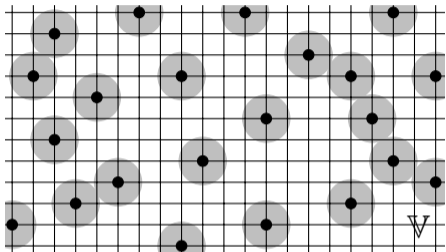


Statistical mechanics of close-packings in 2D lattices

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The hard-core model on a lattice



- A discrete set $\mathbb{L} \subset \mathbb{R}^2$
- A finite volume: $\mathbb{V} \subset \mathbb{L}$
- A configuration of particles: $\psi^{\mathbb{V}} \in \{0, 1\}^{\mathbb{V}}$
- An admissible configuration:
 - $\rho(x, y) \geq D \geq 1$ for any $\psi_x^{\mathbb{V}} = \psi_y^{\mathbb{V}} = 1$
- Activity/Fugacity: $u > 0$

- A boundary condition: an admissible configuration $\phi = \phi^{\mathbb{Z}^2}$
- An additional restriction: $\psi^{\mathbb{V}} \vee \phi^{\mathbb{Z}^2 \setminus \mathbb{V}}$ is admissible, $\psi^{\mathbb{V}} \in \mathcal{A}(\mathbb{V} \parallel \phi)$
- The statistical weight: $w(\psi^{\mathbb{V}} \parallel \phi) = u^{\sharp(\psi^{\mathbb{V}})}$
- The partition function: $\mathbf{Z}(\mathbb{V} \parallel \phi) = \sum_{\psi^{\mathbb{V}} \in \mathcal{A}(\mathbb{V} \parallel \phi)} w(\psi^{\mathbb{V}} \parallel \phi)$

Gibbs measures on \mathbb{L}

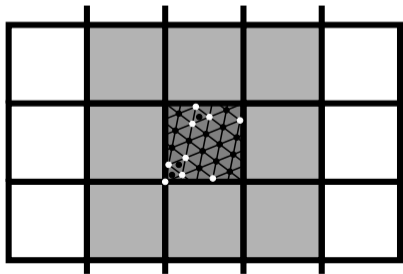
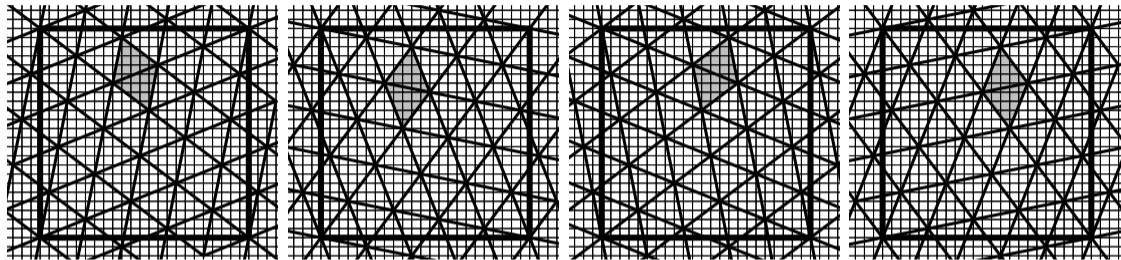
- The Gibbs measure: $\mu_{\mathbb{V}}(\psi^{\mathbb{V}} \parallel \phi) = w(\psi^{\mathbb{V}} \parallel \phi) / \mathbf{Z}(\mathbb{V} \parallel \phi)$
- A probability measure μ on $\mathcal{X} = \{0, 1\}^{\mathbb{L}}$ is called a *D-HC Gibbs/DLR measure* if (i) $\mu(\mathcal{A}) = 1$, (ii) \forall finite $\mathbb{V} \subset \mathbb{L}$ and a function $f : \phi \in \mathcal{X} \mapsto f(\phi) \in \mathbb{C}$ depending only on the restriction $\phi \upharpoonright_{\mathbb{V}}$, the integral $\mu(f) = \int_{\mathcal{X}} f(\phi) d\mu(\phi)$ has the form

$$\mu(f) = \int_{\mathcal{X}} \int_{\{0,1\}^{\mathbb{V}}} f(\psi^{\mathbb{V}} \vee \phi \upharpoonright_{\mathbb{L} \setminus \mathbb{V}}) d\mu_{\mathbb{V}}(\psi^{\mathbb{V}} \parallel \phi) d\mu(\phi).$$

One can say that under such measure μ , the probability of a configuration $\psi^{\mathbb{V}}$ in a finite volume $\mathbb{V} \subset \mathbb{L}$, conditional on a configuration $\phi \upharpoonright_{\mathbb{L} \setminus \mathbb{V}}$, coincides with $\mu_{\mathbb{V}}(\psi^{\mathbb{V}} \parallel \phi)$, for μ -a.a. $\phi \in \{0, 1\}^{\mathbb{L}}$.

