Soft Packing of Spheres in $\mathbb{R}^3$

Toronto 2021

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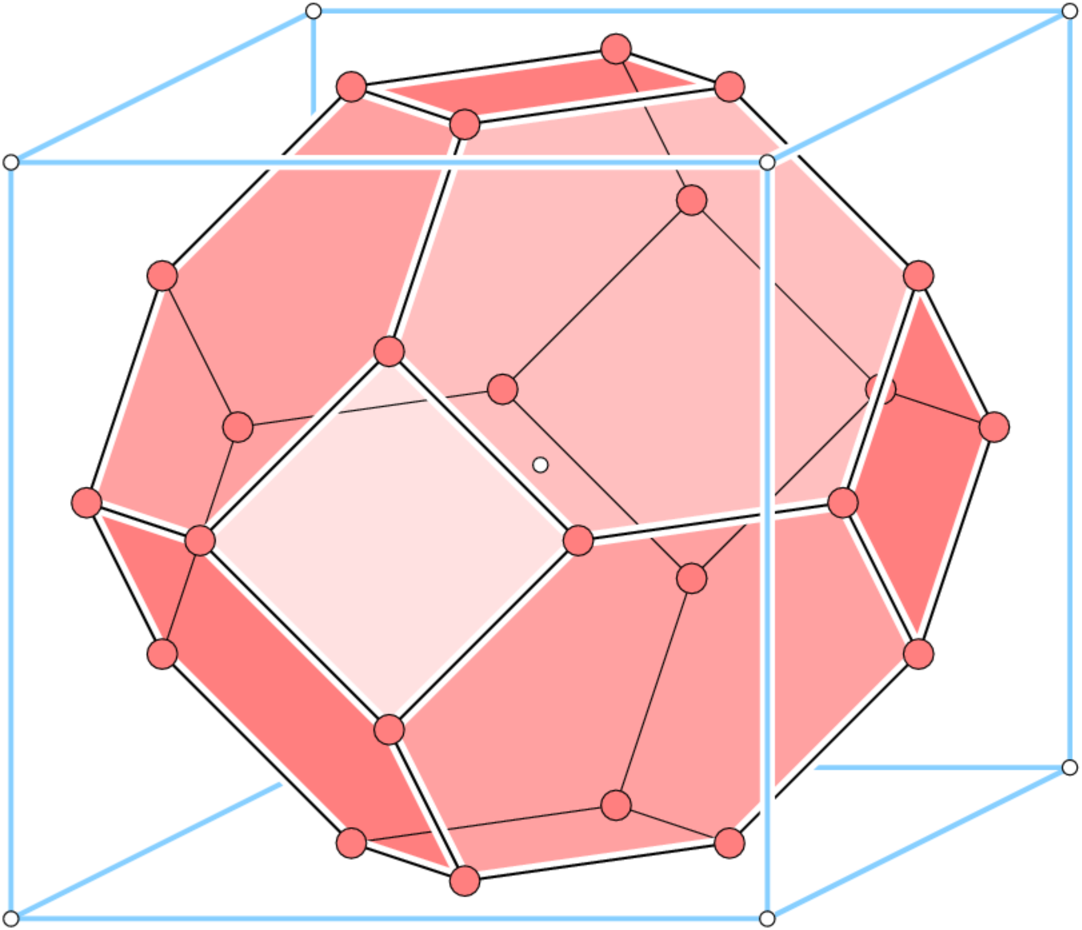
BCC LATTICE

(Body Centered Cubic)

$$\Lambda = \{(2i, 2j, 2k), (2i+1, 2j+1, 2k+1) \mid i, j, k \in \mathbb{Z}\}$$

$$|\Lambda| = 4$$



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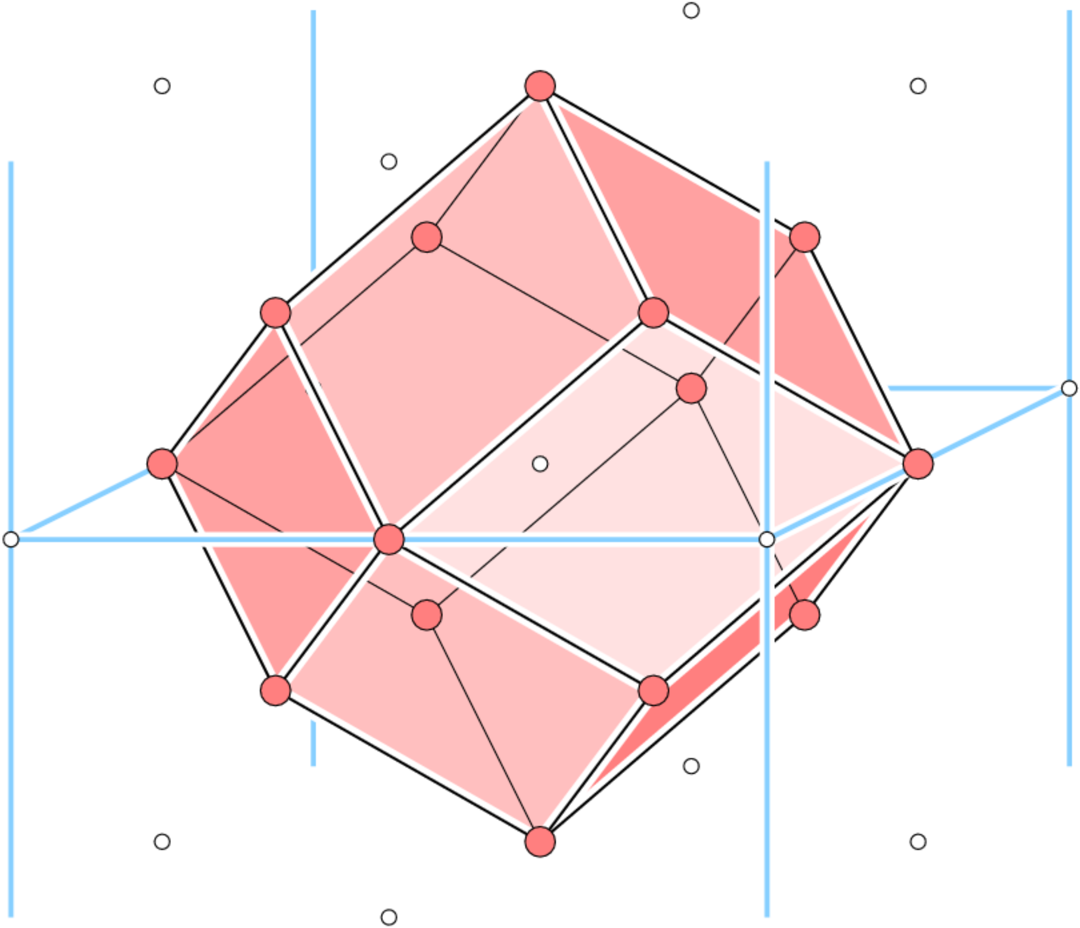
	radius	density
packing	$\sqrt{3}/2$	$0.680\ldots$
covering	$\sqrt{5}/2$	$1.463\ldots$

FCC Lattice

(Face Centered Cubic)

$$\Lambda = \{(2i, 2j, 2k), (2i+1, 2j+1, 2k), (2i+1, 2j, 2k+1), (2i, 2j+1, 2k+1) \mid i, j, k \in \mathbb{Z}\}$$

$$|\Lambda| = 2$$



FCC LATTICE

(Face Centered Cubic)

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$$(2i+1, 2j, 2k+1), (2i, 2j+1, 2k+1) \mid i, j, k \in \mathbb{Z}\}$$

$$|\Lambda| = 2$$

	radius	density
packing	$\sqrt{2}/2$	0.740 ...
covering	1	2.094 ...

Space of Lattices

$\Lambda \sim \Lambda'$ if related by rotation and scaling

5-dimensional

decomposed into 5 cells corresponding to

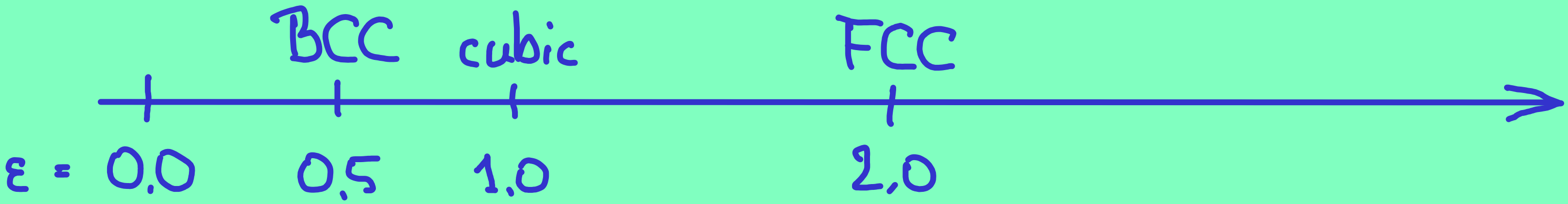
- truncated octahedron
- hexa-rhombic dodecahedron
- rhombic dodecahedron
- hexagonal prism
- cuboid

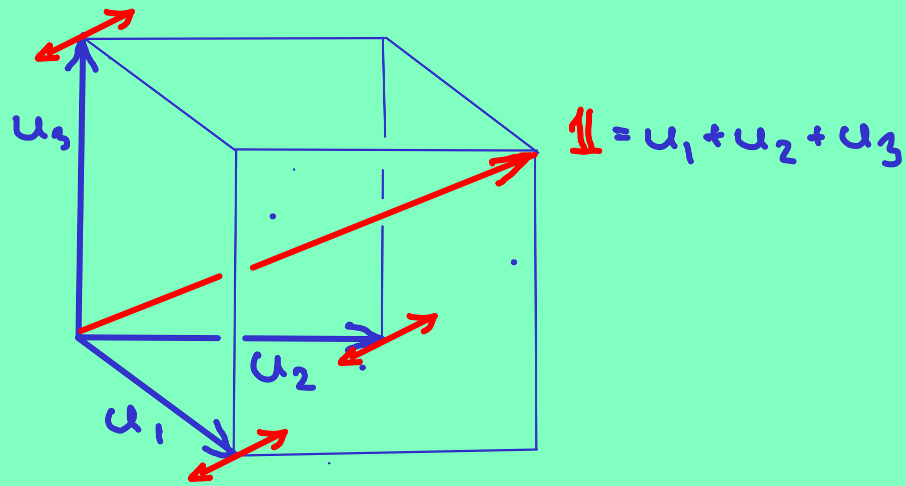
I Diagonal Family of Lattices

II Density and Soft Density

III Optimality of FCC Lattice

1-PARAMETER FAMILY OF DISTORTIONS

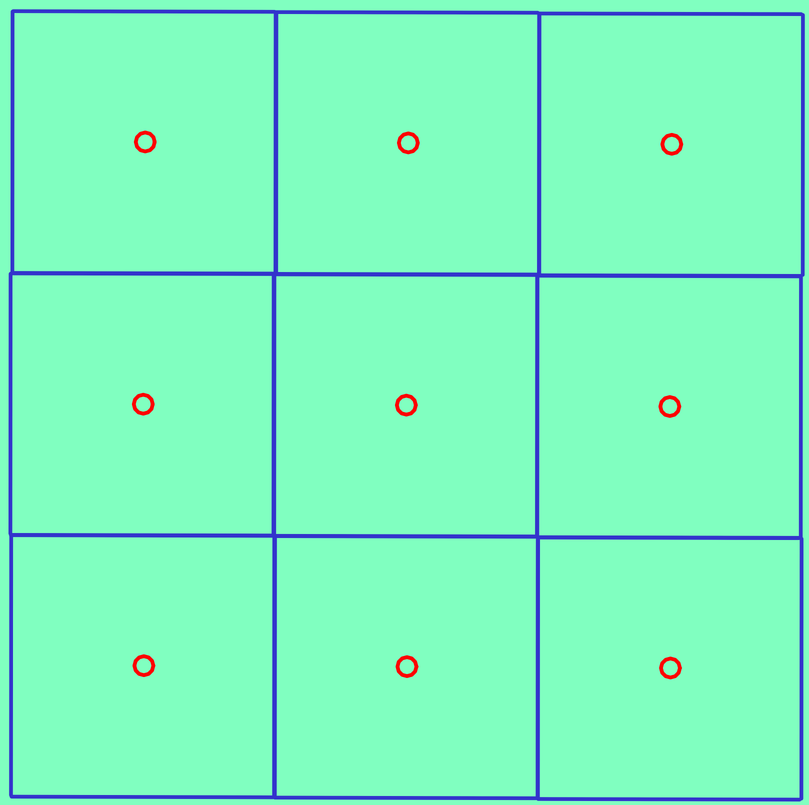




$$u_i(\varepsilon) = u_i + \frac{\varepsilon - 1}{3}\,\mathbb{1}$$

DISTORTION : VORONOI

Distortion : Voronoi



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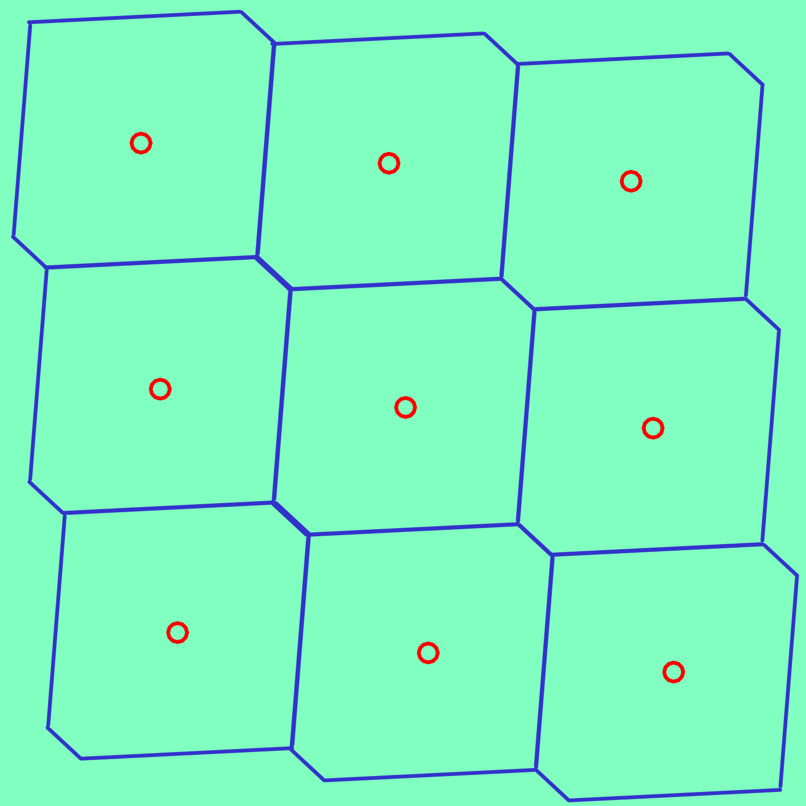

