A criterion for crystallization in
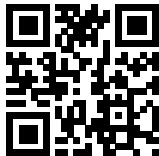# hard-core lattice particle systems

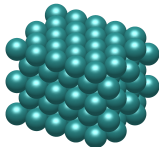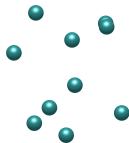**Ian Jauslin**

joint with **Qidong He, Joel L. Lebowitz**

http://ian.jauslin.org

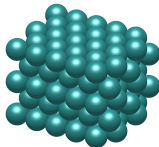# Crystallization

- 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
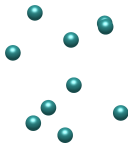
- Very difficult (in the continuum): small fluctuations easily break long-range order.

- 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 $\mathbb{R}^d$. $(d \geqslant 2)$
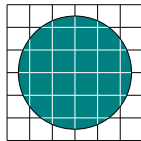
Equilibrium statistical mechanics

- 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 $d \geqslant 2$ 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.
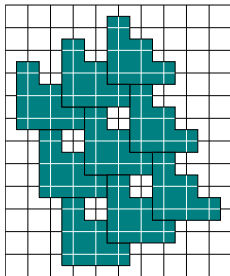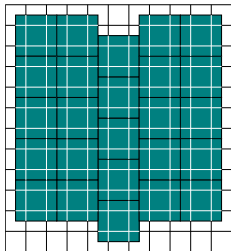
Ground states

- Ground states: closely-packed configurations.

- Periodic uniform density configurations: periodic X in Λ_∞, such that 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:
$$\langle A \rangle_\nu := \lim_{\Lambda \to \Lambda_\infty} \frac{1}{\Xi_{\Lambda,\nu}(z)} \sum_{X \subset \Lambda} A(X) z^{|X|} \mathfrak{B}_\nu(X) \prod_{x \neq y \in X} \varphi(x, y)$$

  - Λ: finite subset of lattice Λ_∞.
  - $z \geqslant 0$: 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:
$$p(z) := \lim_{\Lambda \to \Lambda_\infty} \frac{1}{|\Lambda|} \log \Xi_{\Lambda,\nu}(z).$$

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 $\mathcal{L}_\nu$ for $\nu \in \mathcal{G}$.

If (A1)-(A6) (see below) 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:

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

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 $\leqslant 1$ 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,

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

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

Criterion

- **(A1)** Λ_∞ is $\mathbb{Z}^d$ with $d \geqslant 2$ 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:** $\rho_{\max}^{(\mathrm{loc})} = \rho_{\max}$.

- **(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,

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- For $z \geqslant z_0$, there are at least $|\mathcal{G}|$ distinct Gibbs states:

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

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 $\tilde{R}^{-1}$.