Correlation of clusters

Oleksii Rebenko

Institute of Mathematics, Kyiv, Ukraine

POTSDAM, 02 04 2019

$$\boxed{N \sim\ 10^{23}\ - 10^{27}}$$

Phase space

$$\widetilde{\Gamma} \ni \widetilde{\gamma} := \{(x_1, p_1), ..., (x_n, p_n)...\}, \quad x_n \in \mathbb{R}^d,\ p_n \in \mathbb{R}^d. \tag{1}$$

Hamilton equations:

$$\frac{dx_i^{(\alpha)}}{dt} = \frac{\partial H(\widetilde{\gamma})}{\partial p_i^{(\alpha)}}, \quad \frac{dp_i^{(\alpha)}}{dt} = -\frac{\partial H(\widetilde{\gamma})}{\partial x_i^{(\alpha)}}, \quad i \in \{1, ..., N\},\ \alpha \in \{1, ..., d\} \tag{2}$$

Mean values of observables

$$\overline{F} \approx \frac{1}{T}\int_0^T F(\widetilde{\gamma}(t))dt. \tag{3}$$

2. Gibbs ensembles

Josiah Willard Gibbs
proposed instead of one system to introduce an ensemble of identical systems that each time with some probability occupy some configuration. Such identical systems are called *Gibbs ensembles*.
The **basic postulate of Gibbs** is the existence of some probabilistic measure μ on the phase space $\widetilde{\Gamma}$:

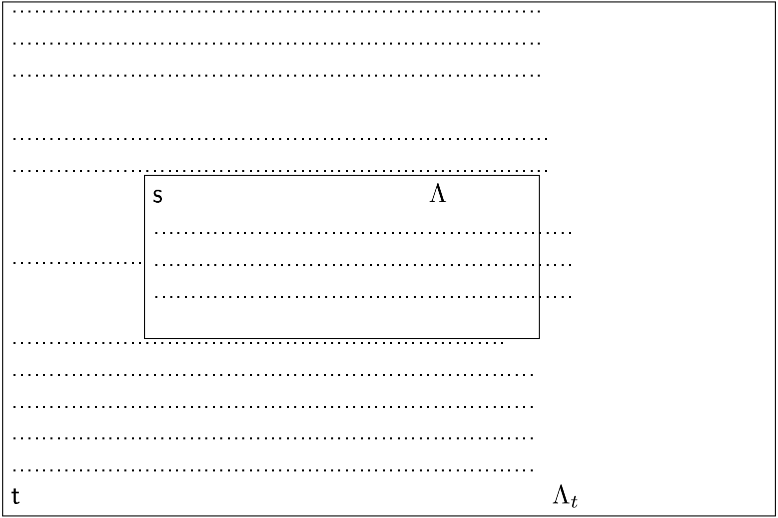
$$\int_{\widetilde{\Gamma}} \mu(d\widetilde{\gamma}) \;=\; 1, \; \overline{F} = \int_{\widetilde{\Gamma}} F(\widetilde{\gamma})\mu(d\widetilde{\gamma}) \tag{4}$$

and the identity

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T F(\widetilde{\gamma}(t))dt = \int_{\widetilde{\Gamma}} F(\widetilde{\gamma})\mu(d\widetilde{\gamma}). \tag{5}$$

which is called *Ergodic hypothesis*, and which is a basic mathematical justification of statistical physics.

3. Gibbs measure



4. Great Canonical Ensemble

Expression for density:

$$D_{gc}^{\Lambda}(\widetilde{\gamma}, N, \beta, \mu) = \frac{1}{\Xi_{\Lambda}(\beta,\mu)} \frac{1}{N!} e^{\beta\mu N - \beta H(\widetilde{\gamma})}, \quad N = |\widetilde{\gamma}|, \beta = \frac{1}{kT}, \qquad (6)$$

where $\Xi_{\Lambda}(\beta,\mu)$ is called *Great Partition Function*:

$$\Xi_{\Lambda}(\beta,\mu) = \sum_{N\geq 0} \frac{1}{N!} \int_{\widetilde{\Gamma}_{\Lambda}^{(N)}} e^{\beta\mu N - \beta H(\widetilde{\gamma})} \frac{d\widetilde{\gamma}}{h^{3N}}, \qquad (7)$$

and

$$H(\widetilde{\gamma}) = \sum_{i=1}^{N} \frac{p_i^2}{2m} + U(x_1, \ldots, x_N). \qquad (8)$$

The physical justification of this formula can be found in:

Yu. B. Rumer, M. Sh. Ryvkin, *Thermodynamics, Statistical Physics and Kinetics*, Mir Publishers, Moscow, 1980.

5. Gibbs distributions in the configuration space

$$D_{gc}^{\Lambda}(\gamma, N, \beta, \mu) = \frac{1}{\Xi_{\Lambda}(\beta,\mu)} \frac{z^N}{N!} e^{-\beta U(\gamma)}, \quad N = |\gamma|, \tag{9}$$

$$\Xi_{\Lambda}(\beta,\mu) = \sum_{N \geq 0} \frac{z^N}{N!} \int_{\Gamma_{\Lambda}^{(N)}} e^{-\beta U(\gamma)} d\gamma, \tag{10}$$

where

$$z \; = \; \frac{e^{\beta\mu}}{h^d} \int_{\mathbb{R}^d} e^{-\frac{p^2}{2m}} dp \; = \; e^{\beta\mu} \left(\frac{2\pi m}{\beta h^2} \right)^{d/2} \tag{11}$$

is called *activity* of the system.

