# Cluster expansion in the canonical ensemble

**Elena Pulvirenti, Università di Roma Tre**
**joint work with D. Tsagkarogiannis**

**Comm. Math. Phys. (to appear)**

## Background

Our initial motivation comes from studying phase transitions for a system of particles in the continuum interacting via a Kac potential, as in the LMP model (Lebowitz, Mazel, Presutti "Liquid-vapor phase transitions for systems with finite-range interactions.", J. Stat. Phys. 94, 955-1025 (1999)), with extra short range interaction.

In such a case the main step is to eliminate some degrees of freedom of the system by partitioning the space into boxes and defining a coarse-grained functional for the order parameter, which brings us in a multi-canonical set-up.

The prototype example of such a case is the *calculation of the free energy functional with respect to the density by cluster expanding the canonical partition function*.

## The model

Configuration $\mathbf{q} \equiv \{q_1, \dots, q_N\}$ of $N$ particles in a box $\Lambda \subset \mathbb{R}^d$ interacting via potential $V : \mathbb{R}^d \to \mathbb{R}$ *stable* and *tempered*:

$$\sum_{1 \le i < j \le N} V(q_i - q_j) \ge -BN$$

$$C(\beta) := \int_{\mathbb{R}^d} |e^{-\beta V(q)} - 1|\, dq < \infty$$

The CANONICAL PARTITION FUNCTION is:

$$Z_{\beta,\Lambda,N} := \frac{1}{N!} \int_{\Lambda^N} dq_1 \dots dq_N\, e^{-\beta H_\Lambda(\mathbf{q})}, \quad H_\Lambda(\mathbf{q}) := \sum_{i<j} V(q_i - q_j)$$

## Mayer's expansion

Mayer's expansion through grand canonical (1940):

$$\beta p_\beta(z) = \sum_{n \ge 1} b_n z^n, \quad \rho_\beta(z) = \sum_{n \ge 1} n b_n z^n \quad (z = e^{\beta\mu}\text{: activity})$$

$$\xRightarrow{z=z(\rho)} \beta p_\beta(\rho) = \rho - \sum_{m \ge 1} \frac{m}{m+1} \beta_m \rho^{m+1} \qquad \text{VIRIAL EXPANSION}$$

$$\beta_n := \lim_{|\Lambda| \to \infty} \frac{1}{|\Lambda| n!} \sum_{g \in \mathcal{B}_{n+1}} w_\Lambda(g), \qquad \text{Mayer's coefficients}$$

$$w_\Lambda(g) := \int_{\Lambda^{|V(g)|}} \prod_{\{i,j\} \in E(g)} f_{i,j} \prod_{i \in V(g)} dq_i, \quad f_{i,j} := e^{-\beta V(q_i - q_j)} - 1$$

$\mathcal{B}_{n+1}$: set 2-connected graphs on $(n+1)$ vertices
$g \equiv (V(g), E(g))$, $V(g)$: vertices, $E(g)$: edges

$$\beta f_\beta(\rho) = \sup_z \{\rho \log z - \beta p_\beta(z)\} = \rho \log z(\rho) - \beta p_\beta(z(\rho))$$

$$= \rho(\log\rho - 1) - \sum_{n \ge 1} \frac{1}{n+1} \beta_n \rho^{n+1}$$

## The problem

**Question:** How to cluster expand: $\frac{1}{|\Lambda|} \log Z_{\beta,\Lambda,N}$?

**Conjecture:** Write the log of the c.p.f. as:

$$\beta f_{\beta,\Lambda}(N) := -\frac{1}{|\Lambda|} \log Z_{\beta,\Lambda,N} = -\frac{1}{|\Lambda|} \log \sum_{\{V_1,\dots,V_k\}_\sim} \prod_{i=1}^k \zeta_\Lambda(V_i)$$

*polymers*: $V_i \in \mathcal{V}(N)$, $\mathcal{V}(N) := \{V : V \subset \{1,\dots,N\}, |V| \ge 2\}$
*incompatibility*: $V_i \sim V_j \Leftrightarrow V_i \cap V_j = \emptyset$, $\forall V_i, V_j \in \mathcal{V}(N)$
*activity*: $\zeta_\Lambda(V) := \sum_{g \in \mathcal{C}_V} w_\Lambda(g) |\Lambda|^{-|V|}$
$\mathcal{C}_V$ : set of *connected graphs* on the vertices $V \in \mathcal{V}(N)$

$$\log \sum_{\{V_1,\dots,V_k\}_\sim} \prod_{i=1}^k \zeta_\Lambda(V_i) = \sum_I c_I \zeta_\Lambda^I, \qquad \text{CLUSTER EXPANSION}$$

$I : \mathcal{V}(N) \to \mathbb{N}$ is a multi-index, $\operatorname{supp} I := \{V \in \mathcal{V}(N) : I(V) > 0\}$, $\zeta_\Lambda^I = \prod_V \zeta_\Lambda(V)^{I(V)}$, $I! = \prod_V I(V)!$ and:

$$c_I = \frac{1}{I!} \frac{\partial^{\sum_V I(V)} \log Z_{\beta,\Lambda,N}}{\partial^{I(V_1)} \zeta_\Lambda(V_1) \cdots \partial^{I(V_n)} \zeta_\Lambda(V_n)} \Big|_{\zeta_\Lambda(V)=0}, \quad c_I \ne 0 \text{ if } I \text{ is a cluster}$$

- Convergence of cluster expansion
- Cancellation of non 2-connected graphs to get in the limit Mayer's result!

## Main result

There exists $c_0 \equiv c_0(\beta, B) > 0$ such that if $\rho C(\beta) < c_0$ then:

$$\frac{1}{|\Lambda|} \log Z_{\beta,\Lambda,N} = \log \frac{|\Lambda|^N}{N!} + \frac{N}{|\Lambda|} \sum_{n \ge 1} F_{\beta,N,\Lambda}(n),$$

with $N = \lfloor \rho|\Lambda| \rfloor$, and for all $n \ge 1$:

$$\lim_{\substack{N,|\Lambda| \to \infty \\ N = \lfloor \rho|\Lambda| \rfloor}} F_{\beta,N,\Lambda}(n) = \frac{1}{n+1} \beta_n \rho^{n+1}, \quad |F_{\beta,N,\Lambda}(n)| \le C e^{-cn}.$$

## Sketch of the proof

$$F_{\beta,N,\Lambda}(n) = \frac{1}{n+1} \binom{N-1}{n} \sum_{I : A(I) = [n+1]} c_I \zeta_\Lambda^I, \qquad A(I) = \bigcup_{V \in \operatorname{supp} I} V$$

$$\frac{1}{|\Lambda|} \log Z_{\beta,\Lambda,N} = \frac{1}{|\Lambda|} \sum_I c_I \zeta_\Lambda^I = \frac{N}{|\Lambda|} \sum_{n \ge 1} F_{N,\Lambda}(n) =$$

$$= \frac{N}{|\Lambda|} \sum_{n \ge 1} \frac{1}{n+1} \frac{(N-1)\dots(N-n)}{|\Lambda|^n} B_{\beta,\Lambda}(n)$$

$$B_{\beta,\Lambda}(n) := \frac{|\Lambda|^n}{n!} \sum_{I : A(I) = [n+1]} c_I \zeta_\Lambda^I \to \beta_n$$

by cancellations of terms both at finite volume and in the limit.