Cluster Expansion in the Canonical Ensemble

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(joint work with Dimitrios Tsagkarogiannis)

Background

- Motivation: 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.
- General technique: eliminate some degrees of freedom of the system by partitioning the space into boxes and defining a coarse-grained functional for the order parameter (multi-canonical set-up).
- Prototype example: calculation of the free energy functional with respect to the density in a single box.
- Method: cluster expansion of the canonical partition function. (new, more direct proof of Mayer's virial expansion)

The Model

Configuration $\mathbf{q} \equiv \{q_1, \ldots, q_N\}$ of N particles in a box $\Lambda \subset \mathbb{R}^d$ which interact with a pair potential $V : \mathbb{R}^d \to \mathbb{R}$, such that:

$$\text{(stable)} \qquad \sum_{1 \le i < j \le N} V(q_i - q_j) \ge -BN, \qquad \forall N, q_1, ..., q_N$$

$$\text{(tempered)} \qquad C(\beta) := \int_{\mathbb{R}^d} |e^{-\beta V(q)} - 1| dq < \infty, \qquad \forall \beta > 0$$

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The hamiltonian is:

$$H_\Lambda(\mathbf{q}) := \sum_{1\le i<j\le N} V(q_i, q_j)$$

The canonical partition function is given by:

$$Z_{\beta,\Lambda,N} := \frac{1}{N!} \int_{\Lambda^N} dq_1 \ldots dq_N \, e^{-\beta H_\Lambda(\mathbf{q})}$$

The Result

Theorem (with D. Tsagkarogiannis):
If $\rho\, C(\beta)$ is small enough then:

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

- $|F_{N,\Lambda}(n)| \leq Ce^{-cn}, \quad \forall n \geq 1;$
- $F_{N,\Lambda}(n) = \frac{1}{n+1}P_{N,|\Lambda|}(n)B_{\beta,|\Lambda|}(n)$, for all $n \geq 1$

$$P_{N,|\Lambda|}(n) = \frac{(N-1)\dots(N-n)}{|\Lambda|^n} \sim \rho^n \quad \text{and} \quad \lim_{\Lambda\to\infty} B_{\beta,\Lambda}(n) = \beta_n$$

$$\Rightarrow \beta f_\beta(\rho) = \rho(\log\rho - 1) - \sum_{n\geq 1}\frac{1}{n+1}\beta_n\rho^{n+1} \qquad (\beta_n : \text{Mayer's coefficients})$$

Mayer's idea

Grand canonical partition function:

$$\Xi_{\beta,\Lambda}(z) := \sum_{N\geq 0} z^N Z_{\beta,\Lambda,N} \qquad z: \text{ activity}$$

$$\beta p_\beta(z) := \lim_{|\Lambda|\to\infty} \frac{1}{|\Lambda|} \log \Xi_{\beta,\Lambda}(z) = \sum_{n\geq 1} b_n z^n \tag{1}$$

$$\rho_\beta(z) := \lim_{|\Lambda|\to\infty} \frac{1}{|\Lambda|} z \frac{\partial}{\partial z} \log \Xi_{\beta,\Lambda}(z) = \sum_{n\geq 1} n b_n z^n \tag{2}$$

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Inverting (2) and replacing $z(\rho)$ in (1):

$$\beta p_\beta(\rho) = \rho \left(1 - \sum_{m\geq 1} \frac{m}{m+1} \beta_m \rho^m \right) \qquad \text{virial expansion}$$

Cluster Expansion for the Canonical Partition Function

1) Normalize the measure with the volume:

$$Z_{\beta,\Lambda,N} = Z^{ideal}_{\Lambda,N} Z^{int}_{\beta,\Lambda,N},$$

$$Z^{ideal}_{\Lambda,N} := \frac{|\Lambda|^N}{N!} \quad \text{and} \quad Z^{int}_{\beta,\Lambda,N} := \int_{\Lambda^N} \frac{dq_1}{|\Lambda|} \dots \frac{dq_N}{|\Lambda|} e^{-\beta H_\Lambda(\mathbf{q})}$$

2) Use the "± 1 trick" (Mayer's idea) for $e^{-\beta H_\Lambda(\mathbf{q})}$:

$$e^{-\beta \sum_{i<j} V(q_i - q_j)} = \prod_{1 \le i < j \le N} (e^{-\beta V(q_i - q_j)} - 1 + 1) = \sum_{g \in \mathcal{G}_N} \prod_{\{i,j\} \in E(g)} f_{i,j}$$

