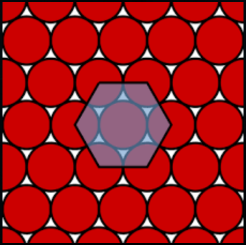
The hard-core model in discrete 2D

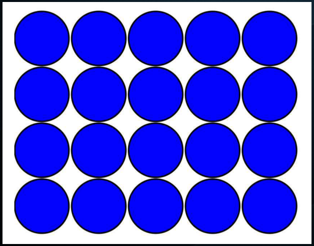
Izabella Stuhl

This is a joint work with **Alexander Mazel** and **Yuri Suhov**

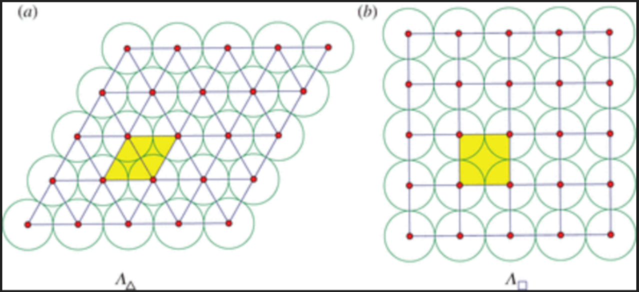
May 18, 2020

Dense disk-packing in a popular culture

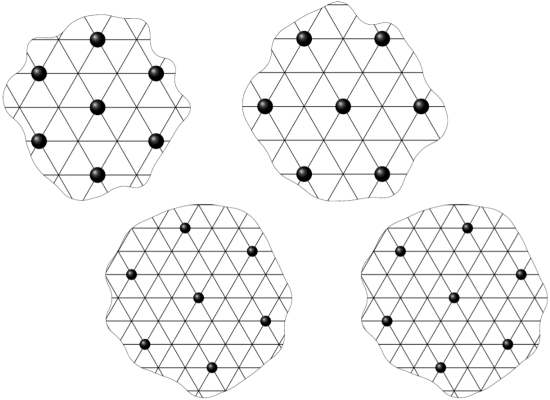




Dense disk-packing on unit lattices: (a) triangular, (b) square



Dense disk-packing on triangular lattice



Fragments of the dense-packed configurations for $D = \sqrt{3}$, $D = 2$ *and* $D = \sqrt{7}$*; the latter case is represented by two configurations obtained from each other by a reflection (about any of the 3 directions constituting* $\mathbb{L}$*).*

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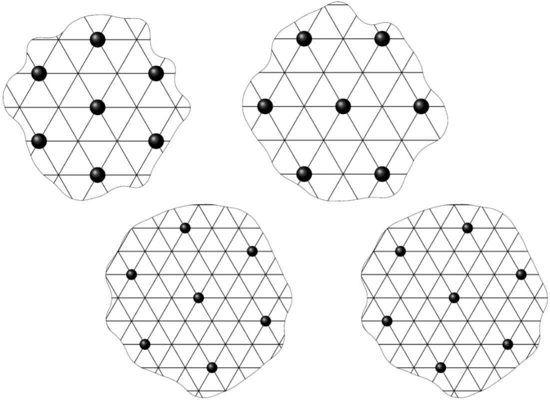

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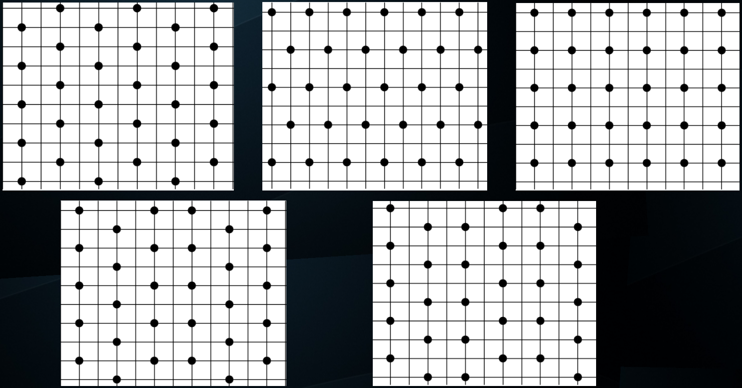
Inscribed/inclined triangular/hexagonal arrangement depending on the value of D.

Dense disk-packing on square lattice

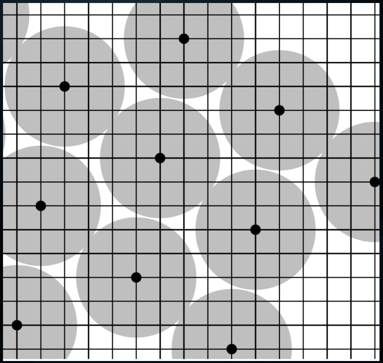


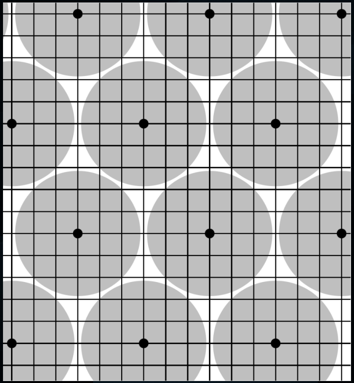
$D = 2$

Lattice and non-lattice: all have the same particle density 1/4.

