

Department of Probability and Mathematical Statistics



FACULTY  
OF MATHEMATICS  
AND PHYSICS  
Charles University

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Daniel Jahn

## Existence of Gibbs-Laguerre-Delaunay Models

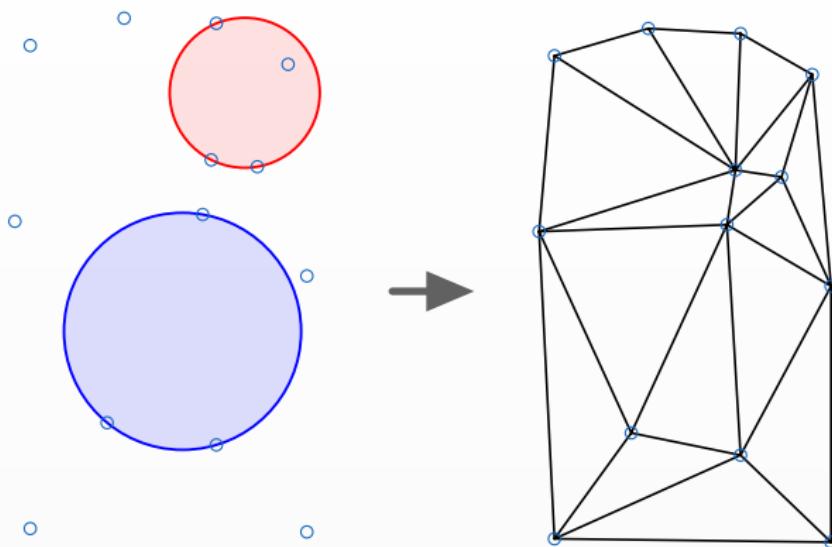
Workshop Devet Skal

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27 February 2019

# Delaunay tetrahedrization

Let  $\gamma$  be a locally finite subset  $\mathbb{R}^3$ .



$$\mathcal{D}_4(\gamma) = \{\eta \subset \gamma : \text{card}(\eta) = 4, \eta \text{ satisfies the empty ball property } \}$$

# Point processes

$\mathcal{B}$  Borel  $\sigma$ -algebra on  $\mathbb{R}^3$ ,  $\mathcal{B}_0$  bounded Borel sets,  $|\cdot|$  is the Lebesgue measure.

**Point process:**  $\Phi : (\Omega, \mathcal{A}, \mathbb{P}) \rightarrow (\mathbf{N}_{lf}, \mathcal{N}_{lf})$  where

- $\mathbf{N}_{lf}$  is the set of all locally finite simple counting measures on  $\mathbb{R}^3$ .
- $\mathcal{N}_{lf}$  is generated by sets of the form

$$\{\nu \in \mathbf{N}_{lf} \mid \nu(\Lambda) = n\}, n \in \mathbf{N}_{lf}, \Lambda \in \mathcal{B}.$$

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**Poisson point process** with intensity  $z > 0$  is a point process  $\Phi$  such that

- $\Phi(B) \sim Pois(z|B|)$  for each  $B \in \mathcal{B}_0$ ,
- $\Phi(B_1), \dots, \Phi(B_n)$  are independent for each  $n \in \mathbb{N}$  and  $B_1, \dots, B_n \in \mathcal{B}_0$  pairwise disjoint.

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For  $\Lambda \in \mathcal{B}_0$  and Poisson point process  $\Phi$  with intensity  $z > 0$ , denote the distribution of  $\Phi_\Lambda := \Phi \cap \Lambda$  as  $\Pi_\Lambda^z$ .

We obtain the probability space  $(\mathbf{N}_{lf}, \mathcal{N}_{lf}, \Pi_\Lambda^z)$ .

# Gibbs point process

Denote

$$\mathbf{N}_\Lambda = \{\nu \in \mathbf{N}_{lf} : \nu(\mathbb{R}^3 \setminus \Lambda) = 0\}.$$

A translation-invariant probability measure  $P$  on  $(\mathbf{N}_{lf}, \mathcal{N}_{lf})$  is a **Gibbs measure** with activity  $z > 0$  if it satisfies the **Dobrushin-Lanford-Ruelle equation**:

$$\int f dP = \int \frac{1}{Z_\Lambda^z(\gamma)} \int_{\mathbf{N}_\Lambda} f(\zeta \cup \gamma_{\Lambda^c}) e^{-H_\Lambda(\zeta \cup \gamma_{\Lambda^c})} \Pi_\Lambda^z(d\zeta) P(d\gamma)$$

for every  $\Lambda \in \mathcal{B}_0$  and every measurable  $f : \mathbf{N}_{lf} \rightarrow [0, \infty)$ .

