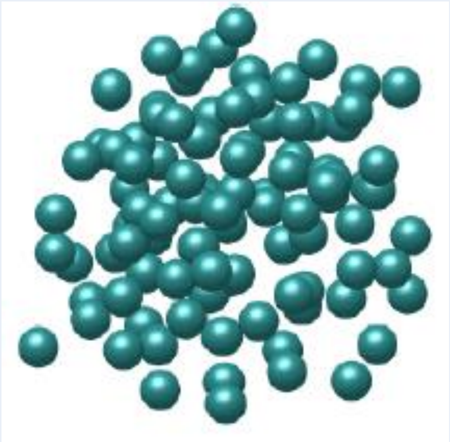
Random Packings and Liquid Crystals



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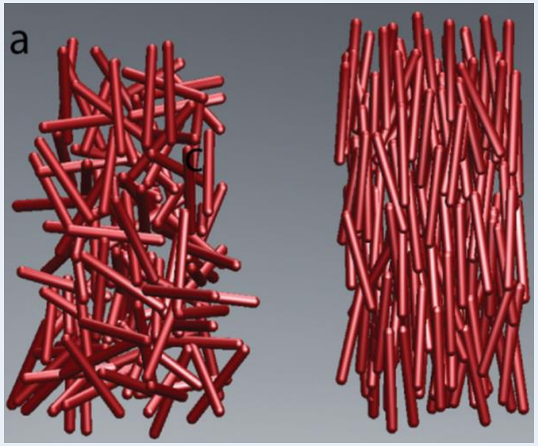

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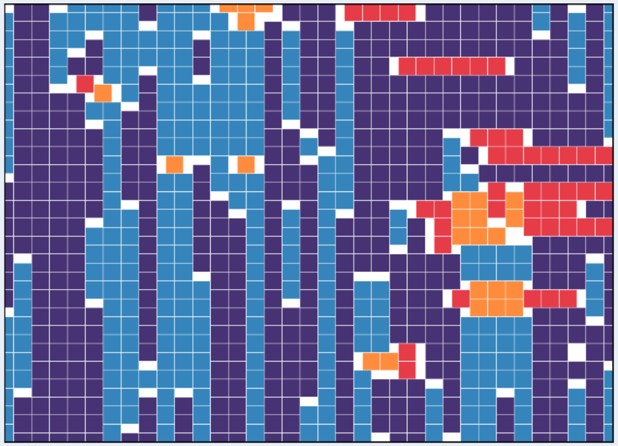


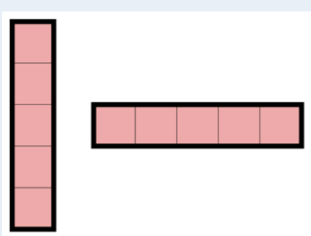
Ron Peled, Tel Aviv University,
on sabbatical at the IAS and Princeton University

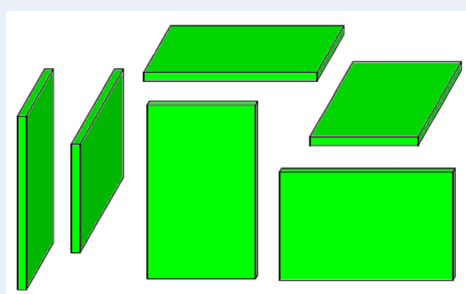
Portions joint with Daniel Hadas

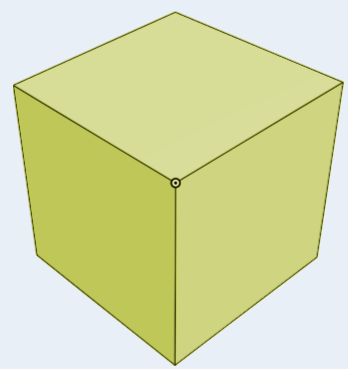
Mathematical Physics Webinar, Rutgers University
January 25, 2023

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 λ – dilute configurations, large λ - dense configurations).
- Hard-core measure $\mu_{\Lambda,\lambda}$: On $\mathbb{Z}^d$, probability of a configuration σ is proportional to $\lambda^{N_\Lambda(\sigma)}$, where $N_\Lambda(\sigma)$ = number of tiles of σ in Λ (with boundary values outside). On $\mathbb{R}^d$, similar construction with respect to suitable Lebesgue measure.
- At small λ, tiles are mostly isolated and hardly interact – disorder.
- Do the configurations order at intermediate and large λ? In which way?



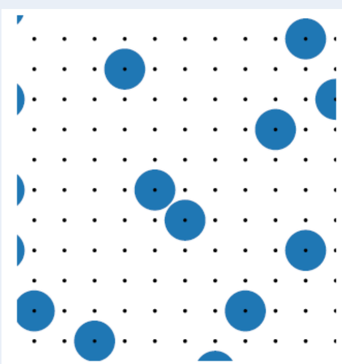




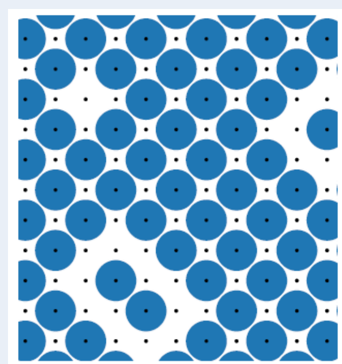
Some pictures based on Disertori-Giuliani-Jauslin 20

Example: Nearest-neighbor hard-core model on $\mathbb{Z}^d$

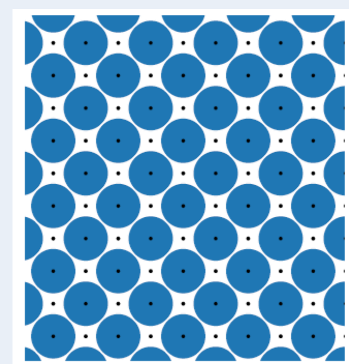
- Tile: an open disk of diameter $\sqrt{2}$ around the origin. Translations in $\mathbb{Z}^d$.
- Small fugacity λ: typical configurations are disordered, as shown by the Dobrushin uniqueness theorem, van den Berg's disagreement percolation or a cluster expansion. In particular, there is a unique Gibbs 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.



