starting from z passing through $\gamma(t)$.

The convexity of V now has the following geometric consequences:

(G1) V surely contains the "cone" delimited by the surfaces $V \cap \Pi_x$ and $\bigcup_{t\in[0,1]}(\ell_t \cap \{x_1 \geq x\})$,
(G2) for any $t \in [0,1]$, the half-line ℓ_t exits V at $\gamma(t)$, that is, $\ell_t \cap \{x_1 < x\} = \emptyset$.

Now let $V_+(x) := V \cap \{x_1 \geq x\}$, and we estimate its volume. By construction, in view of $|z-y| = \max_{z' \in V} |z'-y|$ and observation (G2), it follows that $V \cap \{x_1 < x\}$ must be contained in the truncated cone (that we denote by $\mathcal{C}_-$) delimited by the surfaces $\bigcup_{t\in[0,1]}(\ell_t \cap \{-r \leq x_1 \leq x\})$, $\{x_1 = -r\}$ and Π_x. Let $\mathcal{C}$ be the cone delimited by

$\bigcup_{t\in[0,1]}(\ell_t \cap \{-r \le x_1\})$ and $\{x_1 = -r\}$ and Π_x, and note that the cone $\mathcal{C}_+ := \mathcal{C}\backslash\mathcal{C}_-$ satisfies

$$\frac{|\mathcal{C}_+|}{|\mathcal{C}|} = \left(\frac{r-x}{2r}\right)^3 \implies \frac{|\mathcal{C}_+|}{|\mathcal{C}_-|} = \frac{\left(\frac{r-x}{2r}\right)^3}{1-\left(\frac{r-x}{2r}\right)^3} = \frac{(r-x)^3}{8r^3-(r-x)^3}.$$

Since by construction we have $V \subseteq \mathcal{C}_- \cup V_+$, and $\mathcal{C}_+ \subseteq V_+$, it follows

$$|V| \le |\mathcal{C}_-| + |V_+| \qquad \text{and} \qquad |V_+| \ge |\mathcal{C}_+| = \frac{(r-x)^3}{8r^3-(r-x)^3}|\mathcal{C}_-|.$$

Hence, we have

$$|\mathcal{C}_-| \le |V_+|\frac{8r^3-(r-x)^3}{(r-x)^3} = |V_+|\left[\frac{8r^3}{(r-x)^3} - 1\right] \quad \text{and so} \quad |V| \le |\mathcal{C}_-| + |V_+| \le |V_+|\frac{8r^3}{(r-x)^3}.$$

Thus

$$\frac{|V_+|}{|V|} \ge \frac{(r-x)^3}{8r^3} = \left(\frac{1}{2} - \frac{x}{2r}\right)^3. \tag{19}$$

Now take an arbitrary point $w = (w_1, w_2, w_3) \in V_+$ (hence $w_1 \in [x, r]$), and note that

$$\begin{aligned} &|w-y|^2 = w_1^2 + w_2^2 + w_3^2, \qquad |w-y'|^2 = (w_1-x)^2 + w_2^2 + w_3^2 \\ &\quad \implies |w-y|^2 - |w-y'|^2 = w_1^2 - (w_1-x)^2 = x(2w_1 - x) \ge x^2. \end{aligned} \tag{20}$$

Thus

$$\begin{aligned} \int_V [|w-y|^2 - d^2(w,\{y,y'\})]\,\mathrm{d}w &\ge \int_{V_+} [|w-y|^2 - d^2(w,\{y,y'\})]\,\mathrm{d}w \\ &= \int_{V_+} [|w-y|^2 - |w-y'|^2]\,\mathrm{d}w \\ &\overset{(20)}{\ge} |V_+|x^2 \\ &\overset{(19)}{\ge} |V|\left(\frac{1}{2} - \frac{x}{2r}\right)^3 x^2. \end{aligned}$$

Since the above argument is valid for all $x \in [0, r]$, it follows

$$\int_V [|w-y|^2 - d^2(w,\{y,y'\})]\,\mathrm{d}w \ge |V| \max_{x\in[0,r]} \left(\frac{1}{2} - \frac{x}{2r}\right)^3 x^2.$$

Maximizing the last expression over $x \in [0, r]$ (i.e. taking $x = \frac{2r}{5}$) yields (18).