6. Thermodynamic limit

The transition $N \to \infty$, $\Lambda \uparrow \mathbb{R}^d$ is a necessary operation in studying the macroscopic properties of physical systems. This is due to the fact that at the finite values of volume $V = \sigma(\Lambda)$ the behavior of thermodynamic functions is regular (analytical). Therefore, the point of a phase transition on a rigorously mathematical level can not be detected.
Consequently, from the point of view of physical considerations, an important mathematical problem is the rigorous proof of existence limit in expression for the mean observed value:

$$\overline{F} = \lim_{\Lambda \uparrow \mathbb{R}^d} \int_{\Gamma_\Lambda} F(\gamma) \mu_\Lambda(d\gamma). \tag{12}$$

On the other hand, in terms of a rigorous approach to the mathematical problem of constructing a theory, it is not unreasonable to find out whether there exists a Gibbs measure on the space of infinite configurations Γ.
This is a topic of a separate lecture!

7. Mixing property for measures

This talk is related to such characteristic of probability measures as *mixing property*. In the language of Gibbs distributions for the systems of interacting particles, the property of mixing means that the behavior of subsystems of particles in some volumes, which are located at great distances from each other is statistically independent:

$$\mu(F_1F_2)\ -\mu(F_1)\mu(F_2)\ \to\ 0,$$

$$\mathrm{dist}(\mathrm{supp}\,F_1, \mathrm{supp}\,F_2)\ \to\ \infty. \qquad (13)$$

The mixing property ensures ergogodicity and allows to state that the nonequilibrium distribution will go to equilibrium:

I. P. Cornfeld, S. V. Fomin, Y. G. Sinai,
Ergodic Theory, Springer-Verlag, N.Y., Heidelberg, Berlin, 1982.

8. Mixing property for Correlation functions

It is most convenient from a technical point of view to prove this property by estimating the correlation between clusters of particles, that is, the behavior of correlation functions, in which one group of variables is at a considerable distance from another group.

Theorem

(A.L.R., M.V. Tertychnii, Ukr.Math.J.(2017), v.69, No. 8)
Let $\phi(|x|)$ is continuous on $\mathbb{R}_+ \setminus \{0\}$ strong superstable interaction potential of radius R. Then for any subconfigurations $\eta_1 = \{x_1, ..., x_{m_1}\}$ and $\eta_2 = \{y_1, ..., y_{m_2}\}$, with $\mathrm{dist}(\eta_1, \eta_2) := \min_{\substack{x\in\eta_1 \\ y\in\eta_2}} |x - y| \ > \ R$ *and sufficiently small z, the next inequality is true*

$$|\rho(\eta_1 \cup \eta_2) - \rho(\eta_1)\rho(\eta_2)| \leq C^{m_1+m_2}\lambda^{\frac{\mathbf{dist}(\eta_1,\eta_2)}{R}}, \qquad (14)$$

where $\lambda < 1$, $C > 0$, does not depand on η_1, η_2.

Correlation of Clasters: Partially Truncated Correlation Functions and Their Decay.

T. C. Dorlas[1], A. L. Rebenko[2], B. Savoie[1]

1.– Dublin Institute for Advanced Studies School of Theoretical Physics;
2.– Institute of Mathematics, Ukrainian National Academy of Sciences, Kyiv, Ukraine

Published in: Preprint, arXiv:1811.12342, 2018. (to be published in JMP)

10. Content

1. Mathematical background.
2. Correlation functions.
3. Truncated (connected) correlation functions.
4. Partially truncated correlation functions(PTCF).
5. Equations for PTCF and their solutions.
6. Strong decay properties for PTCF.

$\mathbb{R}^d$ – d-dimensional Euclidean space.
$\gamma = \{x_i\}_{i \in \mathbb{N}}$–set of positions of identical particles ($x_i \in \mathbb{R}^d$).
$\mathcal{B}(\mathbb{R}^d)$–family of all Borel sets. $\mathcal{B}_c(\mathbb{R}^d)$–family of all bounded Borel sets.
Configuration space in $\mathbb{R}^d$:

$$\Gamma = \Gamma_{\mathbb{R}^d} := \left\{ \gamma \subset \mathbb{R}^d \middle| \, |\gamma \cap \Lambda| < \infty, \text{ for all } \Lambda \in \mathcal{B}_c(\mathbb{R}^d) \right\}, \tag{15}$$

Spaces of finite configurations Γ_0 in $\mathbb{R}^d$ and Γ_Λ in Λ:

$$\Gamma_0 = \bigsqcup_{n \in \mathbb{N}_0} \Gamma^{(n)}, \quad \Gamma^{(n)} := \{\eta \in \Gamma \mid |\eta| = n\}, \quad \mathbb{N}_0 = \mathbb{N} \cup \{0\}, \tag{16}$$

$$\Gamma_\Lambda := \left\{ \gamma \in \Gamma_0 \middle| \, \gamma \subset \Lambda \right\}. \tag{17}$$