$Z_\Lambda^z(\gamma) = \int e^{H_\Lambda(\zeta \cup \gamma_{\Lambda^c})} \Pi_\Lambda^z(d\zeta)$  is the **partition function**

$H_\Lambda$  is the **energy function**

$$H_\Lambda(\gamma) = \sum_{\eta \in \mathcal{E}_\Lambda(\gamma)} \varphi(\eta, \gamma),$$

such that  $Z_\Lambda^z(\gamma) < \infty$ .

A point process whose distribution is a Gibbs measure is called a **Gibbs point process**.

D. Dereudre and F. Lavancier. Practical simulation and estimation for Gibbs Delaunay-Voronoi tessellations with geometric hardcore interaction (2011)

Considered Delaunay triangulation in  $\mathbb{R}^2$  using the potential

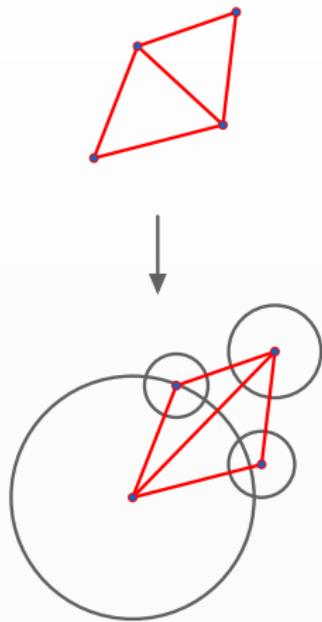
$$\varphi(\eta) = \begin{cases} \infty & \text{if } I(T) \leq \epsilon, \\ \infty & \text{if } \chi(T) \geq \alpha, \\ \theta \text{Per}(T) & \text{otherwise,} \end{cases}$$

where

- $I(T)$  is the length of the shortest edge of the triangle  $T$ .
- $\chi(T)$  is the circumradius of  $T$ .
- $\text{Per}(T)$  is the perimeter of the triangle  $T$ .
- $\theta \in \mathbb{R}$ ,  $\epsilon \geq 0$ ,  $\alpha > 0$  such that  $2\epsilon < \alpha < 1/2$ .

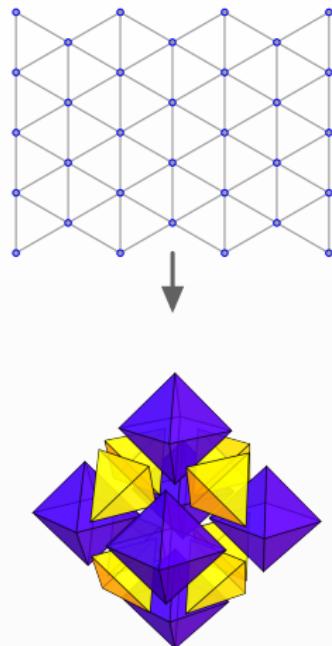
Delaunay → Laguerre

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2D → 3D

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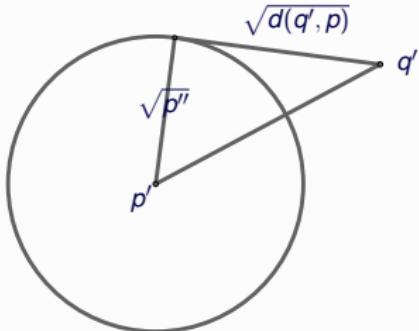


# Laguerre-Delaunay

## Power distance

- Generating points are now both locations and **weights**. Can be geometrically interpreted as **spheres**.
- $\gamma = \{p_1, \dots, p_n\} = \{(p'_1, p''_1), \dots, (p'_n, p''_n)\}$  can be thought of as **marked point process**.
- $\gamma \subset \mathbb{R}^3 \times S$ , where  $S = [0, W]$ ,  $W > 0$ .
- Distance is not Euclidean, but the **power distance**