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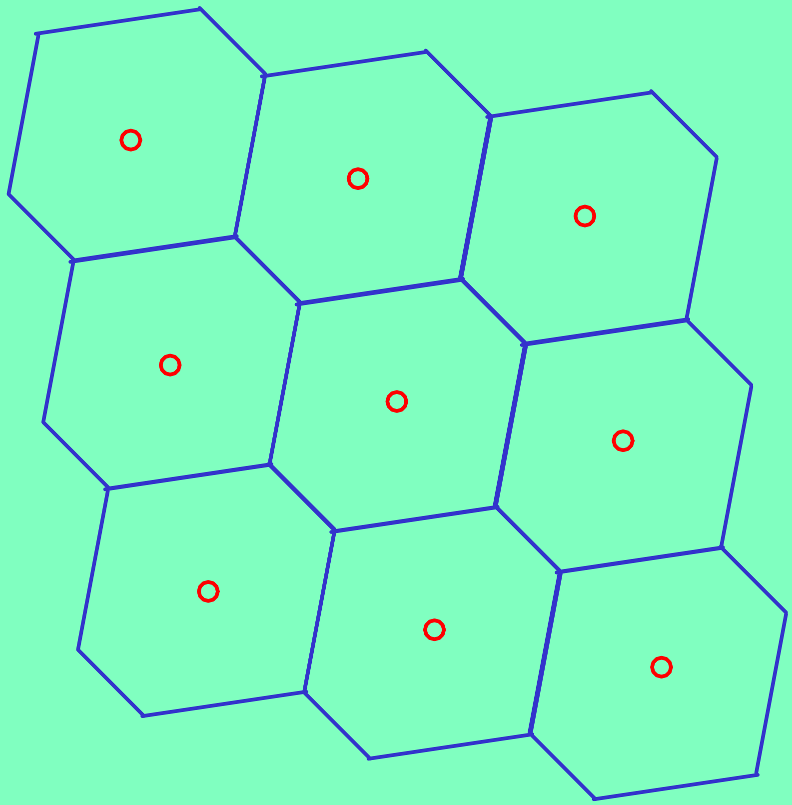

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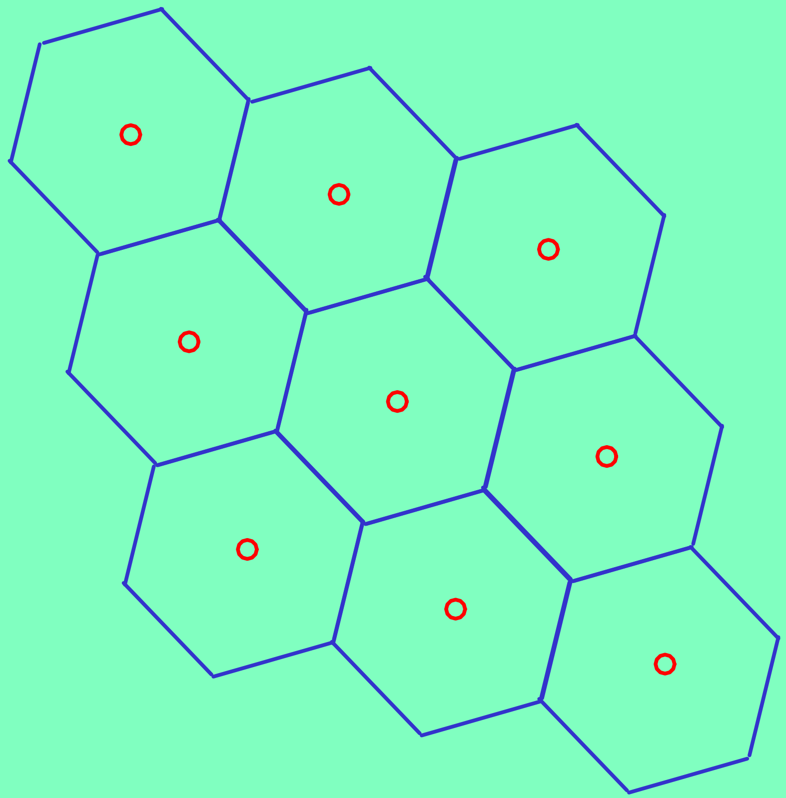

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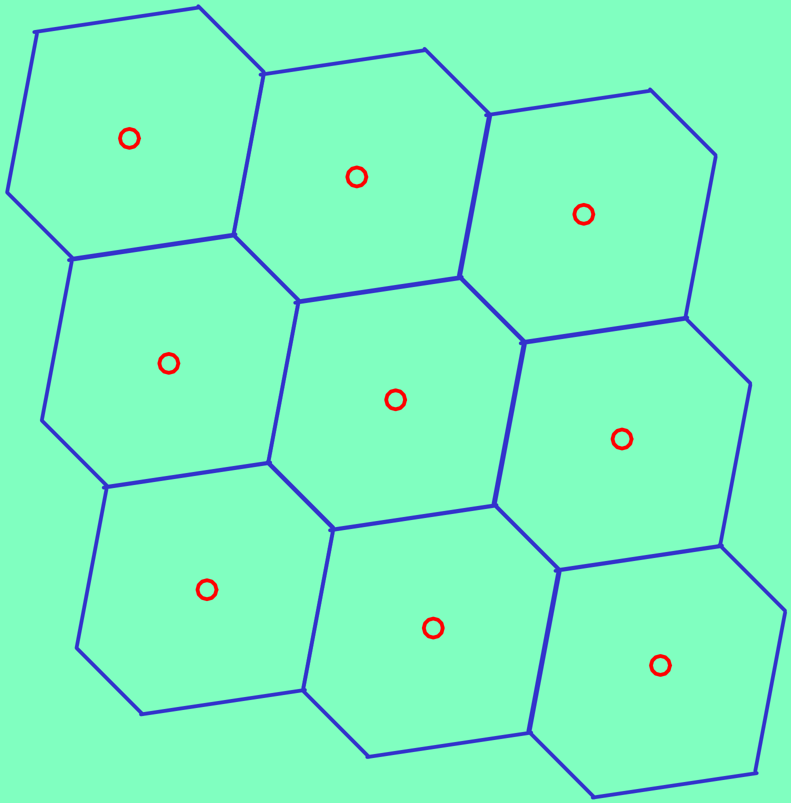

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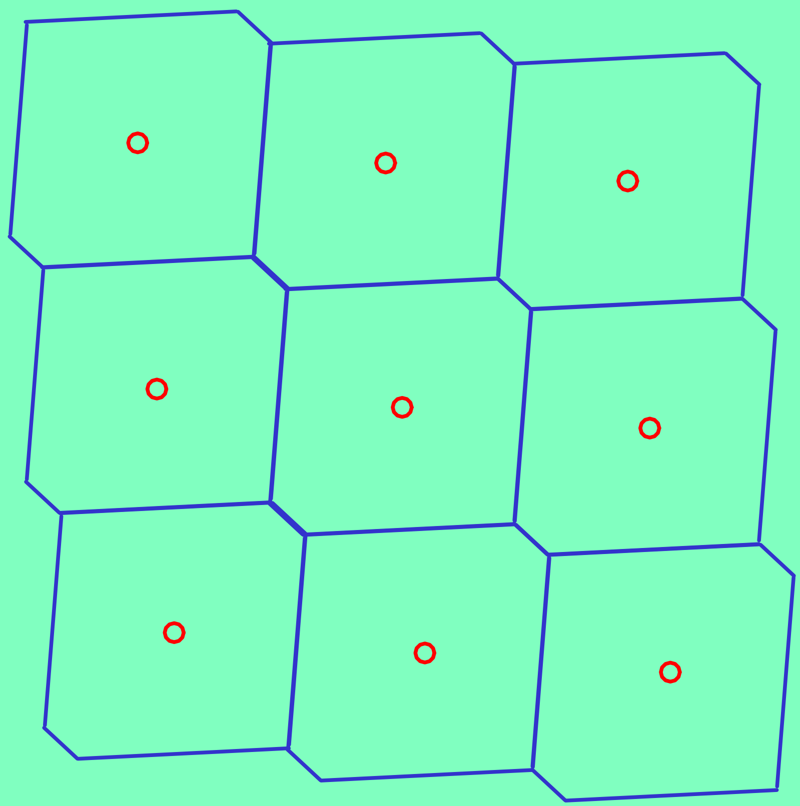

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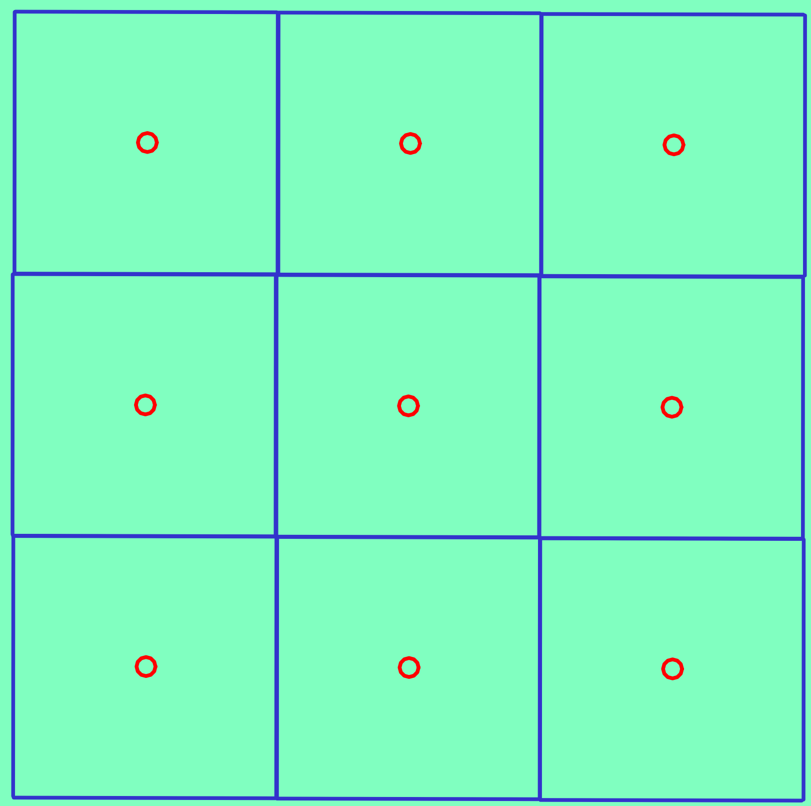

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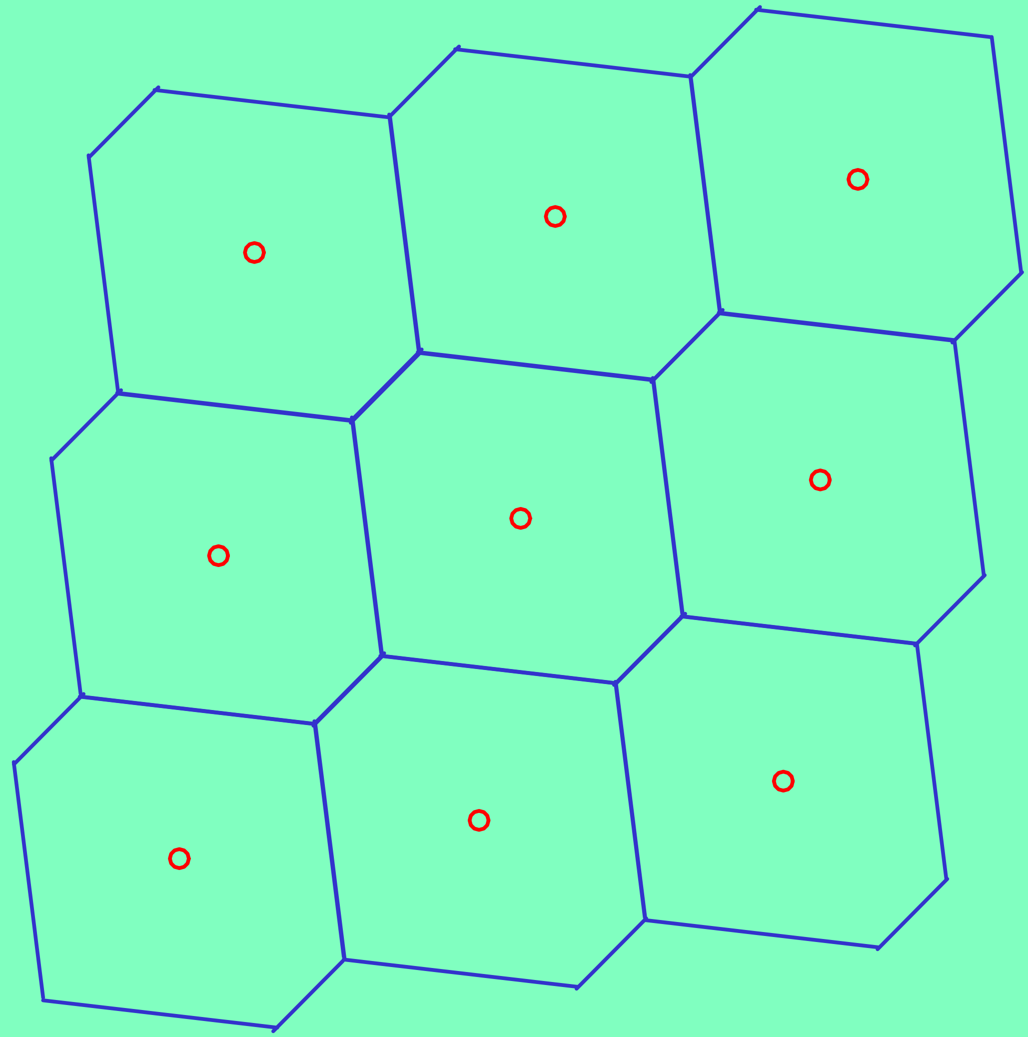

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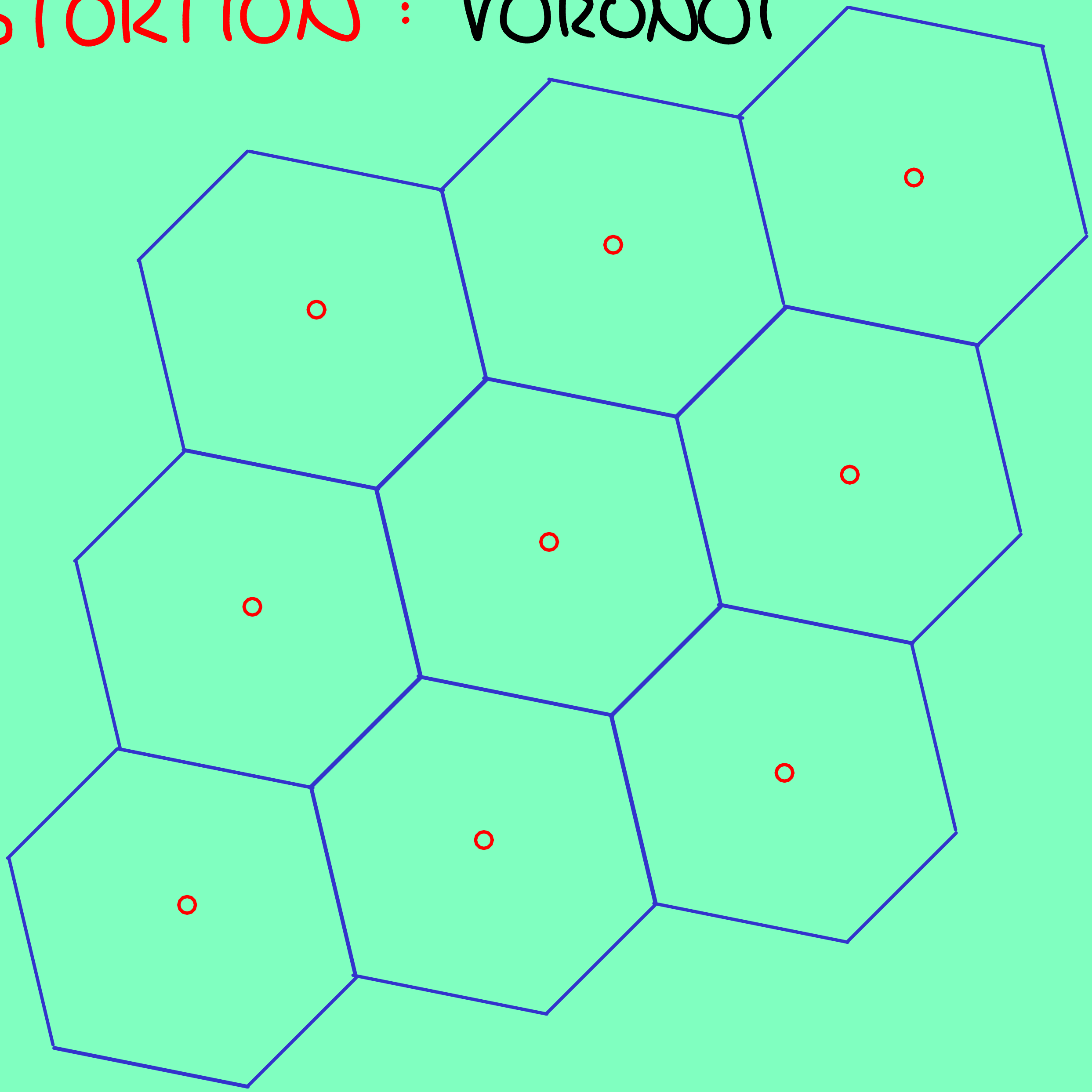

