

# Existence of Gibbs distributions with Delaunay and Laguerre-Delaunay potentials

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## 1 Notation, basic terms

We will restrict ourselves to  $(\mathbb{R}^3, \mathcal{B})$ , where  $\mathcal{B}$  is the Borel  $\sigma$ -algebra on  $\mathbb{R}^3$ . Denote  $\mathcal{B}_0 \subset \mathcal{B}$  the system of bounded Borel sets, Denote  $S$  the mark space with a Borel  $\sigma$ -algebra  $\mathcal{S}$ . In our case,  $S = [0, W]$  for some  $W > 0$ . A *configuration* is a subset  $\mathfrak{x} \in \mathbb{R}^3 \times S$  with a locally finite projection onto  $\mathbb{R}^3$ . Individual points from  $\mathfrak{x}$  will typically denoted  $p = (p', p'')$  where  $p' \in \mathbb{R}^3$  is called the *center* of  $p$  and  $p'' \in S$  is called the *weight* of  $p$ . Given the geometric interpretation (section 2.1.2), the word *point* and *sphere* will be used interchangeably in this text.

Since this text also deals with the Delaunay triangulation, which does not take into account the marks, we will often tacitly identify a point  $p' \in \mathbb{R}^3$  with the marked point  $p = (p', 0)$  with  $p'' = 0$ . In that sense, these “unmarked” points are

still elements of  $\mathbb{R}^3 \times S$  and other terms do not have to be define twice for marked and unmarked configurations. We will use the word “unmarked” to mean *with marks set to 0*. Sometimes it will be useful to denote that a whole configuration is unmarked in this manner. For that purpose we will use the notation  $(\eta', \mathbb{x}')$ .

This is possibly a temporary solution

The space of all configurations on  $\mathbb{R}^3 \times S$  is denoted  $N$ . It is equipped with the standard  $\sigma$ -algebra  $\mathcal{N}$ . Let  $N_f \subset N$  be the space of all configurations with finitely many points with the trace  $\sigma$ -algebra  $\mathcal{N}_f$ . For  $\Lambda \in \mathcal{B}$  we write  $\mathbb{x}_\Lambda = \mathbb{x} \cap (\Lambda \times S)$  and  $N_\Lambda = \{\mathbb{x} \in N : \text{pr}_{\mathbb{R}^3}(\mathbb{x}) \subset \Lambda\}$ , where  $\text{pr}_{\mathbb{R}^3}$  denotes the projection on  $\mathbb{R}^3$ , and write  $\mathcal{N}'_\Lambda$  for the corresponding trace  $\sigma$ -algebra.

Define the sigma algebra

The reference measure on  $(N, \mathcal{N})$  is the Poisson point process  $\Pi^z$  with intensity measure  $z\lambda \otimes \mu$ , where  $z > 0$  is called the *activity*,  $\lambda$  is the Lebesgue measure on  $\mathbb{R}^3$  and  $\mu$  is a  $\sigma$ -finite measure on  $(S, \mathcal{S})$ . For  $(N_\Lambda, \mathcal{N}_\Lambda)$ , the reference measure will be  $\Pi_\Lambda^z := \Pi^z \circ \text{pr}_\Lambda^{-1}$ .

**Definition 1.** • A *hypergraph structure* is a measurable subset  $\mathcal{E}$  of  $(N_f \times N, \mathcal{N}_f \otimes \mathcal{N})$  such that  $\eta \subset \mathbb{x}$  for all  $(\eta, \mathbb{x}) \in \mathcal{E}$ . We call  $\eta$  a *hyperedge* of  $\mathbb{x}$  and write  $\eta \in \mathcal{E}(\mathbb{x})$ .

- A *hyperedge potential* is a measurable function  $\varphi : \mathcal{E} \rightarrow \mathbb{R} \cup \{+\infty\}$ .
- Hyperedge potential is *shift-invariant* if

$$(\vartheta_x \eta, \vartheta_x \mathbb{x}) \in \mathcal{E} \text{ and } \varphi(\vartheta_x \eta, \vartheta_x \mathbb{x}) = \varphi(\eta, \mathbb{x}) \text{ for all } (\eta, \mathbb{x}) \in \mathcal{E} \text{ and } x \in \mathbb{R}^3.$$

For notational convenience, we set  $\varphi = 0$  on  $\mathcal{E}^c$ .

## 2 Delaunay and Laguerre-Delaunay hypergraph structures and potentials

### 2.1 Hypergraph structures

Do we actually need the normal position for points? All definitions work regardless

The two key hypergraph structures used in this text are the Delaunay and Laguerre-Delaunay tetrahedronizations.

#### 2.1.1 Delaunay hypergraph structure

**Definition 2.** We say that  $(\eta, \mathbb{x})$  satisfies the *empty sphere property* if there exists an open ball  $B(\eta, \mathbb{x})$  with  $B(\eta, \mathbb{x}) \cap \text{pr}_{\mathbb{R}^3} \mathbb{x} = \emptyset$  and  $\eta \subset \partial B(\eta, \mathbb{x}) \cap \text{pr}_{\mathbb{R}^3} \mathbb{x}$ . The sphere  $\partial B(\eta, \mathbb{x})$  is called the *circumsphere*.

Note that the definition completely ignores the marks of  $\mathbb{x}$ , which are important only for the Laguerre-Delaunay case.

Is  $B(\eta, \mathbb{x})$  even a good notation

**Definition 3.** The Delaunay hypergraph structure  $\mathcal{D}$  is defined as

$$\mathcal{D} = \{(\eta, \mathbb{x}) \in N_f \times N : \eta \subset \mathbb{x}, \# \eta = 4, (\eta, \mathbb{x}) \text{ satisfies the empty sphere property}\}.$$

Note the differences from [1], namely that we're only considering *tetrahedral hyperedges*, i.e. hyperedges with four points, and that  $\partial B(\eta, \mathbb{x}) \cap \mathbb{x}$  only needs to contain  $\eta$  instead of being equal to it. This definition allows e.g. points in a regular lattice to still define tetrahedral hyperedges. In [1], a regular lattice would still yield a nonempty hyperedge structure, but its hyperedges would not be tetrahedral.

Is this correct?

### 2.1.2 Laguerre-Delaunay hypergraph structure

In order to define the Laguerre-Delaunay hypergraph structure, we need to introduce further concepts.