$\mathcal{G}_N$: set of graphs on up to N vertices (*labels of particles*)

$$f_{i,j} := e^{-\beta V(q_i - q_j)} - 1$$

Cluster Expansion for the Canonical Partition Function

3) Compatibility: $g \sim g' \Leftrightarrow \operatorname{supp} g \cap \operatorname{supp} g' = \emptyset$, ($\operatorname{supp} g$: vertices set)

$$\Longrightarrow g \equiv \{g_1, \ldots, g_k\}_\sim, \; \forall g \in \mathcal{G}_N$$

$$Z^{int}_{\beta,\Lambda,N} = \sum_{\{g_1,\ldots,g_k\}_\sim} \prod_{i=1}^{k} \tilde{\zeta}_\Lambda(g_i)$$

where:

$$\tilde{\zeta}_\Lambda(g) := \int_{\Lambda^{|g|}} \prod_{i \in \operatorname{supp} g} \frac{dq_i}{|\Lambda|} \prod_{\{i,j\} \in E(g)} f_{i,j}$$

$\mathcal{C}(N)$: set of connected graphs on up to N vertices
$g_i \in \mathcal{C}(N)$: polymers of the expansion
($|g|$: cardinality of $\operatorname{supp} g$)

Cluster Expansion for the Canonical Partition Function

3) Compatibility: $g \sim g' \Leftrightarrow \operatorname{supp} g \cap \operatorname{supp} g' = \emptyset$, $(\operatorname{supp} g$: vertices set)

$$V := \operatorname{supp} g, \quad g \in \mathcal{G}_N$$

$$Z^{int}_{\beta,\Lambda,N} = \sum_{\{V_1,\dots,V_k\}_\sim} \prod_{i=1}^{k} \zeta_\Lambda(V_i)$$

where:

$$\zeta_\Lambda(V) := \sum_{g \in \mathcal{C}_V} \tilde{\zeta}_\Lambda(g)$$

$\mathcal{V}(N) := \{V : V \subset \{1, \dots, N\}\}$
$V_i \in \mathcal{V}(N)$: polymers of the expansion
$\mathcal{C}_V$: the set of all connected graphs with support V

Cluster Expansion for the Canonical Partition Function

4) Exponentiation of the partition function. We work in the space of vertices sets: $\mathcal{V}(N) := \{V : V \subset \{1,\ldots,N\}\}$

$$Z^{int}_{\beta,\Lambda,N} = \sum_{\{V_1,\ldots,V_k\}_\sim} \prod_{i=1}^{k} \zeta_\Lambda(V_i) \stackrel{\text{c.e.}}{=} \exp\left\{\sum_I c_I \zeta_\Lambda^I\right\}$$

where: $I : \mathcal{V}(N) \to \{0,1,\ldots\}$ with
$\operatorname{supp} I := \{V \in \mathcal{V}(N) : I(V) > 0\}$ is a multi-index,
$\zeta_\Lambda^I = \prod_V \zeta_\Lambda(V)^{I(V)}$, and

$$c_I = \frac{1}{I!} \frac{\partial^{\sum_V I(V)} \log Z^{int}_{\beta,\Lambda,N}}{\partial^{I(V_1)}\zeta_\Lambda(V_1)\cdots\partial^{I(V_n)}\zeta_\Lambda(V_n)}\Big|_{\zeta_\Lambda(V)=0}$$

$c_I \neq 0 \Leftrightarrow \operatorname{supp} I$ is an incompatible collection of V_i's

Convergence of the Cluster Expansion

Kotecký - Preiss convergence condition:
There exist two positive functions $a, c : \mathcal{V}(N) \to \mathbb{R}$ such that for any $V \in \mathcal{V}(N)$:

$$|\zeta_\Lambda(V)| e^{a(V)} \leq \delta$$

holds for some $\delta > 0$ small. Moreover, for any $V' \in \mathcal{V}(N)$

$$\sum_{V:\ V \not\sim V'} |\zeta_\Lambda(V)| e^{a(V)+c(V)} \leq a(V').$$

Theorem (Cluster expansion)

If the K-P condition holds, convergence is absolute.