We now prove

$$\int_V [|x-y|^2 - d^2(x,\{y,y'\})]\,\mathrm{d}x \ge \Gamma_1|V|^{5/3}. \tag{21}$$

As in the proof of (18), endow $\mathbb{R}^3$ with a Cartesian coordinate system with origin in y. For any $t \in [0, |V|^{1/3}]$, set

$$Q(t) := \{-t/2 \le x_1, x_2, x_3 \le t/2\}, \qquad V_k^{\pm}(t) := V \cap \{\pm x_k \ge t/2\}, \quad k = 1, 2, 3.$$

Note that since

$$V \backslash Q(t) = \bigcup_{k=1}^{3} V_k^{\pm}(t),$$

we have

$$|V \backslash Q(t)| = \left| \bigcup_{k=1}^{3} V_k^{\pm}(t) \right| \ge |V| - t^3.$$

Thus there exists an element $\tilde{V}(t) \in \{V_k^{\pm}(t) : k = 1, 2, 3\}$ such that $|\tilde{V}(t)| \ge (|V| - t^3)/6$. Let y' be the center of the face $\tilde{V}(t) \cap Q(t)$. By (20), any $w \in \tilde{V}(t)$ satisfies $|w - y|^2 - |w - y'|^2 \ge t^2/4$, hence

$$\begin{aligned}\int_V [|w - y|^2 - d^2(w, \{y, y'\})]\,\mathrm{d}w &\ge \int_{\tilde{V}(t)} [|w - y|^2 - d^2(w, \{y, y'\})]\,\mathrm{d}w \\ &\ge \frac{|\tilde{V}(t)|t^2}{4} \\ &\ge \frac{(|V| - t^3)t^2}{24}.\end{aligned}$$

This last inequality holds for all $t \in [0, |V|^{1/3}]$. In particular, direct computation gives that the maximum of $(|V| - t^3)t^2$ is attained at $t^3 = 2|V|/5$, thus

$$\int_V [|w - y|^2 - d^2(w, \{y, y'\})]\,\mathrm{d}w \ge \left.\frac{(|V| - t^3)t^2}{24}\right|_{t^3 = 2|V|/5} = \frac{1}{40}\left(\frac{2}{3}\right)^{2/5} |V|^{5/3}$$

which proves (21). □

Proof. **(of Lemma 3.2)** Although a similar estimate has been proven by Gruber in [16], the lower bound therein was only implicit. Here we give an explicit lower bound. To this end, assume $|V| > 0$, otherwise the thesis is trivial. The main idea of the proof is:

(1) first we show that if Y_n is optimal, then y is in the interior of V,
(2) then we add another point y' in V (the energy difference is estimated using Lemma 3.1),
(3) finally we remove y (energy difference to be estimated by direct computation).

Step 1. Assume by contradiction $y \in \partial V$. Then there exists a plane Π such that V is entirely on one side of Π. Endow $\mathbb{R}^3$ with a cartesian system with $\Pi = \{(x_1, x_2, x_3) : x_1 = 0\}$, $V \subseteq \{x_1 \ge 0\}$, $y = (0, 0, 0)$. Then,

$$\int_V |z - y|^2\,\mathrm{d}z = \int_V [z_1^2 + z_2^2 + z_3^2]\,\mathrm{d}z_1\,\mathrm{d}z_2\,\mathrm{d}z_3,$$

with $z_1 \ge 0$ for all $z \in V$. Therefore,

$$\frac{\partial}{\partial y_1} \int_V [(z_1 - y_1)^2 + z_2^2 + z_3^2]\,\mathrm{d}z_1\,\mathrm{d}z_2\,\mathrm{d}z_3 \bigg|_{y_1 = 0} = -2 \int_V z_1\,\mathrm{d}z_1\,\mathrm{d}z_2\,\mathrm{d}z_3 < 0,$$

and Y_n cannot be a minimizer.

Step 2. In Step 1 we have proven that y must be in the interior of V, thus we are under the hypotheses of Lemma 3.1, which gives that there exists y' such that

$$\int_V [|x-y|^2 - d^2(x,\{y,y'\})]\,\mathrm{d}x \geq |V|\frac{2^2\cdot 3^3}{5^2\cdot 10^3}r^2 \geq \Gamma_1|V|^{5/3}, \quad r := \max_{z'\in\partial V}|y-z'|. \tag{22}$$

This means that adding y' in V, the energy decreases by at least $|V|\frac{2^2\cdot 3^3}{5^2\cdot 10^3}r^2$.