12. Poisson measure on configuration spaces

States of *ideal gas* in equilibrium is described by a *Poisson* random point measure $\pi_{z\sigma}$ on the configuration space Γ, where $z > 0$ is activity(physical parameter which is connected with density of particles) and by σ we denote Lebesgue measure on $\mathbb{R}^d$. $\pi_{z\sigma}$ means Poisson measure with intensity measure $z\sigma$. To define $\pi_{z\sigma}$ on the configuration space Γ, we first introduce a *Lebesgue-Poisson* measure $\lambda_{z\sigma} = \lambda_{z\sigma}^{\Lambda}$ on the space of finite configurations Γ_Λ (or Γ_0) by the formula

$$\int_{\Gamma_\Lambda} F(\gamma)\lambda_{z\sigma}(d\gamma) := \sum_{n=0}^{\infty} \frac{z^n}{n!} \int_\Lambda \cdots \int_\Lambda F_n(x_1, ..., x_n)dx_1 \cdots dx_n, \ F = \{F_n\}_{n\geq 0}. \tag{18}$$

It is clear from (18) that the family of probability measures

$$\pi_{z\sigma}^{\Lambda} := e^{-z\sigma(\Lambda)}\lambda_{z\sigma}^{\Lambda}, \ \Lambda \in \mathcal{B}_c(\mathbb{R}^d) \tag{19}$$

is consistent and by the Kolmogorov theorem there exists a unique probability measure $\pi_{z\sigma}$ on the configuration space Γ.

13. Properties of the $\lambda_{z\sigma}$

Lemma

Let $X_1 \in \mathcal{B}_c(\mathbb{R}^d)$, $X_2 \in \mathcal{B}_c(\mathbb{R}^d)$ and $X_1 \cap X_2 = \emptyset$, $X_1 \cup X_2 = \Lambda$. Functions F_i, $(i = 1, 2)$ are $\mathcal{B}(\Gamma_{X_i})$-measurable. Then

$$\int_{\Gamma_\Lambda} F_1(\gamma)F_2(\gamma)\lambda_{z\sigma}(d\gamma) = \int_{\Gamma_{X_1}} F_1(\gamma)\lambda_{z\sigma}(d\gamma) \int_{\Gamma_{X_2}} F_2(\gamma)\lambda_{z\sigma}(d\gamma). \tag{20}$$

Lemma

For all positive measurable functions $G : \Gamma_0 \mapsto \mathbb{R}$ and $H : \Gamma_0 \times \Gamma_0 \mapsto \mathbb{R}$ the following identity is true:

$$\int_{\Gamma_0} G(\gamma) \sum_{\eta \subset \gamma} H(\eta, \gamma \backslash \eta)\lambda_\sigma(d\gamma) = \int_{\Gamma_0} \int_{\Gamma_0} G(\eta \cup \gamma)H(\eta, \gamma)\lambda_\sigma(d\eta)\lambda_\sigma(d\gamma). \tag{21}$$

14. Some distributions in $\mathcal{D}'(\Gamma_0)$

The space of test functions $\mathcal{D}(\Gamma_0)$ we define in the following way. Any $G:\ \Gamma_0 \mapsto \mathbb{R}$ such that $G \in \mathcal{D}(\Gamma_0)$ and any $\gamma \in \Gamma_0^{(n)}$ $G(\gamma) = G(\{x_1, ..., x_n\}) = G_n(x_1, ..., x_n) \in C_0^\infty(\mathbb{R}^{dn})$. Then for any $\eta \in \Gamma_0$ we define distributions δ_η in such a way that for any $G \in \mathcal{D}(\Gamma_0)$

$$(\delta_\eta, G) := \int_{\Gamma_0} \delta_\eta(\gamma) G(\gamma) \lambda_{z\sigma}(d\gamma) = z^{|\eta|} G(\eta). \tag{22}$$

The identity (21) in the sense of distributions at $H(\eta, \gamma \setminus \eta) = \delta_{\eta_i}(\eta) 1\!\!1_{\Gamma_0}(\gamma \setminus \eta)$:

$$\int_{\Gamma_0} G(\gamma) \sum_{\xi_i \subset \gamma} \delta_{\eta_i}(\xi_i) \lambda_{z\sigma}(d\gamma) = z^{|\eta_i|} \int_{\Gamma_0} G(\eta_i \cup \gamma) \lambda_{z\sigma}(d\gamma), \tag{23}$$

Due to (23) for distribution $\Delta_{(\alpha,\eta)}(\gamma) := 1 + \alpha \sum_{\xi \subset \gamma} \delta_\eta(\xi)$, $\alpha \in \mathbb{R}$, $\eta \neq \emptyset$:

$$\begin{aligned}(\Delta_{(\alpha,\eta)}, G) &= \int_{\Gamma_0} G(\gamma) \Delta_{(\alpha,\eta)}(\gamma) \lambda_{z\sigma}(d\gamma) = \\ &= \int_{\Gamma_0} G(\gamma) \lambda_{z\sigma}(d\gamma) + \alpha z^{|\eta|} \int_{\Gamma_0} G(\eta \cup \gamma) \lambda_{z\sigma}(d\gamma). \end{aligned} \tag{24}$$

15. Interaction energy

We consider a general type of two-body interaction potential $V_2(x,y) = \phi(|x-y|)$. For any $\eta, \gamma \in \Gamma_0$ an energy $U(\gamma)$ of particles in a configuration γ and an interaction energy $W(\eta;\gamma)$ between particles in η and γ have the following forms:

$$U(\gamma) = U_\phi(\gamma) := \sum_{\{x,y\}\subset\gamma} \phi(|x-y|), \tag{25}$$

$$W(\eta;\gamma) := \sum_{\substack{x\in\eta \\ y\in\gamma}} \phi(|x-y|). \tag{26}$$

