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 $\tau$ of tilings $\{\mathcal{L}_1, \cdots, \mathcal{L}_\tau\}$ which are **periodic** and **isometric** to each other.
Non-sliding HCLPs

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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 $Y \supsetneq X$, there is empty space in $Y$ neighboring $X$. 
Example of a sliding HCLP

- $2 \times 2$ squares:
Observables

- Gibbs measure:

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

- $\Lambda$: finite subset of lattice $\Lambda_\infty$.
- $z \geq 0$: fugacity.
- $\varphi(x, x')$: hard-core interaction.
- $\mathfrak{B}_\nu$: 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 analytic functions of $1/z$ for large values of $z$.

• There are $\tau$ distinct Gibbs states:

\[
\langle 1_{x} \rangle_\nu = \begin{cases} 
1 + O(z^{-1}) & \text{if } x \in \mathcal{L}_\nu \\
O(z^{-1}) & \text{if not.}
\end{cases}
\]
Low-fugacity expansion

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

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

• 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

$$
b_k(\Lambda) := \frac{1}{|\Lambda|} \sum_{j=1}^{k} \frac{(-1)^{j+1}}{j} \sum_{k_1, \ldots, k_j \geq 1 \atop k_1 + \cdots + k_j = k} Z_\Lambda(k_1) \cdots Z_\Lambda(k_j)
$$
Low-fugacity expansion

- Partition function:

\[ \Xi_\Lambda(z) = 1 + z Z_\Lambda(1) + z^2 Z_\Lambda(2) + \cdots \]

- 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]: $b_k(\Lambda) \rightarrow b_k$.

- [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:

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

• Inverse fugacity $y \equiv z^{-1}$:

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

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

High-fugacity expansion

• Formally,

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

where \( \rho_m = \frac{N_{\text{max}}}{|\Lambda|} \),

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

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

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

- [Eisenberg, Baram, 2005]: crosses: $c_k(\Lambda) \to c_k$ 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:

$$\Xi_{\Lambda,\nu}(z) = z^{\rho_{m}|\Lambda|} \sum_{\gamma \subset \mathcal{E}_{\nu}(\Lambda)} \left( \prod_{\gamma \neq \gamma' \in \gamma} \Phi(\gamma, \gamma') \right) \prod_{\gamma \in \gamma} \zeta^{(z)}_{\nu}(\gamma)$$

  - $\Phi$: 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.
• 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.
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 $\tilde{R}^{-1}$.