λ small



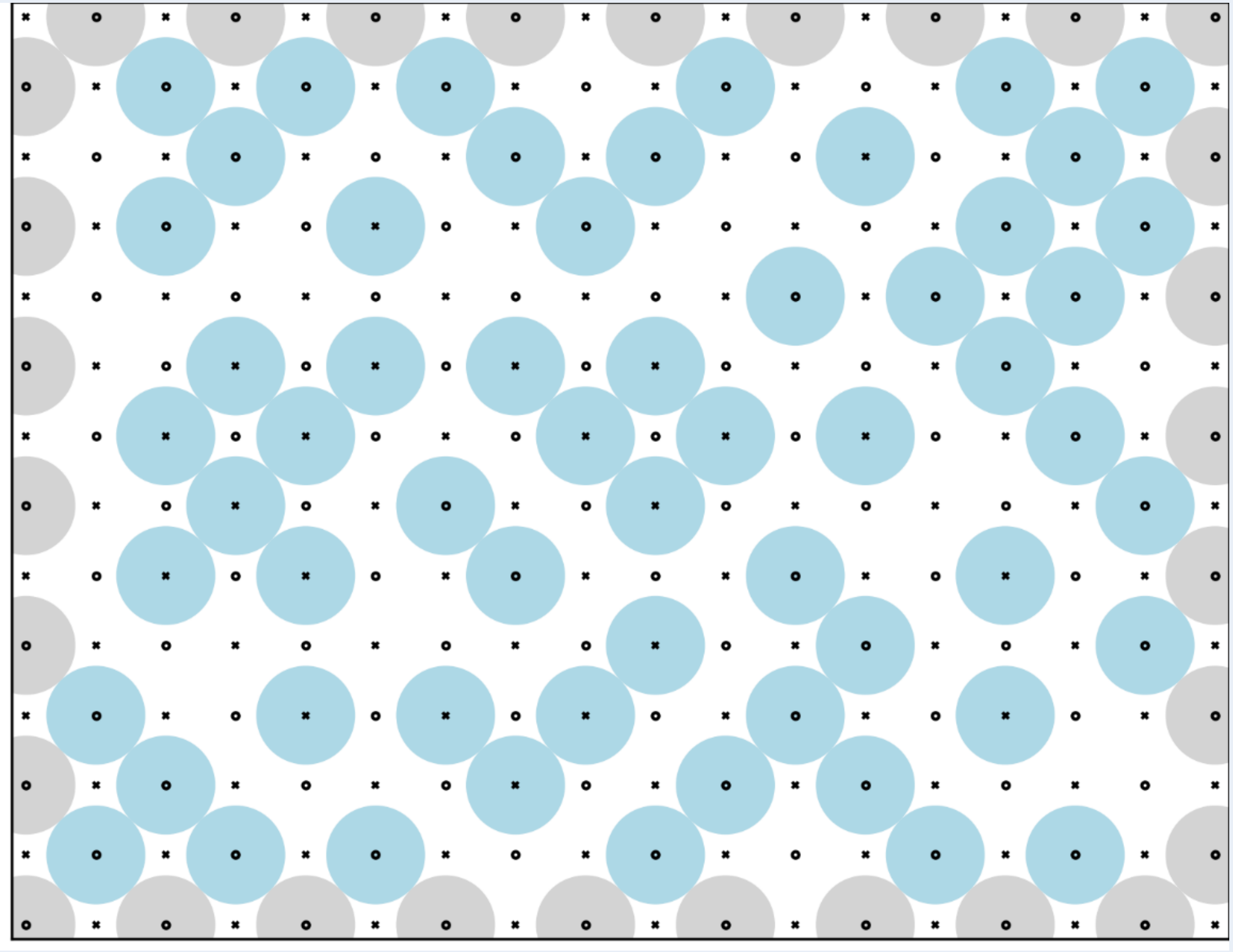
λ large



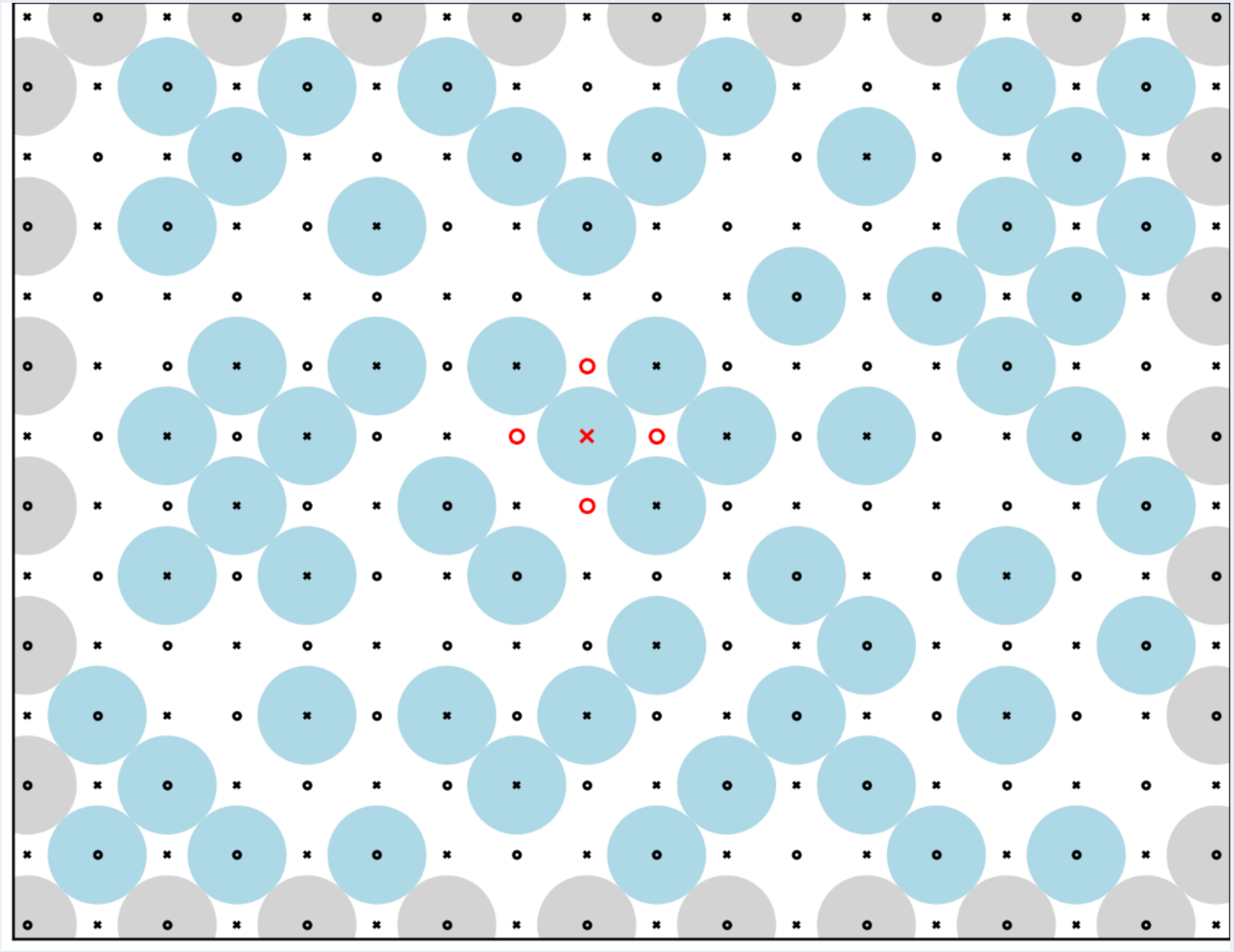
"$\lambda = \infty$"

- 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)