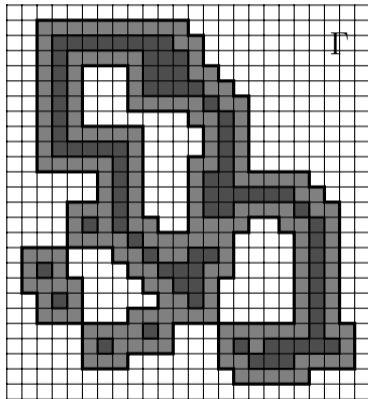
- An extreme Gibbs measure (EGM) = a pure phase: cannot be written as a non-trivial convex combination of other Gibbs measures

Pirogov-Sinai theory: ground states



- Ground states: no local excitation decreases the energy
- Periodic ground states (PGS): energy minimizers on a torus
- A common template
- A correct common template

Pirogov-Sinai theory: contours



- Contours, ensembles of compatible contours

$$\mathbf{Z}(\mathbb{V}||\phi) = \sum_{\{\Gamma_i\}} \prod_i w(\Gamma_i)$$

- A Peierls condition: an excess in energy due to local a defect is proportional to the size of the defect:

$$w(\Gamma) \leq u^{-p(D)||\text{Supp}(\Gamma)||}$$

- A Peierls constant: $p(D) > 0$
- A PGS as a boundary condition: generates a pure phase

Pirogov-Sinai theory: results

Theorem. *Finiteness of the PGS family and a strong enough Peierls condition imply that at least one PGS generates pure phase and any periodic pure phase is generated by some PGS. (Pirogov-Sinai [1976], Zahradnik [1984])*

- Non-periodic ground states

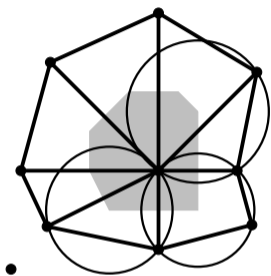
Theorem. *In dimension 2 the finite number of periodic ground states and strong enough Peierls condition imply that all pure phases are periodic. (Dobrushin-Shlosman[1985])*

- Stable and non-stable PGSs (dominance): ensemble of contours with truncated weight, polymer expansion, free energy.
- HC model admits a straightforward application of PS theory but the difficulty is in identifying PGSs and verifying Peierls condition

Local minimizing pattern

- An m -potential (Holztynski-Slawny [1978]):
 - the energy of a configuration is a sum over all translations of a finite set B
 - a minimum of the energy among all configurations in B is achieved at one or more minimizing configurations
 - there exist at least one configuration in entire \mathbb{L} which coincides with one of minimizing configurations on each translation of B in \mathbb{L} .
- A weaker version:
 - a configuration is identified with a partition of \mathbb{R}^2 into bounded sets B_j
 - the energy of a configuration $\{B_j\}$ is the sum of energies attributed to each B_j
 - the variety of B 's contains element(s) with minimal energy
 - there exists a configuration in entire \mathbb{L} formed solely by minimal elements
- A perfect configuration (PC): contains local minimizers only
- All PGSs are PCs
- The minimizing pattern is absent at boundaries between PGSs

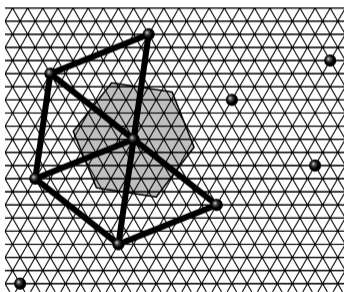
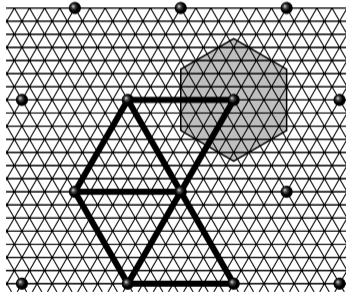
Voronoi cells and disk close-packing in \mathbb{R}^2



- - A Voronoi cell (VC), a convex polygon in \mathbb{R}^2 : defined for each x with $\psi_x = 1$
 - Vertices of a VC: centers of circumcircles
 - A constituting polygon, C-triangle
 - A Delaunay triangulation
- - The area of a VC as a local quantity to minimize:
 - find minimal VCs
 - find all configurations containing minimal VCs only
 - The minimal Voronoi cell in \mathbb{R}^2 is a perfect hexagon

