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Mini-Workshop: Cluster Expansions: From Combinatorics to Analysis through Probability

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Abstract. The workshop addressed the interplay between theory and applications of cluster expansions. These expansions, historically geared towards the study of systems in statistical mechanics, thermodynamics, and physical chemistry, have recently found applications in different areas of current mathematical research, such as point processes, random graphs, coloring issues, logics and inverse problems in numerical analysis. The workshop developed both directions of the theory–application interplay. On the one hand, speakers presented advances in the theoretical foundations of the abstract polymer model and improved tree-graph inequalities, and explored their consequences for the theory of liquids and other applied issues. On the other hand, researchers in stochastic modelisation exposed needs and challenges brought by concrete models of liquids and liquid crystal to the theory of cluster expansions. In addition other complementary methods were discussed, such as disagrement percolation —an expansion-free approach to uniqueness and decay of correlations— and lace expansions —an expansion technique popular for its applications to random walks and percolation problems.

Mathematics Subject Classification (2010): 82B, 60K35, 05A; 05C, 60D05, 65C.

Introduction by the Organisers

Originally, cluster expansions have been devised by Mayer and collaborators in order to derive the equation of state for a non-ideal gas. Rigorous results first appeared in the 60's with convergence proofs built on a combinatorial identity

between graphs and trees. The same decade saw further expansions being developed for correlation functions as a means to describe the liquid state. Subsequent developments took place both in mathematics and applied disciplines.

The abstract polymer model gave a boost to rigorous cluster expansions, establishing a broadly applicable framework and removing the need of case-by-case convergence proofs. The abstract polymer model paved the way for connections with combinatorics, e.g., Lovász lemma and graph enumeration formulas. It inspired similar techniques in probability to calculate two-point functions for self-avoiding random walks, e.g., lace expansions and connectivity functions in Boolean models. Cluster expansions have also been a precious tool in mathematical statistical mechanics, notably in establishing uniqueness of Gibbs states and defining effective potentials.

Numerous applied techniques were built on expansion methods leading to the modern liquid state theory; surprisingly, these approaches are still on a formal level. With the advancement of computational power, methods shifted to direct simulations via Monte Carlo or molecular dynamics. For complex molecules, however, the computational cost of direct simulations spurred the development of new coarse-graining methods, which in turn brings back theoretical treatments of atomistic degrees of freedom in order to define effective potentials.

The meeting brought together scientists from several fields within or outside mathematics, contributing different points of view on problems, challenges and solutions. The workshop program combined forefront research with survey talks, which successfully fostered lively cross-disciplinary discussions that took place around the talks as well as in dedicated discussion sessions.

The meeting started with an introduction to the abstract polymer model by R. Kotecký, one of the founders of this approach. A. Procacci presented a new partition scheme for the tree-graph inequality and deduced an improved radius of convergence for potentials with both attractive and repulsive parts. His proof was spontaneously taken up by D. Ueltschi, who presented possible simplifications, giving us the opportunity to deepen our understanding of technical intricacies.

A second group of talks investigated applications, correlation functions, and liquid state theory, for which direct correlation functions and the Ornstein-Zernike equation are key. Existence and convergence theorems for the latter, albeit in the gas regime, were presented by T. Kuna, including refined combinatorial considerations of graphs and connectivity concepts. Going beyond the reach of current rigorous results, L. Lue surveyed some practical applications of expansion methods and made a case for incorporating modern rigorous developments into modelisation; one challenge raised was how higher order correction terms may help predict clustering of particles from first principles. Continuum models for liquid crystals, object of a significant body of analytical literature, still lack a satisfying atomistic derivation. In this spirit E. Virga presented some elements to make rigorous a program going back to Onsager. M. Hanke addressed the validity of the

inverse Boltzmann iteration, a method underpinning numerical approaches, by formulating an inverse problem and establishing Fréchet differentiability of relevant operators between suitably constructed spaces.

Lace expansions are closely related to, but somewhat different from, cluster expansions, and enjoy a slightly bigger, though more recent, popularity in probability theory. A pioneer in both cluster and lace expansions, D. Brydges explained key concepts and gave a glimpse into selected applications, among them random walks with repulsive self-interaction and the φ^4-model. R. Fitzner reviewed percolation results in higher dimensions and commented on the mean field character attained by the system. T. Helmuth in a similar context discussed the self-attractive and the self-avoiding walk as a model for linear polymers in good/bad solvent.