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



# Laguerre-Delaunay

Characteristic point, regularity

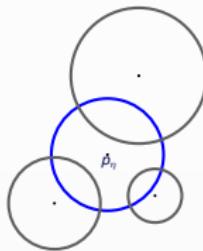
- Instead of circumscribed ball, we have the **characteristic point**  $p_\eta = (p'_\eta, p''_\eta)$ .

$$d(p'_\eta, p_i) = p''_\eta, \quad \text{for each } i = 1, \dots, 4.$$

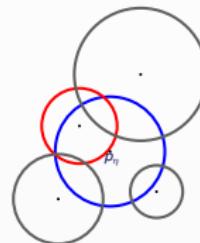
- Instead of the empty sphere property, we have **regularity**

$\eta$  is **regular** if there is no other point  $q \in \gamma$  such that  $d(p'_\eta, q) < p''_\eta$ .

$$\mathcal{LD}_4(\gamma) = \{\eta \subset \gamma : \text{card}(\eta) = 4, \eta \text{ is regular}\}$$



Points of  $\eta$  (gray) and their characteristic point  $p_\eta$  (blue).



A point (red) breaking the regularity of  $\eta$ .

# Practical results

## Implementation

The partition function  $Z_\lambda^z$  is unknown → Birth-Death-Move Metropolis-Hastings algorithm.

Each step has to reconstruct a new tetrahedrization.



- Implemented the MCMC algorithm and relied on Computer Graphics Algorithms Library for handling the tetrahedrization.  
Current version at <https://github.com/DahnJ/Gibbs-Laguerre-Delaunay.git>
- Simulations done in C++, numerical analysis in Python and Mathematica.

# Theoretical results

**Goal:** To prove the existence of the Gibbs-Laguerre-Delaunay models we simulated.

**Results:** Proved the existence of the following two classes of models.

A hyperedge potential  $\phi$  is **unary** for the hypergraph structure  $\mathcal{E}$  if there exists a measurable function  $\hat{\varphi} : \mathbf{N}_f \rightarrow \mathbb{R} \cup \{+\infty\}$  such that

$$\varphi(\eta, \gamma) = \hat{\varphi}(\eta) \text{ for } \eta \in \mathcal{E}(\gamma).$$

**Bounded interaction:** For  $\eta \in \mathcal{LD}_4(\gamma)$  define the potential  $\varphi_S$  as a unary potential such that

$$\varphi_S(\eta, \gamma) \leq K_0 + K_1 \chi(\eta)^\beta$$

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

**Hard-core interaction:** For  $\eta \in \mathcal{LD}_4(\gamma)$  define the potential  $\varphi_{HC}$  as a unary potential such that

$$\sup_{\eta: d_0 \leq \chi(\eta) \leq d_1} \varphi_{HC}(\eta, \gamma) < \infty \text{ and } \varphi_{HC}(\eta, \gamma) = \infty \text{ if } \chi(\eta) > \alpha$$

for some  $0 \leq d_0 < d_1 \leq \alpha$ .

Based on *Dereudre, Drouilhet, Georgii: Existence of gibbsian point processes with geometry-dependent interactions (2012)*.

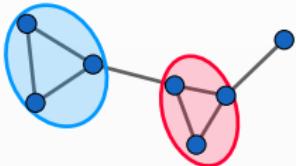
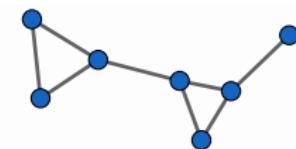
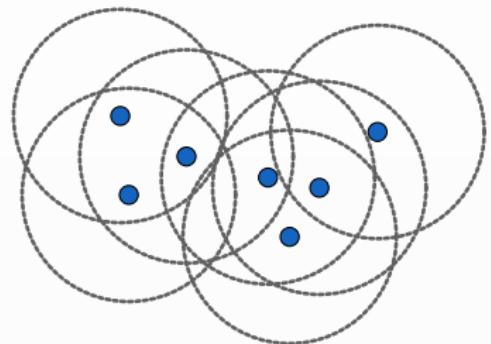
## Definition. Hypergraph structure