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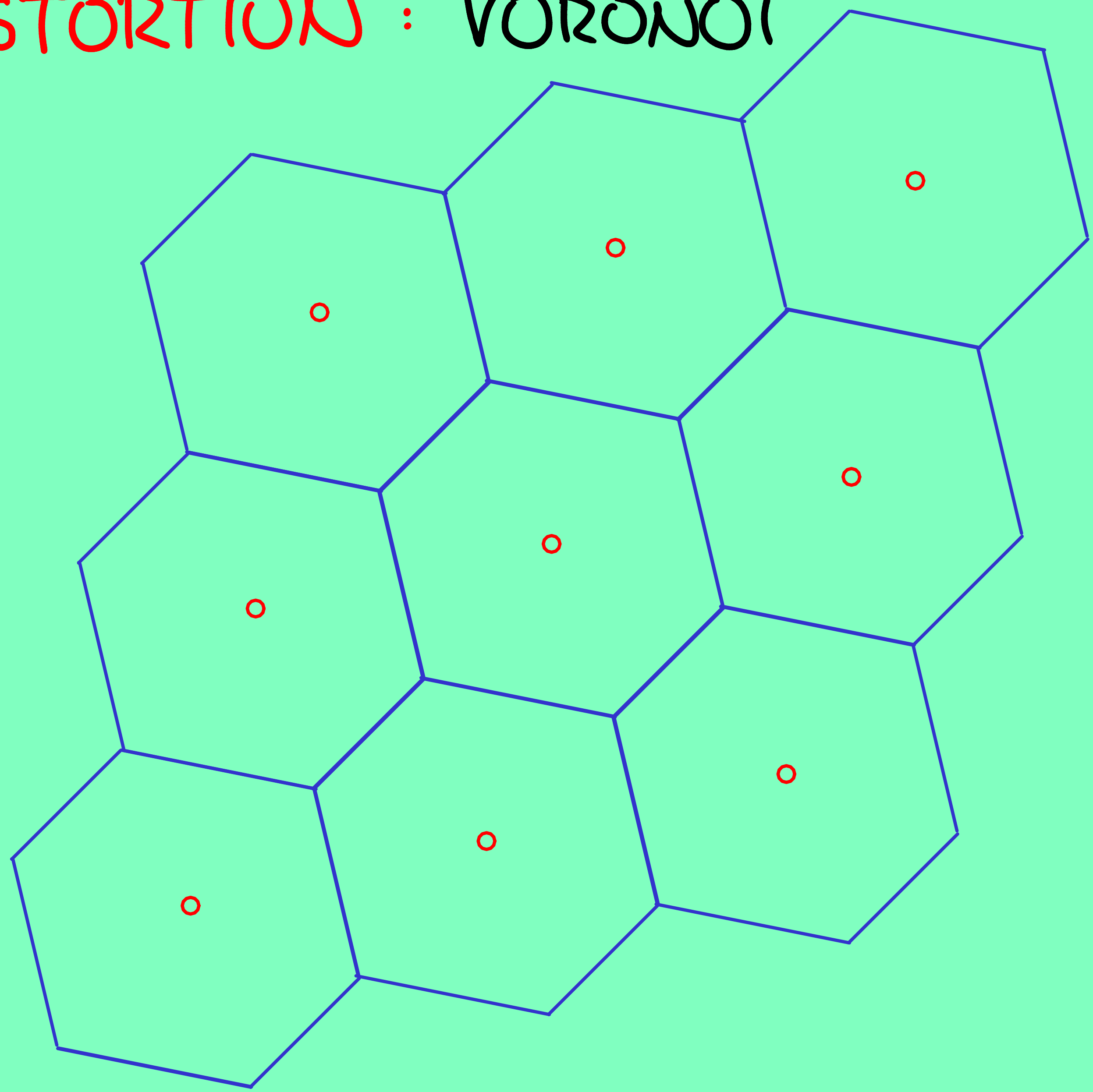

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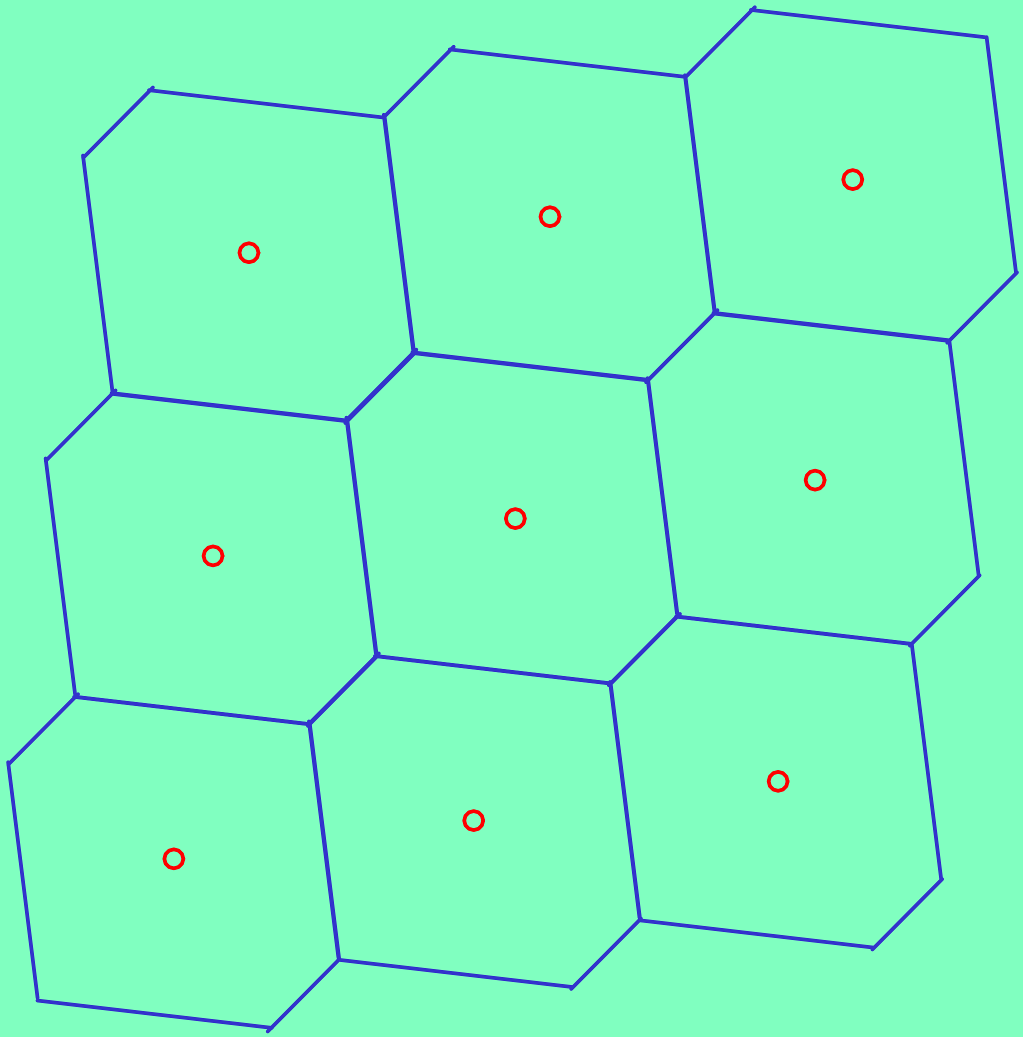

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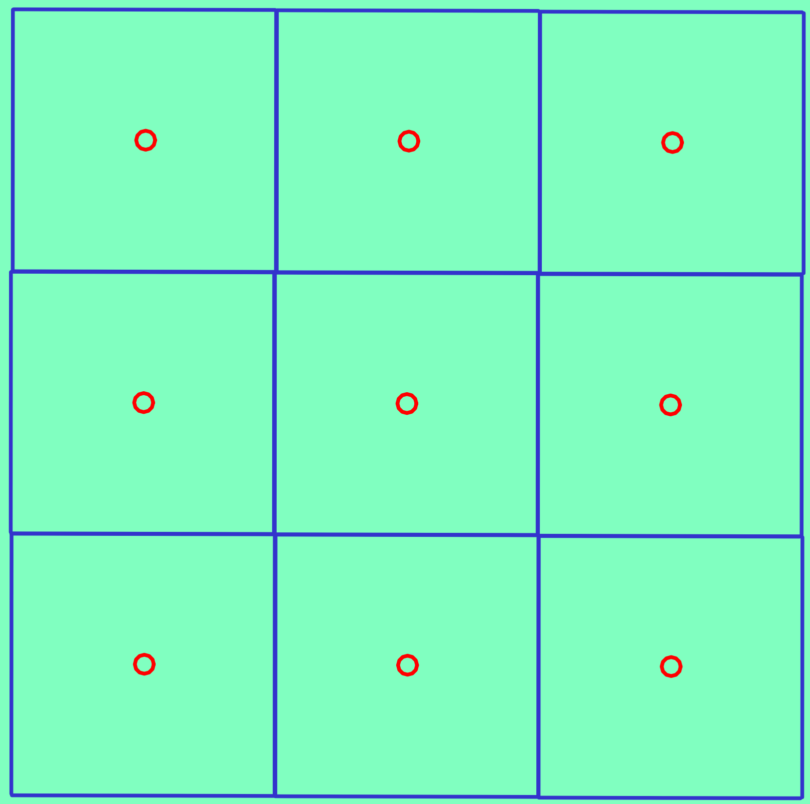

Distortion : Packing

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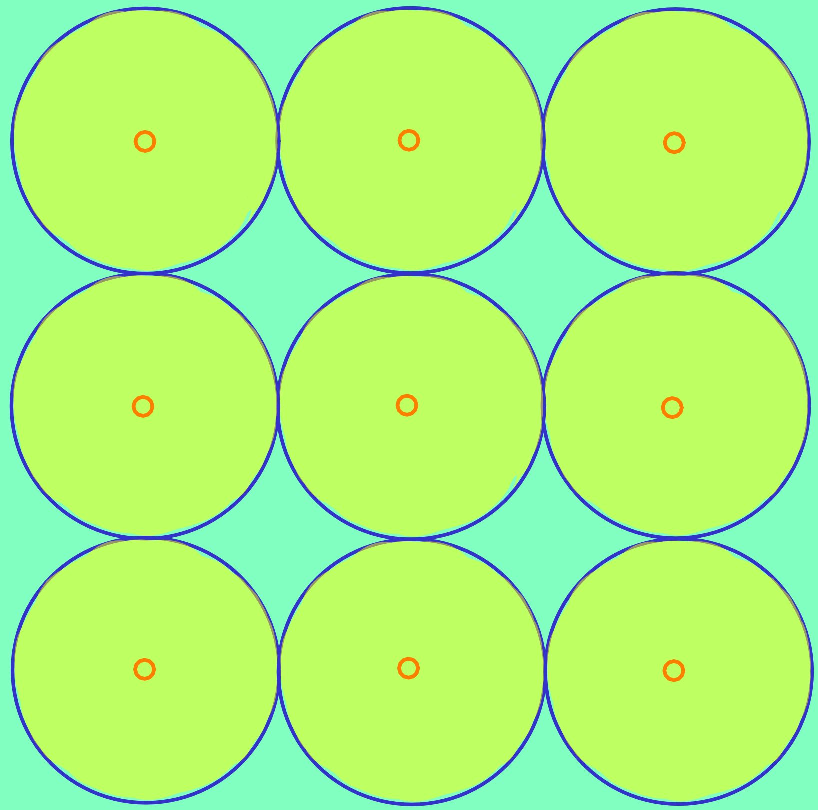

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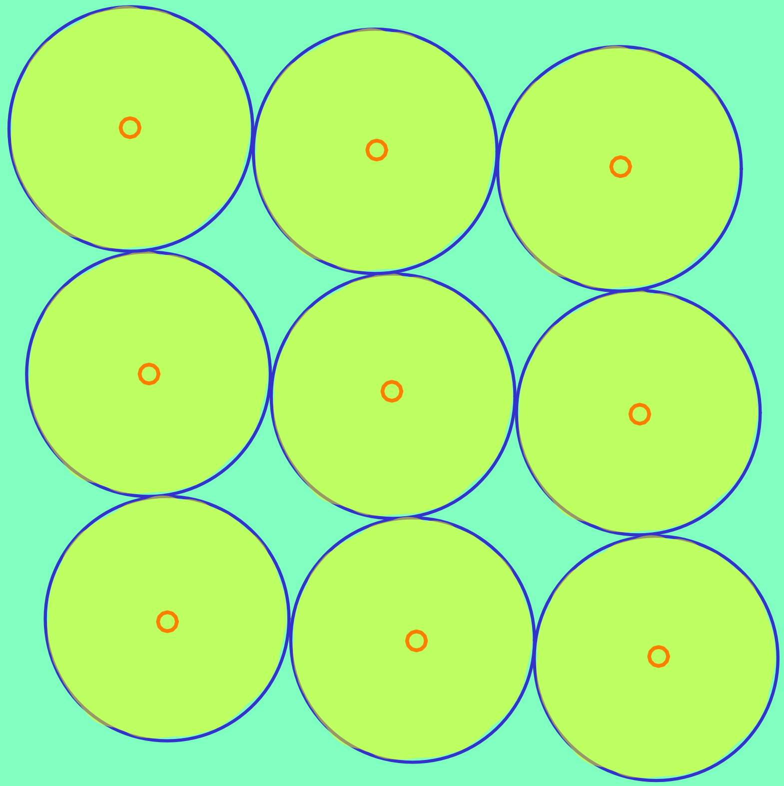

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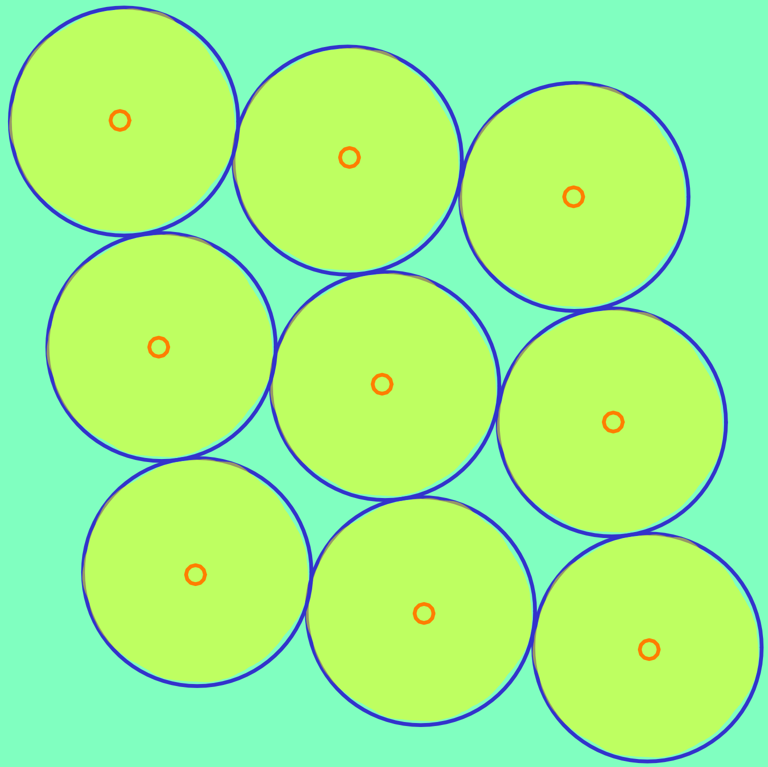

