Random Packings and Liquid Crystals

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Rényi 100 conference, Budapest, Hungary
June 21, 2022

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Hard-core models (random packings)

- A **hard-core model** is a natural **probability distribution** on the ways to place non-overlapping copies of a tile in a domain.
- **Tile (or molecule):** subset $T \subset \mathbb{R}^d$, possibly allowing some of its rotations too.
- **Configuration in $\Lambda \subset X$:** Non-overlapping translations of $T$ (perhaps rotated) by elements of $X$, where we work either with $X = \mathbb{R}^d$ or $X = \mathbb{Z}^d$.
- **Fugacity parameter $\lambda > 0$:** Controls typical number of tiles in a configuration (small $\lambda$ – dilute configurations, large $\lambda$ - dense configurations).
- **Hard-core measure $\mu_{\Lambda, \lambda}$:** On $\mathbb{Z}^d$, probability of a configuration $\sigma$ is proportional to $\lambda^{N_{\Lambda}(\sigma)}$, where $N_{\Lambda}(\sigma) = \text{number of tiles of } \sigma \text{ in } \Lambda$ (with boundary values outside). On $\mathbb{R}^d$, similar construction with respect to suitable Lebesgue measure.
- At **small $\lambda$,** tiles are mostly isolated and hardly interact – disorder.
- Do the configurations **order at intermediate and large $\lambda$?** In which way?

Some pictures based on Disertori-Giuliani-Jauslin 20
Example: Nearest-neighbor hard-core model on $\mathbb{Z}^d$

- **Tile**: an open disk of diameter $\sqrt{2}$ around the origin. Translations in $\mathbb{Z}^d$.
- **Small fugacity $\lambda$**: typical configurations are disordered, as shown by the Dobrushin uniqueness theorem, van den Berg’s disagreement percolation or a cluster expansion. In particular, there is a unique Gibbs measure.
- **Maximal density packings in $\mathbb{Z}^d$**:
  - there are exactly two periodic packings of maximal density, corresponding to the two sublattices of $\mathbb{Z}^d$ (bipartite structure).
- **Theorem (Dobrushin 68)**: $\exists \lambda_0(d)$ such that $\forall \lambda > \lambda_0(d)$, in a typical hard-core configuration with “even-boundary conditions”, most tiles are on even sites. In particular, the model has two periodic Gibbs measures.

- **Open**:
  1) Is there a single transition value $\lambda_c(d)$ from disorder to order?
  2) Behavior of $\lambda_c(d)$ as $d \to \infty$? (Galvin-Kahn 04, Samotij-Peled 14, $\lambda_c(d) \to 0$ as a power of $d$, but optimal power is unknown)
Dobrushin proof idea 1
Dobrushin proof idea 2
Dobrushin proof idea 4
Dobrushin proof idea 5
Dobrushin proof idea 6
Dobrushin proof idea 7
Dobrushin proof idea 8
Dobrushin proof idea 9
Dobrushin proof idea 10
Dobrushin proof idea 11
Other behaviors and liquid crystals

- **Monomer-dimer model**: Tiles are edges of $\mathbb{Z}^d$.
  - **Heilmann-Lieb 70**: The model is disordered at all values of $\lambda$.
  - Alternative proof by **van den Berg 99** using disagreement percolation.

- **Liquid/gas** – invariant in distribution under rotations and translations of $\mathbb{R}^3$.
- **Crystal** – Broken rotation and translation symmetry (invariant only under discrete subgroups of rotations and translations)

- **Liquid crystals**:
  - **Disordered (liquid/gas)**
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  - **Nematic**
    - Broken rotation symmetry, preserved translation symmetry
  - **Smectic**
    - Broken rotation symmetry, translation symmetry broken in only one direction
  - **Columnar**
    - Broken rotation symmetry, translation symmetry broken only in a plane of directions
    - © Termine-Golemme 2021
Nematic liquid crystals: predictions and proofs

• Onsager 49 studied the packing of long rods in $\mathbb{R}^3$ and predicted nematic order at intermediate densities. This remains unproven mathematically.

• Rigorous proofs of nematic phase in other models:
  - Ioffe-Velenik-Zahradník 06: polydispersed rods on $\mathbb{Z}^2$
  - Disertori-Giuliani 13: long rods of fixed length on $\mathbb{Z}^2$, intermediate density range
  - Heilmann-Lieb 79 and Jauslin-Lieb 18: interacting dimers
  - Disertori-Giuliani-Jauslin 20: anisotropic plates in $\mathbb{R}^3$ with finite number of allowed orientations, intermediate density range.