Dense disk-packing on square lattice

First surprises: the disks do not want to touch each other (at least, partially). And they do not want to form squares (for $D^2 \geq 20$).



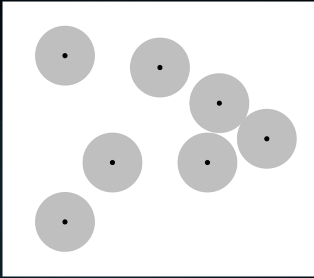


$D = 5, \sqrt{32}$

The object of investigation: the hard-core model

The *hard-core* model was introduced in late 1940s and early 1950s in theoretical chemistry, for a gas where the particles

- have non-negligible diameters,
- cannot overlap.



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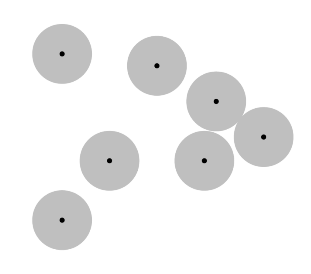

The impact of the model spread out to many areas: theoretical and mathematical physics, dynamical systems, computer science, network theory, social sciences, etc.

The hard-core model

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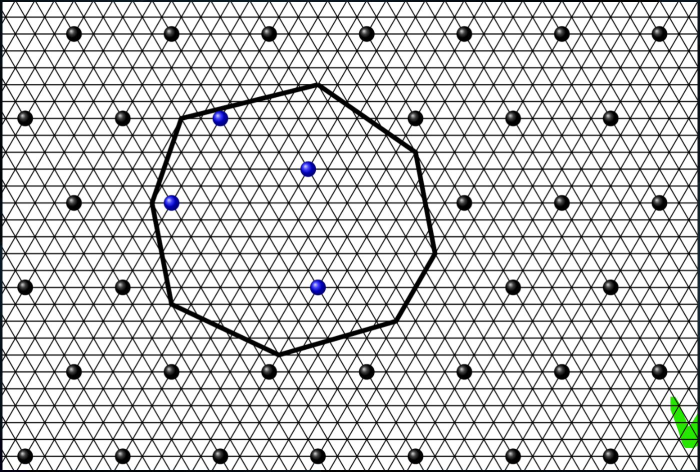
(a)

Let $\mathbb{W} \subset \mathbb{R}^d$ be a countable set. We say that a configuration $\phi \in \{0,1\}^{\mathbb{W}}$ is D-**admissible** if $\rho(x,y) \geq D$ $\forall$ pairs of 'occupied' points $x, y \in \mathbb{W}$ with $\phi(x) = \phi(y) = 1$. The set of D-admissible configurations is denoted by $\mathcal{A} = \mathcal{A}(\mathbb{W}, D)$. The notion of a D-admissible configuration can be given $\forall$ finite set $V \subset \mathbb{R}^d$.

Concatenated configurations, $\mathbb{W}$: a triangular lattice

$D = 5$



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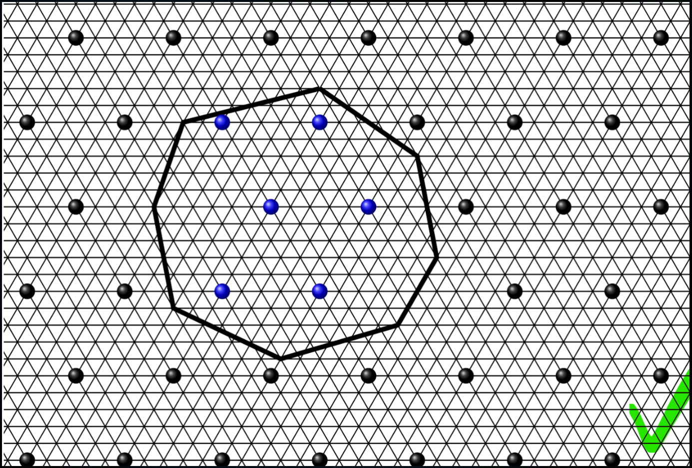

