A criterion for crystallization in hard-core lattice particle systems

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1708.01912
arXiv: 2402.02615

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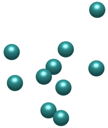
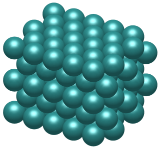
Crystallization

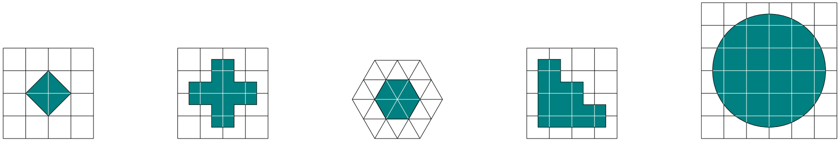




- Crystallization: phase transition from a disordered phase to one with long-range positional order. (For example: freezing in water)
- Hard spheres: identical spherical particles in $\mathbb{R}^3$, may not overlap. Conjecture: gas phase at low densities, crystalline phase at high densities.
- Very difficult (in the continuum): small fluctuations easily break long-range order.

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.

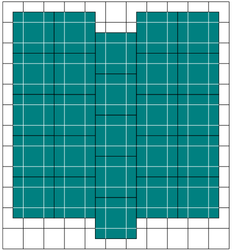
- Question: for large z, are typical configurations ordered?

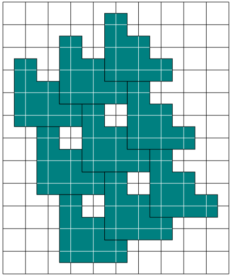
High density crystallization

- [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.





Main result

- Criterion under which configurations are typically crystalline for large (but finite) values of z.
  - The number of close-packed configurations is finite.
  - Disconnected defects are independent (non-sliding).
  - Defects lower the local density.
  - *The maximal local density is equal to the global local density.*
  - *The close-packed configurations are related to each other by isometries.*
- The criterion can be verified based entirely on local considerations.

Theorem

- $\mathbb{P}_\nu(x)$: probability in Gibbs measure with a boundary condition that favors the ν-th close packing of finding a particle at x, in the thermodynamic limit.
- For $z \geqslant z_0$, there are at least as many distinct Gibbs states as there are close-packings:

$$\mathbb{P}_\nu(x) = \begin{cases} 1 + O(z^{-1}) & \text{if } x \text{ is in the } \nu\text{th close packing} \\ O(z^{-1}) & \text{if not.} \end{cases}$$

Main tools

- Analytic expansion in z^{-1}: Mayer expansion and Pirogov-Sinai theory.
- Effective low-density model of defects.
- To identify defects: discrete Voronoi cells to identify neighboring particles.
- Defects are particles whose neighbors are not the same as in a close-packing.

Conclusion and outlook

- Locally verifiable criterion for crystallization in hard-core lattice particle systems that are non-sliding.
- Future work: generalize the criterion (remove technical assumptions).
- Future work: applications to systems in $d \geqslant 2$.
- Future work: generalize to continuum models.