Voronoi cells and disk close-packing in \mathbb{A}_2

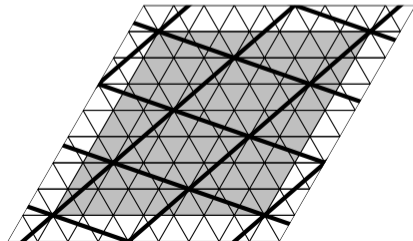
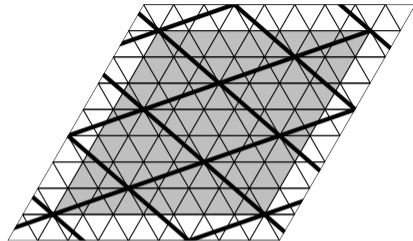
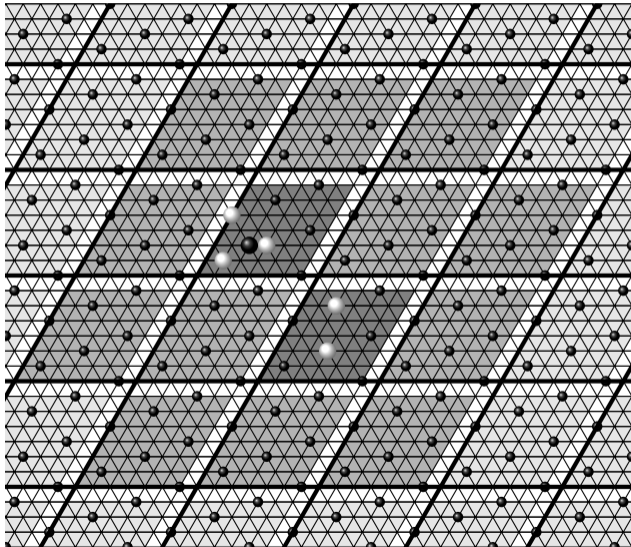
- The minimal Voronoi cell in \mathbb{A}_2 is the same as in \mathbb{R}^2
- For an admissible configuration containing a particle at the origin there are only finitely many possibilities to implement the minimal Voronoi cell centered at this particle



- Each possibility corresponds to the configuration of particles forming a triangular D -sublattice of \mathbb{A}_2
- Each D -sublattice generates a class of PCs which contains its \mathbb{A}_2 -symmetries.

- Depending on arithmetical structure of D^2 , there may be one or more classes
- All PGSs are from classes generated by D -sublattices

Templates and contours on \mathbb{A}_2



Peierls estimate on \mathbb{A}_2 via Voronoi cells

◦ **Theorem.** Define the statistical weight $w(\Gamma)$ of a contour Γ by

$$w(\Gamma) = u^{\#(\psi_\Gamma) - \#(\varphi_\Gamma)} = \prod_{x \in \psi_\Gamma} u^{-S^{-1}(|C_{\psi_\Gamma}(x)| - S)}.$$

Here and below, ψ_Γ stands for the restriction $\psi \upharpoonright_{\text{Supp } \Gamma}$. Then

$$w(\Gamma) \leq u^{-p(D) \|\text{Supp } \Gamma\|}.$$

Next, $S = S(D) = D^2\sqrt{3}/2$ is the area of the minimal Voronoi cell (a perfect hexagon of side length $D\sqrt{3}/2$), $|C_{\psi_\Gamma}(x)|$ is the area of the Voronoi cell $C_{\psi_\Gamma}(x)$ for $x \in \psi_\Gamma$, $p(D) > 0$ is a Peierls constant, and $\|\text{Supp } \Gamma\|$ is the number of templates in $\text{Supp } \Gamma$.

◦ Here $p(D)$ is calculated via the difference $-s(D) < 0$ of areas between minimal and next-to-minimal Voronoi cells

Proof of Peierls estimate on \mathbb{A}_2

Consider x where $|C_{\psi_\Gamma}(x)| > S$; otherwise x does not contribute into $w(\Gamma)$. Observe that

$$\text{if } |C_{\psi_\Gamma}(x)| - S \geq S \text{ then } |C_{\psi_\Gamma}(x)| - S \geq \frac{1}{2} |C_{\psi_\Gamma}(x)| .$$

On the other hand,

$$\text{if } |C_{\psi_\Gamma}(x)| - S < S \text{ then } |C_{\psi_\Gamma}(x)| - S \geq s(D) \geq \frac{s(D)}{2S} |C_{\psi_\Gamma}(x)| .$$