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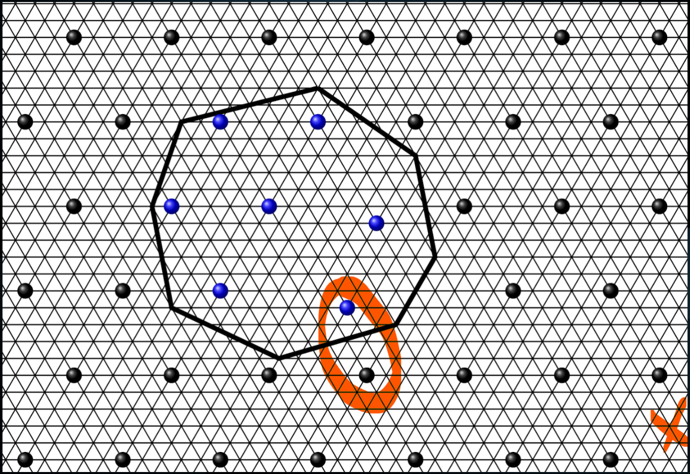

The hard-core model

(b)

Let $V \subset \mathbb{W}$ be a finite set, and $\phi \in \mathcal{A}$ be a D-admissible configuration. We say that a finite configuration $\psi^V \in \{0,1\}^V$ is **compatible** with ϕ if the concatenated configuration $\psi^V \vee (\phi \upharpoonright_{\mathbb{W}\setminus V}) \in \mathcal{A}$.

Given $u > 0$, consider a probability measure $\mu_{V|\mathbb{W}}(\,\cdot\,\|\phi)$ on $\{0,1\}^V$ given by

$$\mu_{V|\mathbb{W}}(\psi^V\|\phi) = \begin{cases} \dfrac{u^{\sharp(\psi^V)}}{Z(V|\mathbb{W};\phi)}, & \text{if } \psi^V \text{ and } \phi \text{ are compatible,} \\ 0, & \text{otherwise.} \end{cases}$$

(i) $\sharp(\psi^V)$ is the number of occupied sites in ψ^V,

(ii) $Z(V|\mathbb{W};\phi) = \sum_{\psi^V \in \{0,1\}^V} u^{\sharp(\psi^V)} \mathbf{1}(\psi^V \text{ compatible with } \phi)$

the *partition function* in V with the boundary condition ϕ.

(c)

A probability measure μ on $\{0,1\}^{\mathbb{W}}$ is called a D-**hard-core Gibbs/DLR-measure** on $\{0,1\}^{\mathbb{W}}$ if $\forall$ finite $V \subset \mathbb{W}$ and a function $f : \phi \in \{0,1\}^{\mathbb{W}} \mapsto f(\phi) \in \mathbb{C}$ depending only on the restriction $\phi \restriction_V$, the integral $\mu(f) = \int_{\{0,1\}^{\mathbb{W}}} f(\phi) \mathrm{d}\mu(\phi)$ has the form

$$\mu(f) = \int_{\{0,1\}^{\mathbb{W}}} \int_{\{0,1\}^V} f(\psi^V \vee \phi \restriction_{\mathbb{W}\setminus V}) \mathrm{d}\mu_{V|\mathbb{W}}(\psi^V \| \phi) \mathrm{d}\mu(\phi).$$

It means that under μ, the probability of a configuration in a finite subset $V \subset \mathbb{W}$ conditional on a configuration $\phi \restriction_{\mathbb{W}\setminus V}$ coincides with $\mu_{V|\mathbb{W}}(\psi^V \| \phi)$, for μ-a.a. ϕ.

Hard-core Gibbs measures: uniqueness *vs* non-uniqueness

One of the main questions: verify, for given $\mathbb{W}$, D and u, whether there is a **unique** hard-core Gibbs measure or **many**.

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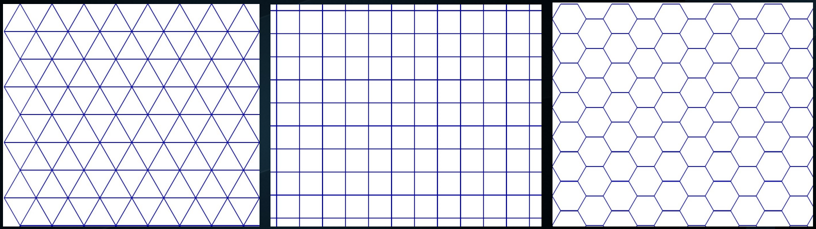
In the latter case it would be interesting to describe **extreme** Gibbs measures since every Gibbs measure is a mixture of these.

We focus upon $\mathbb{W} = \mathbb{A}_2, \mathbb{Z}^2, \mathbb{H}_2$.



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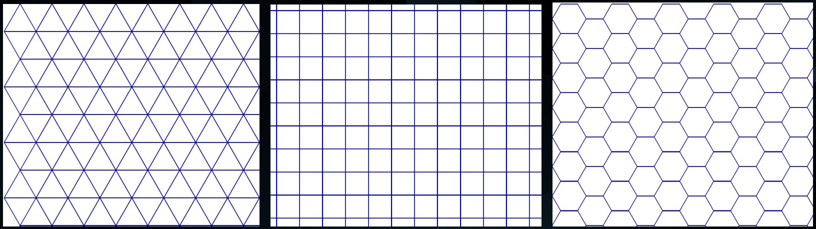

$\diamond$ The exclusion diameter D is measured in the Euclidean metric ρ.