**Definition 4.** Define the *power distance* of the unmarked point  $q' \in \mathbb{R}^3$  from the point  $p = (p', p'') \in \mathbb{R}^3 \times S$  as

$$d(q', p) = \|q' - p'\|^2 - p''.$$

**Definition 5.** For two (marked) points  $p = (p', p'')$  and  $q = (q', q'')$ , define their *power product* by

$$\rho(p, q) = \|p' - q'\|^2 - p'' - q''.$$

Notice that  $\rho(p, q) = d(p, q') - q'' = d(q, p') - p''$  and that  $\rho(p, (q', 0)) = d(p, q')$ .

Talk about the geometric interpretation

**Definition 6.** For a tetrahedral hyperedge  $\eta$ , we define the *characteristic point* of  $\eta$  as the point  $p_\eta = (p'_\eta, p''_\eta)$  such that

$$\rho(p, p_\eta) = 0 \text{ for all } p \in \eta.$$

Note that the characteristic point can be thought of as a ball or sphere with the center  $p'_\eta$  and radius  $\sqrt{p''_\eta}$ . This ball will be referred to as  $B(p'_\eta, \sqrt{p''_\eta})$ .

Comment on uniqueness of this point - e.g. maybe we need to choose one with minimal weight

Again, talk about the geometric interpretation, orthogonality, etc.

**Definition 7.** We say that  $(\eta, \mathbb{x})$  is *regular* if  $\rho(p_\eta, p) \geq 0$  for all  $p \in \mathbb{x}$ .

Again, comment on the geometric interpretation of this property

Using these terms, we are now ready to define the Laguerre-Delaunay hypergraph structure

**Definition 8.** The Laguerre-Delaunay hypergraph structure  $\mathcal{LD}$  is defined as

$$\mathcal{LD} = \{(\eta, \mathbb{x}) \in N_f \times N : \eta \subset \mathbb{x}, \#\eta = 4, (\eta, \mathbb{x}) \text{ is regular} \}.$$

Titles for remarks (and maybe definitions too?)

*Remark 1.* If all the points from  $\mathbb{x}$  have weight 0, then the regularity property of  $(\eta, \mathbb{x})$  becomes the empty sphere property. Similarly, the characteristic point then coincides with the circumsphere. It would have therefore been possible to simply define  $\mathcal{D}$  as a special case of  $\mathcal{LD}$ . We have decided to keep the definitions and related terms separate in order to stress the different properties of these two hypergraph structures.

Finish these remarks

*Remark 2.* Tessellation is invariant in addition in weights  $\Rightarrow$  Delaunay is obtained for any configuration with equal marks **TO BE DONE**

*Remark 3.* Redundant points **TO BE DONE**

Since both of the hyperedge structures only contain tetrahedral edges, that is  $\#\eta = 4$ , we will tacitly assume any  $\eta$  to be tetrahedral for the remained of this text.

## 2.2 Hypergraph potentials

Throughout this text, two potentials will mainly be used for both  $\mathcal{D}$  and  $\mathcal{LD}$ . For a tetrahedral  $\eta$ , denote  $\delta(\eta) = 2\sqrt{p''_\eta}$ , the diameter of the characteristic point.

For now

This is WRONG, since  $p'_\eta$  depends on the marks, too, and won't be the same as the center of  $B(\eta, \mathbb{x})$ . Is the assertion even true?

*Remark 4.* For any  $\eta = \{p_1, p_2, p_3, p_4\}$  and any  $i = 1, 2, 3, 4$ , we have

$$p''_\eta = \|p'_\eta - p'_i\|^2 - p''_i \leq \|p'_\eta - p'_i\|^2 = 1/2 \cdot \text{diam}B(\eta, \mathbb{x})$$

Half diameter is an ugly notation for radius

From this we can see two things. One, the diameter of the characteristic point is bounded by the diameter of the circumsphere. Two, their diameters equal only in the Delaunay case, that is if  $p''_i = 0$  for all  $i = 1, 2, 3, 4$ .

**Definition 9.** The first potential is the *smooth-interaction* potential  $\varphi_S$  satisfying

$$\varphi_S(\eta, \mathbb{x}) \leq K_0 + K_1(\delta(\eta))^\beta$$

for some  $K_0 \geq 0, K_1 \geq 0, \beta > 0$ .

The second is the *hardcore interaction* potential  $\varphi_{HC}$  for which there are constants  $0 \leq d_0 < d_1 \leq \alpha$  such that

$$\sup_{\eta: d_0 \leq \delta(\eta) \leq d_1} \varphi(\eta, \mathbb{x}) < \infty \text{ and } \varphi(\eta, \mathbb{x}) = \infty \text{ if } \delta(\eta) > \alpha.$$

How exactly does this look? Why?

For simplicity, we assume that  $\varphi_{HC}$  depends only on the points of  $\eta$  in the sense of remark 5.

Talk a bit about  $\varphi_{HC}$  - can be  $\infty$  below  $d_0$ , requires infinity later,...

*Remark 5.* The potentials depend on  $\mathbb{x} \setminus \eta$  only in the sense that they equal to 0 if  $\eta \notin \mathcal{E}(\mathbb{x})$ . One implication of this is that the remaining points of  $\mathbb{x}$  can never change the value  $\varphi(\eta, \mathbb{x})$  in other way than setting it to zero if  $\eta \notin \mathcal{E}(\mathbb{x})$ . In other words, if  $\eta \in \mathcal{E}(\mathbb{x})$  and we take another configuration  $\tilde{\mathbb{x}}$ , then  $\varphi(\eta, \tilde{\mathbb{x}}) \neq \varphi(\eta, \mathbb{x})$  precisely only when  $\varphi(\eta, \mathbb{x}) > 0$  and  $\eta \notin \mathcal{E}(\tilde{\mathbb{x}})$ , so that  $\varphi(\eta, \tilde{\mathbb{x}}) = 0$ .

Other potentials. Other characteristics other than circumdiameter. Combinations of potentials. Interaction.

**TO BE DONE**

In the remainder of this text, whenever we say a property holds for  $\mathcal{D}$  we mean that the property holds for the pair  $(\mathcal{D}, \varphi_S)$  and  $(\mathcal{D}, \varphi_{HC})$ . Similarly for  $\mathcal{LD}$  and  $(\mathcal{LD}, \varphi_S)$  and  $(\mathcal{LD}, \varphi_{HC})$ .