Statistical mechanics for point particles in $\mathbb{R}^d$ can benefit from stochastic geometry and point process theory; conversely, equations first devised in statistical mechanics may pop up in genuinely stochastic problems. G. Last gave a helpful tutorial on key concepts from point processes (Palm measure, Campbell formula) and presented existence and analyticity results for the Ornstein-Zernike equation in the context of the random connection model. C. Temmel spoke about disagreement percolation for hard spheres and decay of correlations beyond the radius of convergence of the associated cluster expansion. Still in the continuum, but in a language closer to traditional statistical mechanics, E. Pulvirenti discussed a variant of the LMP model (named after Lebowitz, Mazel, Presutti) and in particular how to derive an effective Hamiltonian for a coarse-grained version. M. Yin brought cluster expansions into yet another area of probability, random graphs, and situated her results within the context of graph limits and graphons.

The workshop included ample time for topical discussions among the participants. Issues discussed include: resummations for two-connected graphs, analytic extensions, limiting regimes in high dimensions, Lee-Yang singularity and existing results for the classical hard-sphere gas. There was also a session on prioritary new directions of research. A consensus emerged on the need to develop cluster and lace expansion techniques for quantum models.

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Abstracts

The Lace expansion for the $|\varphi|^4$ model with $n = 0, 1, 2$ components

David C. Brydges

This is a report on work in progress with *Tyler Helmuth* and *Mark Holmes*. The lace expansion is a standard method for studying critical behaviour in statistical mechanics [5]. It is of possible use in cases where mean field theory is expected to be a good approximation and is a method to prove this in the sense of determining the asymptotics of the decay of the two point function. In this presentation I outline our proof that the critical two-component $|\varphi|^4$ model admits a convergent lace expansion, for weak coupling, or all coupling for high dimensions. In particular the high dimensional $O(2)$ model is also included. This is the first time the lace expansion has been shown to exist and converge for a model with a continuous symmetry.

Akira Sakai has shown that a convergent lace expansion exists for the Ising model [3] and the one component φ^4 model [4]. His derivation uses the current representation for the Ising model to convert the system to a percolation. Our starting point is instead the Symanzik local time isomorphism [6], [1] [2] and it results in expansions that are not the same as those found by Sakai, although we used essential ideas from his work. Our lace expansion exists for $|\varphi|^4$, $O(n)$ models and the continuous time lattice Edwards model ($n = 0$), but we can only prove convergence for $n = 0, 1, 2$ because our proof relies on GHS and Ginibre correlation inequalities that are not known to hold for $n > 2$. As in all lace expansions, for convergence a small parameter is required. Thus the method gives information on critical exponents for the listed models in high dimensions, or for finite but sufficiently long-range coupling, or for weak coupling.

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Mean-field behavior using the lace expansion

Robert Fitzner
(joint work with Remco van der Hofstad)

The lace expansion is a powerful perturbative technique to analyze the critical behavior of random spatial processes. Its major application is to prove that a model shows mean-field behavior in dimensions above the so-called upper critical dimension. We present recent result on the nearest-neighbor square lattice and explain its implication. Most prominently, F. and van der Hofstad proved that nearest-neighbor percolation shows mean field behavior in all dimension d¿10.

In this process we review mean-field behavior of self-avoiding walk and percolation. For these two model mean-field behavior can be loosely translated to the statement that their spatial correlation function behaves asymptotically like the Greens function of the simple random walk. This mean-field behavior can only be expected if the dimension of the underlying lattice is high enough. In the talk we give a heuristic explanation for the upper critical dimension of these models.

The lace expansion creates a characterization of the two-point function as a perturbation of the two-point function of the simple model, in our case the simple random walk. Using a sophisticated analysis one can use bounds on the perturbation terms to obtain information on the original function, which can imply the desired result on mean-field behavior.

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An inverse problem in statistical mechanics

Martin Hanke

Coarse-graining is a standard technique in physical chemistry for reducing the computational burden of numerical simulations of complex materials such as polymers, for example. The idea is to simplify substructures of a given molecule to so-called "beads", and then use effective potentials to evaluate the interaction of these beads in a simulation. There are various techniques to derive effective potentials depending on the data at hand, and we are interested in the case where the given data is the radial distribution function, which is a rescaled pair distribution function.