Rods of length 7 on $\mathbb{Z}^2$ at different density regimes

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Packing balls in the continuum

- An important problem regards the packing of balls in $\mathbb{R}^d$.
- Physicists predict crystal order at high fugacity in dimension $d = 3$, but only nematic order in two dimensions.
- Richthammer 07: No translational order in two dimensions.
- Magazinov 18: Infinite cluster of nearly-touching balls at high fugacity in $d = 2$.
- Other parts of prediction remain unproved.
  No known method to prove continuous-symmetry breaking in such a system.

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Lattice balls and sliding phenomenon

- **Lattice approximation:** Mazel-Stuhl-Suhov 19 considered a hard-core model on $\mathbb{Z}^2$ (and hexagonal and triangular lattices) where the tile is $\{v \in \mathbb{R}^2: \|v\|_2 \leq r\}$ for general $r$.

- Obtained a description of the maximal-density periodic packings.

- For all $r$ with finitely many maximal-density periodic packings, they proved that samples from a high-fugacity state will equal one of these packings at most places.

- **Sliding phenomenon:** Finitely many exceptional $r$ for which there are infinitely many maximal-density periodic packings (Mazel-Stuhl-Suhov 19, Krachun 19). Mazel-Stuhl-Suhov conjecture that there is no long-range order at high fugacity.
The $2 \times 2$ hard-square model

- **Tile:** the square $\{v \in \mathbb{Z}^2: \|v\|_\infty \leq 1\}$ ($r = \sqrt{2}$ of Mazel-Stuhl-Suhov study. Sliding)

**Configurations:** Non-overlapping tiles with centers on the square lattice.

- **Probability measure** $\mu^\rho_{\Lambda, \lambda}$: Let $\Lambda \subset \mathbb{Z}^2$ be finite and $\rho$ be a configuration. Then $\mu^\rho_{\Lambda, \lambda}$ is supported on configurations which agree with $\rho$ outside $\Lambda$ and is defined by $\mu^\rho_{\Lambda, \lambda}(\sigma) \propto \lambda^{N(\sigma)}$, where $N_\Lambda(\sigma)$ is the number of tiles of $\sigma$ in $\Lambda$.

**Gibbs measure:** probability measure over configurations in the entire $\mathbb{Z}^2$ which is “consistent” with the probability measures $\mu^\rho_{\Lambda, \lambda}$ (satisfies DLR condition).

[Simulation of $2 \times 2$ hard-square model at large $\lambda$]
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- **Gibbs measure**: probability measure over configurations in the entire $\mathbb{Z}^2$ which is “consistent” with the probability measures $\mu^{\rho}_{\Lambda, \lambda}$ (satisfies DLR condition).

- **Disordered phase** (unique Gibbs measure) for small $\lambda$, by Dobrushin’s uniqueness theorem or by van den Berg’s disagreement percolation method.

- **Our results clarify the structure of configurations in the high-fugacity regime.**

!”
Columnar order and characterization of periodic Gibbs measures

- **Theorem 1 (Hadas-P. 2022):** There exists $\lambda_0$ such that the $2 \times 2$ hard-square model at each fugacity $\lambda > \lambda_0$ admits a Gibbs measure $\mu_{\text{ver},0}$ satisfying:
  - **Invariance:** $\mu_{\text{ver},0}$ is $2\mathbb{Z} \times \mathbb{Z}$-invariant and extremal (so also $2\mathbb{Z} \times \mathbb{Z}$-ergodic).
  - **Columnar order:**
    $$\mu_{\text{ver},0}(\text{tile at } (x, y)) = \begin{cases} \Theta \left( \frac{1}{\lambda} \right) & x \text{ even} \\ \frac{1}{2} - \Theta \left( \frac{1}{\sqrt{\lambda}} \right) & x \text{ odd} \end{cases}$$
  - **Decay of correlations:**
    $$\left| \text{Cov}_{\mu_{\text{ver},0}}(\text{tile at } (x_1, y_1), \text{tile at } (x_2, y_2)) \right| \leq Ce^{-c|x_1-x_2|-c|y_1-y_2|/\sqrt{\lambda}}$$

- By rotating and translating $\mu_{\text{ver},0}$ we obtain four distinct Gibbs measures
- **Theorem 2 (Hadas-P. 2022):** Every periodic Gibbs measure is a mixture of these four measures
- **Additional result:** version of the chessboard estimate for periodic Gibbs measures
Columnar order ideas 1

- Aim to use a Peierls-type argument: classify regions into “columnar ordered” and “row ordered” and prove that the interfaces between them are rare.
- **Sticks**: Tiles are classified into four types according to the parity of their coordinates. Sticks are the boundaries between tiles of different types.
- Sticks are necessarily **horizontal or vertical segments** and sticks of different orientation cannot meet.
- **Properly-divided rectangles**: A rectangle $R$ is said to be properly divided if there is a stick crossing it and $R^-$, where $R^-$ is a concentric rectangle with $(1 - \epsilon)$ the dimensions of $R$ for some fixed small $\epsilon > 0$. Initially only use this with squares.
Columnar order ideas 3

- **Sticks**: Tiles are classified into four types according to the **parity** of their coordinates. Sticks are the boundaries between tiles of different types.