According to the definition of a φ -correct common parallelogram, we have an inequality

$$\sum_{x \in \psi_\Gamma} |C_{\psi_\Gamma}(x)| \mathbf{1} \left(|C_{\psi_\Gamma}(x)| > S \right) \geq \frac{1}{9D^2} |\text{Supp } \Gamma| .$$

Also, $\|\text{Supp } \Gamma\| = \frac{2}{D^4\sqrt{3}} |\text{Supp } \Gamma|$. Thus, we can take

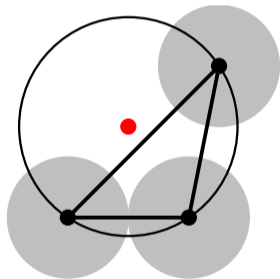
$$p(D) = \frac{1}{9} \min \left(\frac{1}{2}, \frac{s(D)}{\sqrt{3}} D^{-2} \right) . \quad \blacksquare$$

Peierls estimates on \mathbb{H}_2 and \mathbb{Z}^2

- \mathbb{H}_2 can be considered as \mathbb{A}_2 with removed 1/3 of sites (a $\sqrt{3}$ -sublattice)
- For $D^2 \bmod 3 = 0$ the above \mathbb{A}_2 theory is applied to \mathbb{H}_2 verbatim. The PGSs are still triangular D -sublattices and their \mathbb{H}_2 symmetries
- Let $D^* = D_*(D) \geq D$ be the nearest value such that $D_*^2 \bmod 3 = 0$ and $D_*^2 = m^2 + n^2 + mn$.
- For $D^2 \bmod 3 \neq 0$, $D^2 \neq 1, 4, 7, 13, 16, 28, 49, 64, 67, 97, 133, 157, 256$ the PGSs are D_* -sublattices from \mathbb{A}_2 .
- However for $D^2 \bmod 3 \neq 0$ the Voronoi cells do not work.
- The Voronoi cells do not work for \mathbb{Z}^2 either, and we need a different approach

Saturated configurations and minimal triangles

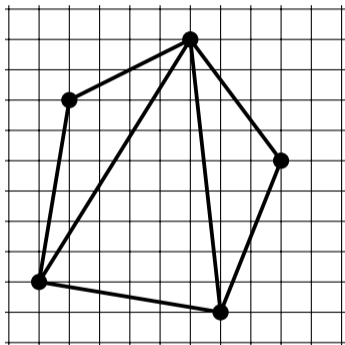
- Saturation of an admissible configuration
- In \mathbb{R}^2 saturation implies (Chang-Wang [2010]):



- all circumradii are $\leq D$ as otherwise a particle can be placed into the circumcenter of the corresponding constituting polygon
- all Delaunay triangles have angles $\leq 2\pi/3$
- amount of triangles is twice the amount of particles

- A minimal triangle (M-triangle): an admissible acute \mathbb{L} -triangle (sides not shorter than D) with a minimal possible area
- M-triangles: better local minimizers than VCs

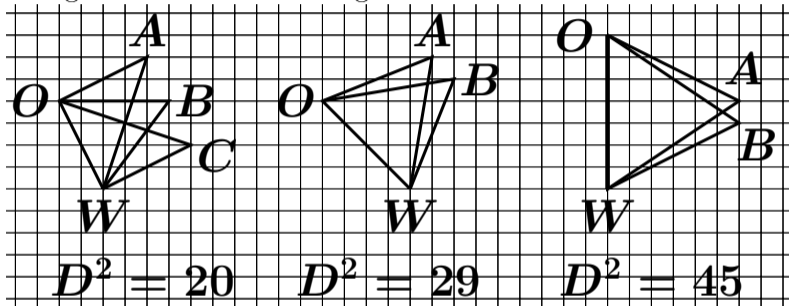
Area-minimization of Delaunay triangles in \mathbb{Z}^2



- All circumradii are $\leq D + \sqrt{2}$
- Obtuse triangles with less than minimal area
- Triangle groups and redistributed area
- Area redistribution is also useful in dealing with other issues, especially on \mathbb{H}_2

M-triangles and sliding in \mathbb{Z}^2

- Sliding in terms of M-triangles



- In absence of sliding:

- an M-triangle generates a unique perfect configuration (PC)
- all PGSs are sublattices or their \mathbb{Z}^2 -symmetries (shifts, rotations, reflections)
- \mathbb{Z}^2 -symmetries define equivalence classes of PCs/PGSs
- the PGS sublattices are non-square for $D^2 > 20$