To be more specific, we work in the thermodynamical limit of a grand canonical ensemble of particles in thermal equilibrium at fixed (inverse) temperature $\beta >$

0 and small activity $z > 0$ (the so-called gas phase). It is assumed that the interaction of the particles is determined by a pair potential u which only depends on the distance r of the particles and satisfies

$$(1) \qquad \begin{aligned} |u(r)| &< C_0 r^{-\alpha}\,, \qquad r \geq r_0\,, \\ u(r) &> c_0 r^{-\alpha}\,, \qquad r \leq r_0\,, \end{aligned}$$

for some fixed $\alpha > 3$, $r_0 > 0$, and constants $C_0 > c_0 > 0$. As such, u belongs to the class of Lennard-Jones type pair potentials, cf. Ruelle [4], which are known to be stable and regular, i.e., there exists $B > 0$ and $c_\beta > 0$ such that

$$\sum_{1 \leq i < j \leq N} u(|R_i - R_j|) \geq -BN$$

for every configuration $(R_1, R_2, \ldots, R_N) \subset (\mathbb{R}^3)^N$ of N particles, $N \in \mathbb{N}$, and

$$\int_{\mathbb{R}^3} |f(R)| \mathrm{d}R < c_\beta\,,$$

where f is the so-called *Mayer function*

$$f(R) = e^{-\beta u(|R|)} - 1\,.$$

Associated with this ensemble are statistical quantities like the local (number) density $\rho^{(1)}(R)$ and the pair distribution function $\rho^{(2)}(R_1, R_2)$, which is a measure for the likelihood that two particles will occupy the positions R_1 and R_2 simultaneously. Working in the thermodynamical limit, $\rho_0 = \rho^{(1)}$ is a constant and $\rho^{(2)}$ only depends on the distance $|R_1 - R_2|$, cf. [4]. Finally, one defines the radial distribution function g as

$$g(r) = \frac{1}{\rho_0^2}\, \rho^{(2)}(R_1, R_2)\,, \qquad |R_1 - R_2| = r\,.$$

In [1] Groeneveld states that

$$(2) \qquad |g(r) - 1| \leq \frac{C_\varrho}{\varrho(r)}\,, \qquad r > 0\,,$$

where $C_\rho > 0$ and

$$\varrho(r) = (1 + r^2)^{\alpha/2}\,, \qquad r > 0\,,$$

but doesn't provide a proof. Our proof of (2) is be based on a tree-graph inequality by Poghosian and Ueltschi [3], and a careful analysis of an associated Ornstein-Zernike equation. We can further show that there are constants $C_1 > c_1 > 0$, such that

$$(3) \qquad c_1 e^{-\beta u(r)} \leq g(r) \leq C_1 e^{-\beta u(r)}\,, \qquad r > 0\,.$$

Consider the operator

$$(4) \qquad F : u \mapsto g\,,$$

which maps a Lennard-Jones type pair potential u onto the associated radial distribution function. On the grounds of (2) we measure perturbations of g in the Banach space $L^\infty_\varrho(\mathbb{R}^+)$ of all measurable functions h, for which the norm

$$\|h\|_{L^\infty_\varrho(\mathbb{R}^+)} \;=\; \|\varrho h\|_{L^\infty(\mathbb{R}^+)}$$

is finite. Concerning the potentials we introduce the Banach space $\mathcal{V}$ of perturbations v, for which the associated norm

$$\|v\|_{\mathcal{V}} \;=\; \max\bigl\{\|v/u\|_{(0,r_0]}, \|\varrho v\|_{[r_0,\infty)}\bigr\}$$

is finite. Note that $\mathcal{V}$ depends on the reference potential u, and that there exists $\delta > 0$ sufficiently small such that $u + v$ also satisfies (1) for every $v \in \mathcal{V}$ with $\|v\|_{\mathcal{V}} \le \delta$.

The following result improves upon our earlier results in [2].

Theorem 1. *If u satisfies (1), and if the activity z is constrained to*

$$0 \;<\; z \;<\; \frac{1}{c_\beta e^{2\beta B+1}}\,, \tag{5}$$

then the operator F of (4) is Fréchet differentiable with respect to $\mathcal{V}$ and $L^\infty_\varrho(\mathbb{R}^+)$, i.e., there exists $F'(u) \in \mathcal{L}(\mathcal{V}, L^\infty_\varrho(\mathbb{R}^+))$ and $\delta > 0$, such that

$$\|F(\widetilde{u}) - F(u) - F'(u)(\widetilde{u} - u)\|_{L^\infty_\varrho(\mathbb{R}^+)} \;=\; O(\|\widetilde{u} - u\|^2_{\mathcal{V}})\,,$$

uniformly for $\widetilde{u}$ with $\|\widetilde{u} - u\|_{\mathcal{V}} \le \delta$.