Interaction potential satisfies the following properties.
(A): 1. *Stability:*

$$U(\gamma) \ \geq \ -B|\gamma|, \ B \geq 0, \ \gamma \in \Gamma_0, \tag{27}$$

2. *Regularity:*

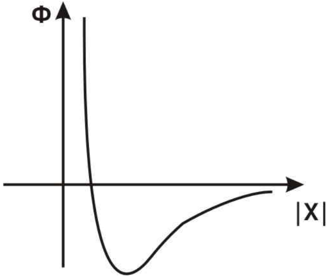
$$C(\beta) \ = \int_{\mathbb{R}^d} dx |e^{-\beta\phi(|x|)} \ - \ 1| \ < \ +\infty, \beta = \frac{1}{kT}. \tag{28}$$

(SSS) *Strong superstability. There exist* $A > 0$, $B \geq 0$, $p > 2$ *and the partition* $\overline{\Delta_{a_0}}$ *such that for any* $\gamma = \{x_1, \ldots, x_N\} \in \Gamma_0$ *the following holds:*

$$U(\gamma) \geq \sum_{\Delta \in \overline{\Delta_a}} \left[A|\gamma_\Delta|^p - B|\gamma_\Delta| \right]. \tag{29}$$

for any $a \leq a_0$, where $\overline{\Delta_a}$ is the partition of the space $\mathbb{R}^d$ into cubes Δ with a rib a and center in $r \in \mathbb{Z}^d$:

$$\Delta = \Delta_a(r) := \left\{ x \in \mathbb{R}^d \ \middle| \ a\left(r^i - 1/2\right) \leq x^i < a\left(r^i + 1/2\right) \right\}. \tag{30}$$



17. Gibbs measure and correlation measure

In the above notations, the Gibbs measure in finite volume Λ has the form:

$$\mu_\Lambda(d\gamma) = \frac{1}{\Xi_\Lambda} e^{-\beta U(\gamma)} \lambda_{z\sigma}(d\gamma), \tag{31}$$

$$\Xi_\Lambda = \int_{\Gamma_\Lambda} e^{-\beta U(\gamma)} \lambda_{z\sigma}(d\gamma), \tag{32}$$

Physical observables are functions on the configuration space Γ. They have the *summatory* form: $F(\gamma) = \sum_{\eta \Subset \gamma} H(\eta)$ (see., for example, the energy (25)). Then one can rewrite mean values of them in the form:

$$\overline{F} = \int_\Gamma \sum_{\eta \Subset \gamma} H(\eta) \mu(d\gamma) = \int_{\Gamma_0} H(\eta)\rho(\eta)\lambda_\sigma(d\eta). \tag{33}$$

In this formula $\rho(\eta)\lambda_\sigma(d\eta)$ is correlation measure and for the case when this measure is absolutely continuous with respect to the Lebesgue-Poisson measure λ_σ the corresponding derivative of Radon-Nicodym is called a correlation function $\rho(\eta)$:

$$\rho_\Lambda(\eta) = \frac{z^{|\eta|}}{\Xi_\Lambda} \int_{\Gamma_\Lambda} e^{-\beta U(\eta \cup \gamma)} \lambda_{z\sigma}(d\gamma). \tag{34}$$

.

18. Justification of the formula (33)

Let $\mathcal{M}^+(\mathbb{R}^d)$ denote the space of nonnegative Radon measures in $\mathcal{B}(\mathbb{R}^d)$. With every configuration $\gamma \in \Gamma$ can be associated an occupation measure

$$\Gamma \ni \gamma \mapsto \sum_{x \in \gamma} \delta_x \in \mathcal{M}^+(\mathbb{R}^d), \tag{35}$$

where δ_x is the Dirac measure. Let $F : \Gamma_0 \to \mathbb{R}$ be a function on the configuration space Γ_0 such that

$$F \restriction \Gamma^{(n)} := F^{(n)}(\{x_1, \dots, x_n\}) = F_n(x_1, \dots, x_n), \quad n \in \mathbb{N}. \tag{36}$$

Then we define the n-th Wick power by

$$\langle F^{(n)}, :\gamma^{\otimes n}: \rangle := \sum_{\substack{x_1, \dots, x_n \in \mathbb{R}^d: \\ \{x_1, \dots, x_n\} \subseteq \gamma}} F_n(x_1, \dots, x_n). \tag{37}$$

19. Correlation measure

The *correlation measures* $\rho^{(n)}$ are defined by

$$\int_{\Gamma^{(n)}} \langle F^{(n)}, :\gamma^{\otimes n}:\rangle\, \mu(d\gamma) := \int_{\mathbb{R}^{dn}} F_n(x_1, \ldots, x_n)\, \rho^{(n)}(dx_1, \ldots, dx_n). \tag{38}$$

In case that the correlation measures $\rho^{(n)}$ are absolutely continuous with respect to the Lebesgue measure in $\mathbb{R}^{dn}$, *correlation functions* are defined as

$$\rho^{(n)}(dx_1, \ldots, dx_n) := \frac{1}{n!}\rho_n(x_1, \ldots, x_n)\, dx_1 \cdots dx_n. \tag{39}$$

Using (37), (38), we can now define the *correlation measure* ρ on the configuration space Γ_Λ by

$$\int_{\Gamma_\Lambda} F(\eta)\, \rho(d\eta) = \sum_{n=0}^{\infty} \int_{\Gamma_\Lambda^{(n)}} \sum_{\substack{x_1,\ldots,x_n \in \mathbb{R}^d: \\ \{x_1,\ldots,x_n\} \subseteq \gamma}} F_n(x_1, \ldots, x_n)\, \mu(d\gamma), \tag{40}$$

which is exactly (33) in the limit $\Lambda \uparrow \mathbb{R}^d$.