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For $\mathbb{W} = \mathbb{A}_2$:

- **Heilmann & Praestgaard** (1973): non-uniqueness for large u, for a large collection of values of D.
- **Baxter** (1980): The critical value for $D = \sqrt{3}$ is $u_{\mathrm{cr}} = \frac{1}{2}(11 + 5\sqrt{5})$.

$\mathbb{W} = \mathbb{A}_2, \mathbb{Z}^2, \mathbb{H}_2$

I'll address the question about the number of extreme hard-core Gibbs/DLR measures on $\mathbb{A}_2$, $\mathbb{Z}^2$ and $\mathbb{H}_2$ in a large fugacity regime ($u >> u_{cr} \vee 1$) for any D.

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◇ As was said, we are interested in the *extreme* Gibbs/DLR measures μ which cannot be written as a non-trivial convex linear combination $\alpha\mu_1 + (1-\alpha)\mu_2$ of Gibbs measures μ_1 and μ_2.

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Pirogov-Sinai theory:

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Dobrushin-Shlosman: in 2D, non-periodic ground states do **not** generate extreme Gibbs measures.

(Periodic) Ground States

A ground state: a D-admissible configuration φ on the lattice which cannot be improved locally: for any D-admissible configuration ψ that differs from φ on a finite set of lattice sites $\mathbb{V}$

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A ground state φ is called **periodic** if there exist linearly independent vectors e_1, e_2 such that φ is invariant under lattice shifts S_{e_i}:

$$S_{e_i}\varphi = \varphi, \quad i = 1, 2.$$

$\mathbb{W} = \mathbb{A}_2$: Periodic ground states = D-sublattices

Any ordered pair of integers (a, b) solving the equation $D^2 = a^2 + b^2 + ab$ defines a D-**sublattice** in $\mathbb{A}_2$ containing the origin and the following 6 sites:
$(a, b); (-b, a + b); (-a - b, a); (-a, -b); (b, -a - b); (a + b, -a)$

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The periodic ground states are obtained from the sublattices by shifts along the **fundamental parallelograms** and rotations.

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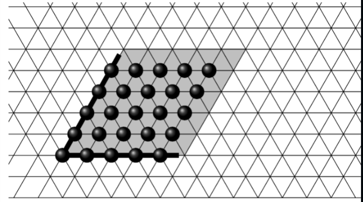

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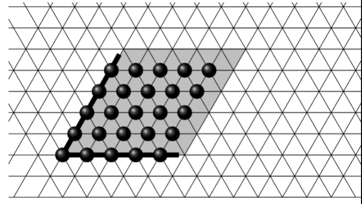

Fundamental parallelogram for $D = 5$

Each periodic ground state is completely determined by just two occupied sites x, y with $\rho(x, y) = D$.

This is a 'rigidity' property of $\mathbb{A}_2$; it simplifies the analysis on $\mathbb{A}_2$ comparing to $\mathbb{Z}^2$.

Eisenstein integer ring

Eisenstein integers:

$$z = a + b\omega \in \mathbb{C}, \text{ where } \omega = -\frac{1}{2} + i\frac{\sqrt{3}}{2}, \quad a, b \in \mathbb{Z}.$$

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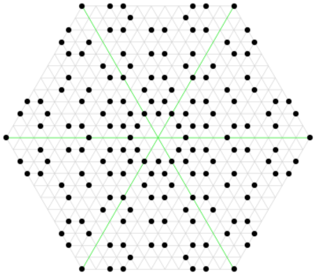

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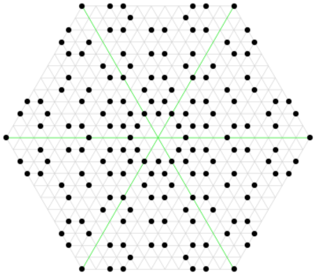

$D^2 = c^2 + d^2 + cd = \varepsilon(1-\omega)^\alpha \prod_{i\geq 0} {p_i}^{\beta_i} \prod_{j\geq 0}(a_j - b_j\omega)^{\gamma_j} \prod_{k\geq 0}(a_k - b_k\omega^2)^{\delta_k}$

$\mathbb{A}_2$: Extreme Gibbs measures

Theorem 1

There are $m \cdot D^2$ periodic ground states, where $m = 1$ or 2 depending on the Eisenstein prime decomposition of D^2. There exists $u^0 \in (1, \infty)$ such that for all $u \geq u^0$ the following properties hold.

