A criterion for crystallization in hard-core lattice particle systems

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1708.01912
arXiv: 2402.02615

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Crystallization

- Crystallization: phase transition from a disordered phase to one with long-range positional order.
- Very difficult (in the continuum): small fluctuations easily break long-range order.
- To this day, there is no proof that there is crystallization in realistic models (models on $\mathbb{R}^3$ at positive temperature).

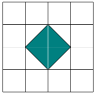
Hard-core models

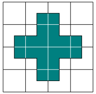
- Paradigmatic model: hard spheres: identical spherical particles in $\mathbb{R}^3$, may not overlap.
- Even at zero-temperature (densest packing): difficult [Hales, 2005] (computer assisted).
- Here: simpler systems: hard-core lattice models: replace $\mathbb{R}^3$ with a lattice Λ_∞ (a periodic graph, examples: $\mathbb{Z}^d$, or triangular lattice, or honeycomb).
- Each particle has a position $x \in \Lambda_\infty$ and a shape $\omega \subset \mathbb{R}^d$, which is a bounded connected subset of $\mathbb{R}^d$. $(d \geqslant 2)$
- Interaction: if $\omega_x := x + \omega$,

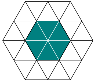
$$\omega_x \cap \omega_y = \emptyset.$$

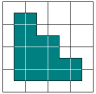
- discrete support: $\sigma_x := \omega_x \cap \Lambda_\infty$.

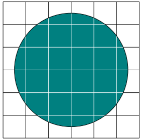
Examples of hard-core lattice models









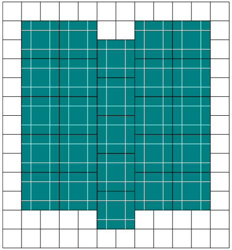


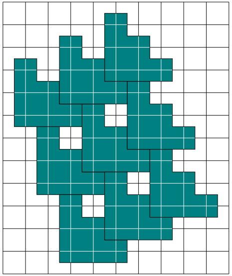
High density crystallization

- [Dobrushin, 1968], [Gaunt, Fisher, 1965]: diamonds on $\mathbb{Z}^2$.
- [Heilmann, Praestgaard, 1974]: crosses on $\mathbb{Z}^2$.
- [Baxter, 1980], [Joyce, 1988]: hexagons on triangular lattice.
- [Jauslin, Lebowitz, 2018]: non-sliding tiling models.
- [Mazel, Stuhl, Suhov, 2018, 2019, 2020, 2021]: hard disks on $\mathbb{Z}^2$, triangular, honeycomb lattice.
- Here: criterion in arbitrary dimension $d \geqslant 2$ for non-sliding model (not necessarily tiling).

Main idea: sliding

- "sliding": in closely-packed configurations, particles are not locked in place.
- non-sliding: defects are localized.





Ground states

- Ground states: closely-packed configurations.
- Uniform density configurations: X in Λ_∞, for all $\Lambda \Subset \Lambda_\infty$, the number of particles in Λ is $\rho|\Lambda| + o(|\Lambda|)$.
- Maximal density: $\rho_{\max} \leftrightarrow$ Maximal density configuration: ground state.
- Set of ground states: $\mathcal{G}$.
- **(A2) $\mathcal{G}$ is finite and non-empty.**

Gibbs measure

- Gibbs measure:

$$\langle A\rangle_\nu := \lim_{\Lambda\to\Lambda_\infty} \frac{1}{\Xi_{\Lambda,\nu}(z)} \sum_{X\subset\Lambda} A(X) z^{|X|} \mathfrak{B}_\nu(X) \prod_{x\neq x'\in X} \varphi(x,x')$$

  - Λ: finite subset of lattice Λ_∞.
  - $z \geqslant 0$: fugacity. $z \gg 1$.
  - $\varphi(x,x')$: hard-core interaction.
  - $\mathfrak{B}_\nu$, $\nu \in \mathcal{G}$: boundary condition: favors the ν-th ground state.
- Pressure:

$$p(z) := \lim_{\Lambda\to\Lambda_\infty} \frac{1}{|\Lambda|} \log \Xi_{\Lambda,\nu}(z).$$

Defects

- Discrete Voronoi cell of a particle at x in a configuration X: $V_X(\sigma_x)$: set of $y \in \Lambda_\infty$ such that y is closer (inclusively) to σ_x than to any other particle.
- Defined in this way, Voronoi cells may overlap.
- The sites in the support σ_x of a particle only belong to the Voronoi cell of that particle.
- Def: The neighbors of a particle x are the particles whose Voronoi cells are at distance $\leqslant 1$ from $V_X(\sigma_x)$.
- Def: Given $\nu \in \mathcal{G}$, a particle $x \in X$ is ν-correct if its neighbors are the same as in the ground state ν.
- Defect: incorrect particle.

Independence of defects

- **(A5)** Given two particles x and y that are neighbors. **If x is ν-correct and y is μ-correct, then $\nu = \mu$.**
- Disconnected defects are independent.