We have to prove:

$$\frac{1}{|\Lambda|}\sum_{I} c_I \zeta_\Lambda^I = \frac{N}{|\Lambda|}\sum_{n\geq 1} F_{N,\Lambda}(n)$$

where:

1. $|F_{N,\Lambda}(n)| \leq Ce^{-cn}, \quad \forall n \geq 1$
2. $F_{N,\Lambda}(n) = \frac{1}{n+1} P_{N,|\Lambda|}(n) B_{\beta,|\Lambda|}(n)$,

$$\lim_{\substack{N,|\Lambda|\to\infty,\\ N/|\Lambda|=\rho}} P_{N,|\Lambda|}(n) = \rho^n \quad \text{and} \quad \lim_{|\Lambda|\to\infty} B_{\beta,|\Lambda|}(n) = \beta_n,$$

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

$\mathcal{B}_{n+1}$: set 2-connected graphs on $(n+1)$ vertices

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

Proof of (2)

Let's work in the space $\mathcal{C}(n+1)$, with: $\tilde{I} : \mathcal{C}(n+1) \to \{0, 1, \dots\}$.
Remark: $\sum_I c_I \zeta_\Lambda^I = \sum_{\tilde{I}} c_{\tilde{I}} \tilde{\zeta}_\Lambda^{\tilde{I}}$.

$$F_{N,\Lambda}(n) = \frac{1}{n+1} \binom{N-1}{n} \sum_{\substack{\tilde{I}: \\ \operatorname{supp} \tilde{I} \equiv \{1,\dots,n+1\}}} c_{\tilde{I}} \tilde{\zeta}_\Lambda^{\tilde{I}} = \frac{1}{n+1} P_{N,|\Lambda|}(n) B_{\beta,\Lambda}(n)$$

where:

$$P_{N,|\Lambda|}(n) := \frac{(N-1)\dots(N-n)}{|\Lambda|^n} \longrightarrow \rho^n$$

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where:

$$P_{N,|\Lambda|}(n) := \frac{(N-1)\dots(N-n)}{|\Lambda|^n} \longrightarrow \rho^n$$

$$B_{\beta,\Lambda}(n) = \frac{|\Lambda|^n}{n!} \sum_{g \in \mathcal{C}_{n+1}} \sum_{\substack{\tilde{I}: \\ \cup_{g' \in \mathrm{supp}\,\tilde{I}} g' = g}} c_{\tilde{I}} \zeta_\Lambda^{\tilde{I}} \longrightarrow \; ?$$

Proof of (2)

Infinite volume cancellations:

Since: $\tilde{\zeta}_\Lambda(g) \sim \frac{1}{|\Lambda|^{|g|-1}}$, then:

$$B_{\beta,\Lambda}(n) = \frac{|\Lambda|^n}{n!} \sum_{g \in \mathcal{C}_{n+1}} \sum^{*}_{\substack{\tilde{I}: \\ \cup_{g' \in \mathrm{supp}\, \tilde{I}} g' = g}} c_{\tilde{I}} \tilde{\zeta}_\Lambda^{\tilde{I}} + O\Big(\frac{1}{|\Lambda|}\Big)$$

where the terms in the $\sum^*$ satisfy the factorization property:

$$\tilde{\zeta}_\Lambda(\cup_{g' \in A} g') = \prod_{g' \in A} \tilde{\zeta}_\Lambda(g'), \quad \forall A \subset \mathrm{supp}\, \tilde{I}$$

and, moreover:

$$\tilde{I}(g') = 1, \quad \forall g' \in \mathrm{supp}\, \tilde{I}$$

Proof of (2)

Finite volume cancellations:

Only 2-connected graphs give non-zero contribution in the $\sum^*$!

Lemma

Given $g \in \mathcal{C}_{n+1} \setminus \mathcal{B}_{n+1}$, then:

$$\sum^{*}_{\substack{\tilde{I}: \\ \cup_{g' \in \mathrm{supp}\, \tilde{I}} g' = g}} c_{\tilde{I}} \tilde{\zeta}_{\Lambda}^{\tilde{I}} = 0$$

We remain with those terms such that: $g \in \mathcal{B}_{n+1}$ and $\tilde{I}(g) = 1$

$$B_{\beta,\Lambda}(n) = \frac{|\Lambda|^n}{n!} \sum_{g \in \mathcal{B}_{n+1}} \tilde{\zeta}_{\Lambda}(g) \longrightarrow \beta_n$$

Next steps

1. Finite volume corrections to the free energy;
2. Optimal radius of convergence of the expansion in powers of the density (also for hard spheres);
3. Applications to the LMP model (coarse-grained Hamiltonians)...