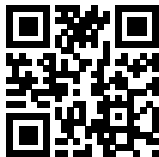


A criterion for crystallization in hard-core lattice particle systems

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Crystallization



- Crystallization: **phase transition** from a **disordered** phase to one with **long-range positional order**.
- Example: Freezing transition in water.
- Simpler example: **hard spheres**: identical spherical particles in \mathbb{R}^3 , may not overlap. Conjecture: gas phase at low densities, crystalline phase at high densities.

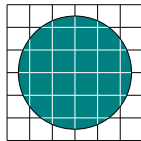
Crystallization



- Very difficult (in the continuum): small fluctuations easily break long-range order.
- To this day, there is **no proof** that there is crystallization in the hard sphere model at positive temperature.

Hard-core lattice models

- 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 . ($d \geq 2$)



Equilibrium statistical mechanics

- Random particle configurations **without overlap**: if $\omega_x := x + \omega$,

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

- Probability of a configuration $X \subset \Lambda_\infty$: proportional to

$$z^{|X|}$$

$|X|$: number of particles, $z > 0$: **fugacity**: controls the density of particles.

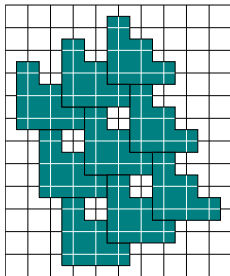
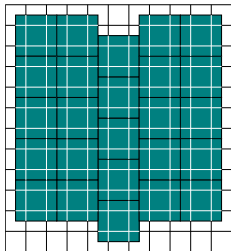
- Question: for large z , are **typical** configurations **ordered**?

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 $d \geq 2$ 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 $\Lambda \in \Lambda_\infty$, 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:**

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

- ▶ Λ : finite subset of lattice Λ_∞ .
- ▶ $z \geq 0$: fugacity. $z \gg 1$.
- ▶ $\varphi(x, y)$: hard-core interaction: = 0 if $\omega_x \cap \omega_y \neq \emptyset$ and 1 otherwise.
- ▶ $\mathfrak{B}_\nu, \nu \in \mathcal{G}$: boundary condition: favors the ν -th ground state.

- **Pressure:**

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

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}_ν for $\nu \in \mathcal{G}$.

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

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

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

Defects

- **Discrete Voronoi cell** of a particle at x in a configuration X : $V_X(\omega_x)$: set of $y \in \Lambda_\infty$ such that y is **closer** (inclusively) to ω_x than to any other particle.
- Defined in this way, Voronoi cells may overlap.
- The sites in the support ω_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 ≤ 1 from $V_X(\omega_x)$.
- 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:

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

- **(A4) The maximal local density is equal to the maximal density:**
 $\rho_{\max}^{(\text{loc})} = \rho_{\max}$.
- 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 ,

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

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

Criterion

- (A1) Λ_∞ is \mathbb{Z}^d with $d \geq 2$ 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 , $\rho_X(y)^{-1} \geq \rho_{\max}^{-1} + \epsilon$.

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

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- For $z \geq z_0$, 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

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

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

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

- 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} .