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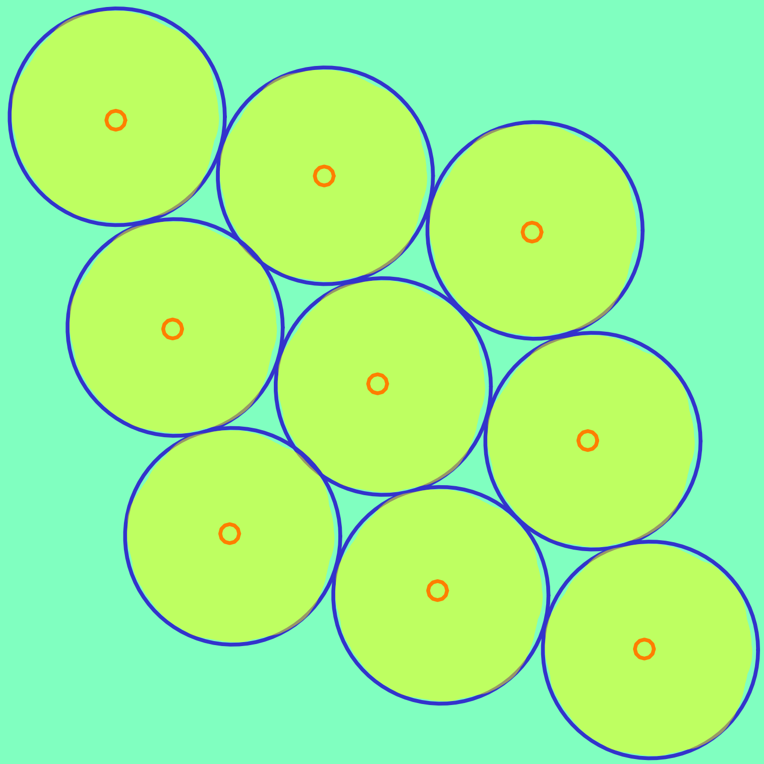

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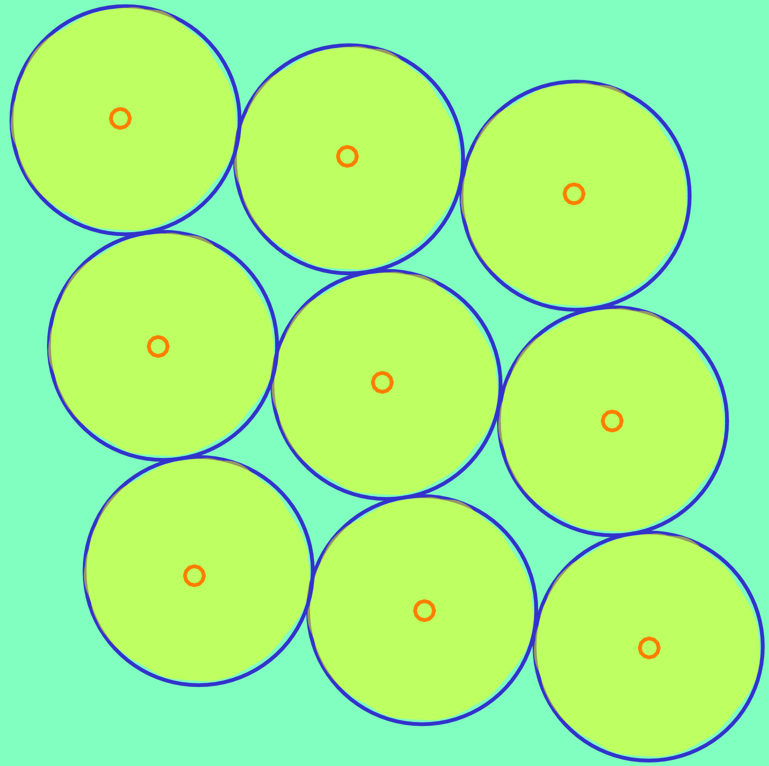

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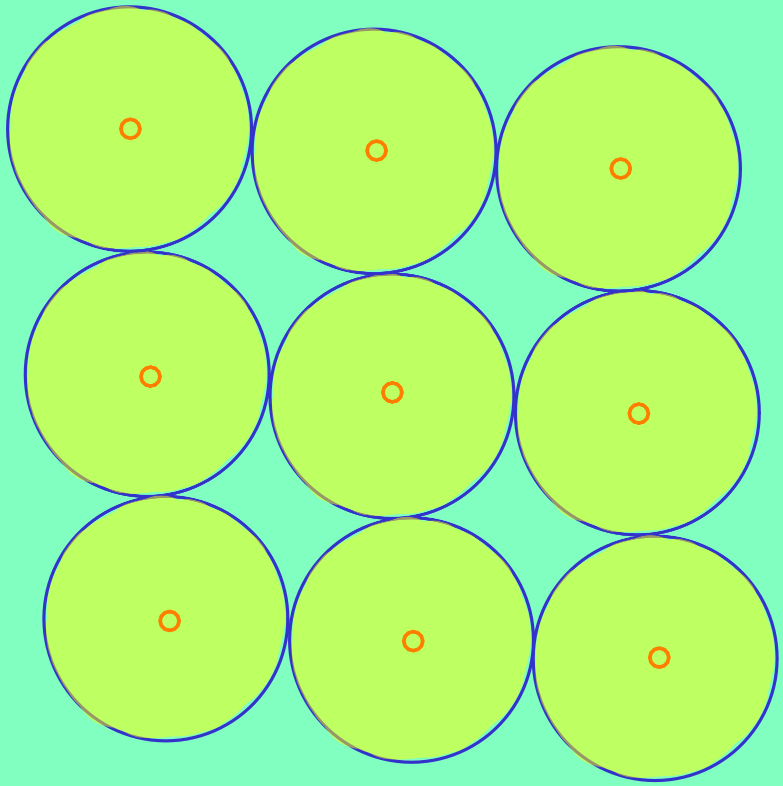

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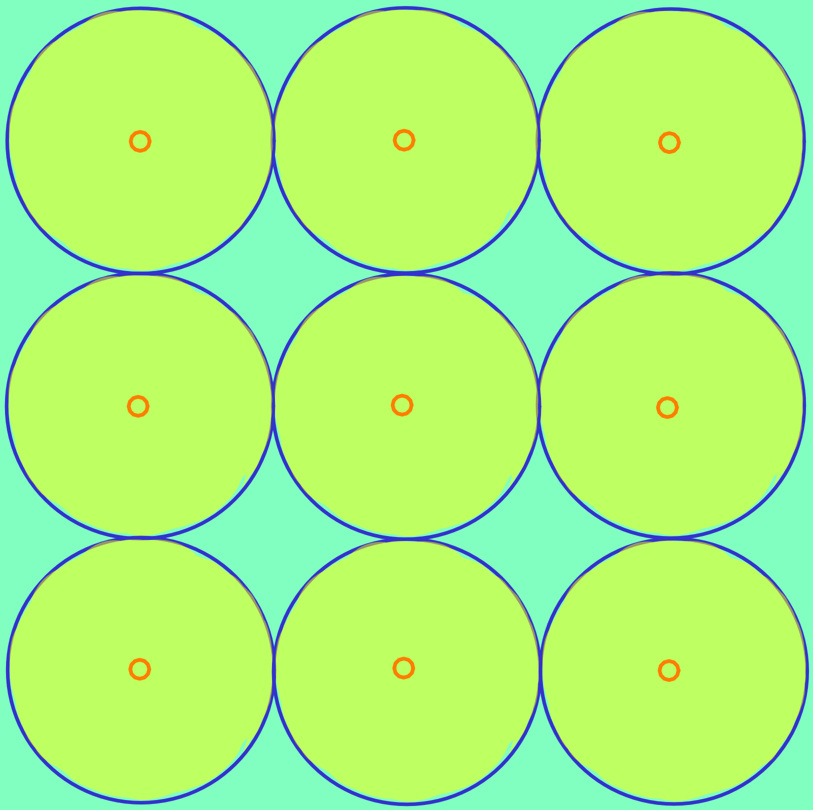

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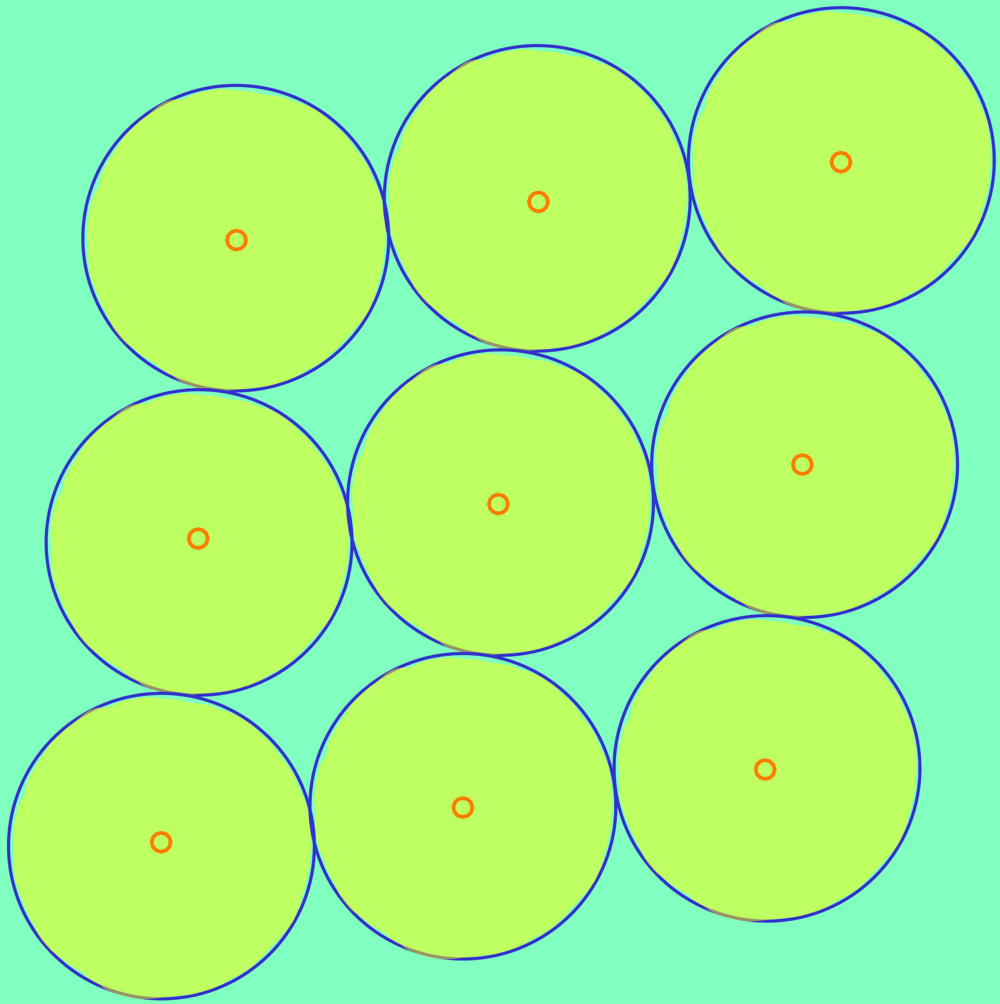

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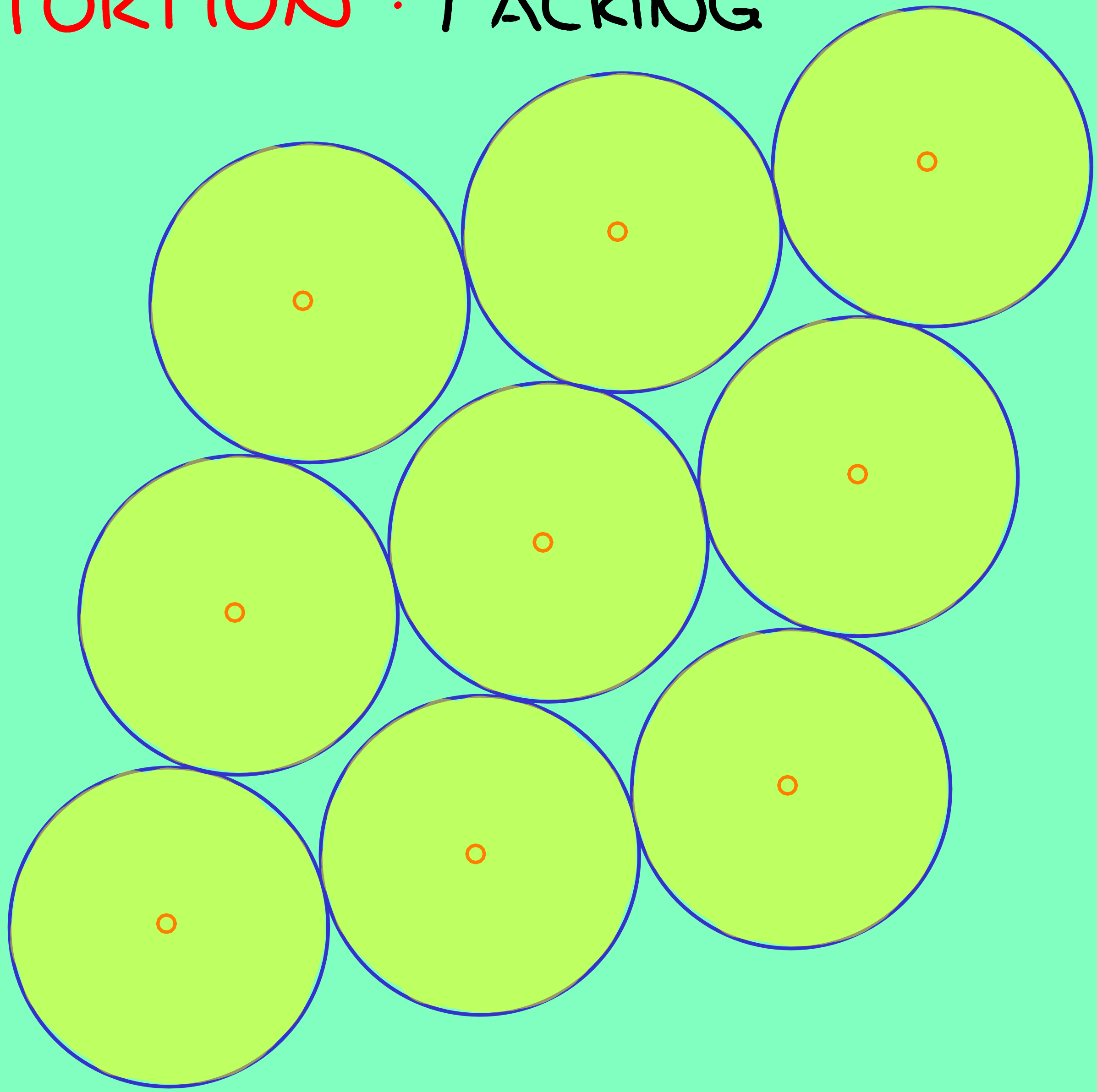