20. Truncated(connected) correlation functions

In fact, correlation functions are the probability densities of the distributions of the correlation measures. N. N. Bogolyubov gave them the name of m-particle distribution functions. Real physical correlations between particles are described by the so-called truncated correlation functions(TCF):

$$\rho^T(\eta) \;=\; \rho(\eta) - \sum_{k=2}^{|\eta|} \sum_{\{\eta_1,\dots,\eta_k\}\subset\eta}^{*} \rho^T(\eta_1)\rho^T(\eta_2)\cdots\rho^T(\eta_k),\;\; \rho^T(\{x_1\}) = \rho(\{x_1\}) \tag{41}$$

where the asterisk over the sum means that the sum is over all partitions of the set η into k non-empty disjoint subsets. They can be also represented by correlation functions $\rho(\eta)$:

$$\rho^T(\eta) \;=\; \sum_{k=1}^{|\eta|}(-1)^{k-1}(k-1)! \sum_{\{\eta_1,\dots,\eta_k\}\subset\eta}^{*} \rho(\eta_1)\rho(\eta_2)\cdots\rho(\eta_k). \tag{42}$$

Two-point correlation function:

$$\rho^T(\{x_1,x_2\}) \;=\; \rho_2^T(x_1,x_2) \;=\; \rho_2(x_1,x_2) \;-\; \rho_1(x_1)\rho_1(x_2). \tag{43}$$

21. Partially truncated correlation functions

Partially truncated(connected) correlation functions(PTCF) describe correlations between clusters of particles. Let the set $\widetilde{\eta} = \{\eta_1, \ldots, \eta_m\}$ is the set of partition of configuration η into m non-empty disjoint subsets($|\eta_1| + \cdots + |\eta_m| = |\eta|$). Then PTCF can be also defined recurrently by:

$$\widetilde{\rho}^T_m(\eta_1; \ldots; \eta_m) = \rho_1(\cup_{i=1}^m \eta_i) - \sum_{k=2}^{m} \sum^{*}_{\{\widetilde{\eta}_1,\ldots,\widetilde{\eta}_k\}\subset\widetilde{\eta}} \widetilde{\rho}^T_{m_1}(\widetilde{\eta}_1)\widetilde{\rho}^T_{m_2}(\widetilde{\eta}_2)\cdots\widetilde{\rho}^T_{m_k}(\widetilde{\eta}_k), \tag{44}$$

where

$$\widetilde{\eta}_i = (\eta_{i_1}; \ldots; \eta_{i_{m_i}}),\ \widetilde{\rho}^T_{m_i}(\widetilde{\eta}_i) = \widetilde{\rho}^T_{m_i}(\eta_{i_1}; \ldots; \eta_{i_{m_i}}),\ \widetilde{\rho}^T_1(\eta) = \rho(\eta). \tag{45}$$

So, this definition coincides with definition (41) when all configurations η_i consist of one point:

$$\widetilde{\rho}^T_m(\eta_1; \ldots; \eta_m) = \sum_{k=1}^{m}(-1)^{k-1}(k-1)! \sum^{*}_{\{\widetilde{\eta}_1,\ldots,\widetilde{\eta}_k\}\subset\widetilde{\eta}} \rho_1(\widetilde{\eta}_1)\rho_1(\widetilde{\eta}_2)\cdots\rho_1(\widetilde{\eta}_k). \tag{46}$$

Two-point PTCF: $\widetilde{\rho}^T_2(\eta_1; \eta_2) = \rho_2(\eta_1 \cup \eta_2) - \rho_1(\eta_1)\rho_1(\eta_2)$.

22. Generating functional of PTCF

To derive equations for these functions we define the generating functional:

$$\widetilde{F}^T_{\rho_j}(\alpha,\eta)_1^m \;=\; \log Z_j(\alpha,\eta)_1^m, \tag{47}$$

$$Z_j(\alpha,\eta)_1^m \;=\; \int_{\Gamma_0} \prod_{i=1}^m \Delta_{(\alpha_i\eta_i)}(\gamma)\chi_j(\gamma)e^{-\beta U(\gamma)}\lambda_{z\sigma}(d\gamma), \tag{48}$$

where $\Delta_{(\alpha,\eta)}(\gamma) \;:=\; 1 \;+\; \alpha\sum_{\xi\subset\gamma}\delta_\eta(\xi)$ and

$$\chi_j(\gamma) \;=\begin{cases} 1, & \gamma=\emptyset \\ \prod_{x\in\gamma} j(x), & |\gamma|\geq 1. \end{cases} \tag{49}$$

with $j\in C_0^\infty(\mathbb{R}^d)$ and $|j|\leq 1$. The product of the distributions $\Delta_{(\alpha_i\eta_i)}(\gamma)$ in (48) is well defined because of all sets $\eta_i,\; i=1,...,m$ are disjoint. Then

$$\widetilde{\rho}^T_{j;m}(\eta_1;...;\eta_m) \;=\; \frac{\partial^m}{\partial\alpha_1\cdots\partial\alpha_m}\widetilde{F}^T_{\rho_j}(\alpha,\eta)_1^m|_{\alpha_1=\cdots=\alpha_m=0}. \tag{50}$$

Note, that at $j(x) \;=\; 1\!\!1_\Lambda(x)$ and $\alpha_1=\alpha_2=\cdots=\alpha_m=0$ the formula (48) is the great partition function (32) and $\widetilde{\rho}^T_{j;m}(\eta_1;...;\eta_m)$, calculated by the formula (51), coincide with (46) in finite volume.

