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 $\psi^\mathbb{V}_x = \psi^\mathbb{V}_y = 1$
- Activity/Fugacity: $u > 0$

- A boundary condition: an admissible configuration $\phi = \phi^{\mathbb{Z}^2}$
- An additional restriction: $\psi^\mathbb{V} \lor \phi^{\mathbb{Z}^2 \setminus \mathbb{V}}$ is admissible, $\psi^\mathbb{V} \in \mathcal{A}(\mathbb{V} || \phi)$
- The statistical weight:
  $$w(\psi^\mathbb{V} || \phi) = u^#(\psi^\mathbb{V})$$
- The partition function:
  $$Z(\mathbb{V} || \phi) = \sum_{\psi^\mathbb{V} \in \mathcal{A}(\mathbb{V} || \phi)} w(\psi^\mathbb{V} || \phi)$$
Gibbs measures on $\mathbb{L}$

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

$$\mu(f) = \int_X \int_{\{0, 1\}^V} f(\psi^V \vee \phi \mid_{\mathbb{L} \setminus V}) d\mu_V(\psi^V\|\phi) d\mu(\phi).$$

One can say that under such measure $\mu$, the probability of a configuration $\psi^V$ in a finite volume $V \subset \mathbb{L}$, conditional on a configuration $\phi \mid_{\mathbb{L} \setminus V}$, coincides with $\mu_V(\psi^V\|\phi)$, for $\mu$-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

\[ Z(\mathcal{V}||\phi) = \sum_{\{\Gamma_i\}} \prod_{i} w(\Gamma_i) \]

- 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 VC$s$
  - find all configurations containing minimal VC$s$ 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 $A_2$
Peierls estimate on $A_2$ via Voronoi cells

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

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

Here and below, $\psi_{\Gamma}$ 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 $|C_{\psi}(x)| > S$; otherwise $x$ does not contribute into $w(\Gamma)$. Observe that

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

On the other hand,

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

According to the definition of a $\varphi$-correct common parallelogram, we have an inequality

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

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

$$p(D) = \frac{1}{9} \min \left( \frac{1}{2}, \frac{s(D)}{\sqrt{3}} D^{-2} \right) .$$
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 $\sqrt{3}$-sublatice)
- For $D^2 \mod 3 = 0$ 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 $D^*_2 = D_*(D) \geq D$ be the nearest value such that $D^*_2 \mod 3 = 0$ and $D^*_2 = m^2 + n^2 + mn$.
- For $D^2 \mod 3 \neq 0$, $D^2 \neq 1, 4, 7, 13, 16, 28, 49, 64, 67, 97, 133, 157, 256$ the PGSs are $D_*$-sublattices from $\mathbb{A}_2$.
- However for $D^2 \mod 3 \neq 0$ 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 $L$-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

\[
\begin{array}{ccc}
O & A & B \\
W & C & O \\
D^2 = 20 & D^2 = 29 & D^2 = 45 \\
\end{array}
\]

- 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 $A_2$ and $H_2$ except for the exceptional values of $D$
Classes of M-triangles on $\mathbb{Z}^2$

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

- **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), $d = 65$, $[65|65|80]$, $[68|68|72]$

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

○ Let $\psi^*$ be a saturation of a given $D$-AC $\psi$.

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

○ Another possibility for a defect is where, in the saturation $\psi^*$, 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 $\psi$). 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 $\psi$).
A Peierls estimate via M-triangles in $\mathbb{Z}^2$

○ **Theorem.** Consider a contour $\Gamma$ 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 $\psi_\Gamma$. Then the amounts $\#(\psi_\Gamma), \#(\varphi_\Gamma)$ of occupied sites in $\psi_\Gamma$ and $\varphi_\Gamma$ satisfy

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

○ Let $\Delta$ be a connected component of $\varphi'$-correct templates enclosed by a connected component of $\varphi''$-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 $\Delta$. This chain constitutes t-defects in the corresponding contour $\Gamma$.

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

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

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 $\Gamma$ 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 $\varphi \in \mathcal{P}(D)$: $\mu = \lim_{V \rightarrow \mathbb{Z}^2} \mu_V (\cdot || \varphi) (= \mu_\varphi)$. The measures $\mu_\varphi$ 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 $\#\mathcal{P}_j(D) = m_jS(D)$ 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 $\mathbb{H}_2$, $j = 1, 2, \ldots, J$. 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 $\varphi$ from a dominant class $\mathcal{P}_j(D)$: $\mu = \lim_{V \uparrow \mathbb{Z}^2} \mu_V(\cdot || \varphi)(= \mu_\varphi)$. The measures $\mu_\varphi$ 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 $\psi_\Gamma$ is $\leq 2^{D^2S(D)} \leq 2^{D^4}$

- 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 $\Gamma$ with $w(\Gamma) = u^{-1}$ is to remove a particle. It does not discriminate between the PGSs.

- There are multiple ways to create $\Gamma$ 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 $\forall y \in \mathbb{A}_2$,
  \[
  F(y) := \sum_{x \in \varphi} f_r 1(\rho(x, y)^2 = r, \text{x removed by y}) = 1.
  \]
- Can define $f_r$ so that
  \[
  G(x) := \sum_{y} f_r 1(\rho(x, y)^2 = r, \text{x removed by y}) \leq 1
  \]
○ The proof is computer-assisted. The bound \( n \leq 6 \) not expected to hold for larger \( D \).

○ \( \forall \) admissible \( n \)-particle insertion \( \Delta \) and \( x \in \varphi \), the deficit \( \delta(x) := 1 - G(x) \geq 0 \)

\[ \sum_{x \in \varphi} \delta(x) = \text{(the difference of the amounts of removed and inserted particles)} \]

○ 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 $D_\ast$-triangles where $D_\ast^2 = 75$, (b) from quadrilaterals, similarly to Class E1. It turns out that type (a) is dominant and type (b) not.

![Diagram](a) ![Diagram](b)