A *hypergraph structure* is a measurable subset  $\mathcal{E}$  of  $(\mathbf{N}_f \times \mathbf{N}_{lf}, \mathcal{N}_f \otimes \mathcal{N}_{lf})$  such that  $\eta \subset \gamma$  for all  $(\eta, \gamma) \in \mathcal{E}$ . We call  $\eta$  a *hyperedge* of  $\gamma$  and write  $\eta \in \mathcal{E}(\gamma)$ , where  $\mathcal{E}(\gamma) = \{\eta : (\eta, \gamma) \in \mathcal{E}\}$ . For a given  $\gamma \in \mathbf{N}_{lf}$ , the pair  $(\gamma, \mathcal{E}(\gamma))$  is called a *hypergraph*.

A *hyperedge potential* is a measurable function  $\varphi : \mathcal{E} \rightarrow \mathbb{R} \cup \{+\infty\}$ . We define  $\varphi = 0$  on  $\mathcal{E}^c$ .

# Many-body interaction

$$\text{LC}_r = \{(\eta, \gamma) : \eta \subset \gamma, \text{diam}(\eta) \leq r, \gamma \in \mathbb{N}_{lf}\}$$

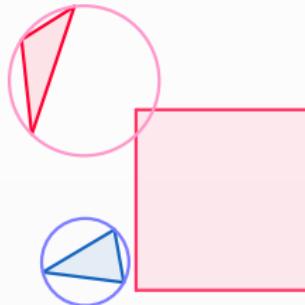


Let  $\Lambda \in \mathcal{B}_0$ . Define the set

$$\mathcal{E}_\Lambda(\gamma) := \{\eta \in \mathcal{E}(\gamma) : \varphi(\eta, \zeta \cup \gamma_{\Lambda^c}) \neq \varphi(\eta, \gamma) \text{ for some } \zeta \in \mathbf{N}_\Lambda\}.$$

For  $\eta \in \mathcal{E}(\gamma)$  such that  $\varphi(\eta, \gamma) \neq 0$  we have the following implication:

$$\eta \notin \mathcal{E}(\zeta \cup \gamma_{\Lambda^c}) \text{ for some } \zeta \in \mathbf{N}_\Lambda \Rightarrow \eta \in \mathcal{E}_\Lambda(\gamma).$$



Finite horizon, range confinement, range condition.

# Pseudo-periodic configurations

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

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

Let  $\Gamma \in \mathcal{N}_C$  be non-empty. Then we define the *pseudo-periodic* configurations  $\bar{\Gamma}$  as

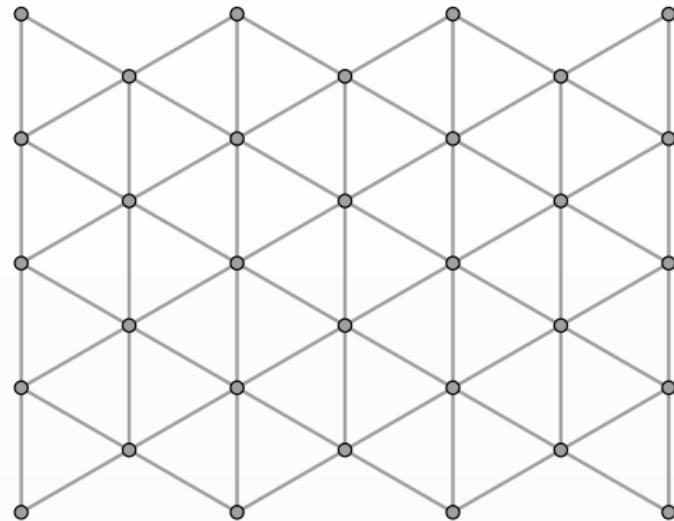
$$\bar{\Gamma} = \{\gamma \in \mathbf{N}_{lf} : \vartheta_{Mk}(\gamma_{C(k)}) \in \Gamma \text{ for all } k \in \mathbb{Z}^3\},$$

