Many-species Tonks gas

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Problem

Problem: Understand cluster and virial expansions better:

- Several sufficient convergence criteria available – are they sharp? what about necessary criteria?
- Is one type of expansion better than the other?

This talk: study these questions for one-dimensional model of non-overlapping rods. Primarily of interest as a control group. But:

- phase transitions for driven 1D systems, zero-range processes...
- 1D polymer partition functions as auxiliary for more interesting 2D systems of hard rods Ioffe, Velenik, Zahradnik.

Connections:

- renewal processes
- counting colored labelled trees
- Lagrange-Good inversion (tool in complex analysis / formal power series / combinatorics).

Overview

Model

Rod lengths: given family $(\ell_k)_{k\in\mathbb{N}}$, $\ell_k > 0$.

Activities $(z_k)_{k\in\mathbb{N}}$, $z_k \geq 0$. Rod of type k has length ℓ_k and activity z_k.
Assumption: stability condition

$$\exists\theta \in \mathbb{R}: \quad \sum_{k=1}^{\infty} z_k \exp(\theta\ell_k) < \infty.$$

Set $\theta^* := \sup\{\theta \in \mathbb{R} \mid \sum_k z_k \exp(\theta\ell_k) < \infty\}$. Think $\exp(\theta^*) =$ radius of convergence. Activities can go to infinity $z_k \to \infty$.

Grand-canonical partition function:

$$\Xi_L(\mathbf{z}) := 1 + \sum_{N_1,N_2,\dots} \frac{z_1^{N_1} z_2^{N_2}}{N_1!N_2!\cdots} \int_{[0,L]^{\sum_k N_k}} \mathrm{d}x_{11}\cdots \mathrm{d}x_{1N_1}\mathrm{d}x_{21}\cdots$$
$$\mathbf{1}\Big(\forall k,m,i,j:\ [x_{kj}, x_{kj}+\ell_k] \cap [x_{mi}, x_{mi}+\ell_m] = \emptyset\Big).$$

Poisson exclusion process. N_k rods of type k, rods do not overlap. Summation over sequences of integers with finitely many non-zero entries.

Pressure:

$$p(\mathbf{z}) := \lim_{L\to\infty} \frac{1}{L} \log \Xi_L(\mathbf{z}).$$

Results: Fixed point equation and packing fraction

Remember $\theta^* := \sup\{\theta \in \mathbb{R} \mid \sum_k z_k \exp(\theta \ell_k) < \infty\}$. Central:

$$p = \sum_{k=1}^{\infty} z_k \exp(-p\ell_k).$$

Theorem (Pressure solves fixed point equation)

1. *If $\sum_k z_k \exp(\ell_k \theta^*) \geq -\theta^*$, the fixed point equation has a unique solution $p \geq -\theta^*$, and this solution is equal to the pressure $p(\mathbf{z})$.*
2. *If $\sum_k z_k \exp(\ell_k \theta^*) < -\theta^*$, the fixed point equation has no solution and $p(\mathbf{z}) = -\theta^*$.*

Grand-canonical Gibbs measure: Poisson rods (Poiss(z_k)) conditioned on non-overlapping. *Packing fraction* $\sum_k N_k(\omega)\ell_k/L$ – random variable.

Theorem (No solution = close-packing)

1. *If $\sum_k z_k \exp(\ell_k \theta^*) > -\theta^*$, then*

$$\frac{1}{L}\sum_k \ell_k N_k \to \sigma(\mathbf{z}) < 1, \quad \frac{\sigma(\mathbf{z})}{1-\sigma(\mathbf{z})} := \sum_k \ell_k \exp[-\ell_k p(\mathbf{z})].$$

2. *If $\sum_k z_k \exp(\ell_k \theta^*) < -\theta^*$, the packing fraction converges to $\sigma = 1$.*

Heuristics 1: renewal theory

Reinterpret:

- line = time axis,
- starting point of rods = events
  (e.g., something breaks and has to be renewed)
- interval between two starting points of rods = waiting times
  ("interarrival" times).

Multiply the grand-canonical partition function with $\exp(-\lambda L)$, distribute the additional factor $\exp(-\lambda L)$ over the rods and empty spaces. After rescaling, a waiting interval of length r has weight $\sum_k z_k \mathbf{1}(r \geq \ell_k) \exp(-\lambda r)$. This weight defines a probability distribution if and only if

$$\int_0^\infty \sum_k z_k \mathbf{1}(r \geq \ell_k) \exp(-\lambda r) \mathrm{d}r = \frac{1}{\lambda} \sum_k z_k \exp(-\lambda \ell_k) = 1,$$

and we recognize the fixed point equation.

If the equation has a solution, the infinite volume-limit of the Gibbs measure can be described in terms of a stationary renewal process.

