Crystalline ordering in hard-core lattice particle systems

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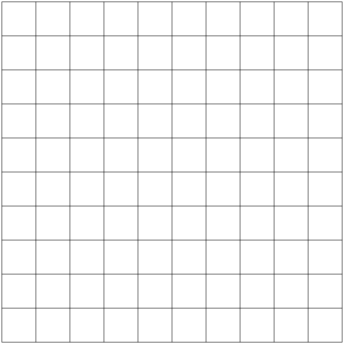
Non-sliding HCLP

- Lattice in $d \geqslant 2$ dimensions.
- Identical particles with pair hard-core interaction.
- Finite number of perfect packings, which are periodic, and related to each other by isometries.
- Non-sliding (defects are full of holes).

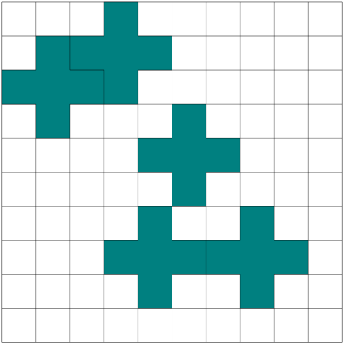
Lattice

- Lattice Λ_∞ of dimension $d \geqslant 2$



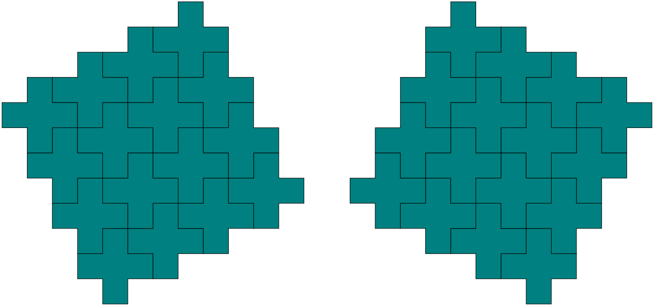
Particles

- Identical particles: shape $\omega \subset \mathbb{R}^d$



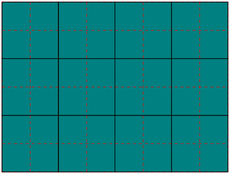
Perfect packings

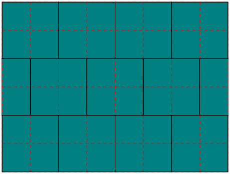
- Perfect packing: $\forall x \in \Lambda_\infty$, $\exists! y$ such that $x \in \omega + y$



Perfect packings

- Example with infinitely many perfect packings: 2×2 squares





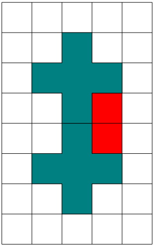
Non-sliding condition

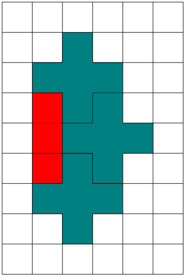
- Defects have an amount of empty space that is proportional to their volume.

- For every *connected* particle configuration X that *cannot* be completed to a perfect packing, and for every particle configuration $Y \supset X$, at least one of the sites *neighboring* X is empty.

Non-sliding condition

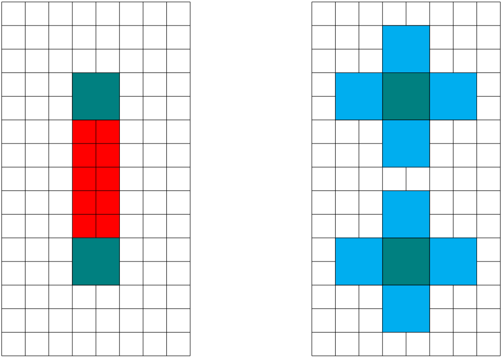
- Example: the red area cannot be entirely covered.





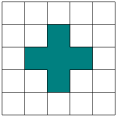
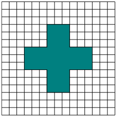
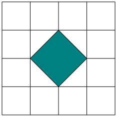
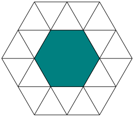
Non-sliding condition

- Counter-example: 2×2 squares.



Examples

- (thick) crosses, diamonds, hexagons...