### 3 Basic notions of hypergraph structures

**Definition 10.** A set  $\Delta \in \mathcal{B}_0$  is a *finite horizon* for the pair  $(\eta, \mathbb{x}) \in \mathcal{E}$  and the hyperedge potential  $\varphi$  if for all  $\tilde{\mathbb{x}} = \mathbb{x}$  on  $\Delta \times S$

$$(\eta, \tilde{\mathbb{x}}) \in \mathcal{E} \text{ and } \varphi(\eta, \tilde{\mathbb{x}}) = \varphi(\eta, \mathbb{x}).$$

The pair  $(\mathcal{E}, \varphi)$  satisfies the *finite-horizon property* if each  $(\eta, \mathbb{x}) \in \mathcal{E}$  has a finite horizon.

The finite horizon of  $(\eta, \mathbb{x})$  delineates the region outside which points can no longer violate the regularity (or the empty sphere property) of  $\eta$ .

*Remark 6.* For  $\mathcal{D}$ , the circumsphere  $\bar{B}(\eta, \mathbb{x})$  itself is a finite horizon for  $(\eta, \mathbb{x})$ .

For  $\mathcal{LD}$ , the situation is slightly more difficult. For one,  $B(p'_\eta, \sqrt{p''_\eta})$  does not contain the points of  $\eta$ . To see this, take two points  $p, q$  with  $p'', q'' > 0$  such that  $\rho(p, q) = 0$ . Then  $q'' = d(q', p) < \|q' - p'\|^2$  and  $\sqrt{q''} < \|q' - p'\|$ . More importantly, however, any point  $s$  outside of  $B(p'_\eta, \sqrt{p''_\eta})$  with a sufficiently large weight can violate the inequality  $\rho(p_\eta, s) = \|p'_\eta - s'\|^2 - p''_\eta - s'' \geq 0$ .

Everything is a circumsphere..

To obtain a finite horizon for  $\mathcal{LD}$ , we need to use the fact that the mark space is bounded,  $S = [0, W]$ . If  $s'' \leq W$ , then  $\Delta = B(p'_\eta, \sqrt{p''_\eta + W})$  is sufficient as a horizon, since any point  $s$  outside  $\Delta$  satisfies

$$\rho(p_\eta, s) = \|p'_\eta - s'\|^2 - p''_\eta - s'' \geq (\sqrt{p''_\eta + W})^2 - p''_\eta - W = 0.$$

From a practical perspective, the maximum weight  $W$  limits the resulting tessellation in the sense that the difference of weights can never be greater than  $W$ . Marks greater than  $W$  are not necessarily a problem, as we can always find an identical tessellation with marks bounded by  $W$ , as long as there no two points  $p, q$  with  $|p'' - q''| > W$  (see remark 2).

Hamiltonians

**Definition 11.** Hamiltonian **TO BE DONE**

Next we must define the set of hyperedges  $\eta$  in  $\mathbb{x}$  for which either  $\eta$  or  $\varphi(\eta, \mathbb{x})$  depends on  $\mathbb{x}_\Lambda$ .

**Definition 12.**

$$\mathcal{E}_\Lambda(\mathbb{x}) := \{\eta \in \mathcal{E}(\mathbb{x}) : \varphi(\eta, \zeta \cup \mathbb{x}_{\Lambda^c}) \neq \varphi(\eta, \mathbb{x}) \text{ for some } \zeta \in N_\Lambda\}$$

Later in the text, these are exactly the sets of tetrahedra used for the calculation, connect those two

For  $\mathcal{D}$ ,  $\eta \in \mathcal{E}_\Lambda(\mathbb{x})$  iff  $B(\eta, \mathbb{x}) \cap \Lambda \neq \emptyset$ . For  $\mathcal{LD}$ ,

characterize it

The final basic term again characterizes a type of finite-range property, this time as a property of the configuration  $\mathbb{x}$ .

**Definition 13.** Let  $\Lambda \in \mathcal{B}_0$  be given. We say a configuration  $\mathbb{x} \in N$  *confines the range of  $\varphi$  from  $\Lambda$*  if there exists a set  $\partial\Lambda(\mathbb{x}) \in \mathcal{B}_0$  such that  $\varphi(\eta, \zeta \cup \tilde{\mathbb{x}}_{\Lambda^c}) = \varphi(\eta, \zeta \cup \mathbb{x}_{\Lambda^c})$  whenever  $\tilde{\mathbb{x}} = \mathbb{x}$  on  $\partial\Lambda(\mathbb{x}) \times S$ ,  $\eta \in N_\Lambda$  and  $\eta \in \mathcal{E}_\Lambda(\zeta \cup \mathbb{x}_{\Lambda^c})$ . In this case we write  $\mathbb{x} \in \Omega_{\text{cr}}^\Lambda$ . We denote  $r_{\Lambda, \mathbb{x}}$  the smallest possible  $r$  such that  $(\Lambda + B(0, r)) \setminus \Lambda$  satisfies the definition of  $\partial\Lambda(\mathbb{x})$ .

Comment on the definition and what it means for  $\mathcal{D}$  and  $\mathcal{LD}$ .

## 4 Existence assumptions and theorems

We will now present the assumptions needed for the existence of the Gibbs measure.

(R) *Range condition.* There exist constants  $\ell_R, n_R \in \mathbb{N}$  and  $\delta_R < \infty$  such that for all  $(\eta, \mathbb{x}) \in \mathcal{E}$  there exists a finite horizon  $\Delta$  satisfying: For every  $x, y \in \Delta$  there exist  $\ell$  open balls  $B_1, \dots, B_\ell$  (with  $\ell \leq \ell_R$ ) such that

- the set  $\cup_{i=1}^\ell \bar{B}_i$  is connected and contains  $x$  and  $y$ , and
- for each  $i$ , either  $\text{diam} B_i \leq \delta_R$  or  $N_{B_i}(\mathbb{x}) \leq n_R$ .

### 4.1 Stability condition

The second assumption is the well-known stability condition.