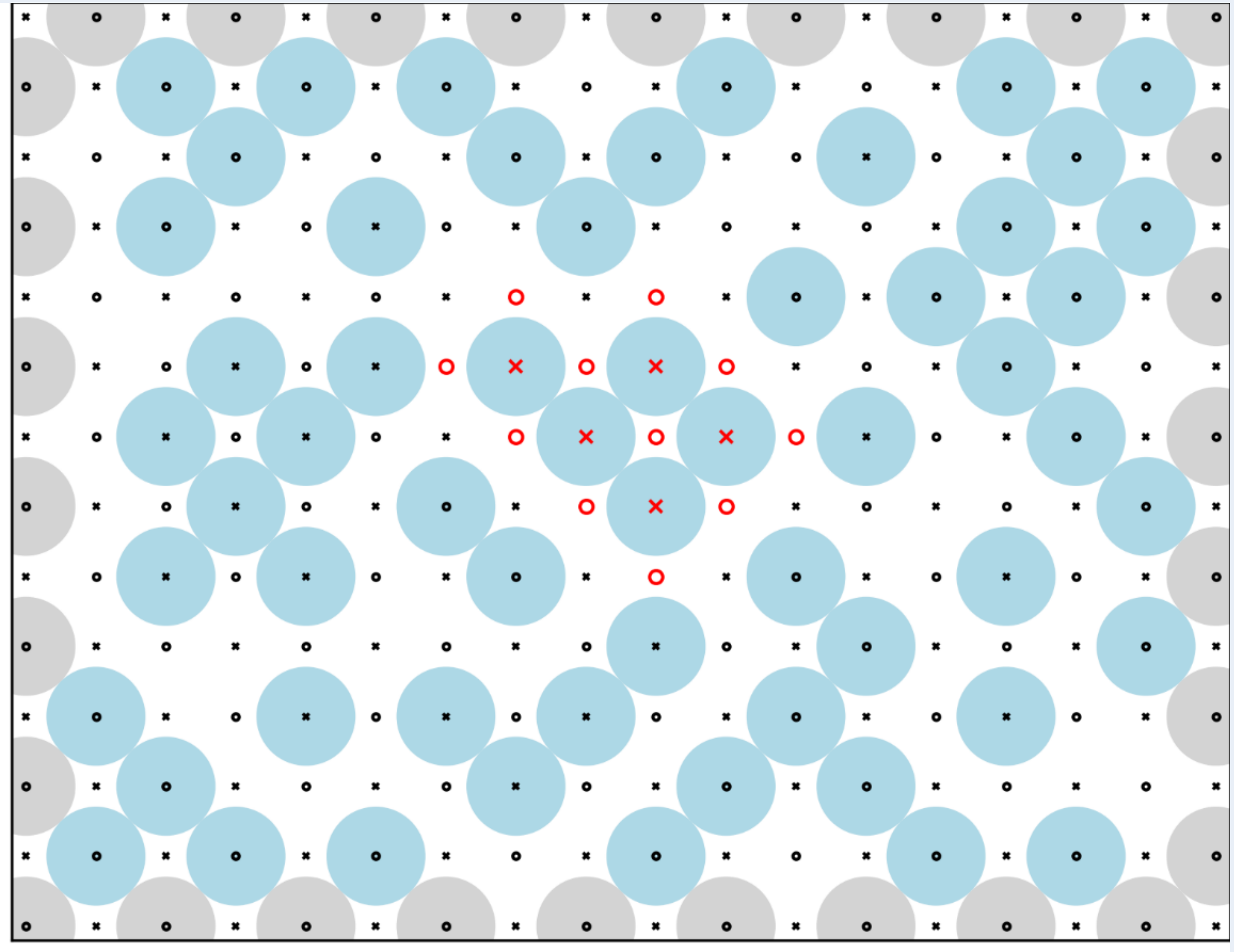
Dobrushin proof idea 1



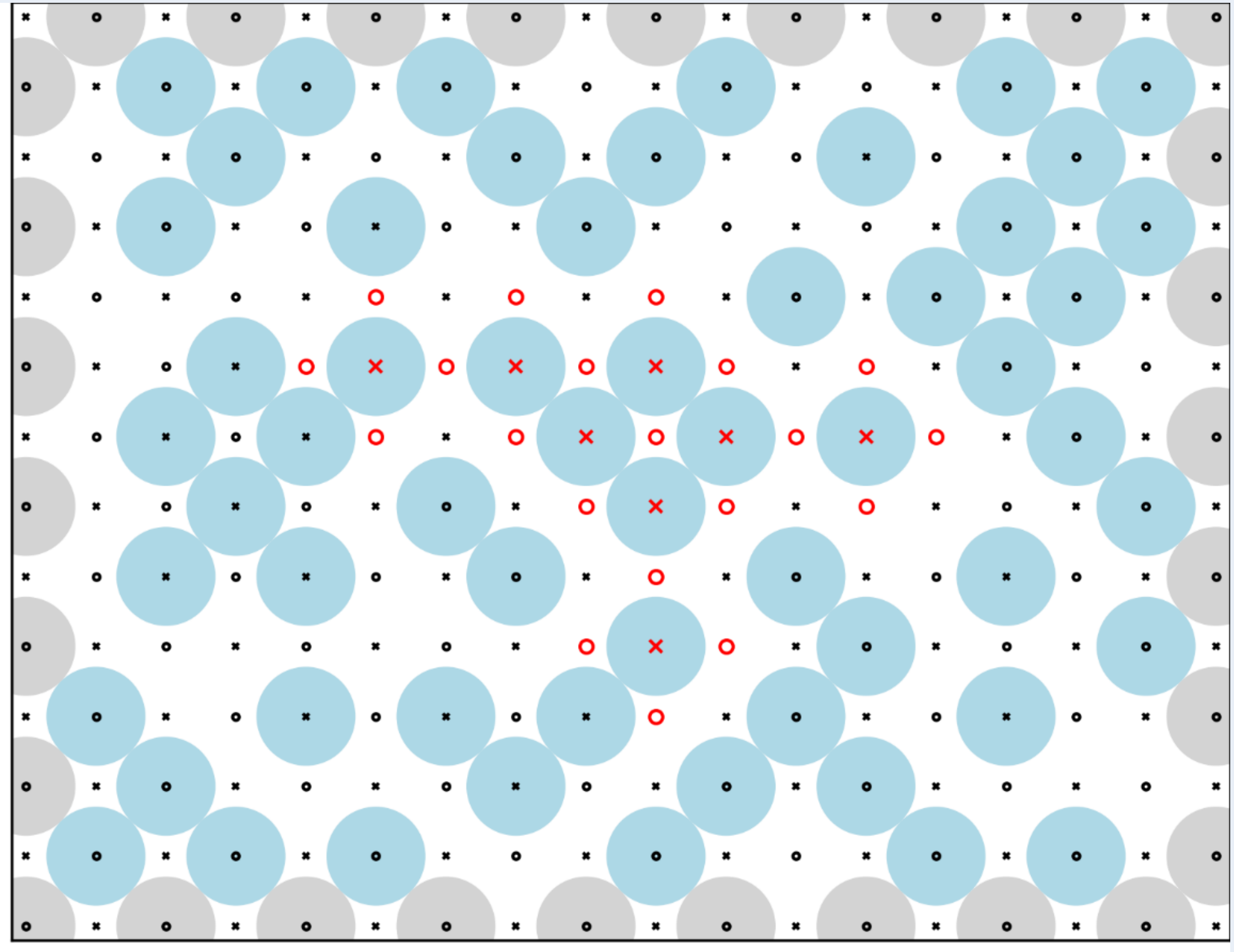
Dobrushin proof idea 2



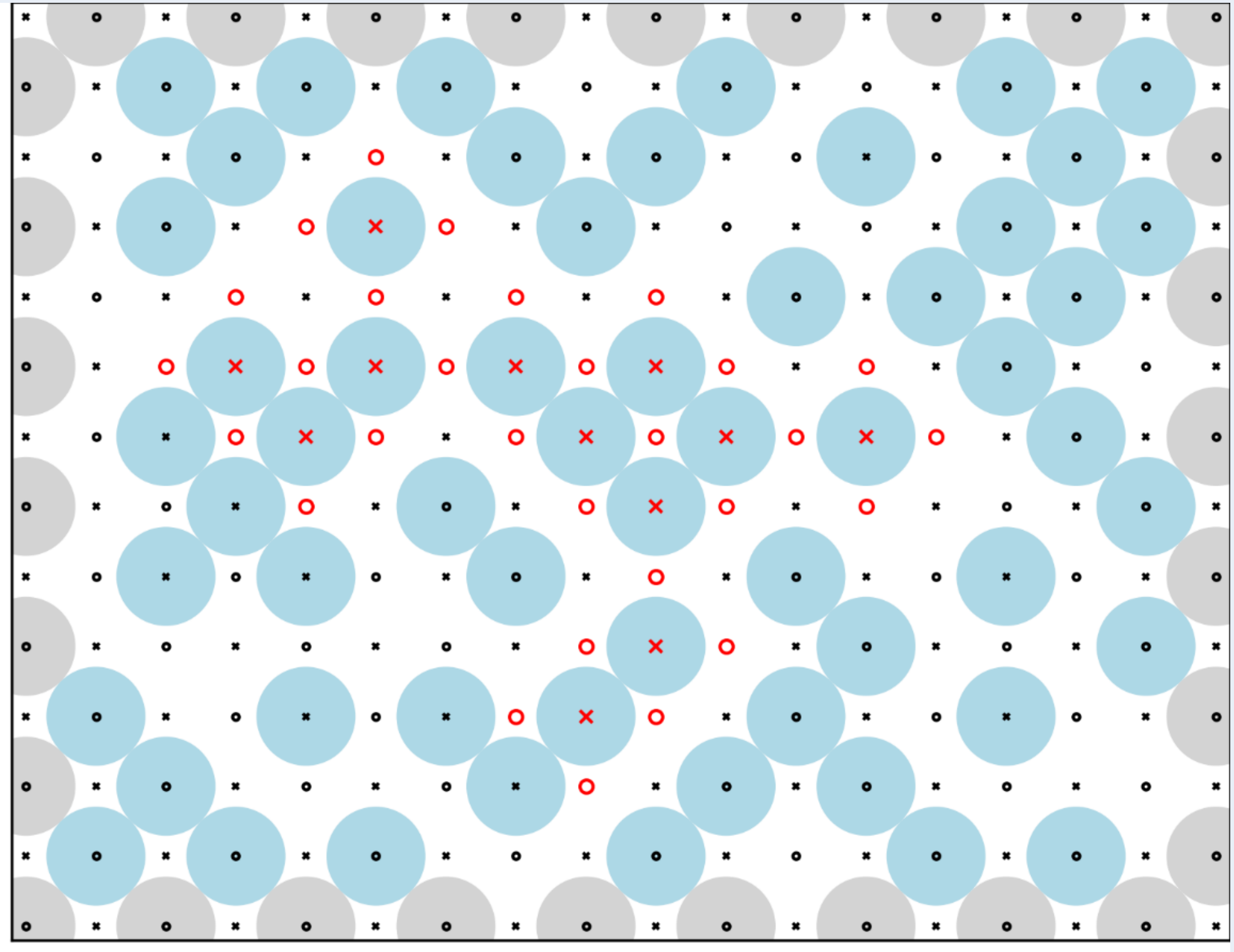
Dobrushin proof idea 3



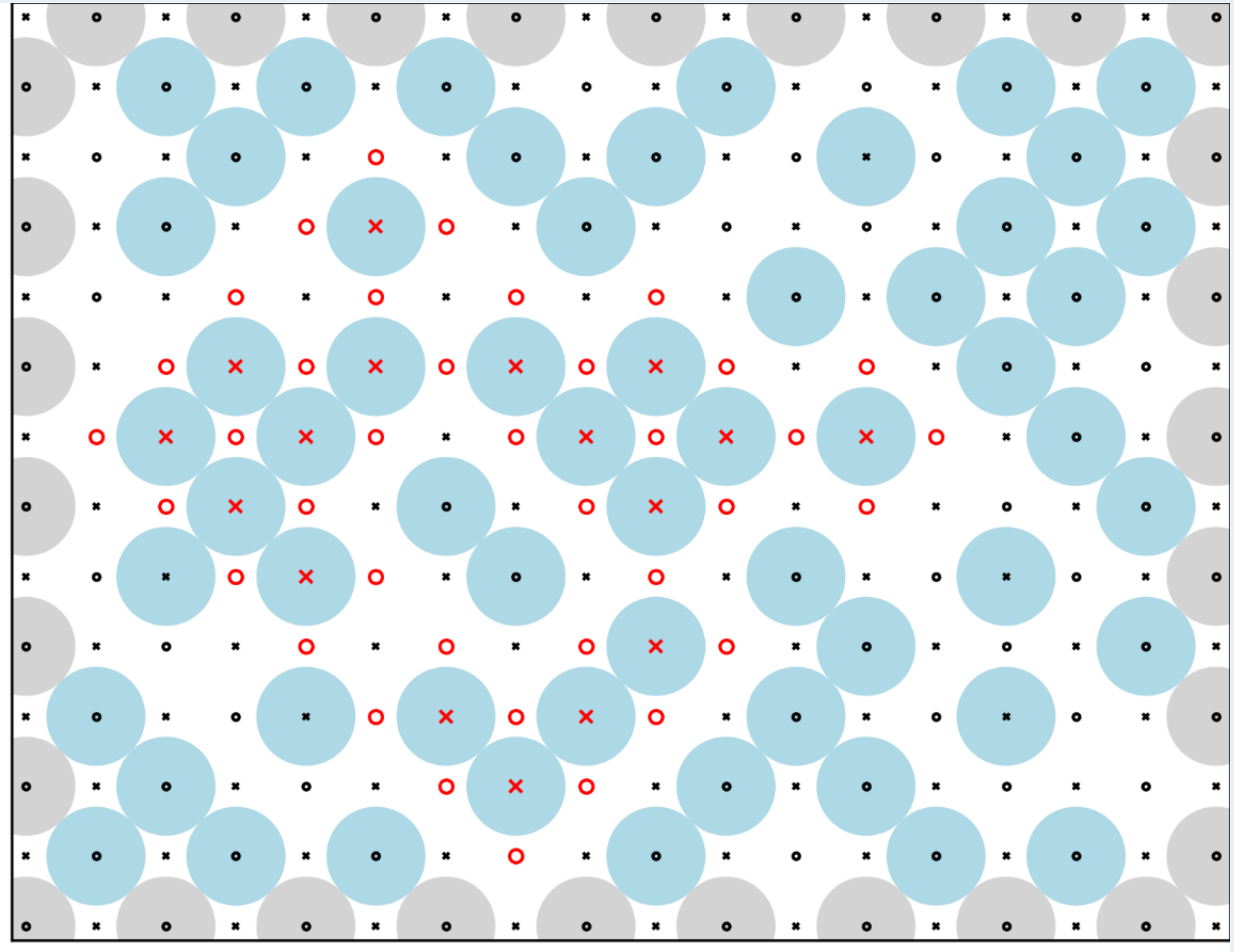
Dobrushin proof idea 4



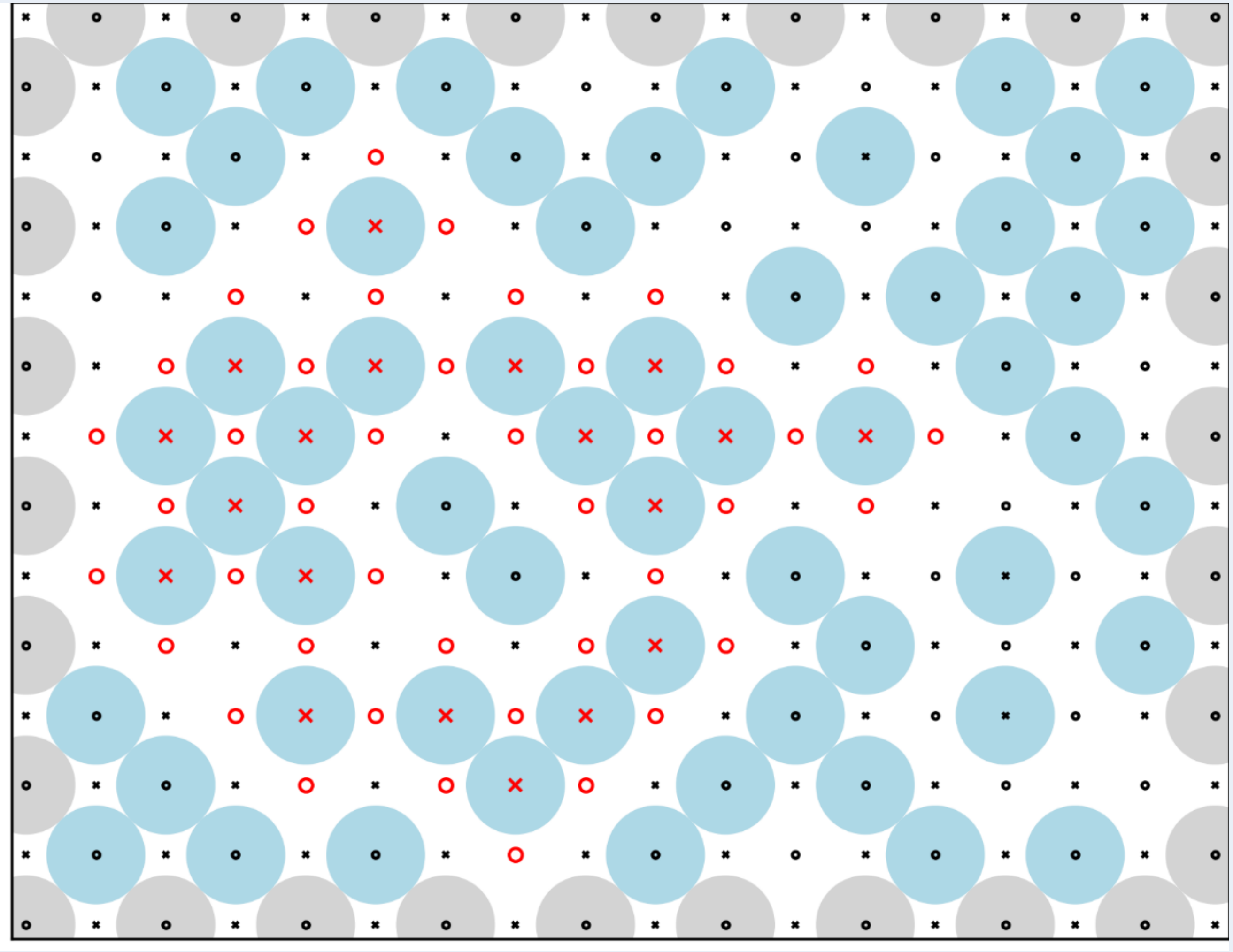
Dobrushin proof idea 5



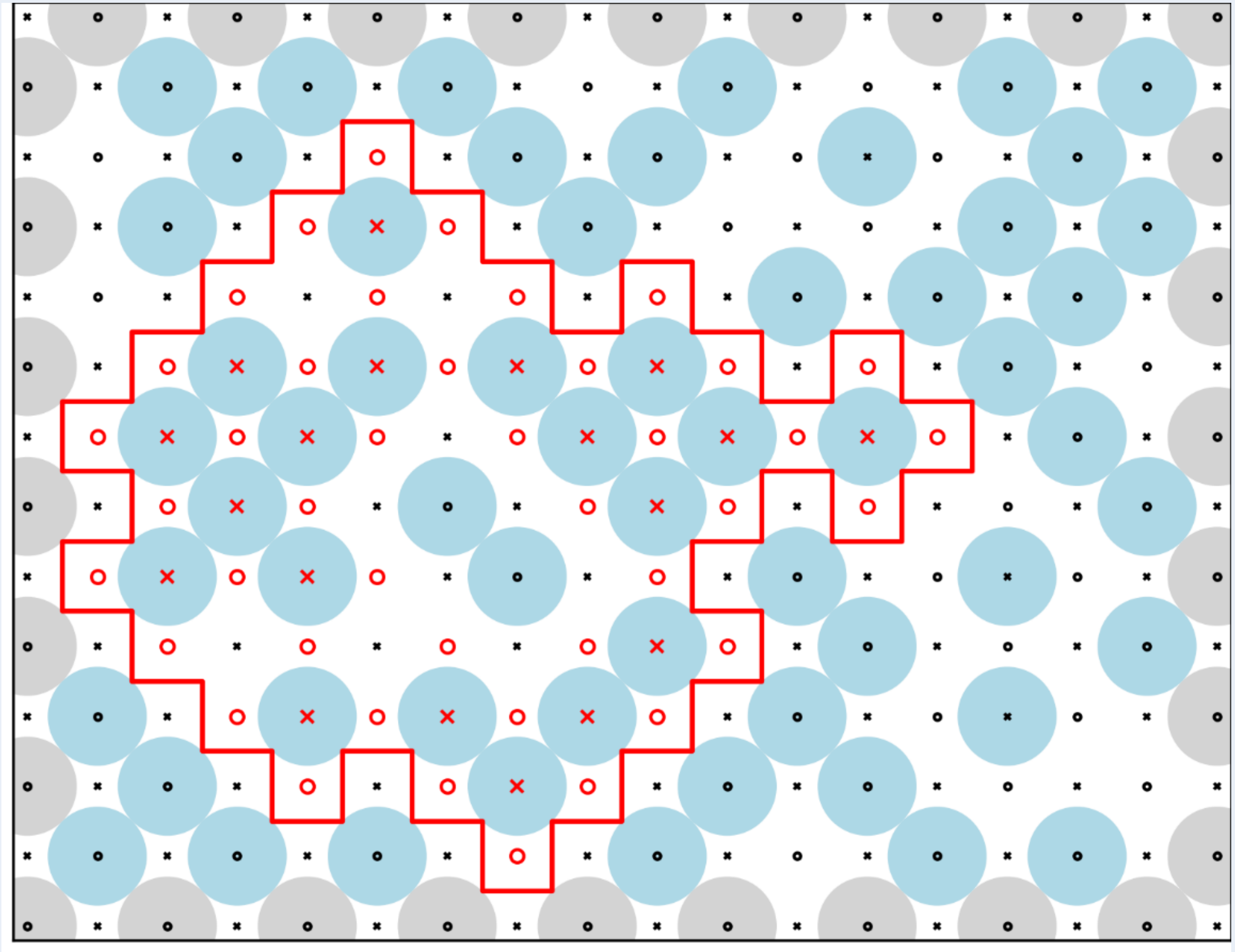
Dobrushin proof idea 6



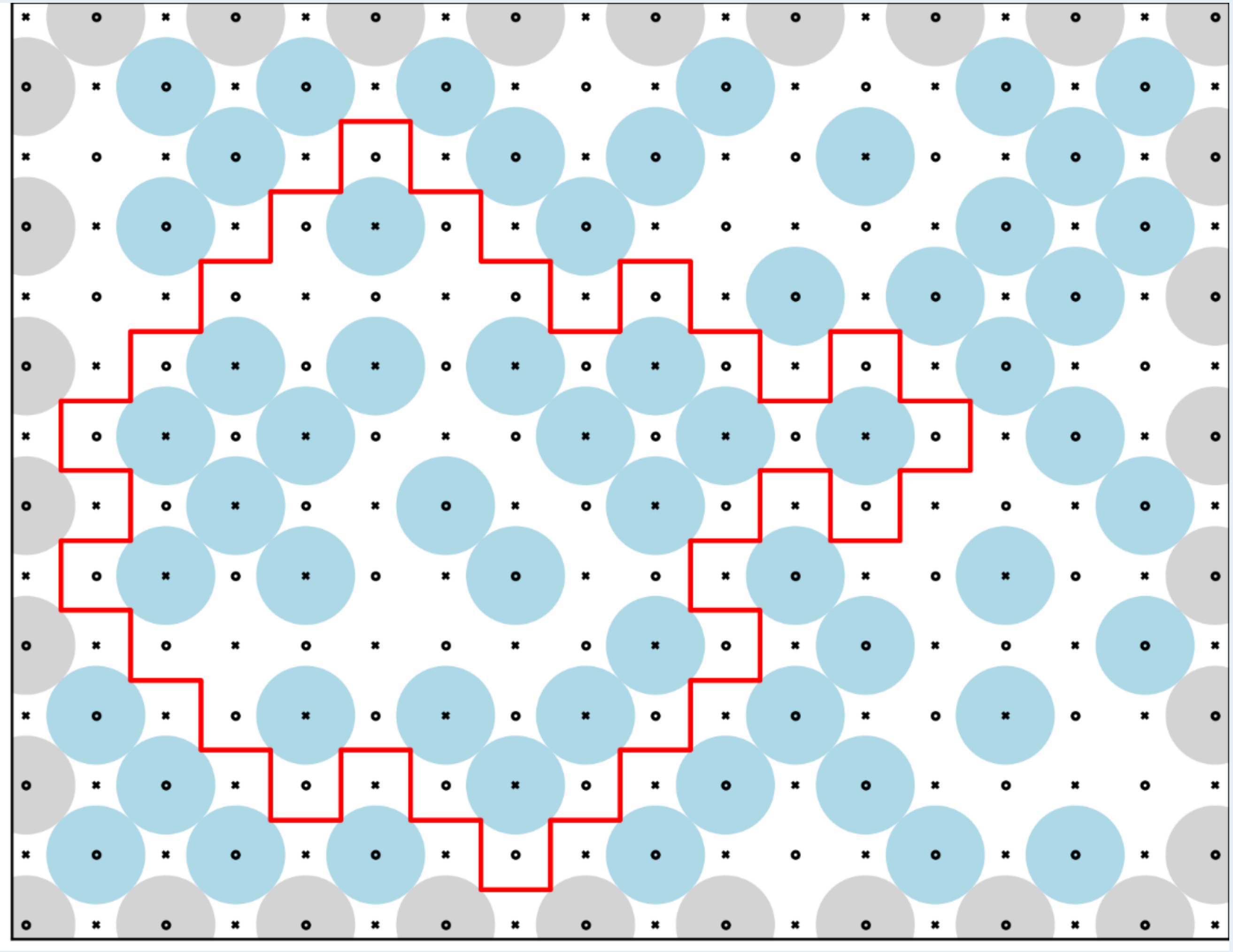
Dobrushin proof idea 7



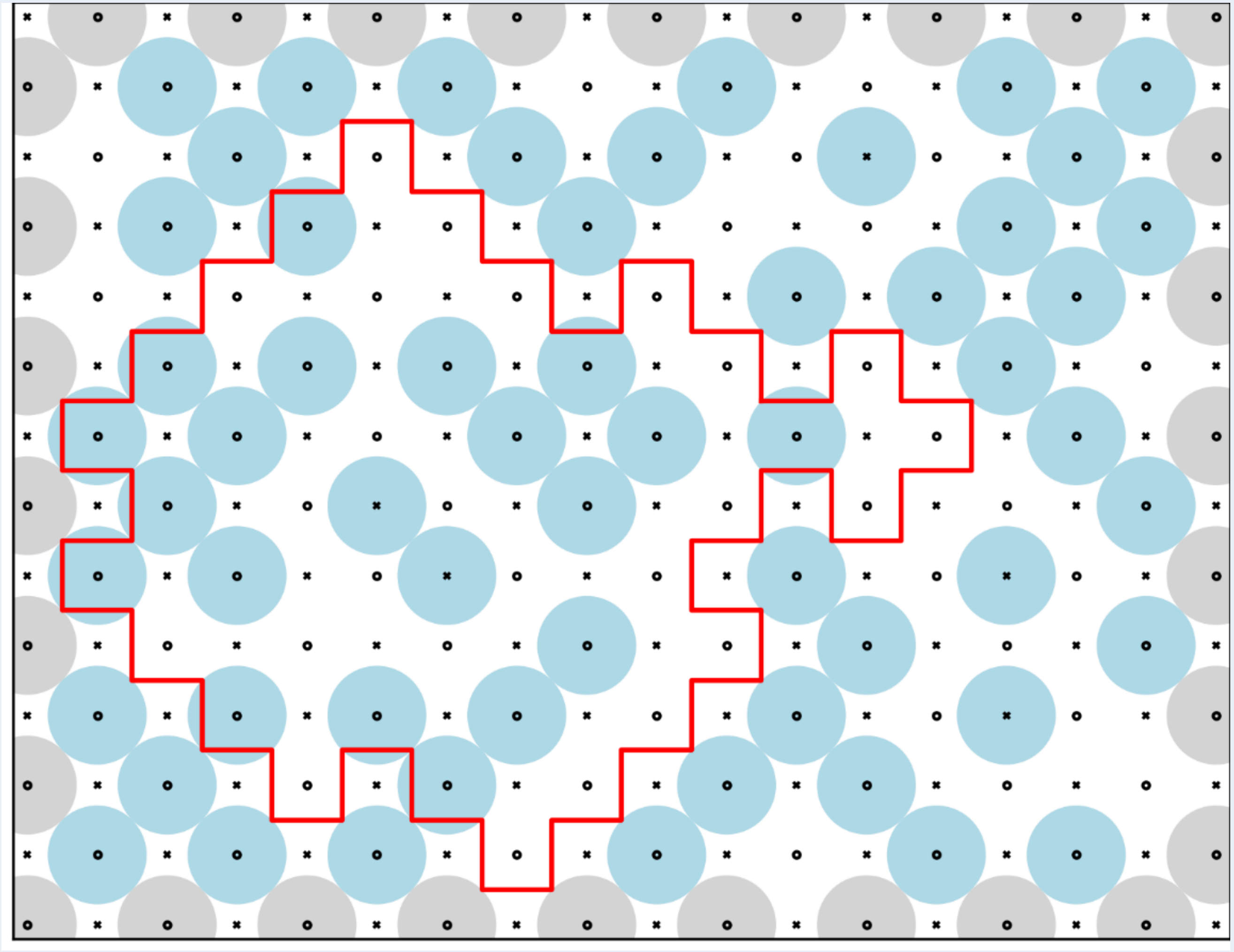