In the physical chemistry literature a standard approach to the inverse problem, i.e., to solve $F(u) = g$ for u when given g, is the inverse Boltzmann iteration

$$u_{n+1} \;=\; \Phi(u_n) \;=\; u_n \;+\; \frac{1}{\beta}\log\frac{F(u_n)}{g}\,, \qquad n = 0, 1, 2, \ldots\,. \tag{6}$$

Here, u_0 is an appropriate initial estimate of u, typically chosen to be the potential of mean force. So far, there is no rigorous mathematical analysis of this iterative scheme, and on a first glance it is not even clear whether the resulting approximations u_n of (6) will stay Lennard-Jones type pair potentials (or anything alike), even when u_0 is known to be one. Using (3) and Theorem 1 we can prove the following result.

Theorem 2. *If u satisfies (1), and if*

$$0 \;<\; z \;<\; \frac{1}{1+e}\,\frac{1}{c_\beta e^{2\beta B+1}}\,, \tag{7}$$

then there exists $\delta > 0$ and some Lipschitz constant $L > 0$ such that

$$\|\Phi(\widetilde{u}) - \Phi(u)\|_{\mathcal{V}} \;\le\; L\|\widetilde{u} - u\|_{\mathcal{V}}\,,$$

provided that $\|\widetilde{u} - u\|_{\mathcal{V}} \le \delta$. Moreover, Φ is Fréchet differentiable with respect to u with $\Phi'(u) \in \mathcal{L}(\mathcal{V}, \mathcal{V})$.

Note that (7) is more restrictive than the classical interval (5) for the activity.

Theorem 2 can be used to establish local well-posedness of the inverse Boltzmann iteration. Assuming that the given data g in (6) is the true radial distribution function associated with a Lennard-Jones type pair potential u, and that $\|u_0 - u\|_{\mathcal{V}} \leq \delta/L$, then it follows from Theorem 2 that the first iterate u_1 of (6) satisfies

$$\|u_1 - u\|_{\mathcal{V}} \;=\; \|\Phi(u_0) - \Phi(u)\|_{\mathcal{V}} \;\leq\; L\|u_0 - u\|_{\mathcal{V}} \;\leq\; \delta\,,$$

and hence, remains in the domain of Φ.

Detailed proofs of Theorems 1 and 2 will be published elsewhere.

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Self-attractive self-avoiding walk

Tyler Helmuth

(joint work with Alan Hammond)

Self-attractive self-avoiding walks are a simple model of linear polymers in poor solvents. For $n \in \mathbb{N}$ and $\kappa > 0$ the model is defined by a probability measure $\mathbb{P}_{n,\kappa}$ on n-step self-avoiding walks ω:

$$\mathbb{P}_{n,\kappa}(\omega) = \frac{(1+\kappa)^{c(\omega)}}{Z_{n,\kappa}}, \qquad \kappa > 0. \tag{1}$$

The walks ω are assumed to begin at the origin of $\mathbb{Z}^d$, and $c(\omega)$ denotes the number of *contacts* contained in a walk ω. A contact occurs when two edges of the walk ω span a plaquette of $\mathbb{Z}^d$, see (1). The walks take steps from a fixed $\mathbb{Z}^d$-symmetric distribution D, and $Z_{n,\kappa}$ is the normalization constant needed to make $\mathbb{P}_{n,\kappa}$ a probability measure.

Suppose that instead of $\kappa > 0$ we take $\kappa = 0$ and assume the step distribution is uniform on the unit vectors of $\mathbb{Z}^d$. Then (1) defines the uniform measure on nearest-neighbour self-avoiding walks; this model has attracted a great deal of interest [1]. A challenging aspect when $\kappa > 0$ is that there is a loss of subadditivity, which is one of the few tools available in the $\kappa = 0$ case. Earlier work on related models with $\kappa > 0$ has been restricted to step distributions D that satisfy a smoothness condition, which allows subadditivity to be recovered when κ is sufficiently small [2]. The smoothness condition has the drawback that it implies that D has infinite range.

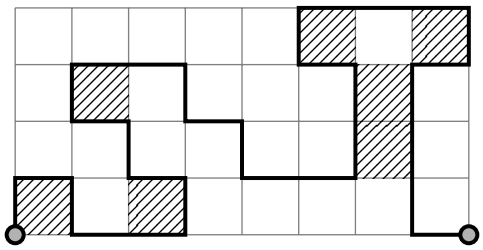

FIGURE 1. A self-avoiding walk ω with its contacts indicated as shaded plaquettes.