Define also:

$$\widetilde{\rho}^{T}_{j;k}(\eta_1; ...; \eta_k | (\alpha,\eta)^{m}_{k+1}) \;=\; \frac{\partial^k}{\partial\alpha_1 \cdots \partial\alpha_k} \widetilde{F}^{T}_{\rho_j}(\alpha,\eta)^{m}_{1}|_{\alpha_1=\cdots=\alpha_k=0},\; 1 \leq k \leq m. \tag{51}$$

For $k = m = 1$, using standard procedure of decomposition:

$$e^{-\beta U(\eta_1 \cup \gamma)} = e^{-\beta W(x_1;\eta_1\setminus\{x_1\})} \sum_{\xi\subset\gamma} K(x_1;\xi) e^{-\beta U(\eta_1\setminus\{x_1\}\cup\gamma)}, \tag{52}$$

where

$$K(x_1;\xi) = \prod_{y\in\xi} \left(e^{-\beta\phi(|x_1-y|)} \;-\; 1 \right),\; W(x_1;\eta_1 \setminus \{x_1\}) \geq -2B, \;\; B \geq 0, \tag{53}$$

24. Kirkwood-Salzburg type equations for PTCF

we obtain:

$$\widetilde{\rho}^{T}_{j;1}(\eta_1) = ze^{-\beta W(x_1;\eta_1\setminus\{x_1\})} j(x_1) \int_{\Gamma_0} K(x_1;\xi)\widetilde{\rho}^{T}_{j;1}(\eta_1 \setminus \{x_1\} \cup \xi)\lambda_\sigma(d\xi) \tag{54}$$

and for $m \geq 2$:

$$\widetilde{\rho}^{T}_{j;m}(\eta_1;\ldots;\eta_m) = z\mathrm{e}^{-\beta W(x_1;\eta_1^{'})} j(x_1) \sum_{I\subset\{2,\ldots,m\}} \sum^{*}_{\xi\subseteq\cup_{i\in I}\eta_i} \int_{\Gamma_0} K(x_1;\xi\cup\gamma)$$
$$\times\, \widetilde{\rho}^{T}_{j;m-|I|}(\eta_1 \setminus \{x_1\} \cup_{i\in I} \eta_i \cup \gamma; \eta_{\{2,\ldots,m\}\setminus I})\, \lambda_\sigma(d\gamma), \tag{55}$$

where $W(x_1;\eta_1^{'}) = W(x_1;\eta_1 \setminus \{x_1\})$ and

$\eta_{\{2,\ldots,m\}\setminus I} := (\eta_{i_2};\ldots;\eta_{i_{m-|I|}})$ if $\{2,\ldots,m\} \setminus I = \{i_2,\ldots,i_{m-|I|}\}$.

25. Solution in the thermodynamic limit

Following the strategy proposed in
Minlos R. A. and Pogosyan S. K., Theor. Math. Phys. **31**(2), 408 (1977), we seek a solution of the equation (73) in the form

$$\widetilde{\rho}^{T}_{j;m}(\eta_1;\ldots;\eta_m) = \int_{\Gamma_0} \chi_j\Big(\bigcup_{i=1}^{m} \eta_i \cup \gamma\Big) T_m(\eta_1;\ldots;\eta_m \mid \gamma)\, \lambda_\sigma(d\gamma), \quad (56)$$

where $T_m(\eta_1;\ldots;\eta_m \mid \gamma)$, $m \geq 2$ and $\gamma \in \Gamma_0$ is a family of kernels such that

$$T_m(\eta_1;\ldots;\eta_m \mid \gamma) = 0 \text{ if } \gamma \cap \bigcup_{i=1}^{m} \eta_i \neq \emptyset. \quad (57)$$

26. Equations for kernels T_m

$$T_m(\eta_1; \ldots; \eta_m \mid \gamma) =$$

$$z\mathrm{e}^{-\beta W(x_1;\eta_1')} \sum_{\xi\subset\gamma} \sum_{I\subset\{2,\ldots,m\}} \sum_{\eta\subset\overline{\eta}_I}^{*} K(x_1; \eta\cup\xi) T_{m-|I|}(\eta_1'\cup\overline{\eta}_I\cup\xi; \eta_{\{2,\ldots,m\}\setminus I} \mid \gamma\setminus\xi), \quad (5$$

where $\eta_1' = \eta_1 \setminus \{x_1\}$ and where we set $\overline{\eta}_I := \bigcup_{i\in I} \eta_i$. Subject to the initial conditions

$$T_1(\emptyset \mid \emptyset) = 1, \quad T_1(\emptyset \mid \gamma) = 0 \text{ if } \gamma \neq \emptyset, \tag{59}$$

and also, for all $m > 1$,

$$T_m(\eta_1; \ldots; \eta_m \mid \gamma) = 0 \text{ if } \gamma \neq \emptyset \text{ and } \eta_j = \emptyset \text{ for some } j = 1, \ldots, m; \tag{60}$$