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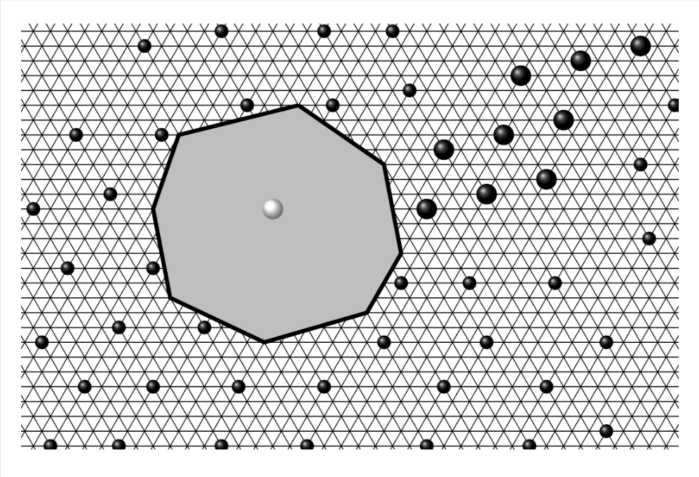
We say that an extreme Gibbs/DLR measure μ is generated by a periodic ground state φ if
$\mu = w - \lim_{V \nearrow \mathbb{A}_2} \mu_{V|\mathbb{A}_2}(\cdot \| \varphi)$.

Physically, it means that μ_φ is supported on configurations that percolate to infinity along φ but **NOT** along any other periodic ground state.



$\mathbb{A}_2$: Extreme Gibbs measures

For a general D, not all periodic ground states generate extreme Gibbs measures only the **dominant** ones.

$\mathbb{A}_2$: Extreme Gibbs measures

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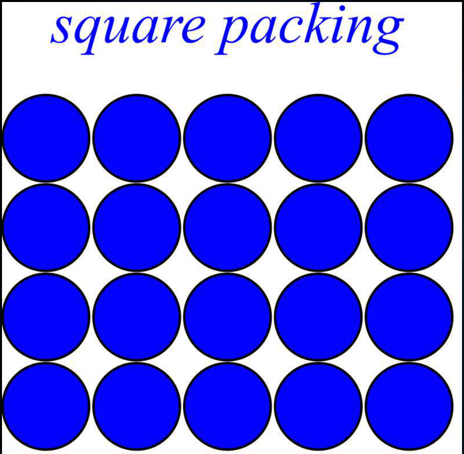
Theorem 2.

If there exist $M \geq 1$ dominant types of periodic ground states then, for a large u, the number of extreme Gibbs/DLR measures is

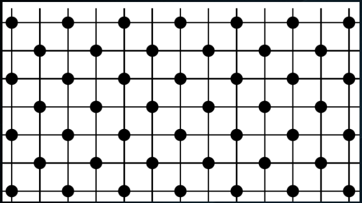
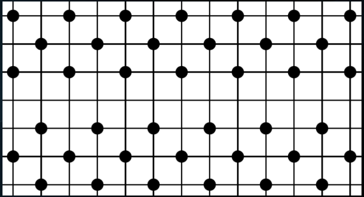
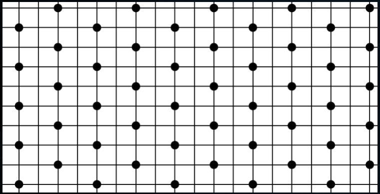
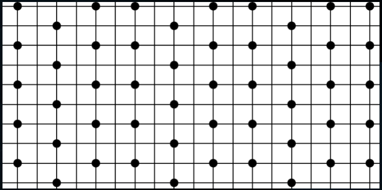
$$D^2 \sum_{j=1}^{M} m_j,$$

where $m_j \in \{1, 2\}$ is determined by the Eisenstein prime decomposition of D^2.

