Crystalline ordering in hard-core lattice particle systems

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Gas-liquid-crystal
Hard-core lattice particle (HCLP) systems
Non-sliding HCLPs

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

• Gibbs measure:

\[ \langle A \rangle_\nu := \lim_{\Lambda \to \Lambda_\infty} \frac{1}{\Xi_{\Lambda,\nu}(z)} \sum_{X \subset \Lambda} A(X) z^{|X|} \mathcal{B}_\nu(X) \prod_{x \neq x' \in X} \varphi(x, x') \]

  ▶ \( \Lambda \): finite subset of lattice \( \Lambda_\infty \).
  ▶ \( z \geq 0 \): fugacity.
  ▶ \( \varphi(x, x') \): hard-core interaction.
  ▶ \( \mathcal{B}_\nu \): boundary condition: favors the \( \nu \)-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 $\langle 1_{x_1} \cdots 1_{x_n} \rangle_\nu$ are \textbf{analytic} functions of $1/z$ for large values of $z$.

• There are $\tau$ distinct Gibbs states:

$$\langle 1_x \rangle_\nu = \begin{cases} 1 + O(y) & \text{if } x \in \mathcal{L}_\nu \\ O(y) & \text{if not} \end{cases}$$
Low-fugacity expansion

- 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

\[
b_k(\Lambda) := \frac{1}{|\Lambda|} \sum_{j=1}^{k} \frac{(-1)^{j+1}}{j} \sum_{\substack{k_1, \ldots, k_j \geq 1 \\ k_1 + \cdots + k_j = k}} Z_\Lambda(k_1) \cdots Z_\Lambda(k_j)
\]
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 $y \equiv z^{-1}$:

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

• Formally,

\[
\frac{1}{|\Lambda|} \log \Xi_\Lambda = \rho m \log z + \sum_{k=1}^{\infty} c_k(\Lambda) y^k + o(1)
\]

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

\[
c_k(\Lambda) := \frac{1}{|\Lambda|} \sum_{j=1}^{k} \left( \frac{-1}{j^j} \right) \sum_{k_1, \ldots, k_j \geq 1} \sum_{k_1 + \cdots + k_j = k} Q_\Lambda(k_1) \cdots Q_\Lambda(k_j)
\]
High-fugacity expansion
High-fugacity expansion

- [Gaunt, Fisher, 1965]: diamonds: $c_k(\Lambda) \rightarrow c_k$ for $k \leq 9$.

- [Joyce, 1988]: hexagons (integrable, [Baxter, 1980]).

- [Eisenberg, Baram, 2005]: crosses: $c_k(\Lambda) \rightarrow c_k$ for $k \leq 6$.

- Cannot be done systematically: there exist counter-examples: e.g. hard $2 \times 2$ 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:

\[ \Xi_{\Lambda,\nu}(z) = z^{p_m|\Lambda|} \sum_{\gamma \subseteq \mathcal{C}_\nu(\Lambda)} \left( \prod_{\gamma \neq \gamma' \in \gamma} \Phi(\gamma, \gamma') \right) \prod_{\gamma \in \gamma} \zeta^{(z)}_{\nu}(\gamma) \]

  ▶ \( \Phi \): hard-core repulsion of defects.
  ▶ \( \zeta^{(z)}_{\nu}(\gamma) \): activity of defect.

• The activity of a defect is exponentially small: \( \exists \epsilon \ll 1 \)

\[ \zeta^{(z)}_{\nu}(\gamma) < \epsilon^{\gamma} \]

• Low-fugacity expansion for defects.
Crystallization

- Peierls argument: in order to have a particle at $x$ that is not compatible with the $\nu$-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.