Dobrushin proof idea 8



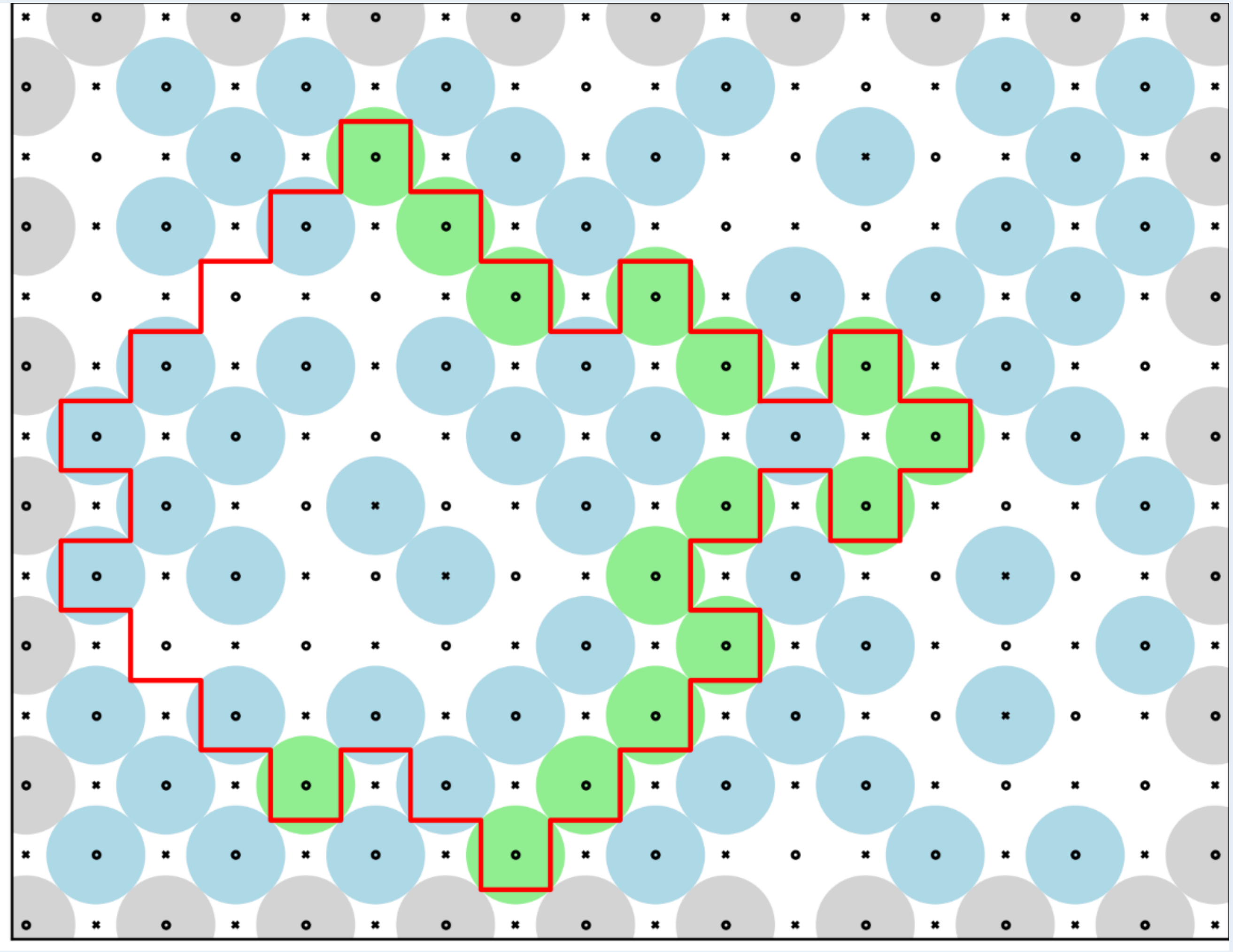
Dobrushin proof idea 9



Dobrushin proof idea 10

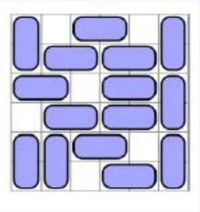


Dobrushin proof idea 11

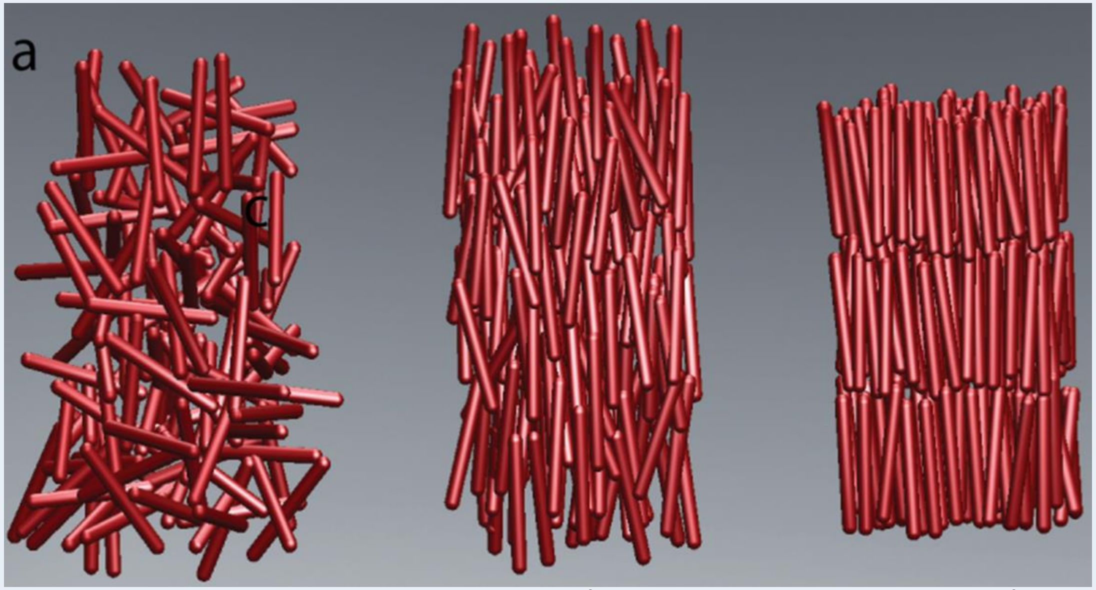


Other behaviors and liquid crystals

- Monomer-dimer model: Tiles are edges of $\mathbb{Z}^d$.
  Heilmann-Lieb 70: The model is disordered at all values of λ.
  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:



Disorderd (liquid/gas)