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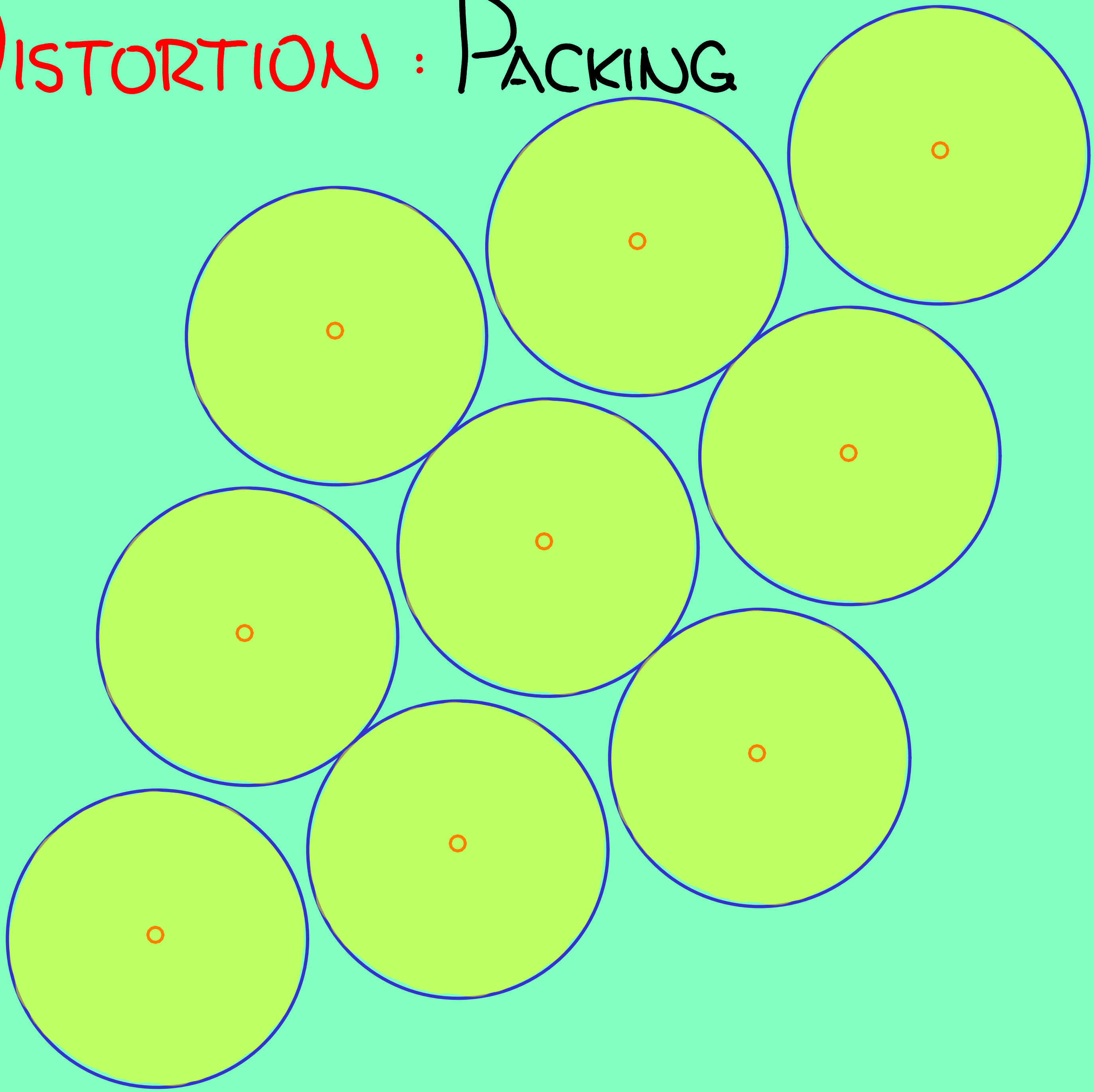

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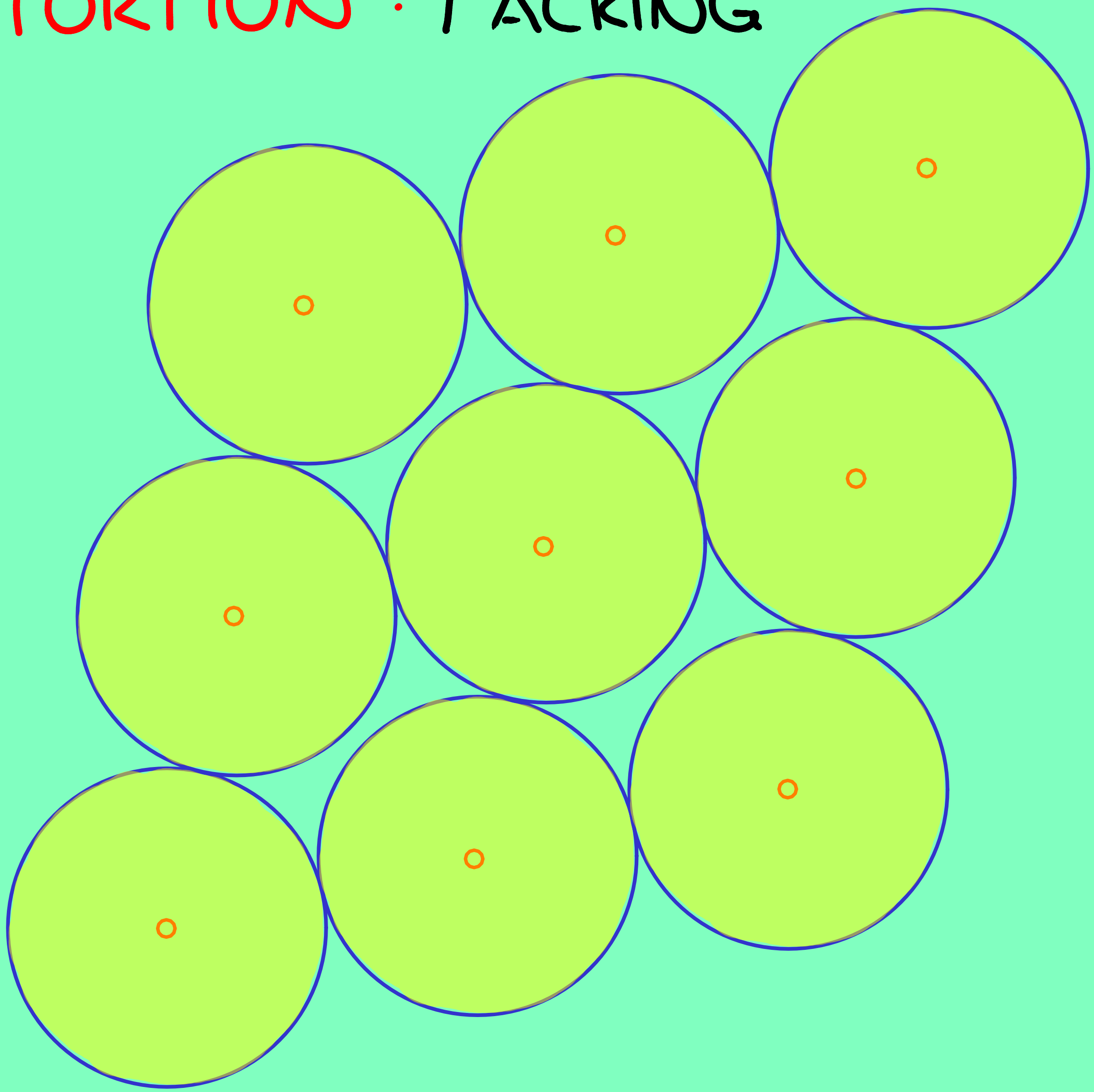

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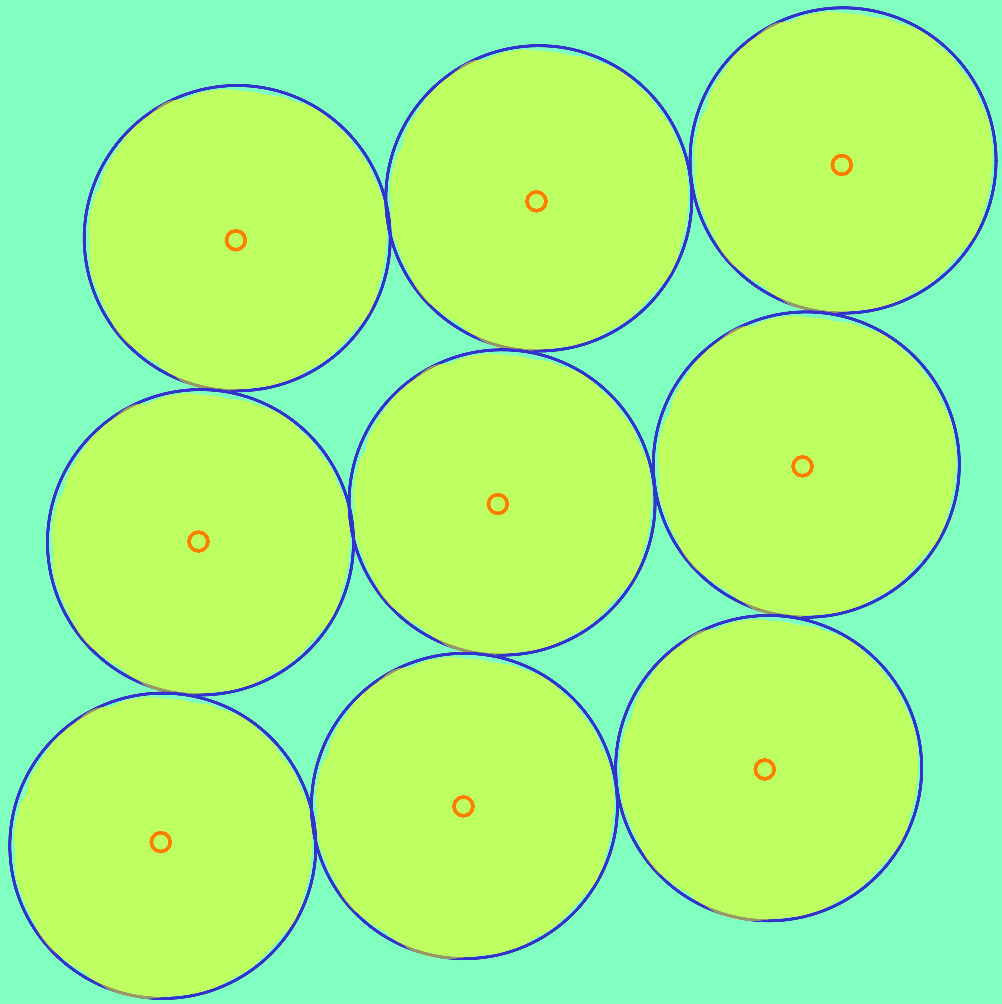

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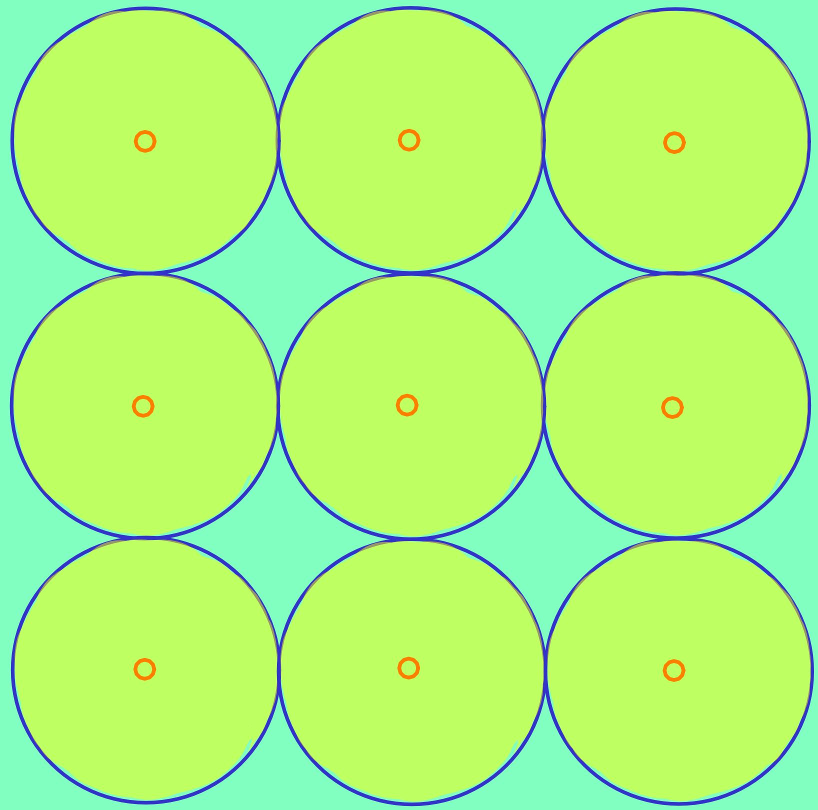
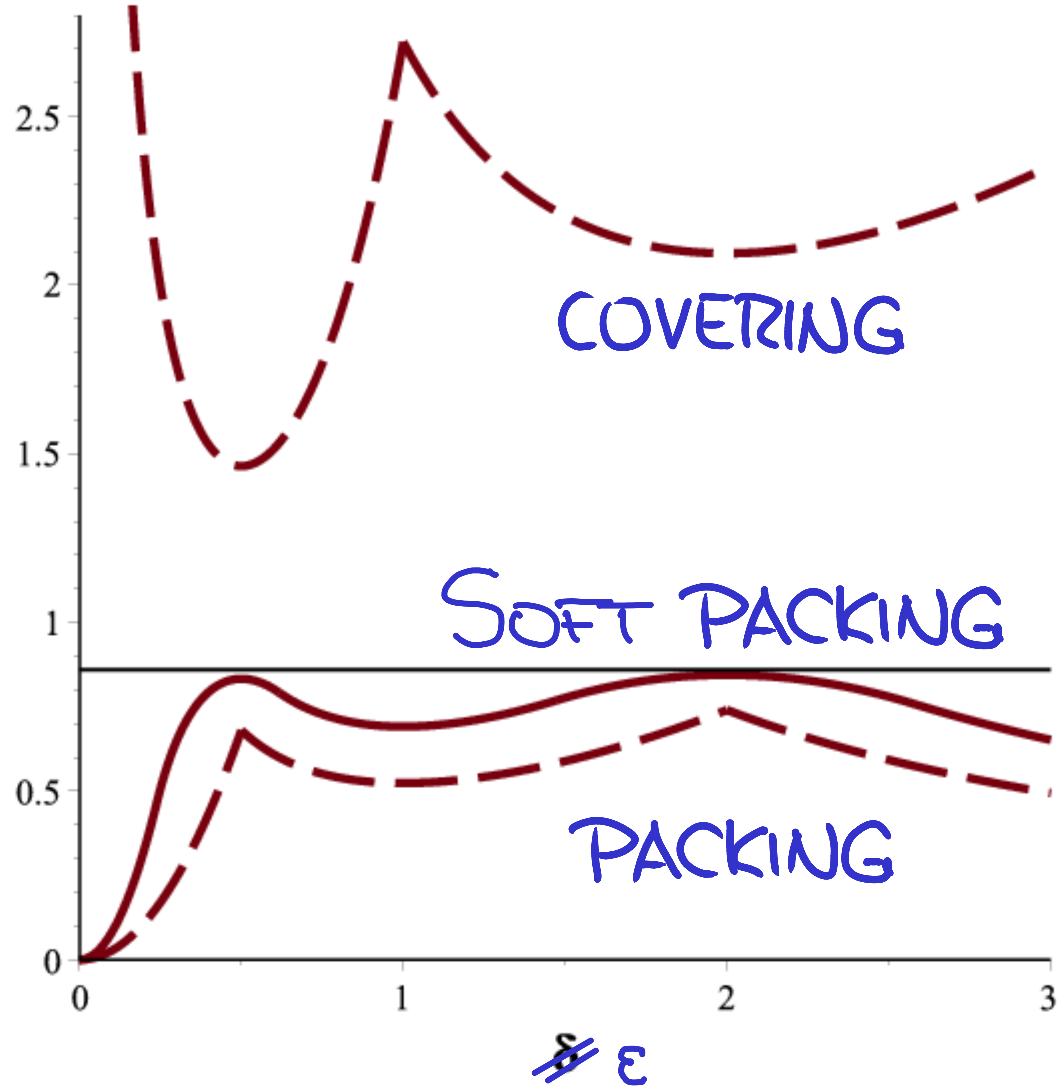