(S) *Stability.* The hyperedge potential  $\varphi$  is called *stable* if there exists a constant  $c_S \geq 0$  such that

$$H_{\Lambda, \mathbb{x}}(\zeta) \geq -c_S \#(\zeta \cup \delta_\Lambda \mathbb{x})$$

for all  $\Lambda \in \mathcal{B}_0, \zeta \in N_\Lambda, \mathbb{x} \in N_{\text{cr}}^\Lambda$ .

The first thing to note that when  $\varphi$  is non-negative, then we can simply choose  $c_S = 0$ . The interesting cases therefore is when  $\varphi$  can attain negative values.

#### 4.1.1 Stability in $\mathbb{R}^2$

In  $\mathbb{R}^2$ , the argument for stability of (Laguerre)-Delaunay hypergraph structures utilizes sublinearity of the hypergraph structure. We say that a hypergraph  $\mathcal{E}$  is *sublinear* if there exists  $C < \infty$  such that  $\#\mathcal{E}(\mathbb{x}) \leq C\#\mathbb{x}$  for all  $\mathbb{x} \in N_f$ . In the case of sublinearity of  $\mathcal{E}$ , it is sufficient that  $\varphi$  is bounded from below,  $\varphi \geq -c_\varphi$  for some  $c_\varphi < \infty$ , since then

$$\varphi(\eta, \mathbb{x}) \geq -c_\varphi \#\mathcal{E}(\mathbb{x}) \geq -c_\varphi \cdot C\#\mathbb{x}$$

and thus  $c_S = c_\varphi \cdot C$ .

Sublinearity of any Laguerre-Delaunay triangulation in  $\mathbb{R}^2$  is easily obtainable in at least two ways. One, using Euler's formula for planar graphs for the number of vertices ( $v$ ), edges ( $e$ ) and faces ( $f$ ):  $v - e + f = 2$ , which establishes a linear relationship between  $v$  and  $f$ . Second, by a direct argument using the fact that any triangulation of  $\mathbb{R}^2$  can be transformed into any other triangulation by a finite series of flips [2]. A point inserted into the triangulation is located within a triangle  $T$ . Three new triangles within  $T$  are then created and  $T$  itself is removed. Any subsequent flips then leave the total number of triangles constant.

### 4.1.2 Stability in $\mathbb{R}^3$

In  $\mathbb{R}^3$ , the situation is more difficult and neither of these approaches work. Any graph can be embedded in  $\mathbb{R}^3$  [3] and thus an analog to Euler's formula in three dimensions cannot exist, as it would have to characterize any finite graph. The number of tetrahedra also no longer remains constant under topological flipping [4].

This is no wonder - it is well known (see e.g. [5]) that the complexity<sup>1</sup> of the Delaunay tetrahedronization of  $n$  points is  $\mathcal{O}(n^2)$  in general. However, this result is not yet dooming to the stability of the Gibbs models. For one, all the known example of point configurations that attain the upper complexity bound are distributed on one-dimensional curves such as the *moment curve* [5]. In fact, in [6], Erickson states that “For all practical purposes, three-dimensional Delaunay triangulations appear to have linear complexity.”. While hardly a proof, this is encouraging to anyone wishing to simulate Delaunay models with potentials that can attain negative values.

More importantly, the fact that Delaunay tetrahedronization *in general* can have  $\mathcal{O}(n^2)$  tetrahedra does not mean that this is the case for the Poisson-Delaunay tetrahedronization, i.e. Delaunay tetrahedronization of a configuration generated by a Poisson point process. If the Poisson-Delaunay tetrahedronization of  $n$  points have  $\mathcal{O}(n)$  tetrahedra almost surely, then the Gibbs-Delaunay tetrahedronization would inherit this property by absolute continuity. Dwyer [7] proved that the expected number of tetrahedra is  $\mathcal{O}(n)$ . More recently, Erickson has provided [6] [8] complexity bounds based on a characteristic of a configuration called *spread* defined as the ratio between the longest and shortest pairwise distance. Delaunay tetrahedronization of point configuration with spread  $\Delta$  has complexity  $\mathcal{O}(\Delta^3)$ . This is a hopeful result, since the spread of point configurations is loosely connected with its dimensionality, in that e.g. regular lattice of in  $\mathbb{R}^d$  with  $n$  points has spread  $\mathcal{O}(n^{1/d})$ . Values such as the nearest neighbor distance are easily tractable with the Poisson process, giving a chance to a simple solution to the stability question. However, to the best of our knowledge, the current literature does not directly give an answer to this problem.

Make  
this  
more  
precise

Simulation study

For now, assume that all potentials used in this text are non-negative.

## 4.2 Upper regularity

In order to present the upper regularity conditions, the notion of *pseudo-periodic* configurations.

Let  $M \in \mathbb{R}^{3 \times 3}$  be an invertible  $3 \times 3$  matrix with column vectors  $(M_1, M_2, M_3)$ . For each  $k \in \mathbb{Z}^3$  define the cell

$$C(k) = \{Mx \in \mathbb{R}^3 : x - k \in [-1/2, 1/2]^3\}.$$

These cells partition  $\mathbb{R}^3$  into parallelotopes. We write  $C = C(0)$ . Let  $\Gamma \in N'_C$  be non-empty. Then we define the *pseudo-periodic* configurations as

$$\bar{\Gamma} = \{\mathbf{x} \in \Omega : \vartheta_{Mk}(\mathbf{x}_{C(k)}) \in \Gamma \text{ for all } k \in \mathbb{Z}^d\},$$

<sup>1</sup>For our purposes, we can define complexity as the number of tetrahedra in the tessellation.

the set of all configurations whose restriction to  $C(k)$ , when shifted back to  $C$ , belongs to  $\Gamma$ . The prefix pseudo- refers to the fact that the configuration itself does not need to be identical in all  $C(k)$ , it merely needs to belong to the same class of configurations.

(U) *Upper regularity.*  $M$  and  $\Gamma$  can be chosen so that the following holds.