- Sticks are necessarily **horizontal or vertical segments** and sticks of different orientation cannot meet.

- **Properly-divided squares**: A square $R$ is said to be properly divided if there is a stick crossing it and $R^-$, where $R^-$ is a concentric square with $(1 - 2\epsilon)$ the dimensions of $R$ for some fixed small $\epsilon > 0$.

- **Separation property**: If two squares overlap enough then it cannot be that they are properly divided by sticks of **different orientations**.
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Separation property: If two squares overlap enough then it cannot be that they are properly divided by sticks of different orientations.

Work with squares of mesoscopic side length $b(\lambda)$ satisfying

$$C\lambda^{1/4} < b(\lambda) < c\lambda^{1/2}$$

The basic estimate: In any periodic Gibbs measure $\mu$, for any such square $R$,

$$\mu(R \text{ is not properly divided}) \leq \exp \left( -c \frac{\text{Area}(R)}{\sqrt{\lambda}} \right)$$

This is moreover multiplicative: The probability that distinct squares $R_1, ..., R_n$ with the dimensions of $R$ are all not properly divided is at most $\exp \left( -c \frac{\text{Area}(R)}{\sqrt{\lambda}} n \right)$.
Basic estimate ideas 1

- Squares of mesoscopic side length $b(\lambda)$ satisfying $C\lambda^{1/4} < b(\lambda) < c\lambda^{1/2}$.
- The basic estimate: In any periodic Gibbs measure $\mu$, for any such square $R$,
  \[ \mu(R \text{ is not properly divided}) \leq \exp\left(-c \frac{\text{Area}(R)}{\sqrt{\lambda}}\right) \]
- Chessboard estimate (consequence of reflection positivity): Work on a discrete torus. For any local event $E$,
  \[ \mu^{\text{torus}}(E) \leq \mu^{\text{torus}}(\overline{E})^{1/N} \]
  where $\overline{E}$ is the event $E$ reflected to fill the whole torus and $N$ is the number of its reflected copies (as in figure).
Basic estimate ideas 2

- Squares of *mesoscopic* side length $b(\lambda)$ satisfying $C \lambda^{1/4} < b(\lambda) < c \lambda^{1/2}$.
- **The basic estimate:** In any periodic Gibbs measure $\mu$, for any such square $R$,
  $$\mu(R \text{ is not properly divided}) \leq \exp \left( -c \frac{\text{Area}(R)}{\sqrt{\lambda}} \right)$$
- **Chessboard estimate (consequence of reflection positivity):** Work on a discrete torus. For any local event $E$,
  $$\mu^{\text{torus}}(E) \leq \mu^{\text{torus}}(\bar{E})^{1/N}$$
  where $\bar{E}$ is the event $E$ reflected to fill the whole torus and $N$ is the number of its reflected copies (as in figure).
- The chessboard estimate, along with minor additional manipulations, reduce the basic estimate to showing that
  $$\mu^{\text{torus}}(E_{b(\lambda)}) \leq \exp \left( -c \frac{\text{Area}(R)}{\sqrt{\lambda}} N \right)$$
  where $E_{b(\lambda)}$ is the event that all sticks on the torus are shorter than $2b(\lambda)$.
- This is proved by *combinatorial counting* of possible “stick components”.
Counting “stick components”

- A main part of the combinatorial proofs involves counting connected components of sticks and vacant faces, with all sticks of length at most $2b(\lambda)$.
- We estimate the number of such components with a fixed number $v$ of vacant faces and a fixed number $d$ of “degrees of freedom” for the length of sticks.

\[ \begin{array}{c|c}
 v & d \\
\hline
 4 & 1 \\
 8 & 3 \\
 12 & 2 \\
\end{array} \]
Open questions

- **Continuous-symmetry breaking**: It is very important to develop methods to prove the breaking of continuous symmetry:
  - Study the high-fugacity behavior of balls in $\mathbb{R}^d$.
  - Study long rods in $\mathbb{R}^d$. Prove the existence of Onsager’s nematic phase at intermediate densities. What is the behavior at high fugacity?

- **Larger cubes and higher dimensions**: We expect columnar order at high fugacity for $k \times k \times \cdots \times k$ cubes with centers in $\mathbb{Z}^d$, for $k, d \geq 2$. Some of our ideas may be relevant to this case (especially for $d = 2$). However, the model is only reflection positive for $k = 2$. Columnar order would entail the existence of $dk^{d-1}$ periodic and extremal Gibbs states.

- Study the high-fugacity behavior of other lattice packing models featuring the sliding phenomenon.

- Approach physics predictions on critical behavior.