M-triangles and PGSs on \mathbb{Z}^2

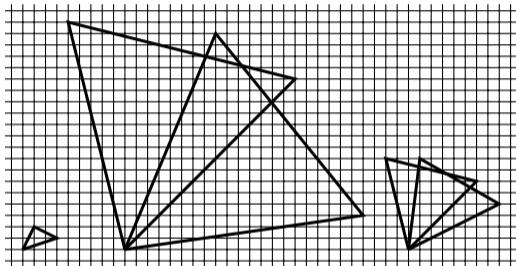
Theorem. (i) *For any attainable D , every PGS is obtained as a tessellation by M-triangles and their \mathbb{Z}^2 -shifts.*

(ii) *Furthermore, if D is non-sliding then every PGS is obtained from a max-dense sub-lattice by means of \mathbb{Z}^2 -congruences. Consequently, for any non-sliding D the PGS set $\mathcal{P}(D)$ is finite.*

○ A similar theorem is true for \mathbb{A}_2 and \mathbb{H}_2 except for the exceptional values of D

Classes of M-triangles on \mathbb{Z}^2

- **Class S** (sliding): finite



- **Class B2** (a non-unique M-triangle, a non-unique implementation), $d = 180610$,
 $[d|d + 60|d + 145]$, $[d|d + 60|d + 145]$, $[d|d + 115|d + 135]$ and $[d|d + 115|d + 135]$
- Classes A, Bx are infinite
- A general strategy: M-triangles \rightarrow PCs \rightarrow PGSs \rightarrow EGMs

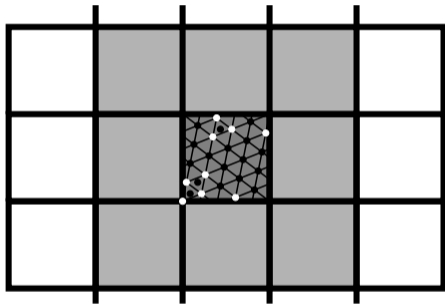
- **Class A** (a unique M-triangle, a unique implementation), $d = 5$, $[5|5|10]$

- **Class B0** (a unique M-triangle, a non-unique implementation), $d = 425$, $[425|425|450]$

- **Class B1** (a non-unique M-triangle, a unique implementation for each), $d = 65$,
 $[65|65|80]$, $[68|68|72]$

C-triangles, M-triangles and defects in \mathbb{Z}^2

○ Let ψ^* be a saturation of a given D -AC ψ .



○ If an added occupied site $x \in \psi^* \setminus \psi$ lies in a template then, clearly, this template is incorrect (more precisely, non- φ -correct in φ for each $\varphi \in \mathcal{P}$). We say that such a template is an *s-defect* (in ψ).

○ Another possibility for a defect is where, in the saturation ψ^* , a template has a non-empty intersection with one of C-triangles that is not an M-triangle. We call it a *t-defect* (again in ψ). C-triangles with obtuse angles $> 2\pi/3$ lead to t-defects by definition.

○ Finally, an incorrect (but actually perfect) template can be simply a neighbor of an s- or a t-defect. We call it an *n-defect* (still in ψ).

A Peierls estimate via M-triangles in \mathbb{Z}^2

◦ **Theorem.** Consider a contour Γ in $\psi \in \mathcal{A}(D)$ containing $\|\text{Supp}\Gamma\| = m$ (incorrect) templates. Set $m = i + j + k$ where i, j, k give the amount of s -, t - and n -defects in ψ_Γ . Then the amounts $\sharp(\psi_\Gamma), \sharp(\varphi_\Gamma)$ of occupied sites in ψ_Γ and φ_Γ satisfy

$$\sharp(\psi_\Gamma) \leq mS(D) - i - \max\left(1, \frac{j}{8S(D)}\right), \quad \sharp(\varphi_\Gamma) = mS(D)$$

◦ Let Δ be a connected component of φ' -correct templates enclosed by a connected component of φ'' -correct templates, $\varphi', \varphi'' \in \mathcal{P}(D)$. Then, in absence of sliding, any extension of this restricted configuration to a $\psi \in \mathcal{A}(D)$ contains a closed chain of adjacent non-minimal C-triangles enclosing Δ . This chain constitutes t -defects in the corresponding contour Γ .

◦ **Theorem.** Assume the value D is non-sliding. For a contour Γ containing $\|\text{Supp}\Gamma\|$ (incorrect) templates

$$w(\Gamma) = u^{\sharp(\psi_\Gamma) - \sharp(\varphi_\Gamma)} \leq u^{-p(D)\|\text{Supp}\Gamma\|}, \quad \text{where } p(D) = 1/(72S(D))$$

and $\frac{\sqrt{3}D^2}{2} < S(D) < \frac{\sqrt{3}D^2}{2} + \sqrt{2}D$

A Peierls estimate via M-triangles in \mathbb{A}_2 and \mathbb{H}_2

◦ **Theorem.** For a contour Γ containing $\|\text{Supp}\Gamma\|$ (incorrect) templates

$$w(\Gamma) \leq u^{-p(D)\|\text{Supp}\Gamma\|}, \quad p(D) = 1/(72S(D)),$$

where $S(D) = \frac{\sqrt{3}D^2}{2}$ for \mathbb{A}_2 , and $\frac{\sqrt{3}D^2}{2} \leq S(D) \leq \frac{\sqrt{3}D_*^2(D)}{2}$ for \mathbb{H}_2 .