(U1) *Uniform confinement:*  $\bar{\Gamma} \subset \Omega_{\text{cr}}^\Lambda$  for all  $\Lambda \in \mathcal{B}_0$  and

$$r_\Gamma := \sup_{\Lambda \in \mathcal{B}_0} \sup_{\mathbf{x} \in \bar{\Gamma}} r_{\Lambda, \mathbf{x}} < \infty$$

(U2) *Uniform summability:*

$$c_\Gamma^+ := \sup_{\mathbf{x} \in \bar{\Gamma}} \sum_{\eta \in \mathcal{E}(\mathbf{x}) : \eta \cap C \neq \emptyset} \frac{\varphi^+(\eta, \mathbf{x})}{\#(\hat{\eta})} < \infty,$$

where  $\hat{\eta} := \{k \in \mathbb{Z}^3 : \eta \cap C(k) \neq \emptyset\}$  and  $\varphi^+ = \max(\varphi, 0)$  is the positive part of  $\varphi$ .

(U3) *Strong non-rigidity:*  $e^{z|C|} \Pi_C^z(\Gamma) > e^{c_\Gamma}$ , where  $c_\Gamma$  is defined as in (U2) with  $\varphi$  in place of  $\varphi^+$ .

*Remark 7.* For  $\mathcal{D}$  and  $\mathcal{LD}$  it always holds that  $\#\{\eta \in \mathcal{E}(\mathbf{x}) : \eta \cap C \neq \emptyset\} < \infty$ . Therefore the only quantity in (U2) which could be infinite is  $\varphi^+(\eta, \mathbf{x})$  and the condition reduces to  $\varphi^+(\eta, \mathbf{x}) < \infty$ . This then means that the condition (U2) is non-trivial only for hardcore-interaction models.

Remark about U3 monotonicity, possibly some other remarks about the assumptions

Get more intuition about U3 and comment on why  $\hat{\mathbf{U}}$  is useful

For some models it is possible to replace the upper regularity assumptions by their alternative and prove the existence for all  $z > 0$ .

( $\hat{\mathbf{U}}$ ) *Alternative upper regularity.*  $M$  and  $\Gamma$  can be chosen so that the following holds.

( $\hat{\mathbf{U}}$ 1) *Lower density bound:* There exist constants  $c, d > 0$  such that  $\#(\zeta) \geq c|\Lambda| - d$  whenever  $\zeta \in \Omega_f \cap \Omega_\Lambda$  is such that  $H_{\Lambda, \mathbf{x}}(\zeta) < \infty$  for some  $\Lambda \in \mathcal{B}_0$  and some  $\mathbf{x} \in \bar{\Gamma}$ .

( $\hat{\mathbf{U}}$ 2) = (U2) *Uniform summability.*

( $\hat{\mathbf{U}}$ 3) *Weak non-rigidity:*  $\Pi_C^z(\Gamma) > 0$ .

Define Gibbs measure

**Theorem 1.** *For every hypergraph structure  $\mathcal{E}$ , hyperedge potential  $\varphi$  and activity  $z > 0$  satisfying (S), (R) and (U) there exists at least one Gibbs measure.*

**Theorem 2.** *For every hypergraph structure  $\mathcal{E}$ , hyperedge potential  $\varphi$  and activity  $z > 0$  satisfying (S), (R) and ( $\hat{\mathbf{U}}$ ) there exists at least one Gibbs measure.*



### 4.3 $M$ and $\Gamma$ for Laguerre-Delaunay models

For the Delaunay and Laguerre-Delaunay models, the choice of  $M$  and  $\Gamma$  will be the following. Fix some  $A \subset C$  and define

$$\Gamma^A = \{\zeta \in N_C : \zeta = \{p\}, p \in A\},$$

the set of configurations consisting of exactly one point in the set  $A$ .

Let  $M$  be such that  $|M_i| = a > 0$  for  $i = 1, 2, 3$  and  $\angle(M_i, M_j) = \pi/3$  for  $i \neq j$ .

In [1],  $A$  is chosen to be  $B(0, b)$  for  $b < \rho_0 a$  for some sufficiently small  $\rho_0 > 0$ . We will use this form aswell - the question, however, is how to choose the mark set. It would be convenient to choose  $A = B(0, b) \times \{w\}$  for some  $w \in S$  and then only deal with a Delaunay triangulation, but this would mean that  $\Pi_C^z(\Gamma) = 0$ , conflicting with both (U3) and  $(\hat{U}3)$ . The choice  $A = B(0, b) \times S$  could, for a small enough  $a$ , result in some spheres being fully contained in their neighboring spheres, possibly resulting in redundant points, thus changing the desired properties of  $\Gamma$ . It is thus necessary to choose the mark space dependent on  $a$ . For given  $a, \rho_0$ , the minimum distance between individual points is  $a - 2\rho_0 a = a(1 - 2\rho_0)$ . We therefore choose  $A = B(0, b) \times [0, \sqrt{\frac{a}{2}(1 - 2\rho_0)}]$  in order for spheres to never overlap .

*Remark 8.* Using the set  $\Gamma^A$ , we can simplify the assumptions (U2) and (U3).

For (U3), we can now directly calculate  $\Pi_C^z(\Gamma)$ .

$$\begin{aligned} \Pi_C^z(\Gamma) &= \Pi_C^z(\{\zeta \in \Omega_C : \zeta = \{p\}, p \in A\}) \\ &= e^{-z|A|} z|A| e^{-z|C \setminus A|} \\ &= e^{-z|C|} z|A|, \end{aligned}$$

and thus (U3) becomes

$$z|A| > e^{c_{\Gamma} A}$$

In the case  $A = B(0, \rho_0 a) \times [0, \sqrt{\frac{a}{2}(1 - 2\rho_0)}]$ , we have

$$|A| = \frac{4}{3}\pi(\rho_0 a)^3 \cdot \sqrt{\frac{a}{2}(1 - 2\rho_0)} = \frac{4\pi}{3\sqrt{2}} \cdot \rho_0^3 \sqrt{1 - 2\rho_0} \cdot a^{7/2}$$

For (U2), we obtain the simplification  $\#(\hat{\eta}) = \#\eta$ , since now each point of  $\eta$  is necessarily in a different set  $C(k)$ .