- Conjecture: k-nearest neighbor exclusion on $\mathbb{Z}^2$ with

$$k \in \{1, 3, 6, 7, 8, 9, 12, 13, \cdots\}.$$

Partition function

$$\Xi_\Lambda^{(\nu)}(z) = \sum_{X\subset\Lambda} z^{|X|} \prod_{x\neq x'\in X} \phi(x,x')$$

- $\Lambda \subset \Lambda_\infty$ is bounded.
- z: *fugacity*, $z = e^{\beta\mu}$.
- ϕ: hard-core repulsion.
- $|X| \leqslant N_{\mathrm{max}}$, maximal density: $\rho_m := \frac{N_{\mathrm{max}}}{|\Lambda|}$.
- Boundary condition: $\Lambda_\infty \setminus \Lambda$ is covered by a perfect covering, indexed by $\nu \in \{1,\cdots,\tau\}$.

Thermodynamical observables

- Pressure:

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

- Correlation functions: for $\underline{x} \equiv \{x_1, \cdots, x_n\} \subset \Lambda_\infty$,

$$\rho_n^{(\nu)}(\underline{x}) := \lim_{\Lambda \to \Lambda_\infty} \frac{1}{\Xi_\Lambda^{(\nu)}(z)} \sum_{\substack{X \subset \Lambda \\ X \supset \underline{x}}} z^{|X|} \prod_{x \neq x' \in X} \phi(x, x')$$

Result

- High fugacity regime: $y \equiv z^{-1} \ll 1$.
- **Analyticity**: $p(z) - \rho_m \log z$ and $\rho_n^{(\nu)}(\underline{x})$ are *analytic* functions of y in a disk in the complex y-plane centered at 0.
- **Crystallization**: If x is compatible with the ν-th perfect packing, then

$$\rho_1^{(\nu)}(x) = 1 + o(1)$$

and if not, then

$$\rho_1^{(\nu)}(x) = o(1)$$

Low-fugacity expansion

- Formally,

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

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

- Second term:

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

- $\frac{1}{2} Z_\Lambda^2(1)$: counts non-interacting particle configurations.

- $Z_\Lambda(2)$: counts interacting particle configurations.

- The terms of order $|\Lambda|^2$ cancel out!

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

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

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

High-fugacity expansion

- Formally,

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

where, if $Q_\Lambda(k_i)$ denotes the number of configurations with $N_{\max} - k_i$ particles, then

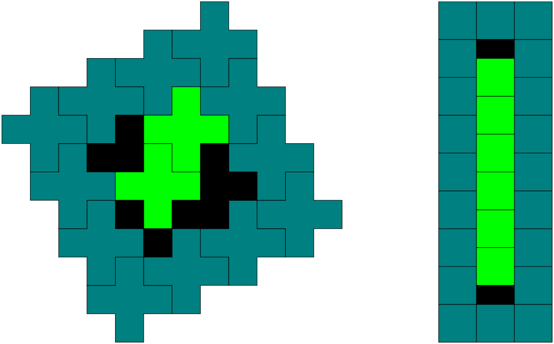
$$c_k(\Lambda) := \frac{1}{|\Lambda|}\sum_{j=1}^{k} \frac{(-1)^{j+1}}{j\tau^j} \sum_{\substack{k_1,\cdots,k_j \geqslant 1 \\ k_1+\cdots+k_j=k}} Q_\Lambda(k_1)\cdots Q_\Lambda(k_j)$$

High-fugacity expansion

- [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. nearest neighbor exclusion in 1 dimension:
$$c_2(\Lambda) = -\frac{1}{192}|\Lambda|(|\Lambda|^2 + 2)$$

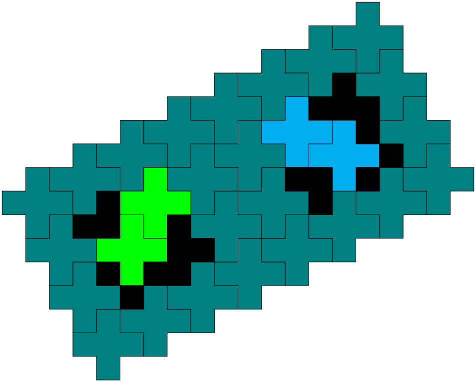
Holes interact

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



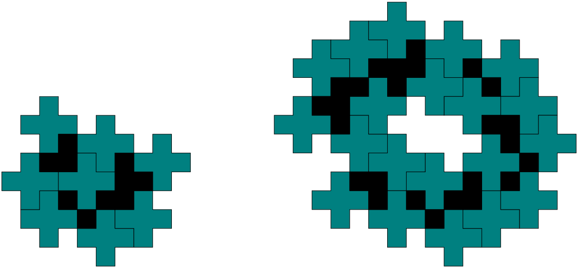
Non-sliding condition

- 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.