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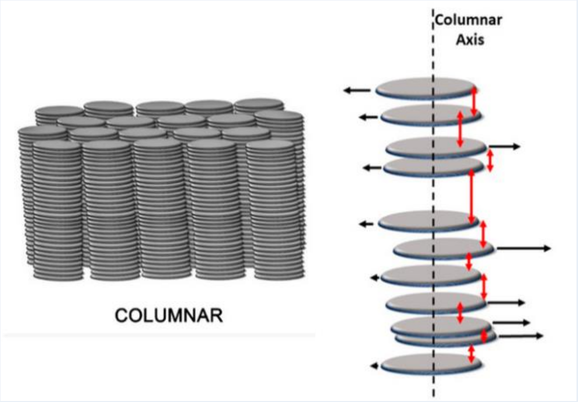
Nematic
Broken rotation symmetry,
preserved translation symmetry

Smectic
Broken rotation symmetry,
Translation symmetry
broken in only one direction



Columnar
Broken rotation symmetry,
Translation symmetry broken
only in a plane of directions

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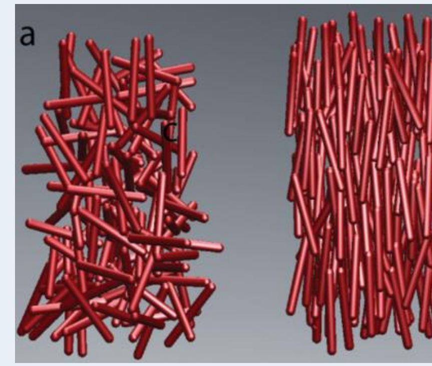
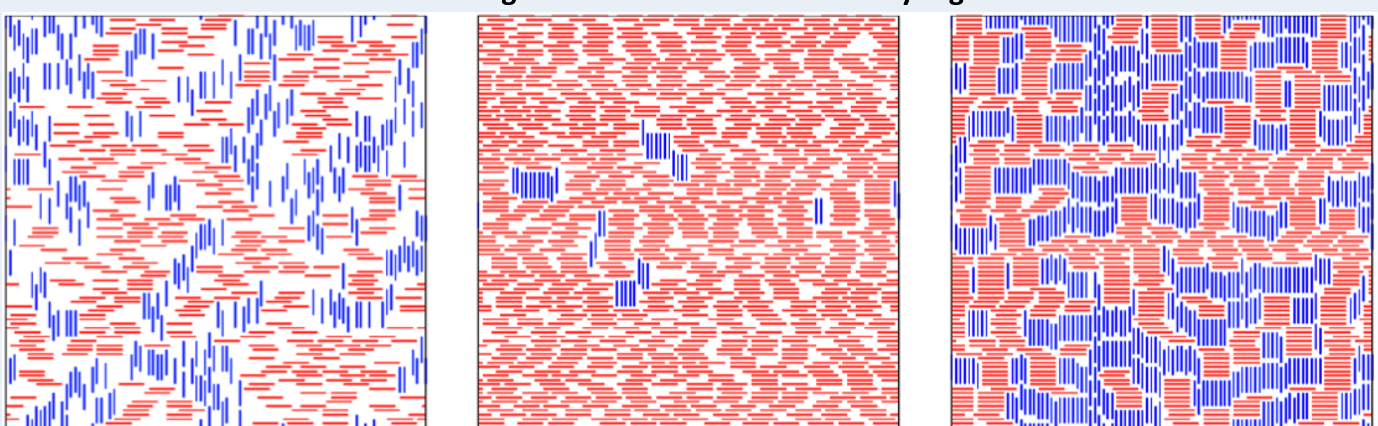
Nematic liquid crystals: predictions and proofs