In joint work with Alan Hammond we have analyzed the behaviour of self-attractive self-avoiding walk when $\kappa > 0$ and the step distribution D has compact support. Our first result establishes the existence of the connective constant in dimensions $d \geq 2$, i.e., the existence of the limit

$$\mu(\kappa) = \lim_{n\to\infty} Z_{n,\kappa}^{1/n},$$

provided $\kappa > 0$ is small enough. The existence of the limit is proved by a modified version of the Hammersley-Welsh unfolding argument [3]. The main idea is to use an energy-entropy estimate to control the loss of attractive contacts during the unfolding procedure. Similar entropic arguments in the context of self-avoiding walks and self-avoiding polygons have previously appeared in [4, 5].

In high dimensions it is reasonable to expect that when $\kappa > 0$ is small the effect of the self-attraction is negligible. We prove that this is true using the lace expansion, a tool which has been developed to prove mean field behaviour for statistical mechanical models like self-avoiding walk. A key step in lace expansion arguments is to establish *diagrammatic bounds* [6]. These bounds are usually established by using a model-specific monotonicity property. Self-attractive self-avoiding walk lacks the monotonicity properties of self-avoiding walk, and this makes obtaining diagrammatic bounds more complicated.

It is possible, however, to use energy-entropy ideas to overcome the lack of monotonicity. The resulting diagrammatic bounds are compatible with the lace expansion analysis of [7]. This allows us to analyze the critical behaviour of the model when $d \geq 5$ for sufficiently spread out step distributions and small enough $\kappa > 0$. One particular conclusion is that the critical two-point function has Gaussian asymptotics, which verifies the mean field behaviour of self-attractive self-avoiding walk under these hypotheses.

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Disagreement percolation for the hard-sphere model

Christoph Hofer-Temmel

Disagreement percolation by van den Berg and Maes [5] is a sufficient condition on the activity of a discrete Gibbs specification on a graph for uniqueness of the Gibbs measure. It implies the absence of phase transitions and the analyticity of the free energy in the high-temperature case. It has also been used to derive the Poincaré inequality in the context of lattice Ising spin systems [1]. I extend disagree percolation to the hard-sphere model on $\mathbb{R}^d$. This results in a sufficient condition lower bound on the activity guaranteeing uniqueness of the Gibbs measure and exponential decay of the reduced pair correlation function in the high temperature regime.

The core idea behind disagreement percolation is to control the competing influence of two differing boundary conditions on the finite volume specification by an iid Bernoulli site percolation. In a second step, it uses the subcriticality of site percolation to derive the uniqueness of the Gibbs measure and additional properties. This approach generalises straightforward to the continuum setting, with the Boolean disc model taking the role of Bernoulli site percolation.

In practice, a lower bound on the critical intensity for percolation of the Boolean model translates into a lower bounds on the extent of the uniqueness region of the infinite volume Gibbs measure. These lower bounds improve upon the radius of the best known cluster expansions [2] and exceed even their theoretically best obtainable radius. In one dimension, where the hard-sphere model is called Tonk's gas, this shows the absence of phase transition for all activities as in [6], whereas cluster expansion has a radius of convergence of $\frac{1}{e}$. In principle, one is be able to use the exponential decay of percolation clusters in the subcritical Boolean model to bound all higher order reduced correlations, too.

In the discrete case, the coupling between the two realisations of the finite volume specification and the controlling site percolation proceeds step-by-step in a recursive fashion along the finite number of sites. It uses a perfect coupling between the disagreement of the two specifications on a site and couples this generically to the site percolation. This approach breaks down in the continuum.

If one turns around the setup, though, one starts with a realisation of the Boolean model, which controls where disagreement may take place. The construction of the coupling then becomes a simultaneous thinning from the Boolean model to the two hard-sphere realisations. The hard-sphere property, already exploited by van den Berg en Steif [4] for the hard-core model, simplifies the construction to a thinning from the Boolean model to a single hard-sphere realisation. The recursive construction of the coupling demands that the thinning is not only recursive in the domain, but also measurable under changes of the boundary condition. The solution is a recursive dependent thinning, where the thinning probability of a point corresponds to the derivative of the free energy of the unexplored part of the domain subject to the already chosen points, as one progresses through the domain.