27. Family of kernels Q_m

$$Q_m(\eta_1;\ldots;\eta_m \mid \gamma) =$$

$$h\sum_{\xi\subset\gamma}\sum_{I\subset\{2,\ldots,m\}}\sum_{\eta\subset\overline{\eta}_I}^{*} K_\nu(x_1;\eta\cup\xi)Q_{m-|I|}(\eta_1'\cup\overline{\eta}_I\cup\xi;\eta_{\{2,\ldots,m\}\setminus I} \mid \gamma\setminus\xi), \tag{61}$$

with initial conditions like (59), (60), and where

$$K_\nu(x_1;\xi) := \begin{cases} 1, & \text{if } \xi=\emptyset, \\ \prod\limits_{x\in\xi}\nu(x_1-x), & \text{if } |\xi|\geq 1. \end{cases} \tag{62}$$

and

$$z\mathrm{e}^{2\beta B} = h \quad \text{and} \quad |\mathrm{e}^{-\beta\phi(|x-y|)}-1| = \nu(x-y). \tag{63}$$

It is clear that if the interaction potential ϕ satisfies (71)–(72), then

$$|T_m(\eta_1;\ldots;\eta_m \mid \gamma)| \leq Q_m(\eta_1;\ldots;\eta_m \mid \gamma). \tag{64}$$

28. The solution for Q_m

The solution $Q_m(\eta_1;\ldots;\eta_m \mid \gamma)$ of the equation (61) with conditions like (59)-(60) can be written with the help of *forest graphs*:
(connected components of every forest graph are *tree graphs*; vertices are points of clusters configurations and points of γ; each edge cannot connect vertices in the same cluster; if we connect all points of each cluster η_i into one point we get the usual tree graph)
The analytical contribution of each configuration point is constant h.
The analytical contribution of each edges is function $\nu(x-y)$.

$$Q_m(\eta_1;\ldots;\eta_m \mid \gamma) = \sum_{\widetilde{f}\in\mathfrak{S}(\eta_1;\ldots;\eta_m|\gamma)} G_\nu(\widetilde{f};\eta_1;\ldots;\eta_m \mid \{y_1,\ldots,y_n\}) = \\ = \sum_{\widetilde{f}\in\mathfrak{S}(\eta_1;\ldots;\eta_m|\gamma)} h^{l+|\gamma|} \prod_{(x,y)\in E(\widetilde{f})} \nu(x-y), \quad (65)$$

where $E(\widetilde{f})$ denotes the set of the edges of $\widetilde{f}$, and where,

$$l := \sum_{i=1}^{m} l_i \ \text{ with } l_i := |\eta_i|, \quad i = 1,\ldots,m. \quad (66)$$

29. Estimates of G_ν

Analytic contributions are easily estimated due to this lemma:

Lemma

Set

$$\nu_0 := \max_{x\in\mathbb{R}^d} \nu(x) < +\infty, \quad \nu_1 := \int_{\mathbb{R}^d} \nu(x)\,dx < +\infty. \tag{67}$$

Then, given a forest graph $\widetilde{f} \in \mathfrak{G}(\eta_1;\ldots;\eta_m \mid \gamma)$ *with* $|\gamma| = n \in \mathbb{N}$,

$$\int_{\mathbb{R}^{dn}} G_\nu(\widetilde{f};\eta_1;\ldots;\eta_m \mid \{y_1,\ldots,y_n\})dy_1\cdots dy_n \le h^{l+n}\nu_0^{|E_{\overline{\eta}}(\widetilde{f})|}\nu_1^n, \tag{68}$$

where l *is defined in* (66), *and*

$$|E_{\overline{\eta}}(\widetilde{f})| \le l - l_1, \quad \overline{\eta} := \bigcup_{i=1}^{m} \eta_i,$$

stands for the number of edges in which one or two ends belong to the set $\bigcup_{i=1}^m \eta_i$.

30. Number of forest graphs

The number of forest graphs $N_n^{(m)}(l_1, \ldots, l_m)$ at fixed configurations $\bigcup_{i=1}^m \eta_i \cup \gamma$ follows from combinatoric lemma.

Lemma

Let $n \in \mathbb{N}_0$ and $m \in \mathbb{N}$, $m \geq 2$. Set $L_i := 2^{l_i} - 1$ for $i = 2, \ldots, m$. Then,

$$N_n^{(m)}(l_1; \ldots; l_m) = l_1 (\prod_{i=2}^m L_i) \left(\sum_{i=1}^m l_i + n \right)^{m+n-2} . \qquad (69)$$

The **proof** follows from recurrent relation

$$N_n^{(m)}(l_1; \ldots; l_m) = \sum_{k=0}^n \binom{n}{k} \sum_{I \subset \{2,\ldots,m\}} L_I N_{n-k}^{(m-|I|)}(l_1 + l_I + k - 1; l_{i_2}; \ldots; l_{i_{m-|I|}}) \qquad (70)$$

where we denote $L_I := \prod_{i \in I} L_i$, $l_I := \sum_{i \in I} l_i$ (with the convention $l_\emptyset := 0$) and $\{i_2, \ldots, i_{m-|I|}\} := \{2, \ldots, m\} \setminus I$.