Fix some  $A \subset C \times S$  and define

$$\Gamma^b = \{\zeta \in \mathbf{N}_C : \zeta = \{p\}, p \in B(0, b)\},$$

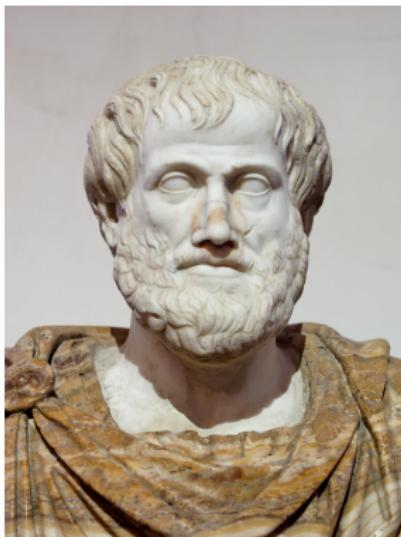
Let  $M$  be such that  $|M_i| = a > 0$  for  $i = 1, 2, 3$  and  $\angle(M_i, M_j) = \pi/3$  for  $i \neq j$ .

## In 2D: Equilateral triangles



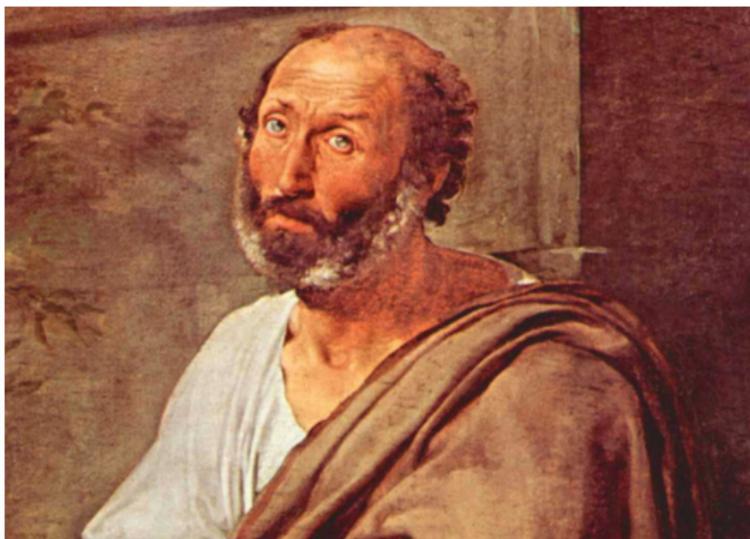
In 3D: Regular tetrahedra?

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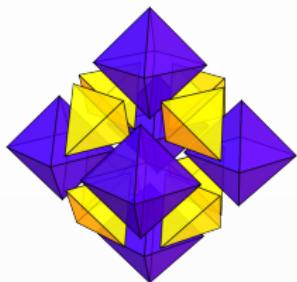
Aristotle

In 3D: Regular tetrahedra

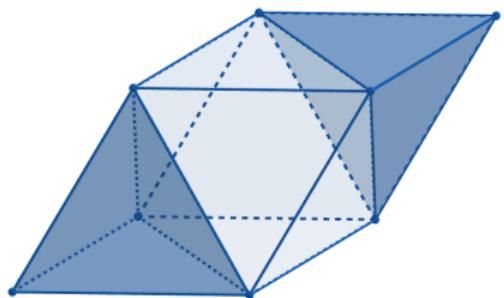


Tetrahedrons do not tessellate.

## In 3D: Tetrahedral-octahedral honeycomb



Tetrahedral-octahedral honeycomb in an exploded view.



A single cell of a tetrahedral-octahedral honeycomb.