Step 3. Now we have to remove y, and estimate how much the energy increases. Set

$$s := |y-y''| = \min_{z\in Y_n,\ z\neq y}|y-z|,$$

and for any $x\in V$ it holds

$$\begin{aligned} |x-y''|^2 - |x-y|^2 &= (|x-y''|-|x-y|)(|x-y''|+|x-y|) \\ &\leq |y-y''|(2|x-y|+|y-y''|) \leq s(2r+s) \\ &\Longrightarrow \int_V [|x-y''|^2 - |x-y|^2]\,\mathrm{d}x \leq |V|s(2r+s). \end{aligned} \tag{23}$$

Combining (22), (23) and the minimality of Y_n then gives

$$s^2 + 2rs - r^2\frac{2^2\cdot 3^3}{5^2\cdot 10^3} \geq 0 \Longrightarrow s \geq r\left(\sqrt{1+\frac{2^4\cdot 3^3}{5^2\cdot 10^3}}-1\right).$$

Finally note that $V\subseteq B(y,r)$, hence $\omega_3 r^3 \geq |V|$, and

$$s \geq r\left(\sqrt{1+\frac{2^4\cdot 3^3}{5^2\cdot 10^3}}-1\right) \geq \left(\sqrt{1+\frac{2^4\cdot 3^3}{5^2\cdot 10^3}}-1\right)\omega_3^{-1/3}|V|^{1/3},$$

and the proof is complete. □

6. Towards a Proof of Gersho's Conjecture in 3D

Let us now address the extension to 3D of Gruber's 2D proof of Gersho's conjecture. The following analogous results are needed.

(1) We first note that the average number of faces (as $n\to+\infty$) of Voronoi cells is some number $\overline{m}\leq 14$. This has been proven in [9]. Note that 14 is the number of faces of truncated octahedra. This is quite promising, since simulations in [8] strongly support the optimality of the BCC lattice, whose Voronoi cells are exactly truncated octahedra.

(2) We **need to verify** that the function

$$m \quad\longmapsto \min_{\substack{V \text{ convex polytope, } |V|=\alpha \\ V \text{ has at most } m \text{ faces}}} \int_V |x-y|^2\,\mathrm{d}x, \qquad y \text{ centroid of } V,$$

is convex for $m\leq N_*$, where N_* is given by Theorem 2.3. This will allow us to extend this function (denoted below by G) to the continuum $m\in[0,N^*]$, so we can then verify its convexity. This step ensures that we can then compute the Hessian matrix of G. Alternatively, we can try to check $G^{**}(a, 14) = G(a, 14)$, with G^{**} denoting the convex envelope of G. However, we do not expect to be able to determine values of G^{**} without any convexity estimates on G.

(3) The optimal polytope V with $\bar{m}$ faces should be space tiling. According to simulations from [8], we should expect $\bar{m} = 14$ and V being the truncated octahedron.

(4) We can dispense with the energetic contributions of the boundary cells. More precisely, as proven in Proposition 6.1 below, the total energetic contributions of the boundary cells is of order $O(n^{-1})$, which is negligible since the total energy is of order $O(n^{-2/3})$.

With these results in hand, Gruber's method would then be as follows: let

$$G(a, m) := \min_{\substack{V \text{ convex polytope, } |V|=a \\ V \text{ has at most } m \text{ faces}}} \int_V |x - y|^2 \, \mathrm{d}x, \qquad y \text{ centroid of } V.$$

Suppose G is jointly convex. Then, for any arbitrary tessellation Y_n (with $\sharp Y_n = n$), of Q, let $\{V_k\}$ be the collection of Voronoi cells, and let α_k be the number of faces of V_k. Then it follows that

$$\begin{aligned} E(Y_n) &= \sum_{k=1}^{n} \int_{V_k} |x - y|^2 \, \mathrm{d}x \\ &\geq \sum_{k=1}^{n} G(|V_k|, \alpha_k) \\ &\geq nG(1/n, \overline{m}) + \text{error due to boundary effects} \\ &\geq nG(1/n, 14) + \text{error due to boundary effects.} \end{aligned}$$

Since the error due to boundary effects is a higher order term (actually of order $O(n^{-1})$, compared to $nG(1/n, m)$, which has order $O(n^{-2/3})$, as $n \to +\infty$) it follows that the optimal tessellation (as $n \to +\infty$) consists of congruent copies of a space tiling polyhedron realizing $G(1/n, 14)$.