◦ M-triangle approach is more technically involved but leads to better estimates

◦ For the case $D^2 = 64$ in \mathbb{H}_2 the corresponding unique M-triangle generates PGSs satisfying above Peierls estimate while the minimal Voronoi cell does not generate an admissible configuration in \mathbb{H}_2 . Consequently, the PGSs consist of next-to-minimal rather than minimal Voronoi cells.

Results for Class A (a unique M-triangle)

○ A complete phase diagram for large u

○ **Theorem.** Assume an attainable value D is of Class A. Then:

- (i) The cardinality $\#\mathcal{P}(D) = mS(D)$ where $m = 1, 2$ or 4 for \mathbb{Z}^2 , $m = 1, 2$ for \mathbb{A}_2 , $m = 2/3, 4/3$ for \mathbb{H}_2 . The PGSs are obtained from each other by \mathbb{L} -congruences.
- (ii) There exists a value $u_* = u_*(D, \mathbb{L}) \in (0, \infty)$ such that for $u \geq u_*$ the following assertions hold true. Every EGM $\mu \in \mathcal{E}(D)$ is generated by a PGS $\varphi \in \mathcal{P}(D)$: $\mu = \lim_{\mathbb{V} \nearrow \mathbb{Z}^2} \mu_{\mathbb{V}}(\cdot \parallel \varphi) (= \mu_{\varphi})$. The measures μ_{φ} are mutually disjoint ($\mu_{\varphi'} \perp \mu_{\varphi''}$ for $\varphi' \neq \varphi''$) and inherit the symmetry properties of their respective PGSs. Moreover, $\#\mathcal{E}(D) = \#\mathcal{P}(D)$.

Results for Class B (a non-unique M-triangle)

- A phase diagram modulo dominance for large u
- **Theorem.** Assume an attainable value D is of Class B with $J = J(D) > 1$ equivalence classes of PGS. Then:
 - (i) The cardinality $\#\mathcal{P}_j(D) = m_j S(D)$ where $m_j = 1, 2$ or 4 for \mathbb{Z}^2 , $m_j = 1, 2$ for \mathbb{A}_2 , $m_j = 2/3, 4/3$ for \mathbb{H}_2 , $j = 1, 2, \dots, J$. The equivalent PGSs are obtained from each other by \mathbb{L} -congruences.
 - (ii) There exists a value $u_* = u_*(D, \mathbb{L}) \in (0, \infty)$ such that for $u \geq u_*$ the following assertions hold true. Every EGM $\mu \in \mathcal{E}(D)$ is generated by a PGS φ from a dominant class $\mathcal{P}_j(D)$: $\mu = \lim_{\mathbb{V} \nearrow \mathbb{Z}^2} \mu_{\mathbb{V}}(\cdot || \varphi) (= \mu_{\varphi})$. The measures μ_{φ} are mutually disjoint ($\mu_{\varphi'} \perp \mu_{\varphi''}$ for $\varphi' \neq \varphi''$) and inherit the symmetry properties of their respective PGSs. Furthermore, $1 \leq \#\mathcal{E}(D) = \sum_{j: \mathcal{P}_j(D) \text{ is dominant}} \#\mathcal{P}_j(D)$.

Polymer series and Dominant PGSs

- The twofold entropy of contours:

- the number of ways to draw $\text{Supp}\Gamma$ with $\|\text{Supp}\Gamma\| = m$ is $\leq 4 \cdot 3^{m-1}$
- the number of ways to select ψ_Γ is $\leq 2^{D^2 S(D)} \leq 2^{D^4}$

