Crystalline ordering in hard-core lattice particle systems

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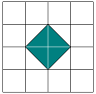
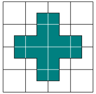
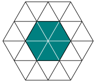
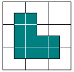
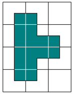
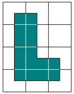
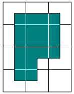
Crystallization in particle systems

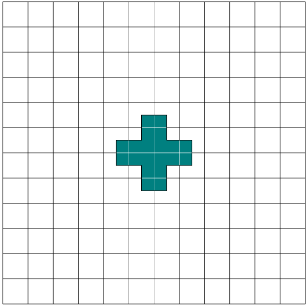
- Gas-liquid-solid paradigm: not yet understood mathematically in realistic particle models.
- Crystallization: long range positional order.
- Here: discuss a class of hard-core lattice particle models for which we can prove crystallization.

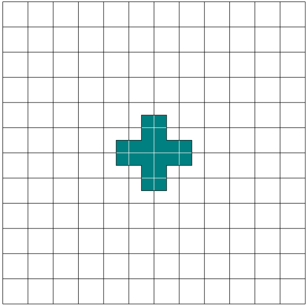
Hard-core lattice particle (HCLP) systems

Non-sliding HCLPs

- There exist a **finite** number τ of tilings $\{\mathcal{L}_1, \cdots, \mathcal{L}_\tau\}$ which are **periodic** and **isometric** to each other.





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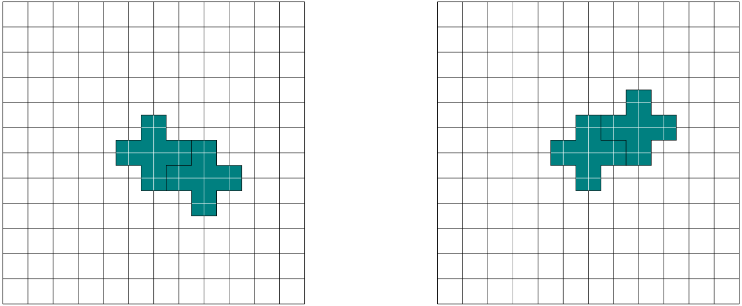

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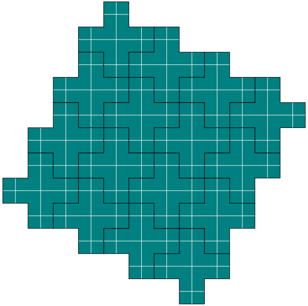
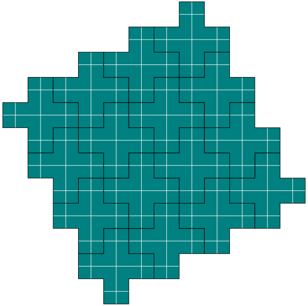
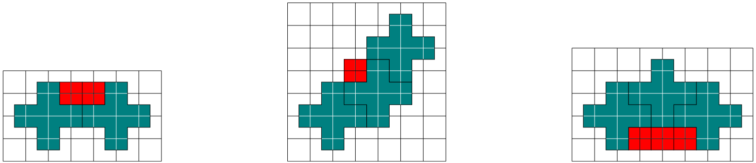




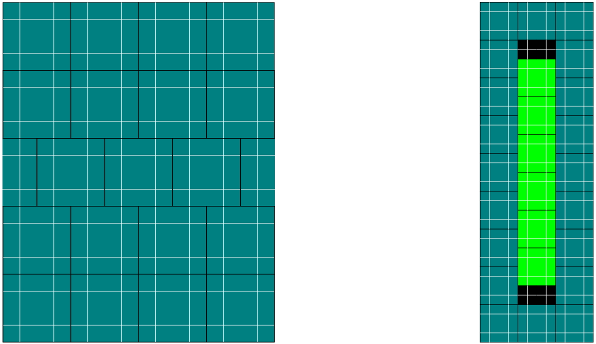
Non-sliding HCLPs

- Defects are **localized**: for every connected particle configuration X that is *not* the subset of a close packing and every $Y \supset X$, there is empty space in Y neighboring X.



Example of a sliding HCLP

- 2×2 squares:



Observables

- 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.
  - $\varphi(x,x')$: hard-core interaction.
  - $\mathfrak{B}_\nu$: boundary condition: favors the ν-th tiling.
- Pressure:

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

Theorem

- $p(z) - \rho_m \log z$ and $\langle \mathbb{1}_{x_1} \cdots \mathbb{1}_{x_n} \rangle_\nu$ are **analytic** functions of $1/z$ for large values of z.

- There are τ 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 expansion

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

$$\Xi_\Lambda(z) = \sum_{X\subset\Lambda} z^{|X|} \prod_{x\neq x'\in X} \varphi(x,x') = \sum_{n=0}^{\infty} z^n Z_\Lambda(n)$$

- Formally,

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

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

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

Low-fugacity expansion

- Partition function:

$$\Xi_\Lambda(z) = 1 + zZ_\Lambda(1) + z^2 Z_\Lambda(2) + \cdots$$

- Second term:

$$b_2(\Lambda) = \frac{1}{|\Lambda|}\left(Z_\Lambda(2) - \frac{1}{2}Z_\Lambda^2(1)\right)$$

- $Z_\Lambda(2)$: counts interacting particle configurations: $O(\Lambda^2)$.
- $\frac{1}{2}Z_\Lambda^2(1)$: counts non-interacting particle configurations: $O(\Lambda^2)$.
- The terms of order $|\Lambda|^2$ cancel out, so $b_2(\Lambda)$ has a limit as $\Lambda \to \Lambda_\infty$.