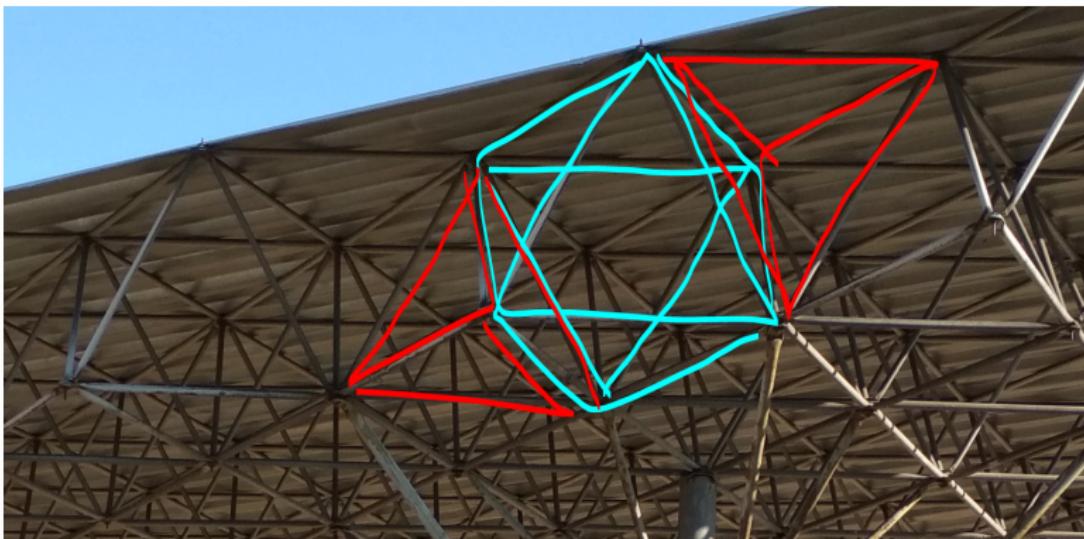


FIGURE 14

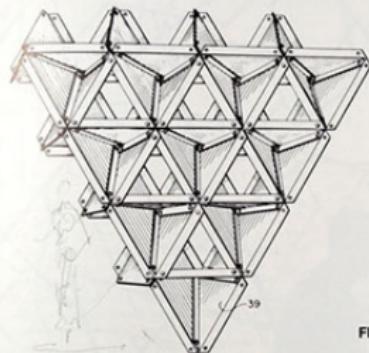


FIGURE 15

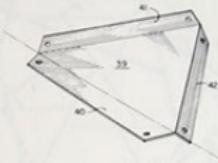
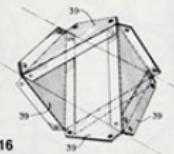
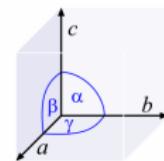
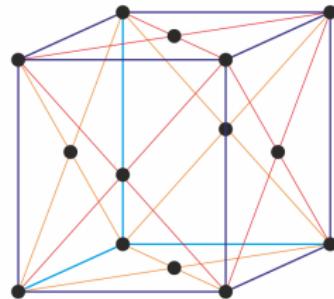