Two questions came up during the workshop. First of all, does an exponential decay of all higher order reduced correlations functions imply analyticity of the free energy, and is this even needed? Second, is there a direct comparison between the pinned series in the cluster expansion of the hard-sphere model and the connection function in the Boolean model, as detailed in recent work on the Ornstein-Zernike function [3]? This would clarify their relation and explain why disagreement percolation admits larger activities than cluster expansions in all known cases.

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Abstract cluster expansion—the simplest proof

Roman Kotecký

I present here a quintessence of cluster expansion for abstract polymer models. The standard Dobrushin statement is proven, adapting from [D] as well as other sources [M, SS]. Notice that a full proof of cluster expansion convergence is given. I leave out, for additional discussions, the further extensions of the standard result proven by Proccaci, Fernández and others.

Abstract polymer models are most easily formulated in terms of a simple graph $G = (V, E)$ (without edges that connect a vertex to itself). Here, *abstract polymers* are the vertices $v \in V$ with $(v, v') \in E$ whenever the corresponding polymers are

incompatible (no loops: only distinct vertices may be incompatible).[1] Given a model *weight* $w : V \to \mathbb{C}$ of the abstract polymers, we define the *partition function*

$$Z_L(w) = \sum_{I \subset L} \prod_{v \in I} w(v) = 1 + \sum_{\emptyset \neq I \subset L} \prod_{v \in I} w(v). \tag{1}$$

The sum is running over all *independent sets* I of vertices in L (no two vertices in I are adjacent). In other words: all collections I of compatible abstract polymers.

The partition function $Z_L(w)$ is an entire function in $w = \{w(v)\}_{v \in L} \in \mathbb{C}^{|L|}$ and $Z_L(0) = 1$. Hence, it is non-vanishing in some neighbourhood of the origin $w = 0$ and its logarithm is, on this neighbourhood, an analytic function yielding a convergent Taylor series

$$\log Z_L(w) = \sum_{X \in \mathcal{X}(L)} a_L(X) w^X. \tag{2}$$

Here, $\mathcal{X}(L)$ is the set of all multi-indices $X : L \to \{0, 1, ...\}$ and $w^X = \prod_v w(v)^{X(v)}$. Inspecting the Taylor formula for the coefficients $a_L(X)$ in terms of corresponding derivatives of $\log Z_L(w)$ at the origin $w = 0$, it is easy to show that the coefficients $a_L(X)$ actually do not depend on L:

$$a_L(X) = a_{\operatorname{supp} X}(X), \text{ where } \operatorname{supp} X = \{v \in V : X(v) \neq 0\}.$$

As a result, one is getting the existence of coefficients $a(X)$ for each $X \in \mathcal{X} = \{X : V \to \{0, 1, \dots\}, |X| = \sum_{v \in V} |X(v)| < \infty\}$ such that, for every finite $L \subset V$,

$$\log Z_L(w) = \sum_{X \in \mathcal{X}(L)} a(X) w^X \tag{3}$$

with convergence on a small neighbourhood of the origin depending on L.

Notice that $a(X) \in \mathbb{R}$ for all X (consider $Z_L(w)$ with real w) and $a(X) = 0$ whenever the graph $G(\operatorname{supp} X)$ (induced by G on $\operatorname{supp} X$) is not connected: just notice that, from definition, $Z_{\operatorname{supp} X}(w) = Z_{L_1}(w) Z_{L_2}(w)$ once $\operatorname{supp} X = L_1 \cup L_2$ with no edges between L_1 and L_2.

The multi-indices X with connected $G(\operatorname{supp} X)$ are called *clusters*.

In addition, the coefficients $a(X)$ have *alternating signs*,

$$(-1)^{|X|+1} a(X) \geq 0 \text{ for any } X \in \mathcal{X}. \tag{4}$$

Rewriting (3) for the weights $-|w|$,

$$-\log Z_L(-|w|) = -\sum_{X \in \mathcal{X}(L)} a(X) (-1)^{|X|} |w|^X$$

and taking into account that every X has $\operatorname{supp} X \subset L$ for some finite L, the condition (4) is equivalent to the claim that for any finite $L \subset V$, *all coefficients of the expansion of* $-\log Z_L(-|w|)$ *in powers* $|w|^X$ *are nonnegative.*

[1] Notice that in applications, typically, such graph has infinite degree—any polymer is incompatible with infinitely many polymers (think about polymers, say, as cycles on $\mathbb{Z}^d$, with two of them incompatible if they intersect).

