Combinatorics in Mayer's theory of cluster and virial expansions

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Stephen James Tate

University of Warwick

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Context of Combinatorics for Cluster and Virial Expansions

- Pressure expansion in terms of activity or fugacity
  $\beta P = \sum_{n \geq 1} b_n \frac{z^n}{n!}$ (Cluster Expansion)
- Pressure expansion in terms of density
  $\beta P = \sum_{n \geq 1} c_n \frac{\rho^n}{n!}$ (Virial Expansion)
- Cluster and virial coefficients as weighted connected and two-connected graphs respectively (Mayer [40])
- Connections with Combinatorial Species of Structure (Ducharme Labelle and Leroux [07])
- Two simple statistical mechanical models (One Particle Hardcore and Tonks Gas) - provide interesting combinatorial identities - want to understand them purely combinatorially
- Bernardi [08] gives the result for the connected graph case

The one-particle hardcore model:

- pair potential: $\varphi(x_i, x_j) = \infty$
- Mayer edge weight: $f_{i,j} := \exp(-\beta\varphi(x_i, x_j)) - 1 = -1$
- Partition Function (all simple graphs) $\Xi(z) = 1 + z$
- Cluster expansion (connected graphs) $\beta P = \log(1+z) = \sum_{n\geq 1} \frac{(-1)^{n+1} z^n}{n}$
- virial expansion (two-connected graphs) $\beta P = -\log(1-\rho) = \sum_{n\geq 1} \frac{\rho^n}{n}$

Two-Connected Graph Combinatorial Identity - One Particle Hardcore Gas

Theorem (T. 14)

If $b_{n,k}$:= *the number of* **two-connected** *graphs with* n *vertices and* k *edges, then:*

$$\sum_{k=n}^{\frac{1}{2}n(n-1)} (-1)^k b_{n,k} = -(n-2)!$$

The cancellations from this alternating sum are explained through a graph involution $\Psi : \mathcal{B} \to \mathcal{B}$, fixing only the two-connected graphs which are formed from an increasing tree on the indices $[1, n-1]$ and has vertex n connected to all other vertices.

The Tonks Gas

The one-particle hardcore model:

- pair potential: $\varphi(x_i, x_j) = \begin{cases} \infty & \text{if } |x_i - x_j| < 1 \\ 0 & \text{otherwise} \end{cases}$
- Mayer edge weight:

  $$f_{i,j} := \exp(-\beta\varphi(x_i, x_j)) - 1 = \begin{cases} -1 & \text{if } |x_i - x_j| < 1 \\ 0 & \text{otherwise} \end{cases}$$
- Can express a graph weight as $w(g) := (-1)^{e(g)} \mathrm{Vol}(\Pi_g)$
- Cluster expansion (connected graphs) $\beta P = W(z) = \sum_{n\geq 1} \frac{(-n)^{n-1} z^n}{n}$
- virial expansion (two-connected graphs) $\beta P = \frac{\rho}{1-\rho} = \sum_{n\geq 1} \rho^n$

Two-Connected Graph Combinatorial Identity - Tonks Gas

Theorem (T. 14)

For the Polytope

$$\Pi_g := \{\mathbf{x}_{[2,n]} \in \mathbb{R}^{n-1} | \, |x_i - x_j| < 1 \, \forall \{i,j\} \in g \text{ with } x_1 = 0\} \qquad (1)$$

We have the combinatorial equation:

$$\sum_{g \in \mathcal{B}[n]} (-1)^{e(g)} \mathrm{Vol}(\Pi_g) = -n(n-2)!$$

Two-connected Graph Combinatorial Identity - Tonks Gas

- The cancellations from this alternating sum are explained through a collection of graph involutions $\Psi_{\mathbf{h}} : \mathcal{B}_{\mathbf{h}} \to \mathcal{B}_{\mathbf{h}}$.
- These fix only the two-connected graphs which are formed from a maximal vertex connected to all other vertices and an increasing tree on the remaining vertices. The order of the vertices depends on the vector **h**.
- The vector $\mathbf{h} \in \mathbb{Z}^{n-1}$ comes from a method of splitting the polytope Π_g into simplices of volume $\frac{1}{(n-1)!}$ attributed to Lass in the paper by Ducharme Labelle and Leroux [07].

Conclusions & Open Questions

- It is possible to obtain a combinatorial interpretation of the cancellations found in the two models of statistical mechanics with the weighted graph interpretation of the coefficients
- Is it possible to generalise the approach to general positive potentials or stable potentials for the two connected case? (analogy with Penrose tree construction and Tree-Graph Inequalities of Brydges Battle Federbush)