$\mathbb{Z}^2$: a misleading picture



Periodic *vs.* non-periodic, lattice *vs.* non-lattice ground states

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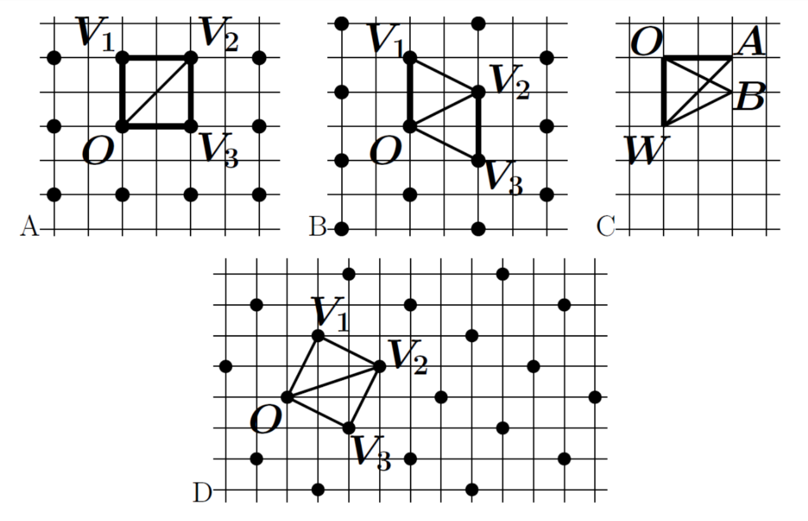
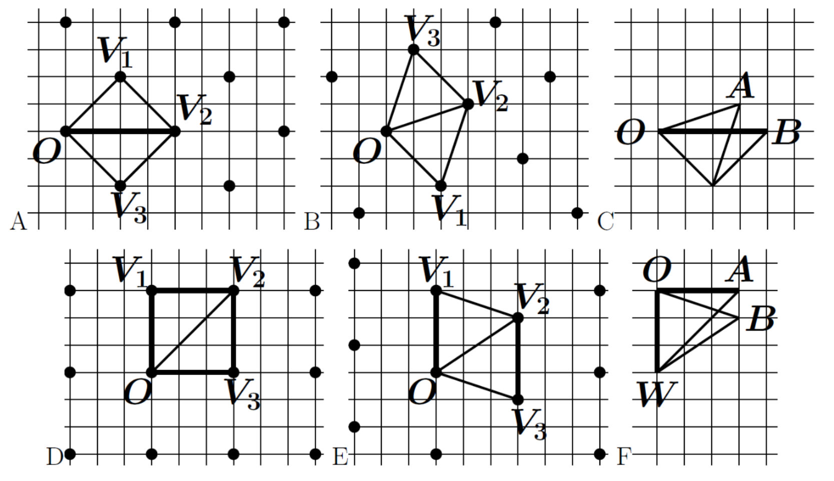
Sliding occurs when we can shift a 1D array of occupied sites without violating the non-overlapping condition. This generates a characteristic pattern of 'competing' fundamental triangles.

$\mathbb{Z}^2$: sliding vs. non-sliding, $D^2 = 4, 5$



$\mathbb{Z}^2$: sliding for $D^2 = 8, 9$



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$$D^2 = 4, 8, 9, 18, 20, 29, 45, 72, 80, 106, 121, 157, 160, 218, 281, 392, 521, 698, 821, 1042, 1325, 1348, 1517, 1565, 2005, 2792, 3034, 3709, 4453, 4756, 6865, 11449, 12740, 13225, 15488, 22784, 29890, 37970.$$

Krachun (2019): proved that the number of sliding instances is finite.

¿ We expect that sliding leads to uniqueness of a Gibbs/DLR measure for large enough u. ?

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For $D \geq \sqrt{20}$, it is a D-min-area sublattice, not a square arrangement, which determines a periodic ground state for a given D on $\mathbb{Z}^2$.

Values D with uniqueness

✓ The D-min-area sub-lattices are obtained from each other via rotations by $\pm\pi/2$ and reflections about the axes.

✓ This defines an **equivalence class** of sub-lattices with a given triple (ℓ_0, ℓ_1, ℓ_2). We say we have uniqueness in $(*)$ if the equivalence class is unique. It may contain a single sublattice ($m = 1$) or two sublattices ($m = 2$) or four ($m = 4$).

Values D with non-uniqueness

The non-uniqueness in $(*)$ has a two-fold character:

(i) There may be more than one triple (ℓ_0, ℓ_1, ℓ_2) solving $(*)$. We found one attainable D with 5 different triples.

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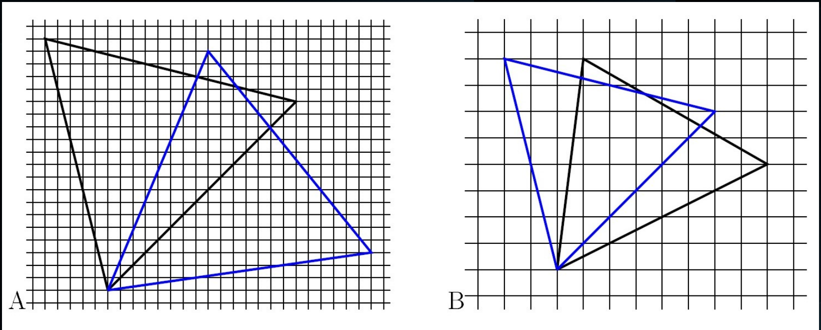
Uniqueness and both non-uniqueness forms have infinite occurrences of D.



- Frame (A): $D^2 = 425$, $(S = 375)$. The optimal squared side lengths are $425, 425, 450$, with two non-equivalent $\mathbb{Z}^2$ implementations.
- Frame (B): $D^2 = 65$, $(S = 60)$. The optimal squared side-lengths are $65, 65, 80$ (blue) and $68, 68, 72$ (black); both triangles admit a unique implementation up to $\mathbb{Z}^2$-symmetries.