31. Generalization of Cayley's formula

It is clear that in the case when every cluster has only one particle ($l_i = 1, i = 1, \ldots, m$) the formula (69) is exactly Cayley's formula for the number of connected tree-graphs with $k = m + n$ vertices:

$$N = k^{k-2} \quad !!!$$

(A): 1. *Stability:*

$$U(\gamma) \;\geq\; -B|\gamma|,\; B \geq 0,\; \gamma \in \Gamma_0, \tag{71}$$

2. *Regularity:*

$$C(\beta) \;=\; \int_{\mathbb{R}^d} dx|e^{-\beta\phi(|x|)} \;-\; 1| \;<\; +\infty, \beta = \frac{1}{kT}. \tag{72}$$

Equation

$$\widetilde{\rho}^T_{j;m}(\eta_1;\ldots;\eta_m) = z\mathrm{e}^{-\beta W(x_1;\eta_1')} j(x_1) \sum_{I\subset\{2,\ldots,m\}} \sum^{*}_{\xi\subseteq\cup_{i\in I}\eta_i} \int_{\Gamma_0} K(x_1;\xi\cup\gamma)$$
$$\times\, \widetilde{\rho}^T_{j;m-|I|}(\eta_1 \setminus \{x_1\} \cup_{i\in I} \eta_i \cup \gamma; \eta_{\{2,\ldots,m\}\setminus I})\, \lambda_\sigma(d\gamma), \tag{73}$$

33. Solution of Eq. for $\widetilde{\rho}_m^T$

Theorem

Assume that the interaction potential ϕ *satisfies* (71)–(72). *Then there exists a unique solution of the equation* (73) *in the thermodynamic limit* $j \to 1$, *which can be written in the form*

$$\widetilde{\rho}_m^T(\eta_1; \ldots; \eta_m) = \int_{\Gamma_0} T_m(\eta_1; \ldots; \eta_m \mid \gamma)\, \lambda_\sigma(d\gamma), \tag{74}$$

$$T_m(\eta_1; \ldots; \eta_m \mid \gamma) = \sum_{\widetilde{f} \in \mathfrak{S}(\eta_1; \ldots; \eta_m | \gamma)} G_\phi(\widetilde{f}), \tag{75}$$

$$G_\phi(\widetilde{f}) = z^{l+n} \prod_{(x,y) \in E(\widetilde{f})} \left(\mathrm{e}^{-\beta\phi(|x-y|)} - 1 \right) \prod_{(x,y) \in S(\widetilde{f})} \mathrm{e}^{-\beta\phi(|x-y|)}, \tag{76}$$

where $S(\widetilde{f})$ *denotes the set of pairs of points of the set* $\bigcup_{i=1}^m \eta_i \cup \gamma$ *for which there are no edges in the graph forest* $\widetilde{f}$ *and* (74) *converges in the region*

$$z\mathrm{e}^{2\beta B + 2}\nu_1(\beta) < 1. \tag{77}$$

34. Strong Decay property of $\widetilde{\rho}^T_m$

Theorem

Suppose that the interaction potential ϕ satisfies (71)–(72). Assume in addition that there exists $\alpha > d$ and $C(\beta) > 0$, such that

$$\nu_\beta(x) := |\mathrm{e}^{-\beta\phi(x)} - 1| \leq \frac{C(\beta)}{1 + |x|^\alpha}, \tag{78}$$

Then, provided that,

$$z\mathrm{e}^{2\beta B}[\nu_1(\beta)\mathrm{e} + \overline{\nu}_1(\beta)(\mathrm{e} + 2^{1+\alpha})] < 1, \tag{79}$$

there exist, constants $A_{m,\sigma} = A_{m,\sigma}(\beta, z, \alpha) > 0$, $m \geq 2$, $1 \leq \sigma \leq m$ such that the PTCF in (74) admit the following bounds

$$|\widetilde{\rho}^T_m(\eta_1; \ldots; \eta_m)| \leq \sum_{\sigma=1}^{m} A_{m,\sigma} \max_{T_m \in \mathcal{T}_m} \overline{\nu}_{T_m}, \tag{80}$$

$$\overline{\nu}_{T_m} := \prod_{(i,j)\in T_m} \max_{x_i\in\eta_i; x_j\in\eta_j} \overline{\nu}(x_i - x_j). \tag{81}$$

35. Constant for $m = 2$

In the case $m = 2$:

$$A_{2,1} = A_{2,2} := \frac{1}{2} l_1 l_2 C (1+C)^{l_2-1} \left(\frac{h}{1 - h\nu_1 \mathrm{e}} \right)^{l} \frac{1 - h\nu_1 \mathrm{e}}{1 - h\nu_1 \mathrm{e} - h\overline{\nu}_1 2^{1+\alpha} C}. \tag{82}$$

36. Constants $A_{m,\sigma}$

In the case $m \geq 4$ and for any $3 \leq \sigma \leq m$:

$$A_{m,\sigma} := (\sigma-2)^{\sigma} \binom{m-1}{\sigma-1} 2^{\alpha(\sigma-1)^2} l^{m-\sigma} C^m (1+C)^{l-l_1-\sigma+1} \left(\frac{h}{1-h\nu_1 \mathrm{e}}\right)^{l} \times \left(\frac{1-h\nu_1\mathrm{e}}{1-h\nu_1\mathrm{e}-h\overline{\nu}_1 2^{1+\alpha}C}\right)^{\sigma} \frac{h\overline{\nu}_1\mathrm{e}(1-h\nu_1\mathrm{e}-h\overline{\nu}_1 2^{1+\alpha}C)}{1-h\nu_1\mathrm{e}-h\overline{\nu}_1(\mathrm{e}+2^{1+\alpha})C}. \quad (83)$$

THANK YOU!