Heuristics 2: statistical mechanics

Constant pressure partition function and Gibbs free energy at given N_k's:

$$Q(N_1, N_2, \ldots; p) = \binom{\sum_k N_k}{N_1, N_2, \ldots} e^{-p \sum_k N_k \ell_k} \left(\int_0^\infty e^{-pr} \mathrm{d}r \right)^{\sum_k N_k}$$

$$G(N_1, N_2, \ldots; p) = \sum_k N_k \left(\log \frac{pN_k}{\sum_j N_j} + p\ell_k \right).$$

The chemical potential is $\log z_k = \partial G / \partial N_k$, which gives

$$z_k = \frac{pN_k}{\sum_j N_j} \exp(p\ell_k), \quad p = \sum_k \frac{pN_k}{\sum_j N_j} = \sum_k z_k \exp(-p\ell_k).$$

The expected volume is $L = -\partial G / \partial p$, which yields the van der Waals-equation

$$p \left(L - \sum_k \ell_k N_k \right) = \sum_k N_k.$$

and

$$z_k = \frac{N_k}{L - \sum_k \ell_k N_k} \exp(p\ell_k).$$

Results continued: Activity expansion

Known: pressure has a power series expansion. Sufficient for absolute convergence:

$$\exists a > 0 \ \forall j \in \mathbb{N}: \ \sum_{k=1}^{\infty} (\ell_j + \ell_k)|z_k| \exp(a\ell_k) < a\ell_j.$$

Kotecký-Preiss-type criterion $\approx$ overlap probability for Poisson rods is small.

Notation: $\mathcal{I} \subset \mathbb{N}_0^{\mathbb{N}}$ set of integer-valued sequences with none or finitely many non-vanishing entries, $\mathcal{I}^* := \mathcal{I} \backslash \{\mathbf{0}\}$. For $\mathbf{n} \in \mathcal{I}$, $\mathbf{z} \in \mathbb{C}^{\mathbb{N}}$, write $\mathbf{n}! := \prod_k (n_k!)$ and $\mathbf{z}^{\mathbf{n}} := \prod_k z_k^{n_k}$,

Theorem

$$p(\mathbf{z}) = \sum_{\mathbf{n} \in \mathcal{I}^*} \frac{\mathbf{z}^{\mathbf{n}}}{\mathbf{n}!} \Big(- \sum_k n_k \ell_k \Big)^{\sum_k n_k - 1}. \qquad (*)$$

- *If $\sum_k |z_k| \exp(a\ell_k) < a$ for some $a > 0$, Eq. (*) holds and the activity expansion converges absolutely.*
- *If $\sum_k |z_k| \exp(a\ell_k) > a$ for all $a > 0$, the right-hand side of Eq. (*) is not absolutely convergent.*

Will use the same letter $p(\mathbf{z})$ for physical pressure (positive activities) and analytic extension to complex activities.

Density (virial) expansion

Density N_k/L of rods of type k in the limit $L \to \infty$ is

$$\rho_k(\mathbf{z}) := z_k \frac{\partial p}{\partial z_k}(\mathbf{z}).$$

Assumption:

- activities positive, stability condition holds, or
- activities complex, $\sum_k |z_k| \exp(a\ell_k) < a$ for some a.

Theorem

The partial derivatives defining $\rho_k(\mathbf{z})$ exist, and we have

$$p(\mathbf{z}) = \frac{\sum_k \rho_k(\mathbf{z})}{1 - \sum_k \ell_k \rho_k(\mathbf{z})}, \quad z_k = \frac{\rho_k(\mathbf{z})}{1 - \sum_j \ell_j \rho_j(\mathbf{z})} \exp\Big(\ell_k p(\mathbf{z})\Big),$$

and $\sum_k \ell_k |\rho_k(\mathbf{z})| < 1$.

Remark If fixed point equation has a solution, not only is the packing fraction strictly smaller than 1, but in addition there is no mass that escapes to large labels k (no condensation, no dust):

$$\sum_k \ell_k \rho_k(\mathbf{z}) = \sigma(\mathbf{z}) = \lim_{L\to\infty} \frac{1}{L} \sum_k \ell_k N_k(\omega).$$

Comparison of activity and density expansions

To fix ideas, take $\ell_k = k$.

Necessary for convergence of activity expansion: $z_k \to 0$ as $\exp(-ak)$ for some $a > 0$ – activities have to go to zero exponentially fast. Convergence of density expansion only requires $\sum_k k|\rho_k| < 1$ – densities can go to zero slowly. Because of the relation

$$z_k = \frac{1}{1-\sigma} \rho_k \exp(kp), \quad \sigma = \sum_k k\rho_k,$$

there will be a region where the density expansion converges but the activities diverge exponentially.

Corollary

Let

$$\mathcal{D}_{\mathrm{May}} := \{\mathbf{z} \in \mathbb{C}^{\mathbb{N}} \mid \exists a > 0 : \sum_k |z_k| \exp(a\ell_k) < a\},$$

$$\mathcal{D}_{\mathrm{vir}} := \{\mathbf{z} \in \mathbb{C}^{\mathbb{N}} \mid \rho_k(\mathbf{z}) \text{ exists for all } k, \text{ and } \sum_k \ell_k|\rho_k(\mathbf{z})| < 1\}.$$

$\mathcal{D}_{\mathrm{May}}$ *is a strict subset of* $\mathcal{D}_{\mathrm{vir}}$*.*

The virial expansion converges in a domain much bigger than the activity expansion.