$\mathbb{Z}^2$: Solutions to the optimization problem

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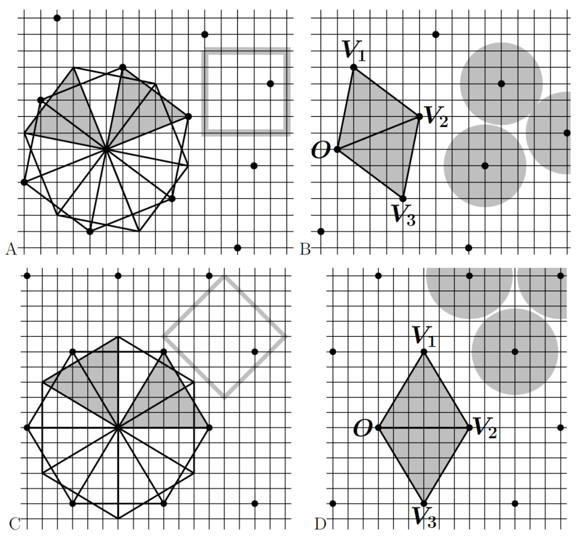
- ✓ Another feature is that side-length l_3 is often $> D$: we call the value of D with this property *non-tessellating*.

$\mathbb{Z}^2$: A count of periodic ground states.



For $D^2 = 25$: $l_1^2 = 29$, $l_2^2 = 26$, $l_3^2 = 25$. For $D^2 = 32$: $l_1^2 = 36$, $l_2^2 = l_3^2 = 34$.

$\mathbb{Z}^2$: Extreme Gibbs measures: uniqueness in $(*)$

Theorem 3.

Suppose that for a given D, the optimization problem $(*)$ produces a **unique triple** (ℓ_0, ℓ_1, ℓ_2), **unique** equivalence class (hence **no sliding**). Then the number of extreme Gibbs measures for u large enough matches the number of the periodic ground states: it equals

$$mS$$

where

(a) $m = 1$ if $D = 1, \sqrt{2}$ (here the fundamental parallelogram is a square),

(b) $m = 2$ if the fundamental triangle is isosceles,

(c) $m = 4$ if the fundamental triangle is non-isosceles.

The extreme Gibbs measures are generated by periodic ground states.

$\mathbb{Z}^2$: Extreme Gibbs measures: non-uniqueness in $(*)$

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$\mathbb{Z}^2$: Extreme Gibbs measures: non-uniqueness in $(*)$

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Theorem 4.

Suppose that D is non-sliding and generates non-uniqueness in $(*)$. If there exist $M \geq 1$ dominant types of periodic ground states then, for a large u, the number of extreme Gibbs/DLR measures is

$$S \sum_{j=1}^{M} m_j,$$

where $m_j \in \{2, 4\}$ is determined by the shape of the dominant fundamental triangle (isosceles or not).

The queen of math, again

We can prove that the classes of D^2 which are referred to in Theorems 3 and 4 are both **infinite**.

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The idea is to approximate an equilateral triangle by $\mathbb{Z}^2$-triangles. It leads to **norm equations** in the cyclotomic integer ring $\mathbb{Z}[\zeta]$, where ζ is a primitive 12th root of unity.

$$t^2 = 3s^2 + r, \quad s, t \in \mathbb{Z}.$$

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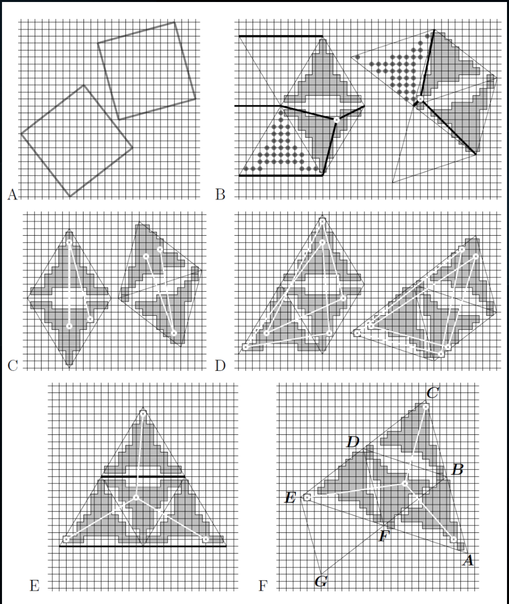
The solutions to the norm equation have to be analyzed both geometrically and algebraically. This leads to infinite sequences of values of D of both types.

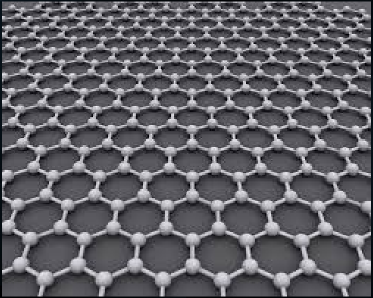
$\mathbb{Z}^2$: Extreme Gibbs measures: non-uniqueness in $(*)$

The smallest values of D^2 from Theorem 4 are $D^2 = 65, 130, 324$. The analysis of dominance can be done on a case-by-case basis, by counting local **excitations** where we vacate some occupied sites in a periodic ground state and attempt to insert 'new particles' while maintaining admissibility.