Number some equations for reference

#### 4.3.1 Geometrical structure of the tessellation defined by $M$ and $\Gamma^A$

Better description and arguments of nearly everything in this section

In order to be able to check the assumptions of the existence theorems, we must investigate the structure of the tessellations formed from  $\bar{\Gamma}_A$  further. Namely there are two main quantities of interest, both coming from the term  $c_{\Gamma}$ :

1. The number of tetrahedra adjacent to the point in  $C$ ,

$$n_T := \#\{\eta \in \mathcal{E}(\mathbb{X}) : \eta \cap C \neq \emptyset\}.$$

Comment better on why this choice

$\rho_0$  possibly conflicts with  $\rho$  for the power product

The vagueness about  $\rho_0$  is not satisfactory, though it's the way DDG did it. If possible, change this

This is perhaps unnecessarily conservative, we could widen it

2. The behaviour of the circumdiameter  $\delta(\eta)$  for  $\eta \in \mathcal{LD}(\mathfrak{x})$  and  $\mathfrak{x} \in \Gamma^A$ .

Let  $\mathfrak{x}' \in \Gamma_A$  such that each point is in the center of  $A$  with marks set to 0. In  $\mathbb{R}^2$ , such configuration generates a tessellation composed of equilateral triangles with side lengths  $a$ . In  $\mathbb{R}^3$ , the situation is more complex. The vectors  $M_1, M_2, M_3$  do in fact form a regular tetrahedron, as all its faces are necessarily equilateral triangles, but the entire tessellation cannot be composed of merely regular tetrahedra, as they alone do not tessellate, as Aristotle famously claimed [9]. To be able to characterize the tessellation  $\mathcal{LD}(\mathfrak{x}') = \mathcal{D}(\mathfrak{x}')$ , it will be useful to use a concrete example of  $M$ :

$$\begin{pmatrix} 1 & \frac{1}{2} & \frac{1}{2} \\ 0 & \frac{\sqrt{3}}{2} & \frac{1}{2\sqrt{3}} \\ 0 & 0 & \sqrt{\frac{2}{3}} \end{pmatrix}.$$

Under this transformation the points of the unit cube get mapped in the following way:

$$\begin{aligned} p_1 : (0, 0, 0) &\rightarrow (0, 0, 0) \\ p_2 : (1, 0, 0) &\rightarrow (1, 0, 0) \\ p_3 : (0, 1, 0) &\rightarrow (1/2, \sqrt{3}/2, 0) \\ p_4 : (1, 1, 0) &\rightarrow (3/2, \sqrt{3}/2, 0) \\ p_5 : (0, 0, 1) &\rightarrow (1/2, 1/(2\sqrt{3}), \sqrt{2/3}) \\ p_6 : (1, 0, 1) &\rightarrow (3/2, 1/(2\sqrt{3}), \sqrt{2/3}) \\ p_7 : (0, 1, 1) &\rightarrow (1, 2/\sqrt{3}, \sqrt{2/3}) \\ p_8 : (1, 1, 1) &\rightarrow (2, 2/\sqrt{3}, \sqrt{2/3}) \end{aligned}$$

If we connect all the nearest-neighbors, we will obtain a tessellation of  $\mathbb{R}^3$ . The resulting structure is that of two regular tetrahedra ( $p_1, p_2, p_3, p_5$  and  $p_4, p_6, p_7, p_8$ ) and a regular octahedron ( $p_2, \dots, p_7$ ), which are well known to tessellate<sup>2</sup>. Figure 1 shows an exploded view of the resulting tessellation and figure 2 shows the cell  $C$  with the two tetrahedra and one octahedron outlined.

However, this tessellation is not yet a Delaunay tetrahedronization, as we still have to tetrahedronize the octahedron  $O = (p_2, \dots, p_7)$ . An octahedron is a Platonic solid and as such all of its vertices are cocircular. As a result, all of  $\binom{6}{4} = 15$  quadruples for a tetrahedron, resulting in a degenerate case which is nevertheless allowed in our definition of  $\mathcal{D}$ . In most (in fact almost surely w.r.t.  $\Pi^z$ ) configurations in  $\Gamma^A$ , this won't be the case, as the tetrahedron won't be regular. However, since we're interested in the supremum, we must consider this extreme case.

In  $\mathcal{D}(\mathfrak{x}')$ , we therefore have two types of tetrahedra. The first is the regular tetrahedron itself. The second is the tetrahedron used to tessellate the octahedron with all side lengths equal to  $a$  except for the diagonal which is equal to  $\sqrt{2}a$ .

The circumdiameter of each of the tetrahedra can be calculated by imagining

<sup>2</sup>The tessellation is of great importance to many fields and thus is known under many names. In mathematics, it is most commonly called the *tetrahedral-octahedral honeycomb*, or the *alternated cubic honeycomb*. In structural engineering, it is known as the *octet truss*, as named by Buckminster Fuller, or the *isotropic vector matrix*. It is stored as *fcu* in the Reticular Chemistry Structure Resource [10]. It is also the nearest-neighbor-graph of the face-centered cubic crystal in crystallography [11].

This is an important point, probably come back to it later. It's quite likely it will be possible to turn this into a formal argument..

Possibly comment on this more

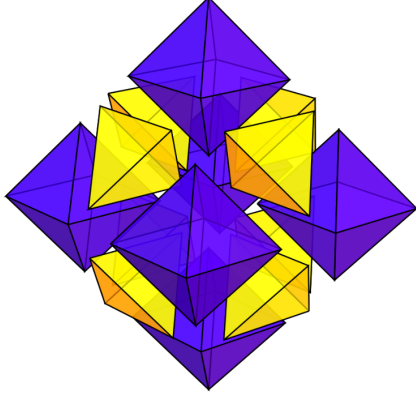


Figure 1: The tessellation in an exploded view.

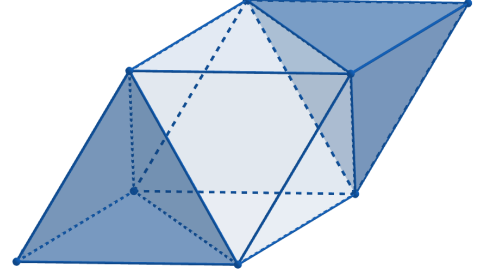


Figure 2: The set  $C$  tessellated by two tetrahedra and an octahedron.

an additional vertex equidistant from the vertices of the tetrahedron and setting the Cayley-Menger determinant [12] [13]<sup>3</sup> equal to zero. This gives the results  $\sqrt{6}/4 \cdot a$  for the regular tetrahedron and  $1/\sqrt{2} \cdot a$  for the other tetrahedron.

Most importantly: what is the supremum of the potential over  $\mathfrak{x} \in \bar{\Gamma}^A$ ?