Local density

- Local density: inverse of the "weighted size" of the Voronoi cell:

$$\frac{1}{\rho_X^{(\mathrm{loc})}(x)} := \sum_{y \in V_X(\sigma_x)} \frac{1}{|\{z \in X : \ y \in V_X(z)\}|}.$$

- **(A4) The maximal local density is equal to the maximal density:** $\rho_{\max}^{(\mathrm{loc})} = \rho_{\max}$.
- It must not be possible for a few particles to be packed more closely than a ground state locally, at the expense of the global density.

Gains from defects

- A dip in the local density should be unlikely when $z \gg 1$.
- **(A6)** $\exists \epsilon > 0$ **such that, for any incorrect particle** x**,**

$$\rho_X(y)^{-1} \geqslant \rho_{\max}^{-1} + \epsilon.$$

- (This condition can actually be made more general.)

Criterion

- **(A1)** Λ_∞ is $\mathbb{Z}^d$ with $g \geqslant 2$ or the triangular or honeycomb lattices (our result is actually more general than this).
- **(A2) $\mathcal{G}$ is finite and non-empty.**
- **(A3)** the ground states are isometric to each other.
- **(A4) The maximal local density is equal to the maximal density:** $\rho_{\max}^{(\text{loc})} = \rho_{\max}$**.**
- **(A5)** Given two particles x and y that are neighbors. **If x is ν-correct and y is μ-correct, then $\nu = \mu$.**
- **(A6)** $\exists \epsilon > 0$ **such that, for any incorrect particle** x**,** $\rho_X(y)^{-1} \geqslant \rho_{\max}^{-1} + \epsilon$.

Theorem

We define $\mathbb{1}_x$ as the function that returns 1 if $x \in X$ and 0 if not, and denote the ground states by $\mathcal{L}_\nu$ for $\nu \in \mathcal{G}$.

If (A1)-(A6) are satisfied, then there exists $z_0 > 0$ such that,

- for $|z| \geqslant z_0$, $p(z) - \rho_{\max} \log z$ and $\langle \mathbb{1}_{x_1} \cdots \mathbb{1}_{x_n} \rangle_\nu$ are analytic functions of $1/z$.
- For $z \geqslant z_0$, there are at least $|\mathcal{G}|$ distinct Gibbs states:

$$\langle \mathbb{1}_x \rangle_\nu = \begin{cases} 1 + O(z^{-1}) & \text{if } x \in \mathcal{L}_\nu \\ O(z^{-1}) & \text{if not.} \end{cases}$$

Low-fugacity (Mayer) expansion

- Partition function: $Z_\Lambda(n)$: number of configurations with n particles:

$$\Xi_\Lambda(z) = \sum_{n=0}^{\infty} z^n Z_\Lambda(n)$$

- Formally, (converges if z is small enough)

$$\frac{1}{|\Lambda|}\log \Xi_\Lambda(z) = \sum_{k=1}^{\infty} b_k(\Lambda) z^k$$

where, if $Z_\Lambda(k_i)$ denotes the number of configurations with k_i particles, then

$$b_k(\Lambda) := \frac{1}{|\Lambda|}\sum_{j=1}^{k}\frac{(-1)^{j+1}}{j}\sum_{\substack{k_1,\cdots,k_j\geqslant 1\\ k_1+\cdots+k_j=k}} Z_\Lambda(k_1)\cdots Z_\Lambda(k_j)$$

High-fugacity expansion

- Partition function: $Z_\Lambda(n)$: number of configurations with n particles:

$$\Xi_\Lambda(z) = \sum_{n=0}^{N_{\max}} z^n Z_\Lambda(n)$$

- Inverse fugacity $y \equiv z^{-1}$:

$$\Xi_\Lambda(z) = z^{N_{\max}} \sum_{n=0}^{N_{\max}} y^n Q_\Lambda(n)$$

with $Q_\Lambda(n) \equiv Z_\Lambda(N_{\max} - n)$.

High-fugacity expansion

- Formally,

$$\frac{1}{|\Lambda|}\log \Xi_\Lambda = \rho_{\max}\log z + \sum_{k=1}^{\infty} c_k(\Lambda) y^k$$

where $\rho_{\max} = \frac{N_{\max}}{|\Lambda|}$,

$$c_k(\Lambda) := \frac{1}{|\Lambda|}\sum_{j=1}^{k}\frac{(-1)^{j+1}}{j\tau^j}\sum_{\substack{k_1,\cdots,k_j\geqslant 1\\ k_1+\cdots+k_j=k}} Q_\Lambda(k_1)\cdots Q_\Lambda(k_j)$$

- Does not always converge for large z. We prove it does under (A1)-(A6) using Pirogov-Sinai theory.

Pirogov-Sinai theory

- Switch to a contour model made up of defects.
- The contours interact via a hard-core repulsion (not really, but they can be made to do so with some work).
- The density of contours is small: they contain dips in the local density whose number is proportional to the size of the contour.
- Use cluster expansion for the contour model.
- (Extra complications: contours must be thickened, for various technical reasons; nested contours interact, which we deal with using the Minlos-Sinai trick.)

Lee-Yang zeros

- Lee-Yang zeros: roots of $\Xi_\Lambda(z) \iff$ singularities of $p_\Lambda(z)$.
- Whenever the high fugacity expansion has a radius of convergence $\tilde{R}$, there are no Lee-Yang zeros outside of a disc of radius $\tilde{R}^{-1}$.