$\mathbb{Z}^2$, $D^2 = 130 = 11^2 + 3^2 = 9^2 + 7^2$: local excitations



$\mathbb{W} = \mathbb{H}_2$



$\mathbb{W} = \mathbb{H}_2$, Class I

First we divide the attainable values $D^2 = a^2 + b^2 + ab$ into two classes:

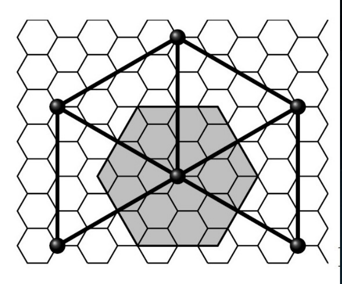
I. $3 \mid D^2$,

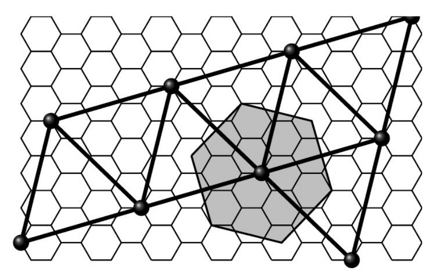
II. $3 \nmid D^2$.

In Class I the problem reduces to the case of the triangular lattice $\mathbb{A}_2$. It leads to a further division into 3 subclasses based on the same Eisenstein prime decomposition of D. It yields the respective formulas for the number of extreme Gibbs measures

$$\frac{2}{3}D^2, \qquad \frac{4}{3}D^2, \qquad \frac{2}{3}D^2 \sum_{j=1}^{M} m_j, \text{ with } m_j \in \{1, 2\}.$$

$\mathbb{W} = \mathbb{H}_2$, Class I





$D^2 = 48$ left frame, $D^2 = 39$ right frame.

$\mathbb{W} = \mathbb{H}_2$, Class II

Class II admits a further partition.

- There are 13 exceptional values forming a finite subclass:

$$D^2 = 1, 4, 7, 13, 16, 28, 49, 64, 67, 97, 133, 157, 256.$$

- And there is an infinite subclass containing all remaining Löschian numbers not divisible by 3.

For non-exceptional values D, minimal-area triangles can be found via a discrete optimization problem. However, they do not generate a tiling of $\mathbb{H}_2$. Hence, one needs to consider sub-optimal triangles which tessellate $\mathbb{H}_2$. The first among them is an equilateral D^*-triangle, where $D^* > D$ is the closest value with $3 \mid D^*$. Then the formulas for Class I apply with D^* replacing D.

$\mathbb{W} = \mathbb{H}_2$, Exceptional non-sliding values

Exceptional non-sliding values of D

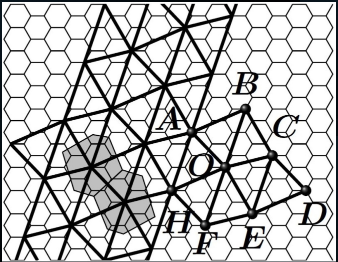
$$D^2 = 1, 13, 28, 49, 64, 97, 157, 16, 256, 67.$$

Ground states: involve non-equilateral and equilateral triangles in specific combinations/arrangements.

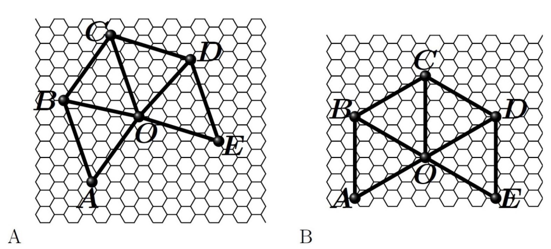
These values of D require a case-by-case analysis, with the help of a computer. (Informally we call them a Zoo.)

Each ground state generates an extreme Gibbs measure for u large enough. Except for $D^2 = 67$: here again we have an issue of dominance, and some periodic ground states are suppressed.

$\mathbb{W} = \mathbb{H}_2$, Exceptional non-sliding examples



$D^2 = 13$

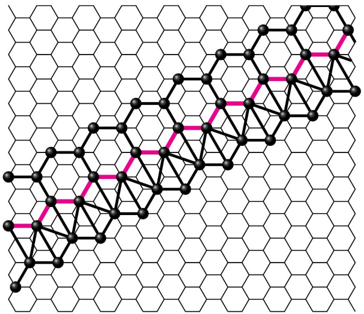


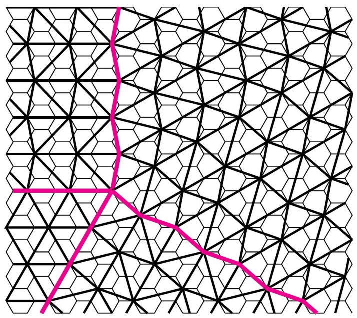
$D^2 = 67$

$\mathbb{W} = \mathbb{H}_2$, Exceptional values: sliding

Sliding

$$D^2 = 4, 7, 133.$$





$D^2 = 4$ left frame

$D^2 = 7$ right frame