2.5
2
1.5
1
0.5
0
0
1
2
3
COVERING
SOFT PACKING
PACKING
~~δ~~ ε

Soft Packing Theorem

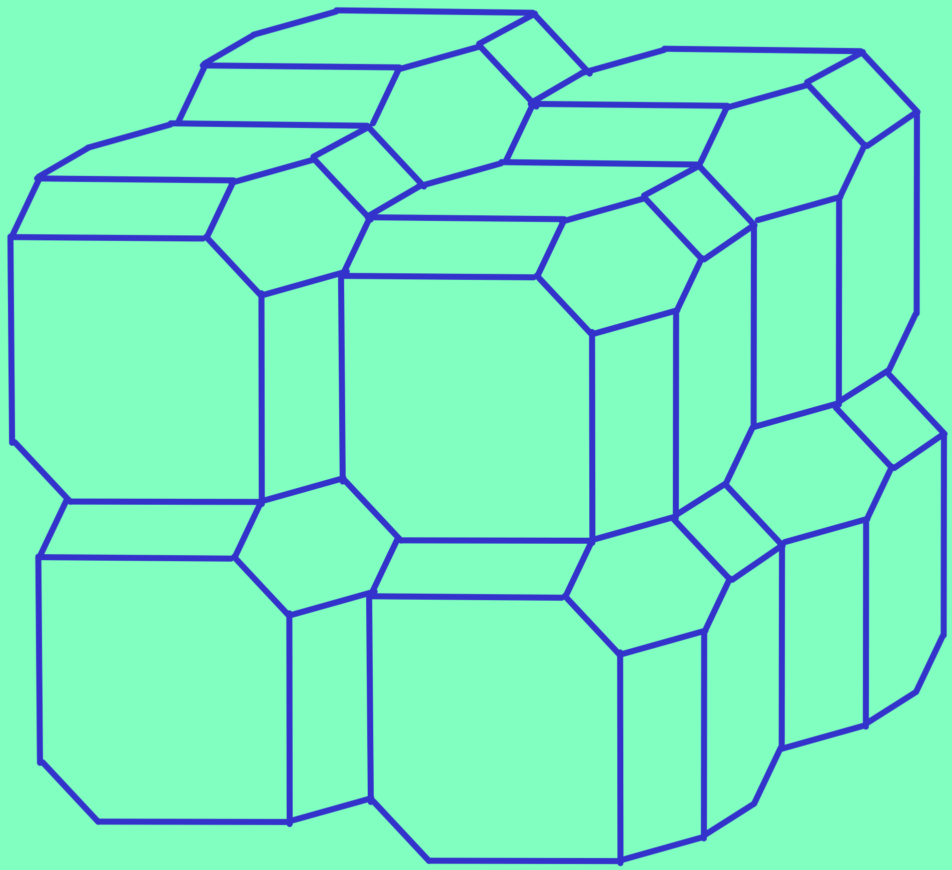
Among the lattices in the diagonal family in $\mathbb{R}^3$, the FCC lattice with spheres of radius $1.090\ldots$ times the packing radius maximizes the soft density at $\delta_1 = 0.844\ldots$.

Combinatorially constant Delaunay mosaic

for $0 < \varepsilon < 1$

and $1 < \varepsilon < \infty$

Compressed Integer Grid



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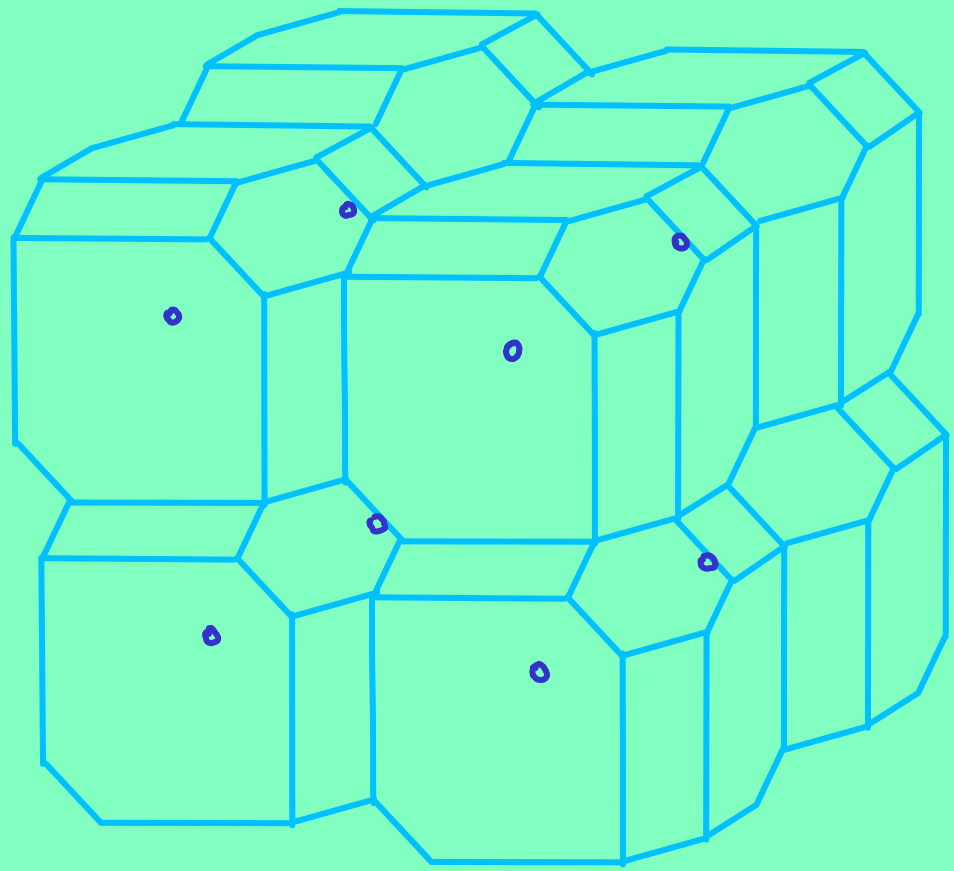

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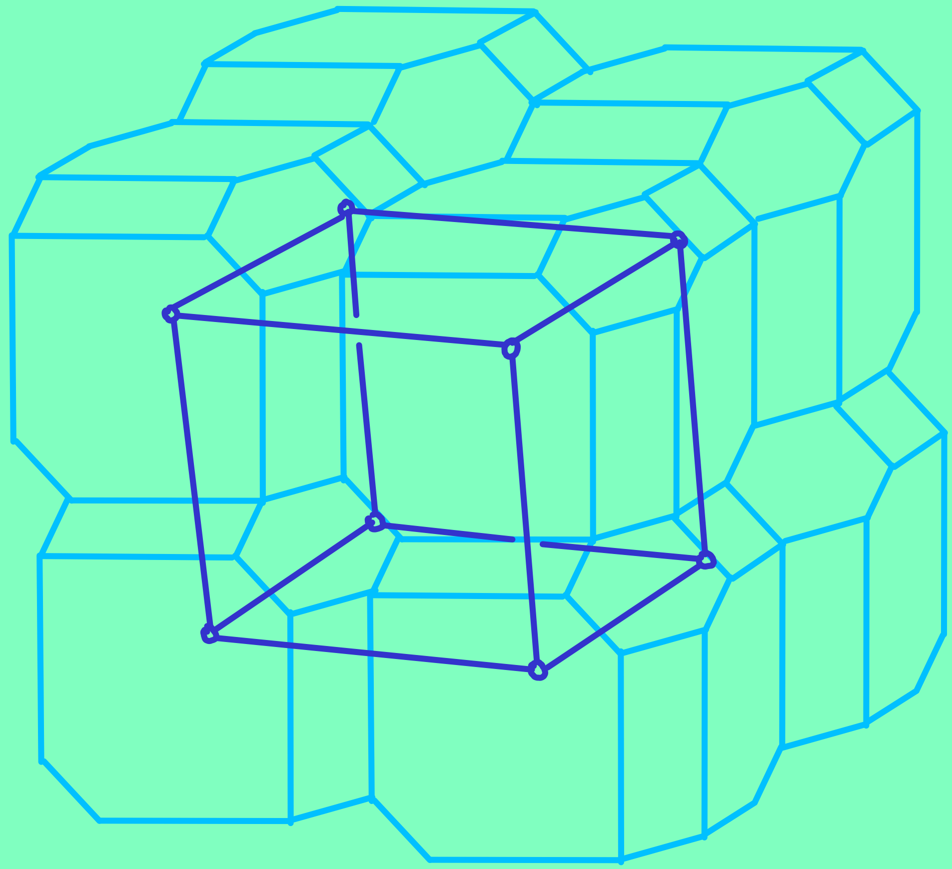

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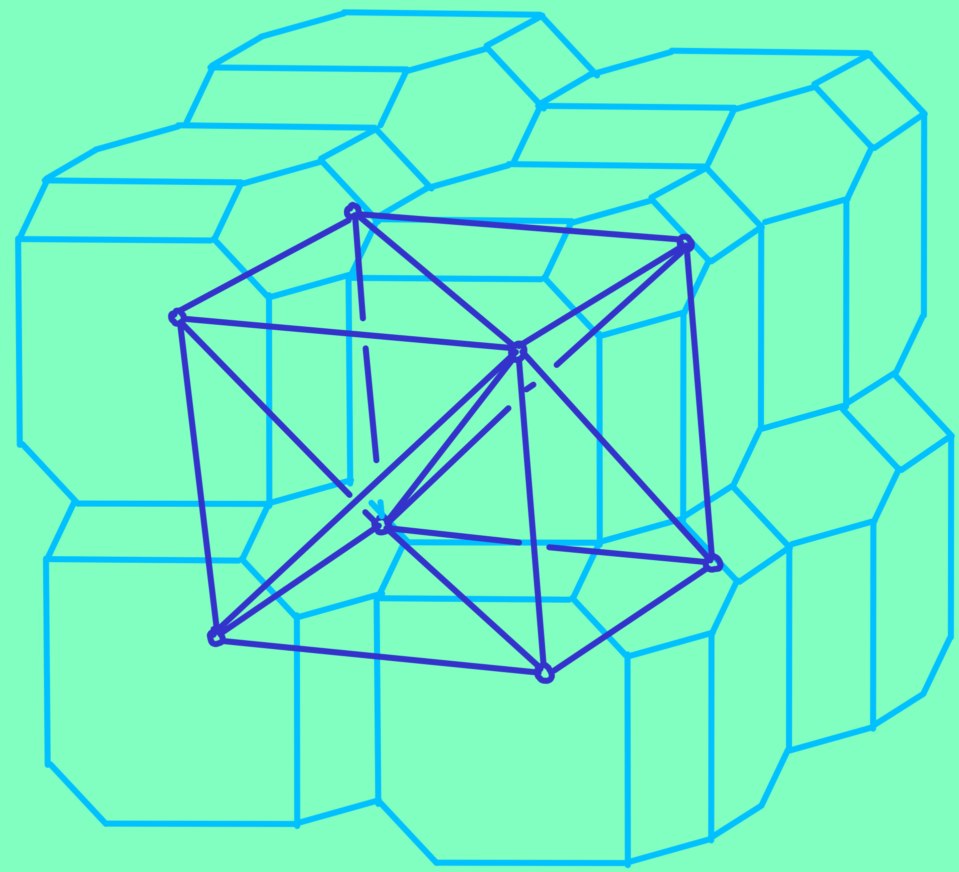
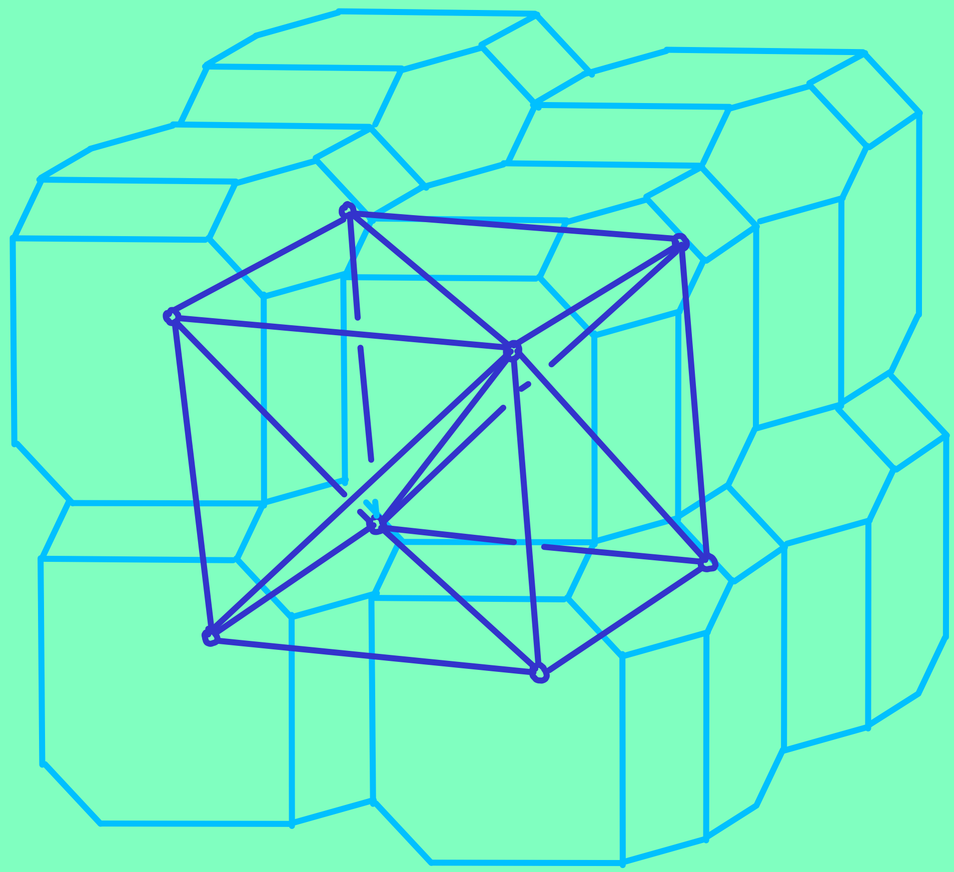
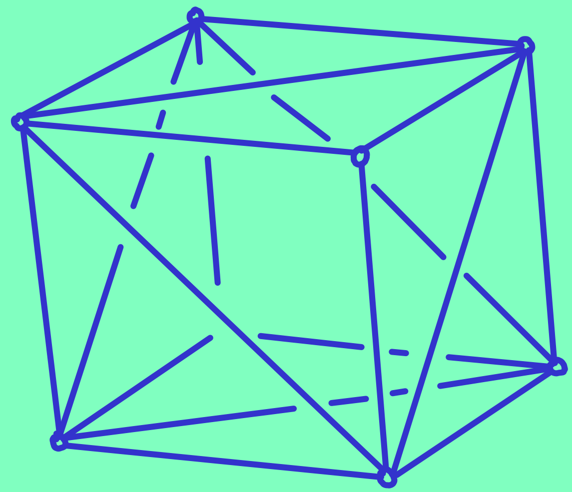


Compressed Integer Grid

$\varepsilon < 1$: Delaunay mosaic is Freudenthal triangulation

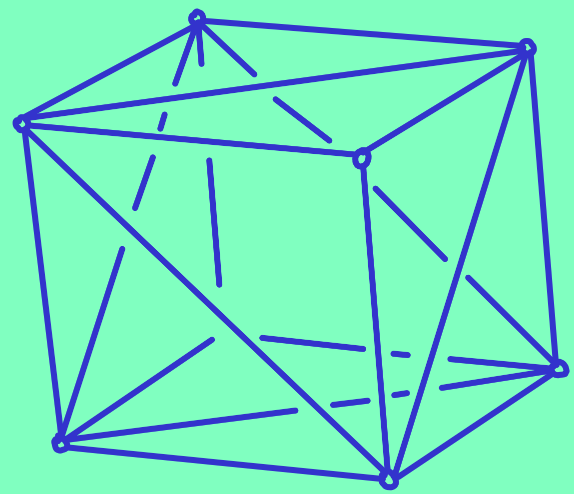


Stretched Integer Grid



Stretched Integer Grid

$\varepsilon > 1$: Delaunay mosaic is slice decomposition



I Diagonal Family of Lattices

II Density and Soft Density

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Density

$\Lambda \subseteq \mathbb{R}^3$, $\quad r \geq 0$, $\quad$ density is $\delta = \dfrac{\mathrm{vol}[B_r]}{|\Lambda|}$