- The statistical weight $w(\pi)$ of a polymer $\pi = \{\Gamma_i\}$ satisfies

$$|w(\pi)| \leq u^{(\log_u c(D) - p(D)) \sum_i \|\text{Supp}\Gamma_i\|}$$

- The polymer series for the free energy has the following form

$$\sum_{k=1}^{\infty} a_k u^{-k}, \text{ where } |a_k| \leq c(D)^k$$

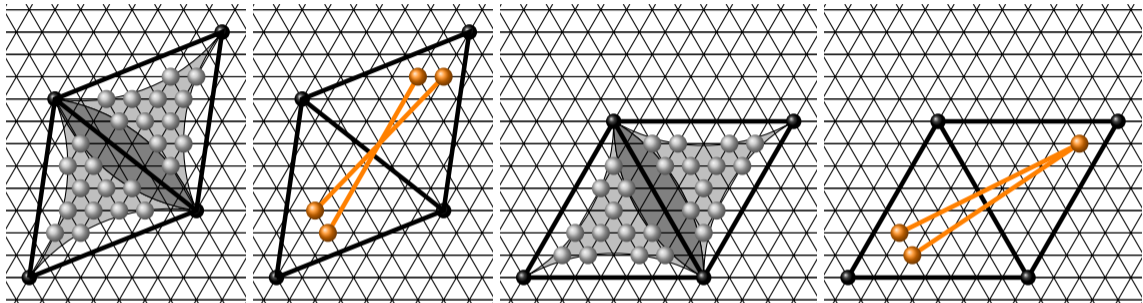
- Dominance of a PGS: the truncated free energy is minimal (and consequently equal to free energy)

- We expect that for our models the dominance can always be seen at the second order u^{-2} in the polymer series

Dominant PGSs: orders of perturbations

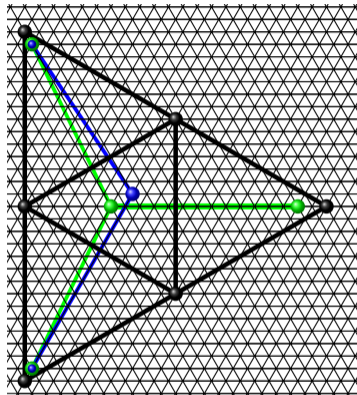
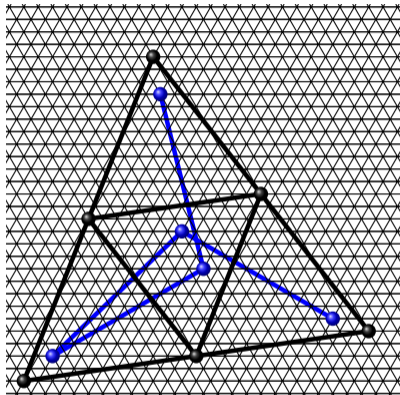
- The constant $p(D)$ is too small to be practical. Need an alternative approach to contour enumeration
- By construction $w(\Gamma) = u^{-k}$, $k \in \mathbb{N}$
- It is possible to show that the only way to create Γ with $w(\Gamma) = u^{-1}$ is to remove a particle. It does not discriminate between the PGSs
- There are multiple ways to create Γ with $w(\Gamma) = u^{-2}$ by removing $n \geq 3$ particles and inserting $n - 2$ particles, without violating admissibility.
- In analyzed examples for $D^2 = 49, 147, 169$ on \mathbb{A}_2 we verified that $n \leq 6$

Perturbation examples: $D^2 = 49$



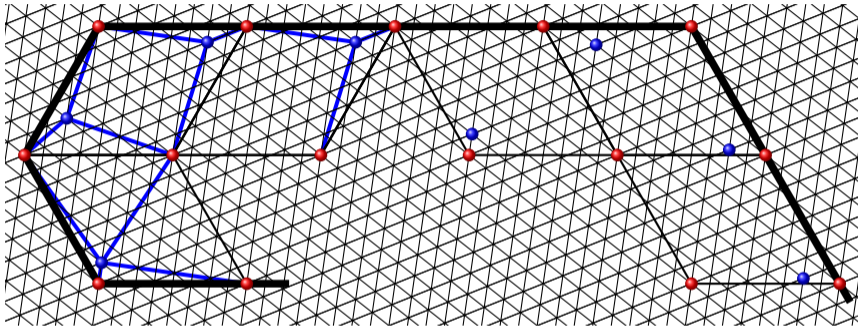
- Gray single-particle insertions ($n = 3$) do not discriminate between PGSs
- Orange pair insertions ($n = 4$) discriminate: the PGS class on the RHS dominates (non-inclined)

Perturbation examples: $D^2 = 147$



- Blue triples represent 3-particle insertions ($n = 5$). A green quadruple represents a 4-particle insertion ($n = 6$)
- In total, for $D^2 = 147$ the PGS class on the RHS dominates

The bound $n \leq 6$ for $D^2 \leq 169$: the proof



○ For $\varphi \in \mathcal{P}(D)$, we assign, to a pair (an insertion at site y , a particle removed by this insertion at site $x \in \varphi$), a repelling force $f_r \geq 0$, $r = \rho(x, y)^2$, so that $\forall y \in \mathbb{A}_2$,

$$F(y) := \sum_{x \in \varphi} f_r \mathbf{1}(\rho(x, y)^2 = r, x \text{ removed by } y) = 1.$$