- 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.

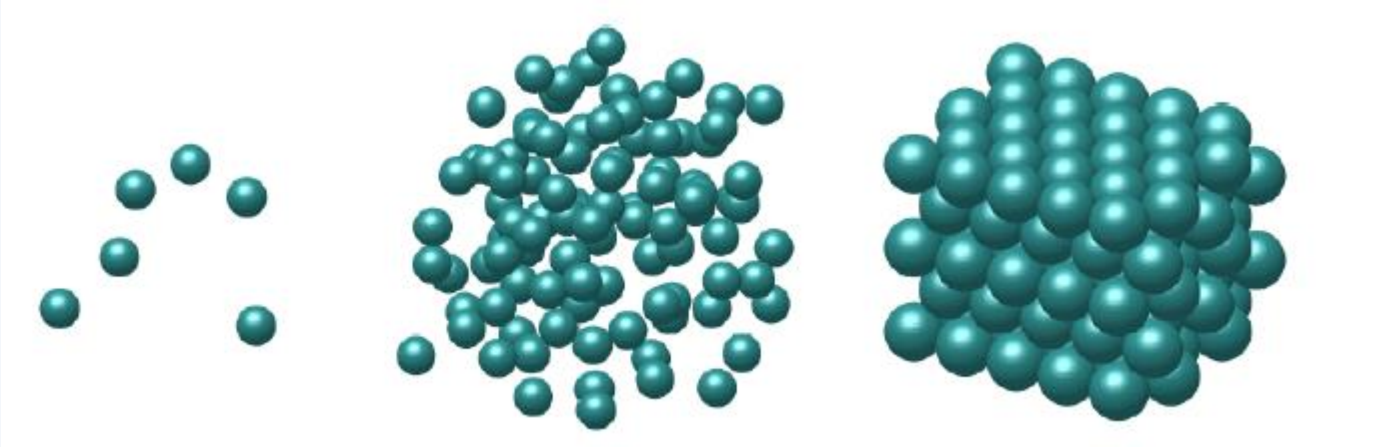
Rods of length 7 on $\mathbb{Z}^2$ at different density regimes



Low density disordered phase **Intermediate density nematic phase** **High-density HDD phase**

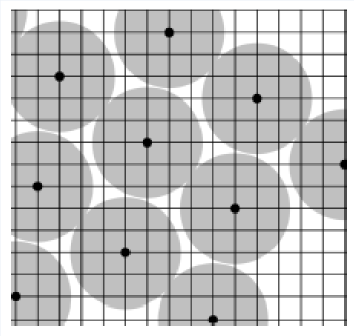
Packing balls in the continuum

- An important problem regards the packing of balls in $\mathbb{R}^d$.
- Physicists predict crystalline 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.