DENSITY

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$\pi_k = \mathrm{Prob}[x \text{ contained in exactly } k \text{ spheres}]$

$\varphi_k = \mathrm{Prob}[x \text{ contained in at least } k \text{ spheres}]$

$= \pi_k + \pi_{k+1} + \pi_{k+2} + \dots$

$\delta = \varphi_1 + \varphi_2 + \varphi_3 + \dots = \pi_1 + 2\pi_2 + 3\pi_3 + \dots$

Soft Density

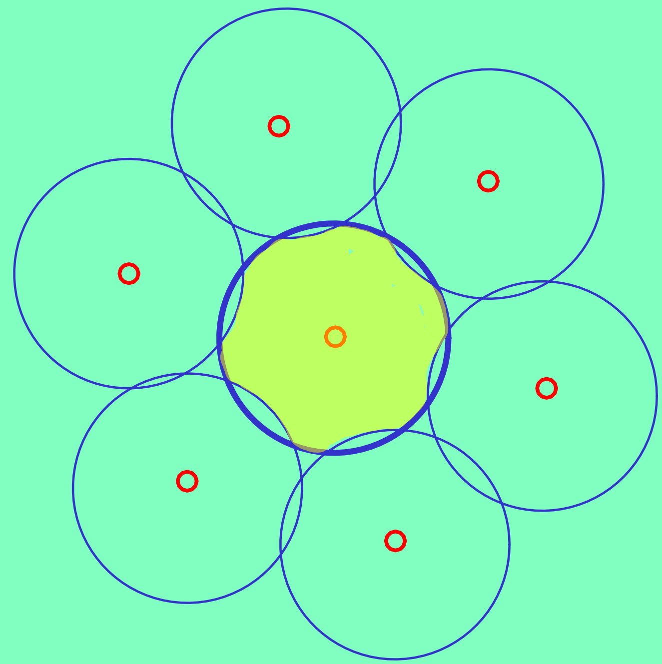
$$\delta_1 = \varphi_1 - \varphi_2 - \varphi_3 - \dots = \pi_1 - \pi_3 - 2\pi_4 - \dots$$

Soft Density

$$\delta_1 = \varphi_1 - \varphi_2 - \varphi_3 - \dots = \pi_1 - \pi_3 - 2\pi_4 - \dots$$

maximized by hexagonal lattice in $\mathbb{R}^2$:

$$\delta_1 = \pi_1 = 0.928\dots$$



[Balázs 1973]

[Bleind, Bleind 1986]

Volume Formulas

k-th Voronoi cell is $V_k(0) = \{x \mid \|x-p\| < \|x\| \text{ for } \leq k-1 \text{ pts } p \in \Lambda\}$

k-th Brillouin zone is $Z_k(0) = V_k(0) \setminus V_{k-1}(0)$

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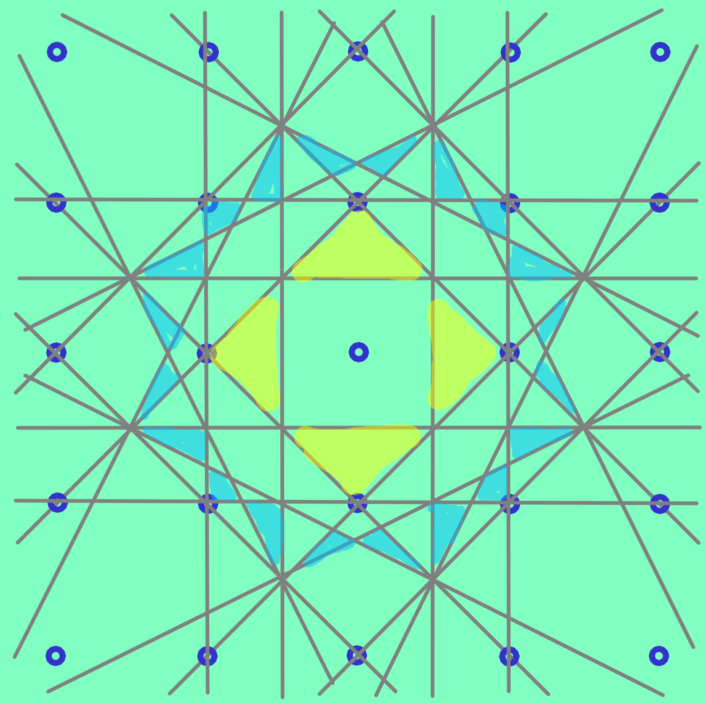

Volume Formulas

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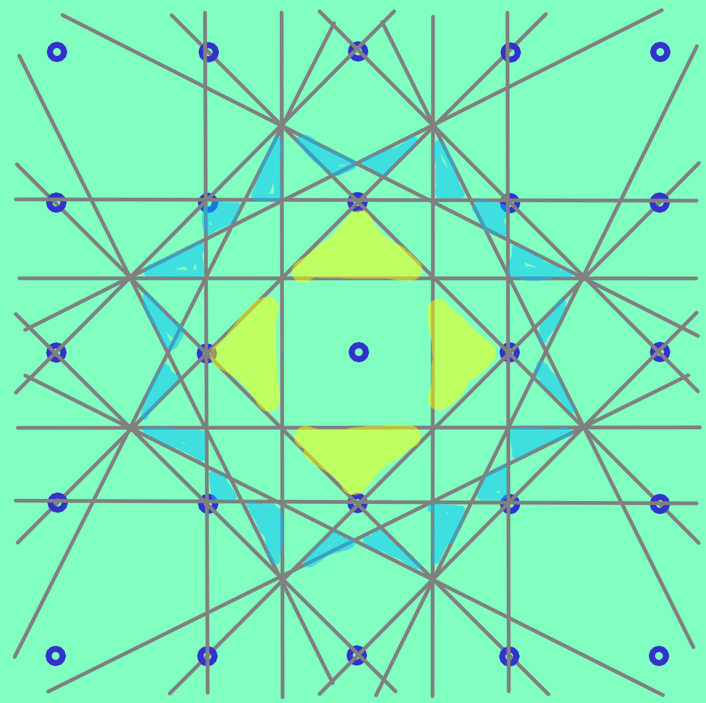
k-th Brillouin zone is $Z_k(0) = V_k(0) \setminus V_{k-1}(0)$

- $\mathrm{vol}[Z_k(p)] = |\Lambda| \qquad \forall k, p$
- $\varphi_k(r) = \dfrac{\mathrm{vol}[Z_k \cap B_r]}{|\Lambda|}$
- $\delta_1(r) = 2\varphi_1 - (\varphi_1 + \varphi_2 + \dots)$

$$= \frac{2\mathrm{vol}[Z_1 \cap B_r] - \mathrm{vol}[B_r]}{|\Lambda|}$$



UNIMODALITY

$f : \mathbb{R}_+ \to \mathbb{R}$ is unimodal if $\exists\, \varrho > 0$ s.t. $\frac{\partial f}{\partial r}(r) \begin{cases} > 0 & \text{if } r < \varrho \\ = 0 & \text{if } r = \varrho \\ < 0 & \text{if } r > \varrho \end{cases}$

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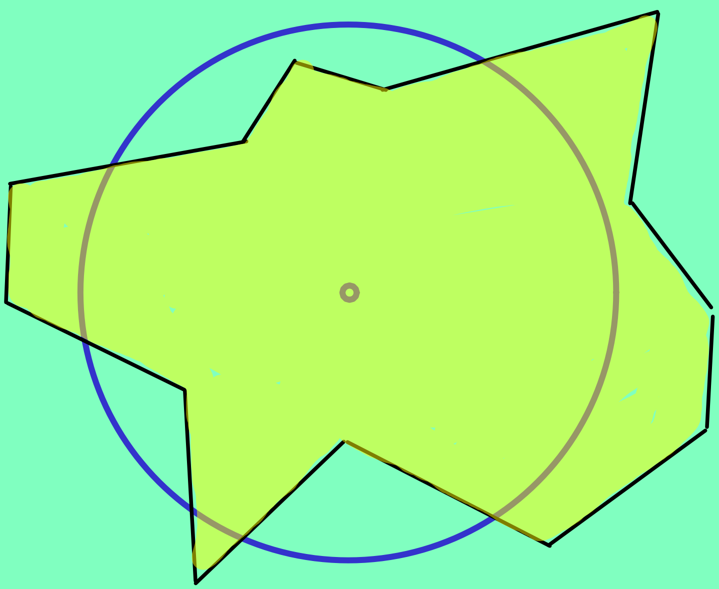
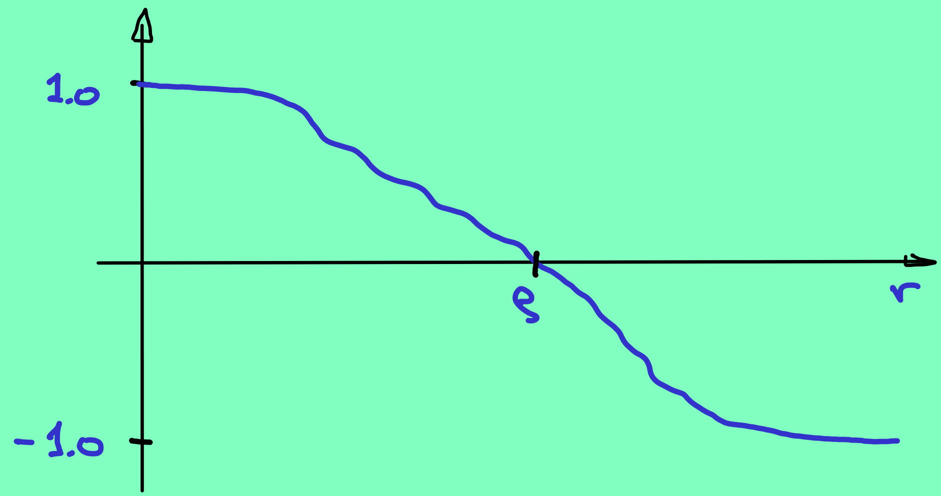
for example $f(r) = \dfrac{|S^{in}_{(r)} - S^{out}_{(r)}|}{|S(r)|}$





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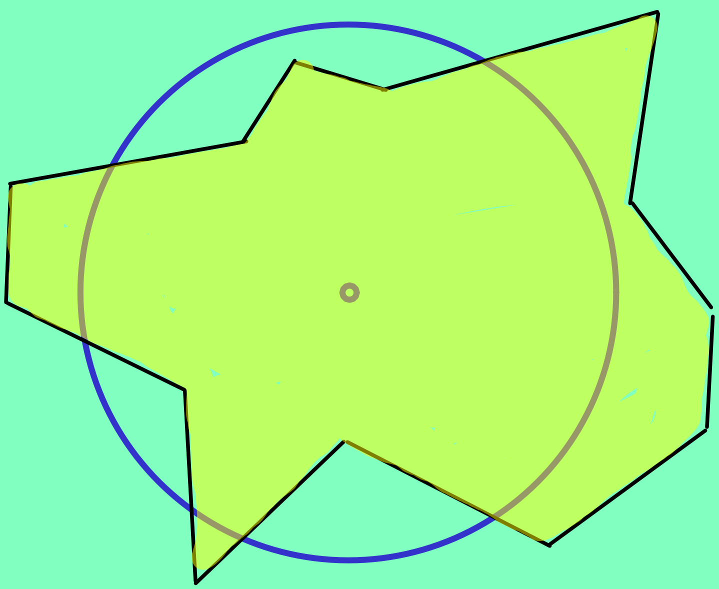
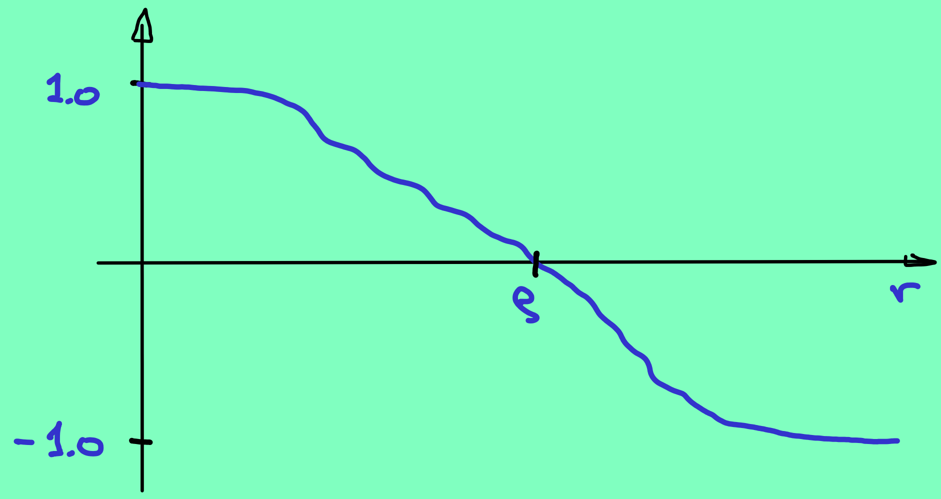
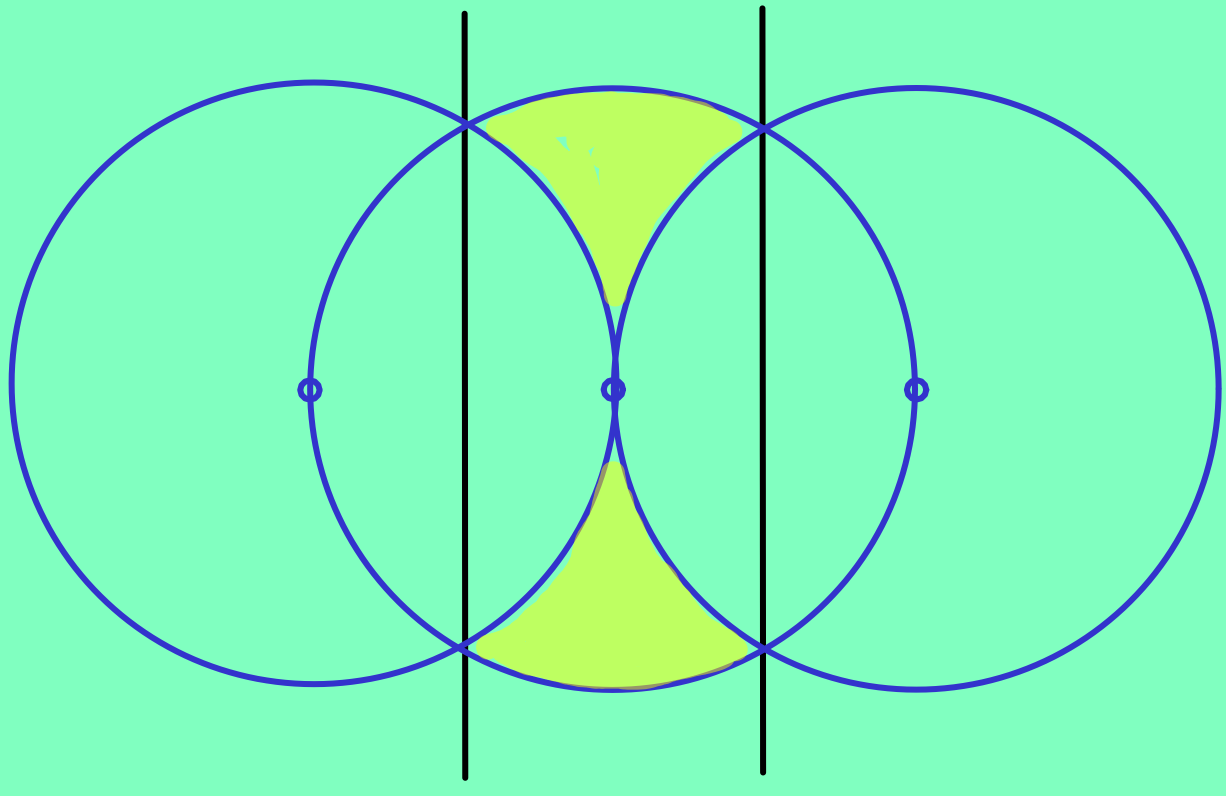




- φ_1 is unimodal.