○ Can define f_r so that

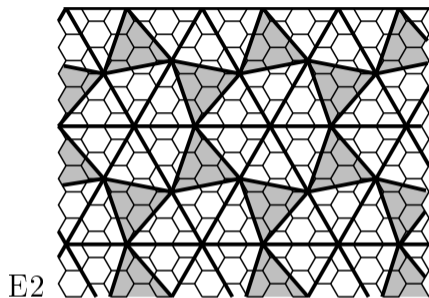
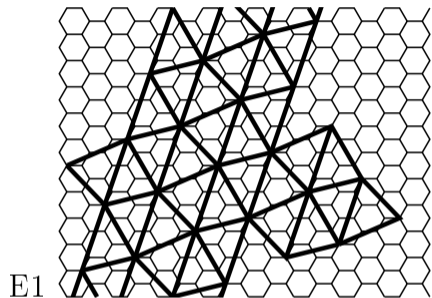
$$G(x) := \sum_y f_r \mathbf{1}(\rho(x, y)^2 = r, x \text{ removed by } y) \leq 1$$

- The proof is computer-assisted. The bound $n \leq 6$ not expected to hold for larger D
- \forall admissible n -particle insertion Δ and $x \in \varphi$, the deficit $\delta(x) := 1 - G(x) \geq 0$
 $\sum_{x \in \varphi} \delta(x) =$ (the difference of the amounts of removed and inserted particles).
- The selection of f_r is not unique but it is possible to choose f_r such that $\delta(x) \geq 1/3$ for $x \in \varphi \cap \partial\Delta$.
- An implication is that on \mathbb{A}_2 , an admissible insertion of order u^{-2} with $n \geq 7$ for $D^2 \leq 169$ is impossible
- We expect that on \mathbb{Z}^2 and \mathbb{H}_2 the future theory will go along similar lines.

PGSs and EGMs for exceptional values of D^2 on \mathbb{H}_2

- Recall: the exceptional values on \mathbb{H}_2 are $D^2 = 1, 4, 7, 13, 16, 28, 49, 64, 67, 97, 133, 157, 256$.
- For $D^2 = 4, 7, 133$: have sliding, offer no results, expect uniqueness of an EGM.
- The case $D^2 = 1$ is trivial: here the only PGS is the whole of \mathbb{H}_2 . The EGM is unique for all $u > 0$: a Bernoulli measure with probability of occupied/vacant site $u/(1+u)$ and $1/(1+u)$.
- The remaining values are divided into 3 classes E1: $D^2 = 13, 16, 28, 49, 64, 97, 157$; E2: $D^2 = 16, 256$; E3: $D^2 = 67$.
- For values D^2 from E1: the PGSs are constructed from quadrilaterals formed by two adjacent D -admissible \mathbb{H}_2 -triangles with the minimal squared side-length D^2 , one of which is an M-triangle. (For $D^2 = 64$ the two triangles are congruent.)

PGSs and EGMs for Classes E1, E2

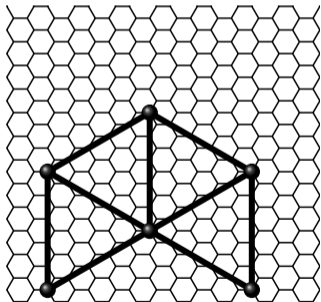


○ For values $D^2 = 16, 256$ from E2: the PGSs are constructed from equilateral triangles of squared side-lengths $(2D + 1)^2$ (outer) and $D^2 + D + 1$ (inner)

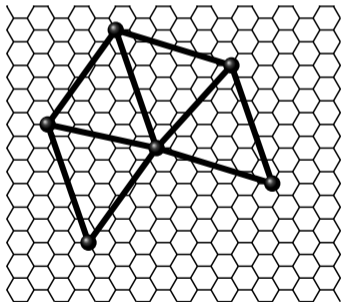
○ **Theorem.** *Let D be from Class E1 or E1. Then each EGM is generated by a PGS and each PGS generates an EGM. All assertions stated for Class A hold true.*

PGSs and EGMs for Class E3

○ For the remaining value $D^2 = 67$ the situation is as in Class B: we have a competition between two groups of PGSs. They are build (a) from equilateral D_* -triangles where $D_*^2 = 75$, (b) from quadrilaterals, similarly to Class E1. It turns out that type (a) is dominant and type (b) not.



(a)



(b)