FIGURE 16



CRYSTAL LATTICE  
face-centered cubic



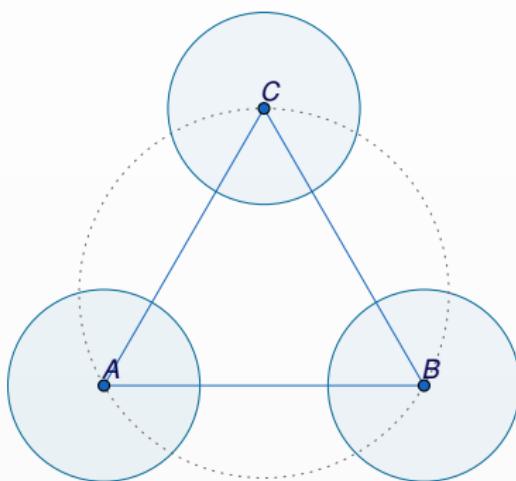
$$a = b = c$$

$$\alpha = \beta = \gamma = 90^\circ$$

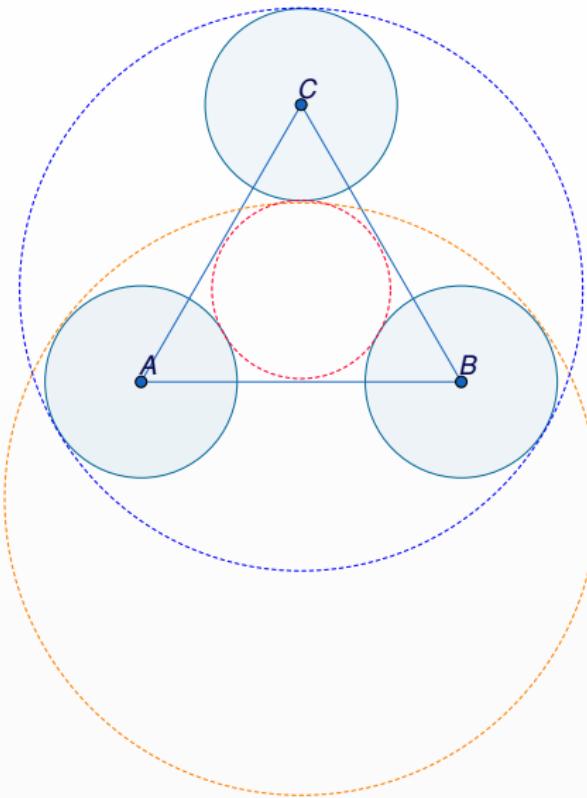
# Bounding the diameter

$$\varphi_S(\eta, \gamma) \leq K_0 + K_1 \chi(\eta)^\beta$$

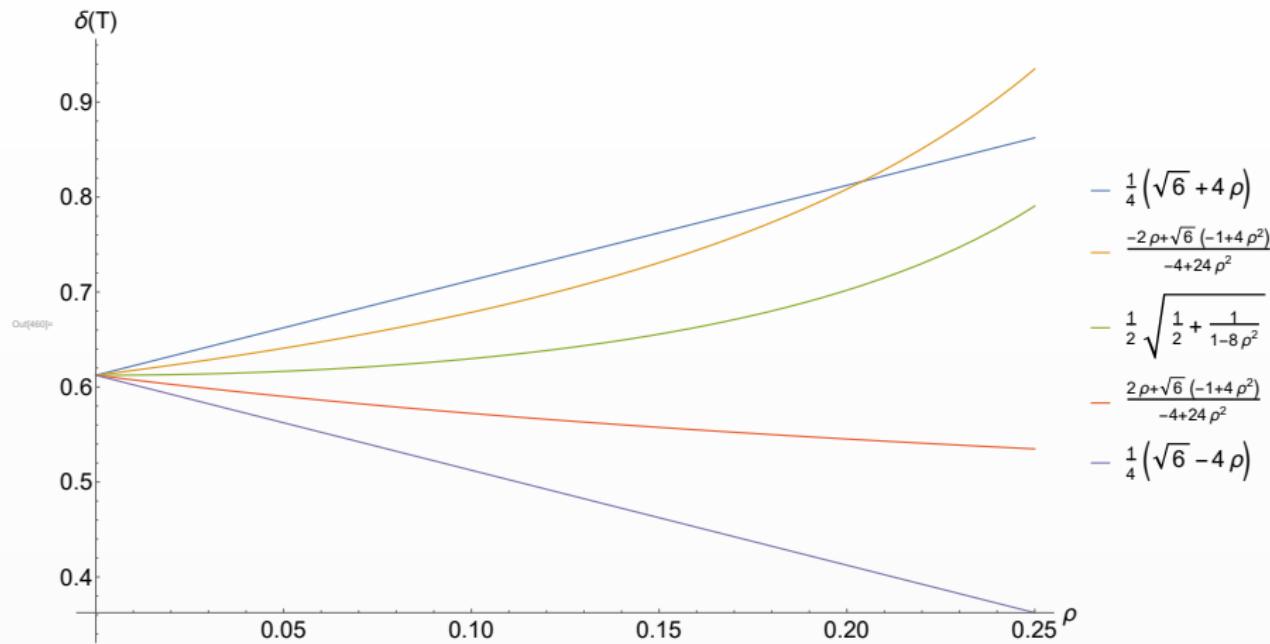
Need to bound the potential on the pseudo-periodic configurations  $\tilde{\Gamma}$ .



# Problem of Apollonius



# Apollonius spheres



$\delta(T)$  - circumdiameter of the tetrahedron

$\rho$  - radius of the sphere in which the points can move

- ① D. Dereudre and F. Lavancier. Practical simulation and estimation for Gibbs Delaunay-Voronoi tessellations with geometric hardcore interaction. *Computational Statistics and Data Analysis*, 55(1):498-519, 2011.
- ② D. Dereudre, R. Drouilhet, and H.O. Georgii. Existence of gibbsian point processes with geometry-dependent interactions. *Probability Theory and Related Fields*, 153(3):643-670, 2012
- ③ Fropuff. The vertex configuration of a tetrahedral-octahedral honeycomb., 2006. URL  
<https://en.wikipedia.org/wiki/File:TetraOctaHoneycomb-VertexConfig.svg>