Now we turn to the combinatorial structure of  $\mathcal{D}(\mathfrak{x})$ . In the tetrahedronized regular octahedron, each vertex is adjacent to  $\binom{5}{3} = 10$  tetrahedra. In the tetrahedron-octahedron tessellation, each vertex is adjacent to eight regular tetrahedra and six regular octahedra. This gives us  $n_T = 8 + 6 \cdot 10 = 68$ . While still large, this is less than half of  $4 \cdot \binom{7}{3}$  for the case of regular cube tessellation induced by the choice  $M = aE$ .

Reference, possibly using Schläfli symbols

## 5 Checking the assumptions for our models

Until the exact bounds for  $\varphi_S$  over  $\bar{\Gamma}^A$  are found, it will be more illustrative to use a universal unary  $\varphi_U(\eta, \mathfrak{x}) = f(\eta)$ , where  $f$  is nonnegative and finite and e.g. equal to or bounded by (a power of, etc.) circumradius, volume, surface area, sum of edge lengths, ...

It might be useful to have such a general theorem anyway, but formulated properly

**Proposition 1.** *The exists at least one gibbs measure for the model  $(\mathcal{D}, \varphi_U)$  and every activity*

$$z > \frac{3\sqrt{2}}{4\pi \cdot \rho_0^3 \sqrt{1 - 2\rho_0}} e^{17\varphi_{\max}(a_{\max})} / a_{\max}^{7/2}.$$

*Proof.* **(R)** The finite-horizon  $\Lambda = \bar{B}(\eta, \mathfrak{x})$  with  $\ell_R = 1, n_R = 0$  and  $\delta_R$  arbitrary can be used. This is because it itself contains no points of  $\mathfrak{x}$  by definition of  $\mathcal{D}$  and acts as the open ball from the definition of the range condition.

**(S)** Stability is satisfied because of  $\varphi$  is non-negative.

**(U)** We choose  $M$  and  $\Gamma$  as in section 4.3.

<sup>3</sup>A nice derivation in English can be found in [14]. It turns out that the Cayley-Menger determinant is basically derived from squaring the INCIRCLE determinant used to calculate the circumcenter.

(U1) For a small enough  $\rho_0$ , such that any three points in  $\bar{\Gamma}$  cannot be coplanar, the class  $\bar{\Gamma}$  provides an upper bound  $d_{\max}$  for  $\text{diam}B(\eta, \mathfrak{x})$  for all  $\eta \in \mathcal{D}(\mathfrak{x})$  for all  $\mathfrak{x} \in \bar{\Gamma}$  and we have  $r_{\Gamma^A} \leq d_{\max}/2$ .

Talk about this more clearly

(U2) Is trivially satisfied since  $n_T < \infty$  and  $\varphi(\eta, \mathfrak{x}) < \infty$  for all  $(\eta, \mathfrak{x}) \in \mathcal{D}$  (see remark 7).

(U3) Using remark 8, we want to find  $z$  as small as possible such that  $z|A| > e^{c_{\Gamma^A}}$ . We can bound  $c_{\Gamma^A} \leq \frac{n_T}{4}\varphi_{\max}(a)$  where  $\varphi_{\max}(a) = \sup_{(\eta, \mathfrak{x}) \in D} \varphi_U(\eta, \mathfrak{x})$  where  $D = \{(\eta, \mathfrak{x}) : \mathfrak{x} \in \bar{\Gamma}^A, \eta \in \mathcal{D}(\mathfrak{x}) : \eta \cap C \neq \emptyset\}$ . This gives us the bound

$$z > Ke^{\frac{n_T}{4}\varphi_{\max}(a)}/a^{7/2} \quad (1)$$

where  $K = \frac{3\sqrt{2}}{4\pi\rho_0^3\sqrt{1-2\rho_0}}$  and  $n_T = 68$ . We then find  $a_{\max}$  that maximizes the right-hand-side of 1.

□

**Proposition 2.** *The exists at least one gibbs measure for the model  $(\mathcal{D}, \varphi_{HC})$  and every activity  $z > 0$ .*

*Proof.* **(R)** Again,  $\Lambda = \bar{B}(\eta, \mathfrak{x})$  with  $\ell_R = 1, n_R = 0$ . Because of the hard-core condition, we can also take  $\delta_R = 2\alpha$ .

**(S)** Stability is satisfied because of  $\varphi$  is non-negative.

**(U)** We choose  $M$  and  $\Gamma$  as in section 4.3.

(U1) The fact that the circumdiameter is limited enforces a minimum density of points.

(U2) is satisfied as long as we choose  $a$  such that  $1/\sqrt{2}a$  is much smaller than the maximum circumradius  $\alpha$  (see remark 7).

(U3)  $\Pi_C^z(\Gamma) > 0$  due to the calculation in remark 8.

□

**Proposition 3.** *The exists at least one gibbs measure for the model  $(\mathcal{LD}, \varphi_S)$  and every activity*

$$z > ?$$

*Proof.* **(R)** Take the horizon set  $\Delta = B(p'_\eta, \sqrt{p''_\eta + W})$ .  $\Delta$  can be decomposed into the sphere  $p_\eta$  and  $\Delta \setminus p_\eta$ , a 3-dimensional annulus with width  $\sqrt{p''_\eta + W} - \sqrt{p''_\eta} = W/(\sqrt{p''_\eta + W} + \sqrt{p''_\eta})$ . By definition of  $\mathcal{LD}$  and remark,  $p_\eta$  cannot contain any points of  $\mathfrak{x}$ . Although the annulus  $\Delta \setminus p_\eta$  does not have any bound on the number of points, its width is bounded by  $\sqrt{W} \geq W/(\sqrt{p''_\eta + W} + \sqrt{p''_\eta})$ . This means that any  $x, y \in \Delta$  can be connected by the spheres  $B(x, \sqrt{W}), p_\eta, B(y, \sqrt{W})$ , yielding the parameters  $\ell_R = 3, n_R = 0, \delta_R = 2\sqrt{W}$ .

Again, this is very vague. Make the argument using exact expressions and the fact that regular tetrahedron minimizes the circumdiameter.