Proof ideas

Fixed point equation: partition function satisfies *renewal equation*

$$\Xi_L(\mathbf{z}) = 1 + \sum_k z_k \int_{\ell_k}^{L} \Xi_{L-x}(\mathbf{z})\mathrm{d}x.$$

Laplace transform $F(\lambda) = \int_0^\infty \exp(-\lambda L)\Xi_L(\mathbf{z})$ satisfies

$$\Big(\lambda - \sum_k z_k \exp(-\ell_k \lambda)\Big) F(\lambda) = \lambda.$$

Pressure $p(\mathbf{z})$ = the critical λ at which $F(\lambda)$ starts to diverge.

Packing fraction: Compute

$$\Xi_L(\mathbf{z}) = 1 + \sum_{\mathbf{N}\in\mathcal{I}^*} \frac{\mathbf{z}^{\mathbf{N}}}{\mathbf{N}!} \Big(L - \sum_k N_k \ell_k\Big)^{\sum_k N_k} \mathbf{1}\big(\sum_k N_k \ell_k < L\big).$$

Large deviations analysis yields

$$p(\mathbf{z}) = \sup_{\sigma\in[0,1]} \inf_{\theta<\theta^*} \Big((1-\sigma)\sum_k z_k e^{\theta \ell_k} - \theta\sigma\Big),$$

find minimizing σ.

Computation of the pressure-activity expansion

Let $F(\mathbf{z}) := -p(-\mathbf{z})$ (get rid of minus signs). Satisfies

$$F(\mathbf{z}) = \sum_k z_k \exp(\ell_k F(\mathbf{z})).$$

Two ways of extracting exact formula from fixed point equation:

1. Lagrange-Good inversion: write $w_k(\mathbf{z}) := z_k \exp(\ell_k F(\mathbf{z}))$. We have

$$z_k = w_k \exp(-\ell_k \sum_j w_j), \quad k \in \mathbb{N}.$$

   Expansion of $F(\mathbf{z}) = \sum_j w_j(\mathbf{z})$ in powers of the z_k's.

$$[\mathbf{z}^{\mathbf{n}}](\sum_j w_j(\mathbf{z})) = [\mathbf{w}^{\mathbf{n}}]\Big\{(\sum_j w_j) e^{\sum_k (n_k+1)\ell_k \sum_j w_j} \det\Big(\big(\frac{\partial z_k}{\partial w_j}\big)_{k,j\in \mathrm{supp}\,\mathbf{n}}\Big)\Big\}.$$

2. Combinatorics: identify $F(\mathbf{z})$ as the exponential generating function of colored labelled weighted trees, count them.

Convergence domain for the activity expansion

Have shown

$$F(\mathbf{z}) = \sum_{\mathbf{n}\in\mathcal{I}^*} \frac{\mathbf{z}^{\mathbf{n}}}{\mathbf{n}!} \Big(\sum_k \ell_k n_k\Big)^{\sum_k n_k - 1}.$$

Necessary convergence criterion: Take $z_k \geq 0$. If $F(\mathbf{z})$ is finite, have $F = \sum_k z_k \exp(\ell_k F)$ hence $\sum_k z_k \exp(a\ell_k) \leq a$ for $a = F$.

Sufficient convergence criterion: Take $z_k \geq 0$. For $V > 0$, set

$$h_V := \sum_{\mathbf{n}\in\mathcal{I}^*} \frac{\mathbf{z}^{\mathbf{n}}}{\mathbf{n}!} V^{\sum_k n_k} \mathbf{1}\Big(\sum_k n_k \ell_k = V\Big).$$

Fix $a > 0$ such that $\sum_k |z_k| \exp(a\ell_k) < a$. Let $R_k \sim \mathrm{Poiss}(Vz_k \exp(a\ell_k))$, $k \in \mathbb{N}$ be independent Poisson random variables, space $(\Omega, \mathbb{P}_V)$. Have

$$h_V = e^{-\alpha V} \mathbb{P}_V\Big(\sum_k kR_k = V\Big), \quad \alpha := a - \sum_k |z_k| \exp(a\ell_k) > 0.$$

Therefore $F(\mathbf{z}) = \sum_V h_V / V$ is finite.

Conclusion

For specific one-dimensional model, improved understanding of expansions.

How much is true in greater generality?

- For non-negative interactions, is it true in general that the density expansion is better than the activity expansion?
- If yes, there should be a way of getting density expansions directly, without the grand-canonical detour. Single-type models: Pulvirenti, Tsagkarogiannis '12; does not work for infinitely many species.

Note: in our example, virial expansion converges all the way up to close-packing transition. Not true in general: hard hexagons on a triangular lattice Baxter, Joyce.

Application to phenomenological fragmentation-coagulation models for nucleation...?