Concerning issue (3), we expect the optimal polytope to be the regular truncated octahedron, since:

- it is the tessellation corresponding to the BCC lattice, which has been proven to be pretty optimal from numerical simulations (see [8]),
- it is the *only* convex polytope to tile the space by translation, with 14 faces (see [17, pp. 471–473]). Although this property is valid for some irregular truncated octahedra too, we expect that for any fixed volume constraint a, irregular truncated octahedra should not realize the minimum in $G(a, 14)$.

Moreover, since a periodic CVT should have generators distributed on a lattice, by [1] such a lattice should be the BCC one. However, a priori Gersho's conjecture requires only the existence of such a unique "seed" polytope for Voronoi cells, without any geometric description.

For issue (4), we have the following proposition which proves that, given any cube $\Omega \subseteq Q$, the energy contribution of Voronoi cells intersecting $\partial\Omega$ is negligible compared to the energy contribution of Voronoi cells not intersecting $\partial\Omega$.

Proposition 6.1. *For any n, let Y_n be a minimizer with $\sharp Y_n = n$. Then let $\Omega \subseteq Q$ be an arbitrary cube with positive volume, then for any sufficiently large n it holds:*

(1) the contribution to the energy of Voronoi cells intersecting $\partial\Omega$ is of order $O(n^{-1})$,
(2) the contribution to the energy of Voronoi cells in Ω but not intersecting $\partial\Omega$ is of order $O(n^{-2/3})$.

Consequently, the energy contribution of Voronoi cells intersecting $\partial\Omega$ is negligible compared to the energy contribution of Voronoi cells in Ω not intersecting $\partial\Omega$.

Proof. Choose $n \gg 1$, and a minimizer Y_n with $\sharp Y_n = n$. We will establish (from Claims 1–3) that the energy contribution of Voronoi cells intersecting $\partial\Omega$ is negligible as $n \to +\infty$. In the following Γ_i $(i = 1, 3, 4)$ will be constants from Theorem 2.3.

- Claim 1: at most $\frac{6\Gamma_4}{\omega_3\Gamma_5^3} n^{2/3}$ Voronoi cells can intersect $\partial\Omega$.

To prove this claim, estimate (6) gives that the diameter of each Voronoi cell is at most $\Gamma_4 n^{-1/3}$, hence all the Voronoi cells intersecting $\partial\Omega$ are contained in

$$\{x : d(x, \partial\Omega) \leq \Gamma_4 n^{-1/3}\}.$$

Estimate (5) gives that the volume of any Voronoi cell is at least $\omega_3\Gamma_5^3 n^{-1}$, hence at most

$$\frac{|\{x : d(x, \partial K) \leq \Gamma_4 n^{-1/3}\}|}{\omega_3\Gamma_5^3 n^{-1}} \leq \frac{6\Gamma_4}{\omega_3\Gamma_5^3} n^{2/3}$$

can intersect $\partial\Omega$. Thus Claim 1 is proven.

- Claim 2: the energy contribution of all Voronoi cells intersecting $\partial\Omega$ is at most

$$\frac{3\Gamma_4^6 n^{-5/3}}{4\Gamma_5^3} = O(n^{-1}).$$

Let $(y_k)_k \subseteq Y_n$ be the (finite) collection of atoms such that their Voronoi cells $(V_k)_k$ intersect $\partial\Omega$. Estimate (6) proves that, for any k, $\mathrm{diam}(V_k) \leq \Gamma_4 n^{-1/3}$, hence $V_k \subseteq B(y_k, \Gamma_4 n^{-1/3}/2)$ and

$$\int_{V_k} |x - y_k|^2 \, \mathrm{d}x \leq |V_k| \, \mathrm{diam}^2(V_k) \leq |B(y_k, \Gamma_4 n^{-1/3}/2)| \, \mathrm{diam}^2(V_k) \leq \frac{\omega_3\Gamma_4^5 n^{-5/3}}{8}.$$

Since Claim 1 proves that at most $\frac{6\Gamma_4^3}{\Gamma_1} n^{2/3}$ Voronoi cells can intersect $\partial\Omega$, the energy contribution of all such cells is at most

$$\frac{6\Gamma_4}{\omega_3\Gamma_5^3} n^{2/3} \cdot \frac{\omega_3\Gamma_4^5 n^{-5/3}}{8} = \frac{3\Gamma_4^6 n^{-1}}{4\Gamma_5^3}$$

and Claim 2 is proven.