COUNTER-EXAMPLE

π_1 is not unimodal in $\mathbb{R}^3$



I Diagonal Family of Lattices

II Density and Soft Density

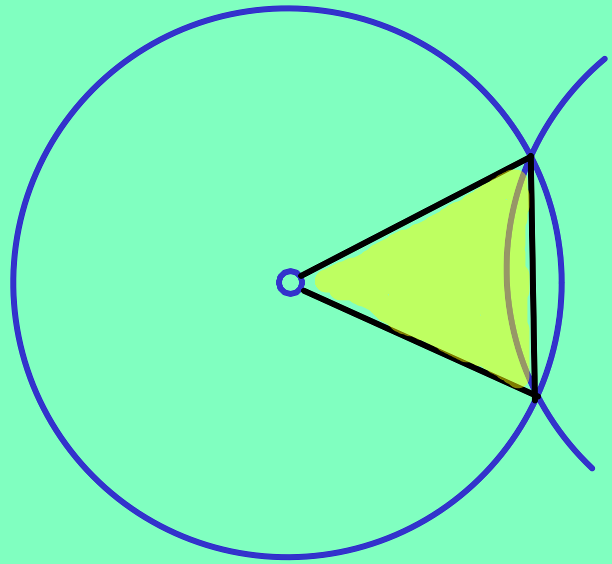
III **Optimality of FCC Lattice**

Soft Density for FCC

$|\Lambda| = 2, \quad r = \sqrt{2}/2$

$\rho = \frac{12}{11} r$

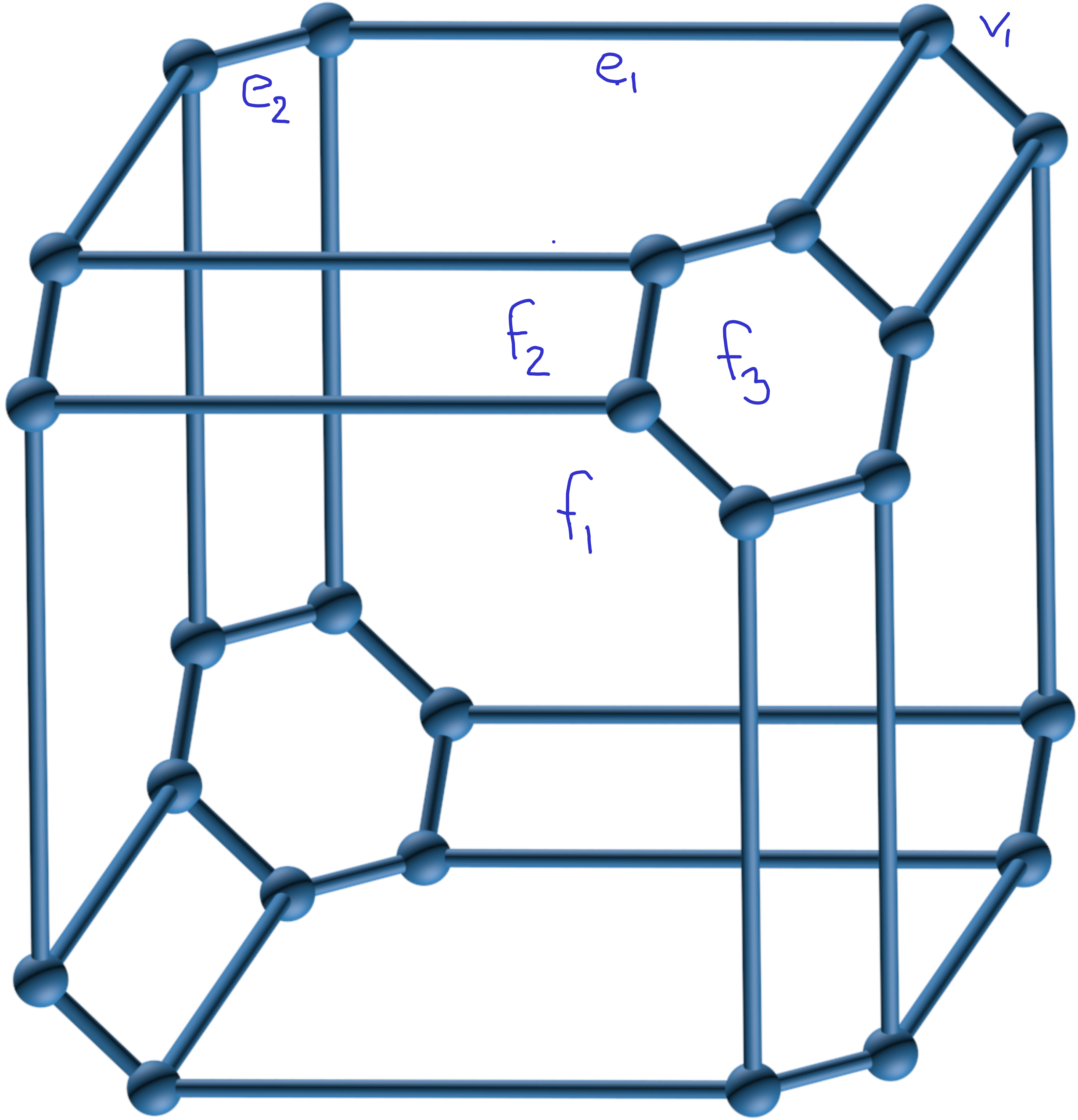
$R = 1$

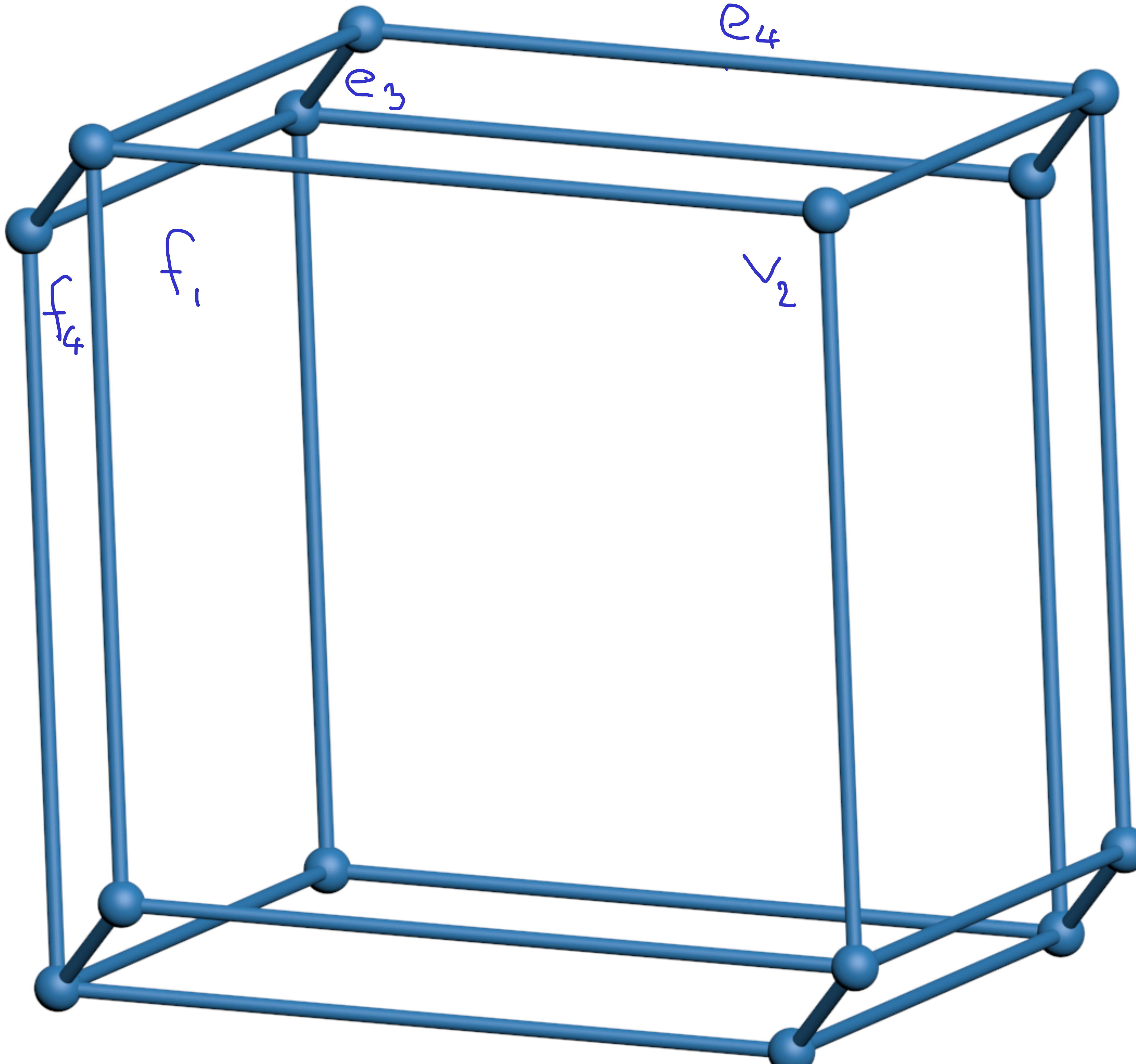


$$\varphi_1 = \frac{1}{2}\left(\frac{\mathrm{vol}[B_r]}{2} + 12\,\mathrm{vol}[\mathrm{Cone}]\right)$$

$$\varphi_2 = \frac{1}{2}\left(\frac{\mathrm{vol}[B_r]}{2} - 12\,\mathrm{vol}[\mathrm{Cone}]\right)$$

$$\delta = \varphi_1 - \varphi_2 = 12\,\mathrm{vol}[\mathrm{Cone}] = 0.844\ldots$$


v_1
e_1
e_2
f_2
f_3
f_1



e_4
e_3
f_1
f_4
v_2

Critical Radii

$$f_1(\varepsilon) = \sqrt{(\varepsilon^2+2)/12}$$

$$f_2(\varepsilon) = \sqrt{(2\varepsilon^2+1)/6}$$

$$f_3(\varepsilon) = \sqrt{3}\,\varepsilon/2$$

$$e_1(\varepsilon) = (\varepsilon^2+2)/(3\sqrt{2})$$

$$e_2(\varepsilon) = \sqrt{(\varepsilon^2+2)(2\varepsilon^2+1)}/(2\sqrt{3})$$

$$v_1(\varepsilon) = \sqrt{8\varepsilon^4+11\varepsilon^2+8}/6$$

$$f_4(\varepsilon) = \sqrt{2}/2$$

$$e_3(\varepsilon) = \sqrt{6}/3$$

$$e_4(\varepsilon) = (\varepsilon^2+2)/\sqrt{12\varepsilon^2+6}$$

$$v_2(\varepsilon) = (\varepsilon^2+2)/(2\sqrt{3}\,\varepsilon)$$

$$v_3(\varepsilon) = \sqrt{\varepsilon^2+8}/(2\sqrt{3})$$

Simplified Soft Density

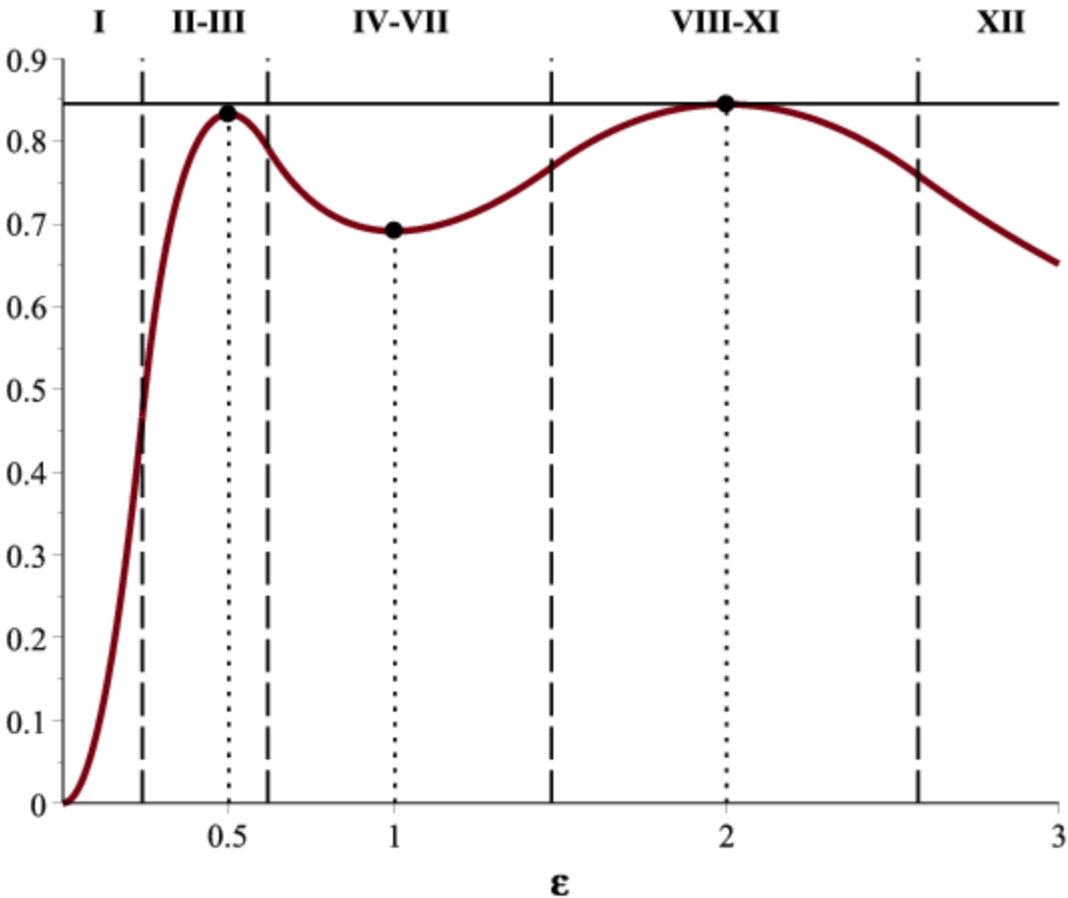
The simplified soft density is

$$\delta_{1s} = \sum_{i=1}^{\infty} (3-2i)\varphi_i = \varphi_1 - \varphi_2 - 3\varphi_3 - \ldots$$

can be computed from pairwise overlaps only.

- $\delta_{1s}(r) \leq \delta_1(r)$
- $\delta_{1s}(r) = \delta_1(r)$ whenever $\varphi_3(r) = 0$

I	$f_3 \leq \rho \leq \ldots$	$0.000 \leq \varepsilon \leq 0.239$
II - III	$f_1, f_3 \leq \rho \leq \ldots$	$0.239 \leq \varepsilon \leq 0.671$
IV - VII	$f_1 \leq \rho \leq \ldots$	$0.671 \leq \varepsilon \leq 1.471$
VIII - IX	$f_1, f_4 \leq \rho \leq \ldots$	$1.471 \leq \varepsilon \leq 2.342$
X - XI	$f_1, f_4, e_3 \leq \rho \leq \ldots$	$2.342 \leq \varepsilon \leq 2{,}576$
XII	$f_4, e_3 \leq \rho \leq \ldots$	$2{,}576 \leq \varepsilon$


I
II-III
IV-VII
VIII-XI
XII
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0.5
1
2
3
ε

THANK YOU