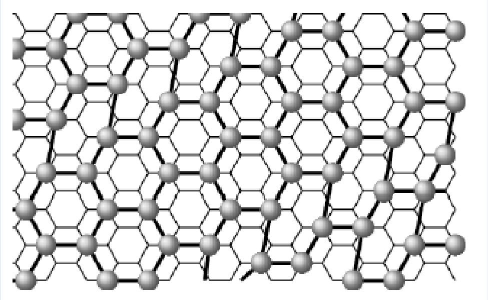


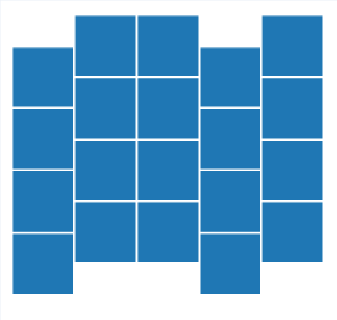
Lattice balls and sliding phenomenon

- Lattice approximation: Mazel-Stuhl-Suhov 19 (related to Jauslin-Lebowitz 18) considered a hard-core model on $\mathbb{Z}^2$ (and hexagonal and triangular lattices) where the tile is $\{v \in \mathbb{R}^2\colon \|v\|_2 \leq r\}$ 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.

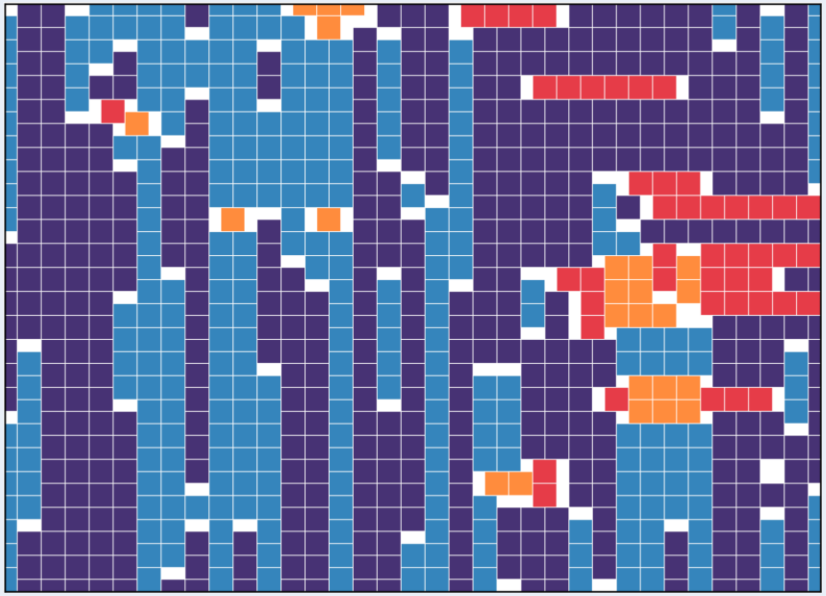




The 2×2 hard-square model

- 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 $\mu_{\Lambda,\lambda}^{\rho}$: Let $\Lambda \subset \mathbb{Z}^2$ be finite and ρ be a configuration.
  Then $\mu_{\Lambda,\lambda}^{\rho}$ is supported on configurations which agree with ρ outside Λ and is defined by $\mu_{\Lambda,\lambda}^{\rho}(\sigma) \propto \lambda^{N(\sigma)}$, where $N_\Lambda(\sigma)$ is the number of tiles of σ in Λ.
  Gibbs measure: probability measure over configurations in the entire $\mathbb{Z}^2$ which is "consistent" with the probability measures $\mu_{\Lambda,\lambda}^{\rho}$ (satisfies DLR condition).



Simulation of 2×2 hard-square model at large λ

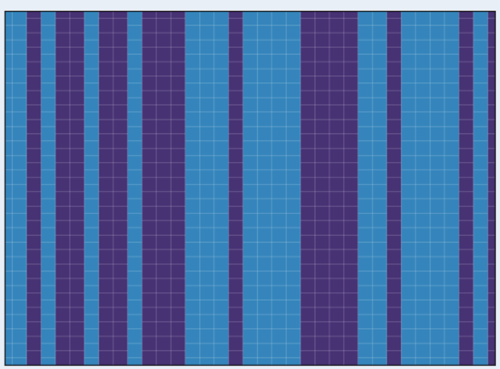
The 2×2 hard-square model

- Tile: the square $\{v \in \mathbb{Z}^2 \colon \|v\|_\infty \le 1\}$ ($r = \sqrt{2}$ of Mazel-Stuhl-Suhov study. Sliding)
  Configurations: Non-overlapping tiles with centers on the square lattice.

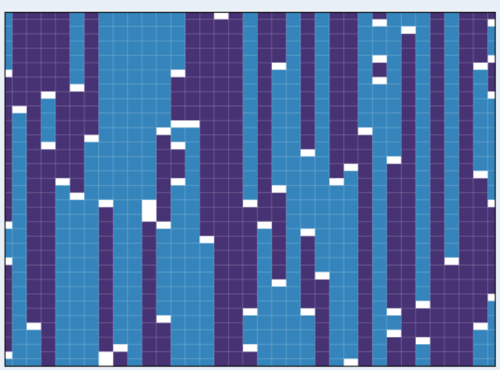
- Probability measure $\mu^{\rho}_{\Lambda,\lambda}$: Let $\Lambda \subset \mathbb{Z}^2$ be finite and ρ be a configuration.
  Then $\mu^{\rho}_{\Lambda,\lambda}$ is supported on configurations which agree with ρ outside Λ and is defined by $\mu^{\rho}_{\Lambda,\lambda}(\sigma) \propto \lambda^{N(\sigma)}$, where $N_\Lambda(\sigma)$ is the number of tiles of σ in Λ.
  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 λ, by Dobrushin's uniqueness theorem or by van den Berg's disagreement percolation method.

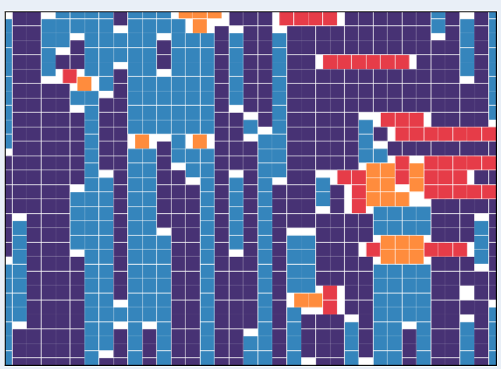
- Our results clarify the structure of configurations in the high-fugacity regime.



"$\lambda = \infty$" – fully-packed (order in columns)



***Independent columns* with large $\lambda < \infty$**

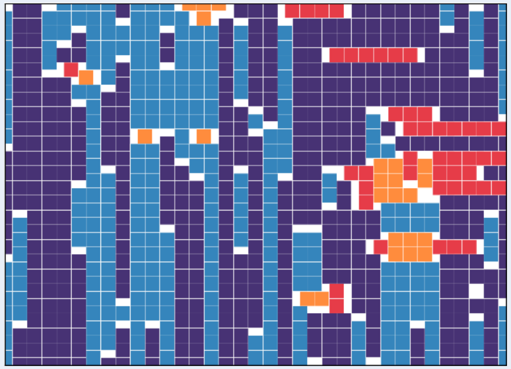


Simulation of 2×2 hard-square model at large λ

Columnar order and characterization of periodic Gibbs measures

- Theorem 1 (Hadas-P. 2022): There exists λ_0 such that the 2×2 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:

$$\mu_{\text{ver},0}(\text{tile at } (x,y)) = \begin{cases} \Theta\left(\frac{1}{\lambda}\right) & x \text{ even} \\ \frac{1}{2} - \Theta\left(\frac{1}{\sqrt{\lambda}}\right) & x \text{ odd} \end{cases}$$



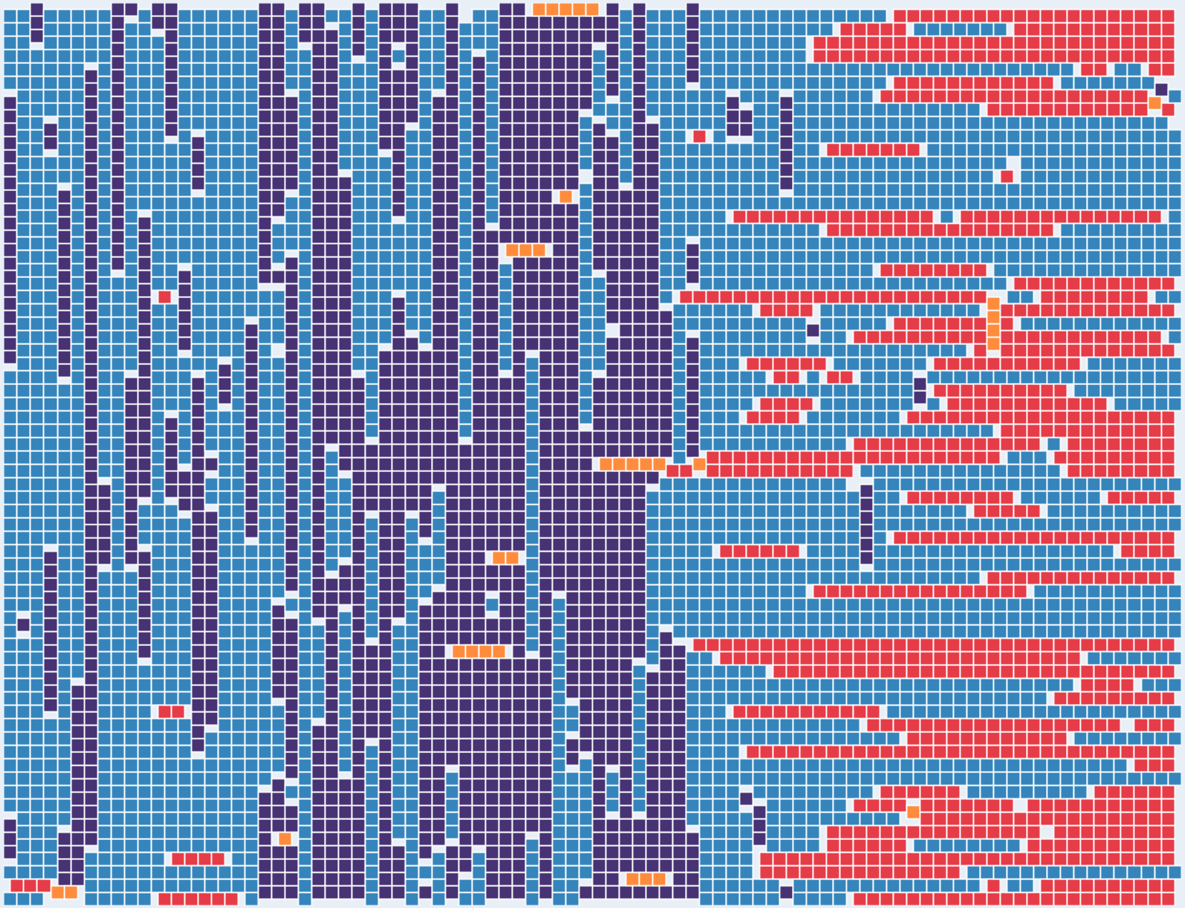
  - Decay of correlations:

$$\left|\text{Cov}_{\mu_{\text{ver},0}}(\text{tile at } (x_1,y_1), \text{tile at } (x_2,y_2))\right| \le Ce^{-c|x_1-x_2|-\frac{c|y_1-y_2|}{\sqrt{\lambda}}}$$

- 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

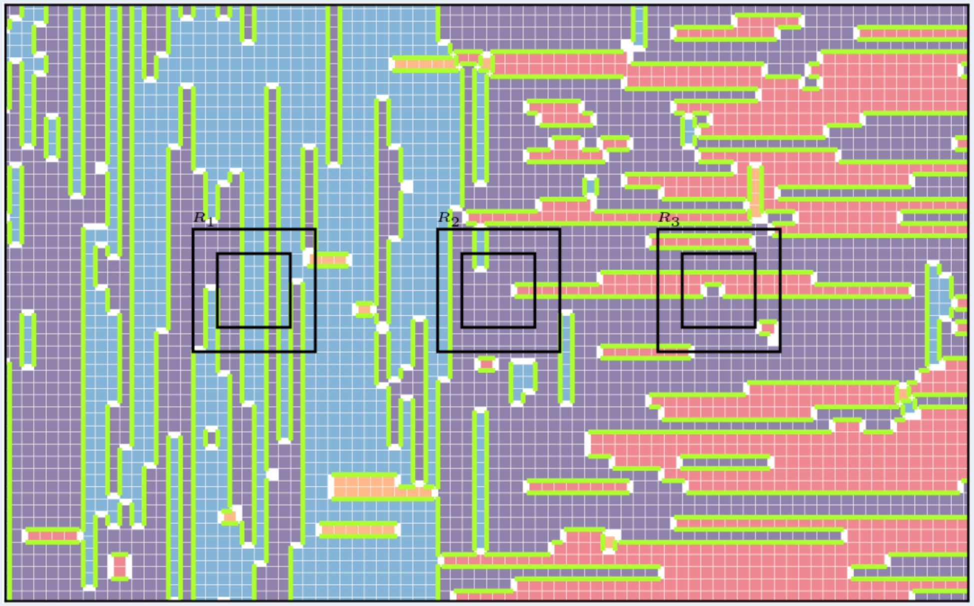
Columnar order ideas 1

- Aim to use a Peierls-type argument: classify regions into "columnar ordered" and "row ordered" and prove that the interfaces between them are rare.



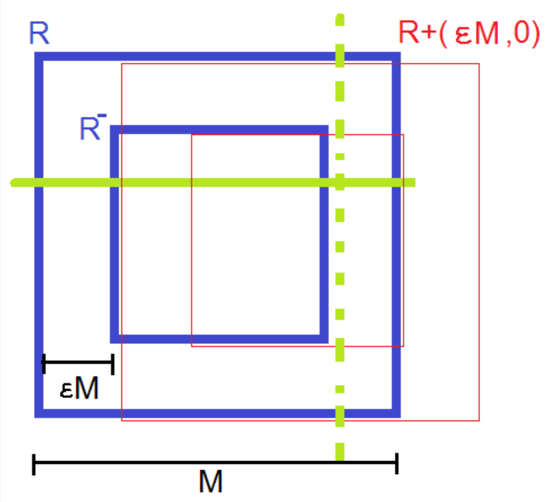
Columnar order ideas 2

- 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 both it and R^{-}, where R^{-} is a concentric square with $(1-2\epsilon)$ the dimensions of R for some fixed small $\epsilon > 0$.



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 both 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.



Columnar order ideas 4

- 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 both 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.
- 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 μ, 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 $R_1, \ldots, R_n$ with the dimensions of R are all not properly divided is at most $\exp\left(-c\frac{Area(R)}{\sqrt{\lambda}}n\right)$.

Basic estimate ideas 1

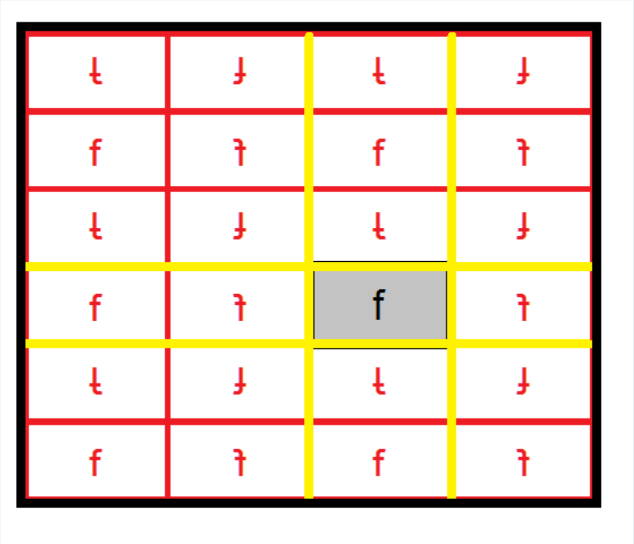
- Squares of mesoscopic side length $b(\lambda)$ satisfying $C\lambda^{1/4} < b(\lambda) < c\lambda^{1/2}$.
- The basic estimate: In any periodic Gibbs measure μ, for any such square R,

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

- Chessboard estimate (consequence of reflection positivity): Work on a discrete torus. For any local event E,

$$\mu^{torus}(E) \leq \mu^{torus}(\bar{E})^{1/N}$$

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).

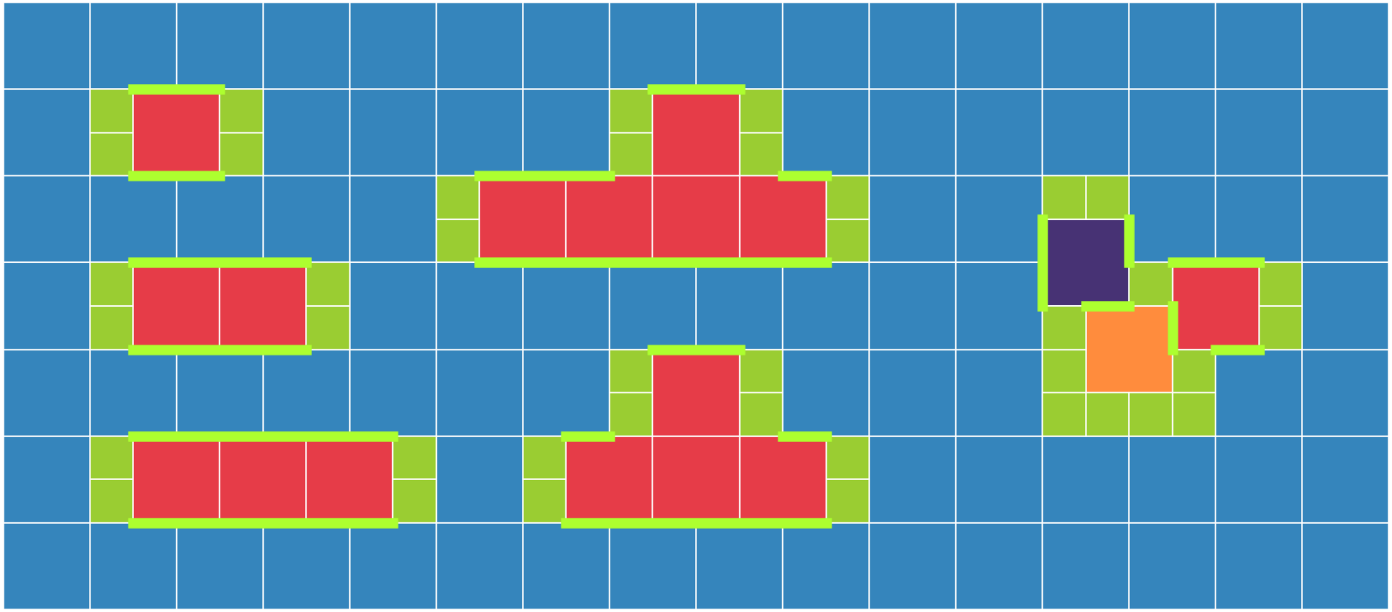


Basic estimate ideas 2

- 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 μ, 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,
$$\mu^{torus}(E) \leq \mu^{torus}(\bar{E})^{1/N}$$
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
$$\mu^{torus}(E_{b(\lambda)}) \leq \exp\left(-c\frac{\text{Area}(R)}{\sqrt{\lambda}}N\right)$$
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.



v=4 d=1 v=8 d=3 v=12 d=2

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.