- Claim 3: the energy contribution of all Voronoi cells in Ω which do not intersect $\partial\Omega$ is at least

$$\frac{\pi}{5}\omega_3^{-5/3} n^{-2/3} - \frac{3\Gamma_4^6 n^{-1}}{4\Gamma_5^3} = O(n^{-2/3}).$$

Zador's asymptotic estimate proved that there exists $\tau > 0$ such that $n^{2/3}E(Y_n) \to \tau$. Thus, for n large we have

$$2\tau n^{-2/3} \geq E(Y_n) \geq \frac{\tau}{2} n^{-2/3},$$

and the contribution of cells not intersection $\partial\Omega$ is estimated by

$$2\tau n^{-2/3} \geq E(Y_n) - \frac{3\Gamma_4^6 n^{-5/3}}{4\Gamma_5^3} \geq \frac{\tau}{2} n^{-2/3} - \frac{3\Gamma_4^6 n^{-1}}{4\Gamma_5^3},$$

and since we proved $\tau \geq \frac{2\pi}{5}\omega_3^{-5/3}$, Claim 3 follows. □

Thus the fundamental remaining issue for the proof of Gersho's conjecture in 3D is (2). Note that the convexity of G in the volume variable is almost trivial due to scaling: without loss of generality assume the centroid is $y = 0$, and by using a scaling of ratio r we obtain

$$\int_{rV} |x|^2 \, \mathrm{d}x = r^5 \int_V |x|^2 \, \mathrm{d}x,$$

independently of the number of faces of V. With this is hand, the Hessian calculation will establish joint convexity once we establish (2).

To prove (2), the convexity of G in the other variable (i.e. the number of faces), note that the bound on the number of faces implies also an uniform bound on the number of vertices. Since we need only the convexity of G for polytopes with up to N_* faces, let M_* be the maximum number of vertices of all such polytopes. Thus one can write the integral

$$\int_V |x - y|^2 \, \mathrm{d}x$$

as a function of the vertices $\{v_1, \cdots, v_m\}$ only ($v_i \in \mathbb{R}^3$, $m \leq N_*$): the cell V is indeed the convex combination of its vertices, hence any $x \in V$ is of the form $x = \sum_{k=1}^m a_k v_k$. Similarly, the centroid $y := |V|^{-1} \int_V x dx$ can be also expressed in terms of the vertices:

$$\begin{aligned} y &= \frac{1}{|V|} \int_V x \, dx \\ &= \frac{1}{|V|} \int_{\{\mathbf{a}\,:\,a_k \geq 0,\ \sum_{k=1}^m a_k = 1\}} \sum_{k=1}^m a_k v_k \ \, \mathrm{d}\mathbf{a} \qquad \mathbf{a} := (a_1, \cdots, a_m). \end{aligned}$$

Hence, if we define

$$\begin{aligned} I(v_1, \cdots, v_m) &:= \int_V |x - y|^2 \, \mathrm{d}x \\ &= \int_{\{\mathbf{a}\,:\,a_k \geq 0,\ \sum_{k=1}^m a_k = 1\}} \left| \sum_{k=1}^m a_k v_k - \frac{1}{|V|} \int_{\{\tilde{\mathbf{a}}\,:\,\tilde{a}_k \geq 0,\ \sum_{k=1}^m \tilde{a}_k = 1\}} \sum_{k=1}^m \tilde{a}_k v_k \ \, \mathrm{d}\tilde{\mathbf{a}} \right|^2 \mathrm{d}\mathbf{a}, \end{aligned}$$

we see that problem reduces to convex minimization in $3m$ variables over a convex constraint; That is, we solve

$$\min_{v_1, \cdots, v_m} I(v_1, \cdots, v_m)$$

under the constraint that V is a convex polytope with unit volume.

7. Conclusion and Future Directions

In this paper we have shown that Voronoi cells in optimal CVTs have at most N_* faces, with N_* independent of the number of generators. This allowed us to reduce Gersho's conjecture in 3D, which is intrinsically nonlocal and infinite dimensional (as it requires the number of generators to tend to infinity), to a local and finite dimensional problem of studying the convexity of G on convex polytopes with at most N_* faces. In our opinion, this alone is an achievement. However, the issue remains that the current bound on N_* is far too big for computer verification. Note that the fact that we are interested only in the convexity of G allows us to have computational errors, as long as these are sufficiently small not to influence the convexity. While we have tried to optimize constants within the framework of our method, one should seek different more optimal techniques for our bounds to lower the threshold for N_*.

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