Vague, improve

Ugly line placements, improve

**(S)** Stability is satisfied because of  $\varphi$  is non-negative.

**(U)** We choose  $M$  and  $\Gamma$  as in section 4.3.

(U1) Similarly to proposition 1, as long as  $\rho_0$  is small enough for any three points to never be coplanar, the weight  $p''_\eta$  of the characteristic point is bounded and therefore also  $r_{\Lambda, \mathfrak{x}}$  is bounded for all  $\Lambda \in \mathcal{B}_0$  and all  $\mathfrak{x} \in \bar{\Gamma}$ .

Vague, improve

(U2) is trivially satisfied since  $n_T < \infty$  and  $\varphi(\eta, \mathfrak{x}) < \infty$  for all  $(\eta, \mathfrak{x}) \in \mathcal{LD}$  (see remark 7).

(U3) **TO BE DONE** (as soon as I have bounds on  $\varphi_S$ , calculation is otherwise simple and is outlined in Proposition 1)

□

**Proposition 4.** *The exists at least one gibbs measure for the model  $(\mathcal{LD}, \varphi_{HC})$  and every activity  $z > 0$ .*

*Proof.* **(R)** The horizon set is  $\Delta = B(p'_\eta, \sqrt{p''_\eta + W})$ . Parameters can be chosen as in proposition 3. Alternatively we have  $\sqrt{p''_\eta} \leq \alpha/2$  because of the hard-core condition, and thus we can also use  $\ell_R = 1, \delta_R = 2\sqrt{\alpha^2 + W}$  with  $n_R$  arbitrary.

**(S)** Stability is satisfied because of  $\varphi$  is non-negative.

**( $\hat{U}$ )** We choose  $M$  and  $\Gamma$  as in section 4.3.

**( $\hat{U}1$ )** The fact that the circumdiameter is limited enforces a minimum density of points.

**( $\hat{U}2$ )** is satisfied as long as we choose  $a$  such that  $1/\sqrt{2}a$  is much smaller than the maximum circumradius  $\alpha$  (see remark 7).

**( $\hat{U}3$ )**  $\Pi_C^z(\Gamma^A) > 0$  due to the calculation in remark 8.

□

Is it a problem that there's no  $n_R$  circle? Cause the proof suggested something like that?

Vague, improve

Vague, improve

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## Todo list

|                                                                                                                                                                    |   |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------|---|
| ■ This is possibly a temporary solution . . . . .                                                                                                                  | 2 |
| ■ Define the sigma algebra . . . . .                                                                                                                               | 2 |
| ■ Do we actually need the normal position for points? All definitions work regardless . . . . .                                                                    | 2 |
| ■ Is $B(\eta, \mathfrak{x})$ even a good notation . . . . .                                                                                                        | 2 |
| ■ Is this correct? . . . . .                                                                                                                                       | 3 |
| ■ Talk about the geometric interpretation . . . . .                                                                                                                | 3 |
| ■ Comment on uniqueness of this point - e.g. maybe we need to choose one with minimal weight . . . . .                                                             | 3 |
| ■ Again, talk about the geometric interpretation, orthogonality, etc. . . .                                                                                        | 3 |
| ■ Again, comment on the geometric interpretation of this property . . . .                                                                                          | 3 |
| ■ Titles for remarks (and maybe definitions too?) . . . . .                                                                                                        | 3 |
| ■ Finish these remarks . . . . .                                                                                                                                   | 4 |
| ■ For now . . . . .                                                                                                                                                | 4 |
| ■ This is WRONG, since $p'_\eta$ depends on the marks, too, and won't be the same as the center of $B(\eta, \mathfrak{x})$ . Is the assertion even true? . . . . . | 4 |
| ■ Half diameter is an ugly notation for radius . . . . .                                                                                                           | 4 |
| ■ How exactly does this look? Why? . . . . .                                                                                                                       | 4 |
| ■ Talk a bit about $\varphi_{HC}$ - can be $\infty$ below $d_0$ , requires infinity later,.. . .                                                                   | 4 |
| ■ Other potentials. Other characteristics other than circumdiameter. Combinations of potentials. Interaction. . . . .                                              | 4 |

|                                                                                                                                          |    |
|------------------------------------------------------------------------------------------------------------------------------------------|----|
| Everything is a circumsphere..                                                                                                           | 5  |
| Hamiltonians                                                                                                                             | 5  |
| Later in the text, these are exactly the sets of tetrahedra used for the calculation, connect those two                                  | 5  |
| characterize it                                                                                                                          | 5  |
| Comment on the definition and what it means for $\mathcal{D}$ and $\mathcal{LD}$ .                                                       | 5  |
| Make this more precise                                                                                                                   | 7  |
| Simulation study                                                                                                                         | 7  |
| Remark about U3 monotonicity, possibly some other remarks about the assumptions                                                          | 8  |
| Get more intuition about U3 and comment on why $\hat{U}$ is useful                                                                       | 8  |
| Define Gibbs measure                                                                                                                     | 8  |
| Comment better on why this choice                                                                                                        | 9  |
| $\rho_0$ possibly conflicts with $\rho$ for the power product                                                                            | 9  |
| The vagueness about $\rho_0$ is not satisfactory, though it's the way DDG did it. If possible, change this                               | 9  |
| This is perhaps unnecessarily conservative, we could widen it                                                                            | 9  |
| Number some equations for reference                                                                                                      | 9  |
| Better description and arguments of nearly everything in this section                                                                    | 9  |
| This is an important point, probably come back to it later. It's quite likely it will be possible to turn this into a formal argument..  | 10 |
| Possibly comment on this more                                                                                                            | 10 |
| Most importantly: what is the supremum of the potential over $\mathfrak{x} \in \bar{\Gamma}^A$ ?                                         | 11 |
| Reference, possibly using Schläfli symbols                                                                                               | 11 |
| It might be useful to have such a general theorem anyway, but formulated properly                                                        | 11 |
| Talk about this more clearly                                                                                                             | 12 |
| Again, this is very vague. Make the argument using exact expressions and the fact that regular tetrahedron minimizes the circumdiameter. | 12 |
| Vague, improve                                                                                                                           | 12 |
| Ugly line placements, improve                                                                                                            | 12 |
| Vague, improve                                                                                                                           | 12 |
| Is it a problem that there's no $n_R$ circle? Cause the proof suggested something like that?                                             | 13 |
| Vague, improve                                                                                                                           | 13 |
| Vague, improve                                                                                                                           | 13 |