Low-fugacity expansion

- [Ursell, 1927], [Mayer, 1937]: $b_k(\Lambda) \to b_k$.

- [Groeneveld, 1962], [Ruelle, 1963], [Penrose, 1963]:

$$p(z) = \sum_{k=1}^{\infty} b_k z^k$$

which has a positive radius of convergence.

High-fugacity expansion

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

$$\Xi_\Lambda(z) = \sum_{X \subset \Lambda} z^{|X|} \prod_{x \neq x' \in X} \varphi(x, x') = \sum_{n=0}^{N_{\max}} z^n Z_\Lambda(n)$$

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

$$\Xi_\Lambda(z) = z^{N_{\max}} \sum_{X \subset \Lambda} y^{N_{\max} - |X|} \prod_{x \neq x' \in X} \varphi(x, x') = z^{N_{\max}} \sum_{n=0}^{N_{\max}} y^n Q_\Lambda(n)$$

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

High-fugacity expansion

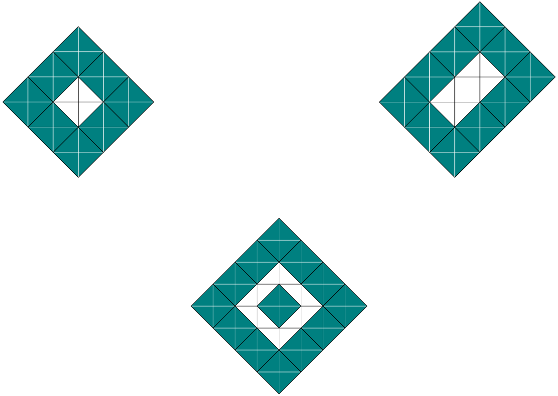
- Formally,

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

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

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

High-fugacity expansion



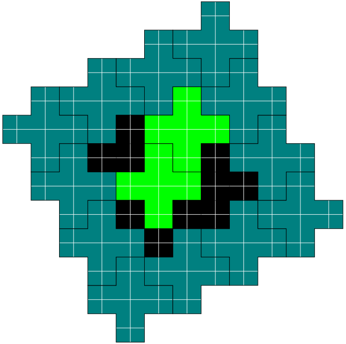
High-fugacity expansion

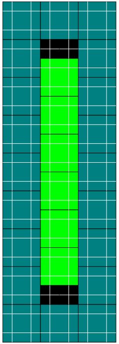
- [Gaunt, Fisher, 1965]: diamonds: $c_k(\Lambda) \to c_k$ for $k \leqslant 9$.
- [Joyce, 1988]: hexagons (integrable, [Baxter, 1980]).
- [Eisenberg, Baram, 2005]: crosses: $c_k(\Lambda) \to c_k$ for $k \leqslant 6$.
- Cannot be done *systematically*: there exist counter-examples: e.g. hard 2×2 squares on $\mathbb{Z}^2$:

$$c_1(\Lambda) \propto \sqrt{|\Lambda|}$$

Holes interact

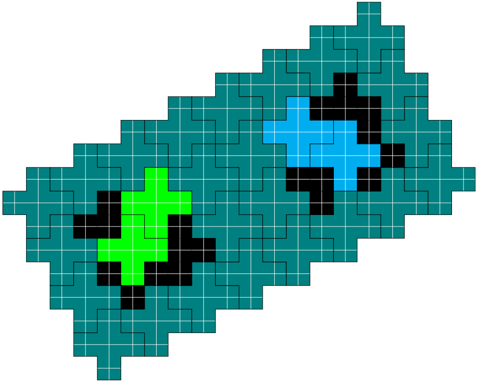
- Total volume of holes: $\in \rho_m^{-1}\mathbb{N}$.





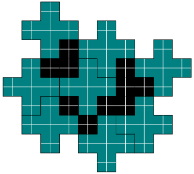
Non-sliding condition

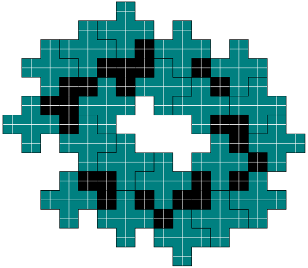
- Distinct defects are decorrelated.



Gaunt-Fisher configurations

- Group together empty space and neighboring particles.





Defect model

- Map particle system to a model of defects:

$$\Xi_{\Lambda,\nu}(z) = z^{\rho_m|\Lambda|} \sum_{\underline{\gamma}\subset\mathfrak{C}_\nu(\Lambda)} \left(\prod_{\gamma\neq\gamma'\in\underline{\gamma}} \Phi(\gamma,\gamma')\right) \prod_{\gamma\in\underline{\gamma}} \zeta_\nu^{(z)}(\gamma)$$

  - Φ: hard-core repulsion of defects.
  - $\zeta_\nu^{(z)}(\gamma)$: activity of defect.

- The activity of a defect is exponentially small: $\exists\epsilon \ll 1$

$$\zeta_\nu^{(z)}(\gamma) < \epsilon^{|\gamma|}$$

- Low-fugacity expansion for defects.

Crystallization

- Peierls argument: in order to have a particle at x that is not compatible with the ν-th perfect packing, it must be part of or surrounded by a defect.

- Note: a naive Peierls argument requires the partition function to be independent from the boundary condition. This is not necessarily the case here, and we need elements from Pirogov-Sinai theory.

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