The latter claim is easy to prove by induction in $|L|$. Indeed, for $|L| = 0$ and $L = 1$, we have $Z_\emptyset(-|w|) = 1$ and $Z_{\{v\}}(-|w|) = 1 - |w(v)|$ with

$$-\log Z_\emptyset(-|w|) = 0 \quad \text{and} \quad -\log Z_{\{v\}}(-|w|) = \sum_{n=1}^{\infty} \frac{|w(v)|^n}{n}$$

(the latter valid for sufficiently small $|w(v)|$). For $|L| \geq 1$ and $v \notin L$, we use $\mathcal{N}(v)$ to denote the set of vertices adjacent to the vertex v in graph G. From the definition (1), we have $Z_{L\cup\{v\}}(-|w|) = Z_L(-|w|) - |w(v)|Z_{L\setminus\mathcal{N}(v)}(-|w|)$ yielding

$$-\log Z_{L\cup\{v\}}(-|w|) = -\log Z_L(-|w|) - \log\left(1 - |w(v)|\frac{Z_{L\setminus\mathcal{N}(v)}(-|w|)}{Z_L(-|w|)}\right)$$

(here we consider $|w|$ sufficiently small on $L \cup \{v\}$ so that all concerned Taylor expansions for $\log Z_W(-|w|)$ with $W \subset L \cup \{v\}$ converge). The first term on the RHS has nonnegative coefficients by induction hypothesis. Taking into account that $-\log(1 - z)$ has only nonnegative coefficients and that

$$\frac{Z_{L\setminus\mathcal{N}(v)}(-|w|)}{Z_L(-|w|)} = \exp\left\{\sum_{X\in\mathcal{X}(L)\setminus\mathcal{X}(L\setminus\mathcal{N}(v))} |a(X)||w|^X\right\}$$

has also only nonegative coefficients, all the expression on the RHS has necessarily only nonnegative coefficients.

What can we say about the *diameter of convergence* of series (3)?

For each finite $L \subset V$, consider the *polydiscs*

$$\mathcal{D}_{L,\boldsymbol{R}} = \{w : |w(v)| \leq R(v) \text{ for } v \in L\} \text{ with the set of radii } \boldsymbol{R} = \{R(v); v \in V\}.$$

The most natural for the inductive proof is the Dobrushin's condition[2]:

There exists a function $r : V \to [0, 1)$ such that, for each $v \in V$,

$$(*) \qquad R(v) \leq r(v) \prod_{v'\in\mathcal{N}(v)} \big(1 - r(v')\big).$$

Using this, we can summarise the cluster expansion claim for an abstract polymer model in the following way:

Theorem (Cluster expansion). *There exists a function $a : \mathcal{X} \to \mathbb{R}$ that is nonvanishing only on* clusters*, so that for any sequence of diameters $\boldsymbol{R}$ satisfying the condition $(*)$ with a sequence $\{r(v)\}$, the following holds true:*

(i) *For every finite $L \subset V$, and any contour weight $w \in \mathcal{D}_{L,\boldsymbol{R}}$, one has $Z_L(w) \neq 0$ and*

$$\log Z_L(w) = \sum_{X\in\mathcal{X}(L)} a(X)w^X;$$

(ii) $\sum_{X\in\mathcal{X}:\operatorname{supp} X\ni v} |a(X)||w|^X \leq -\log\big(1 - r(v)\big)$.

[2]Observe that choosing $r(v) = 1 - \exp(-R(v)\alpha(v))$ and using $e^x - 1 \geq x$, the condition $(*)$ is implied by the assumption that for any $v \in V$ we have $R(v)e^{\alpha(v)} + \sum_{v'\in\mathcal{N}(v')} R(v)e^{\alpha(v')} \leq \alpha(v)$ (which is the condition from [KP]), making thus the claim from [KP] weaker then that from [D].

Proof. Again, by induction in $|L|$ we prove (i) and $(\mathrm{ii})_L$ obtained from (ii) by restricting the sum to $X \in \mathcal{X}(L)$:

Assuming $Z_L \neq 0$ and

$$\sum_{X\in\mathcal{X}(L):\operatorname{supp} X\cap\mathcal{N}(v)\neq\emptyset} |a(X)||w|^X \leq -\sum_{v'\in\mathcal{N}(v)} \log\bigl(1-r(v')\bigr)$$

obtained by iterating $(\mathrm{ii})_L$, we use

$$Z_{L\cup\{v\}}(w) = Z_L\biggl(1+w(v)\frac{Z_{L\setminus\mathcal{N}(v)}(w)}{Z_L(w)}\biggr)$$

and the bound

$$\biggl|1+w(v)\frac{Z_{L\setminus\mathcal{N}(v)}(w)}{Z_L(w)}\biggr| \geq 1-|w(v)|\exp\Biggl\{\sum_{X\in\mathcal{X}(L)\setminus\mathcal{X}(L\setminus\mathcal{N}(v))}|a(X)||w|^X\Biggr\} \geq$$
$$\geq 1-|w(v)|\prod_{v'\in\mathcal{N}(v)}(1-r(v'))^{-1} \geq 1-r(v) > 0$$

to conclude that $Z_{L\cup\{v\}} \neq 0$. To verify $(\mathrm{ii})_{L\cup\{v\}}$, we write

$$\sum_{X\in\mathcal{X}(L\cup\{v\}),\operatorname{supp} X\ni v}|a(X)||w|^X = -\log Z_{L\cup\{v\}}(-|w|)+\log Z_L(-|w|) =$$
$$-\log\biggl(1-|w(v)|\frac{Z_{L\setminus\mathcal{N}(v)}(-|w|)}{Z_L(-|w|)}\biggr) \leq -\log(1-r(v)).$$

□

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Density expansion of the truncated and the direct correlation function

Tobias Kuna

(joint work with Dimitrios Tsagkarogiannis)

Particle systems interacting via translation invariant pair potentials are among the most intractable point processes if one is outside the high temperature low activity regime (HTLAR), cf. the talks of Christoph Hofer-Temmel and Daniel Ueltschi for approximation theorems for recent progress. In particular, the liquid regime is of paramount interest in chemistry and engineering, but the available theory is

phenomenological. Chemists and physicists have derived a rather satisfactory description for the thermodynamics of simple liquids which is far outside the HTLAR exploiting correlation functions and postulation relations between them based on formal expansion in the density, cf. the talk of Leo Lue. A candidate for deriving such relations is the Ornstein-Zernike (OZ) equation, which, however, cannot be solved as an equation as it contains two unknown quantities, namely the second correlation function and the direct correlation function, cf. also the talk by Günter Last. Hence one has to postulate a relation between them, that is a closure scheme. A lot of effort has been made in this direction and various suggestions have appeared. In [7], G. Stell relates the most popular closure schemes (such as the Born-Green-Yvon (BGY) hierarchy, the Hyper-Netted Chain (HNC) and the Percus-Yevick (PY) equation to graphical expansions and tries to motivate them in this way. However, it is also acknowledged that *"the manipulations involved in obtaining these infinite sums ... have been carried out in a purely formal way and we have not examined the important but difficult questions of convergence and the legitimacy of the rearrangement of terms"*.

Following techniques of Elena Pulvirenti and Dimitros Tsagkarogiannis, we derived the convergence of the expansion in the density in the high temperature regime for the direct and the truncated correlation function. As the density is the natural parameter in the canonical ensemble, it is natural to start the expansion from the canonical ensemble, cf. [3]. We show that the series is absolutely convergent with respect to a norm in the argument. An indirect approach could be based on [2] but would require a careful investigation of inversion theorems in infinite dimensional convex analysis which may be more difficult than one may think at a first glance, cf. [1].

The main difficulty for making this approximation scheme rigorous and even just to establish the order of approximation in ρ is that the nth-term in the graphical expansion is the sum of e^{cn^2} $3n$-dimensional integrals, one for each graph. To show convergence, one has to bound this term by an expression of the order $e^{n \ln n + c'n}$. To achieve that, one has to show that a large group of graphs cancel exactly due to a combinatorial relation among the graphs exploiting the tree structure. The slightest violation of the cancelation may easily destroy any attempt to control the expansion. Hence, as pointed out by the previously cited comment of Stell, it is a priori far from clear, if a re-summation has any meaning even when it converges but not absolutely converge in a suitable sense. Thus even deep in the gas phase the convergence of this alternative expansion is far from clear and requires careful estimations and exact combinatorial identities. We see in our treatment, that the combinatorial structure slightly changes and in the case of the direct correlation function we have to consider an integral norm in the distance variable in order to restore the cancelation.

The convergence is essentially nothing else than a rigorous estimation of the error terms of the expansion, that is the contribution of the graphs one neglects in the expansion, either because one tries to approximate the correlation functions by a few terms or one tries to use one of the closure schemes.

A very intriguing question would be whether some expansions have a better radius of convergence than others.

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The Ornstein-Zernike equation for stationary cluster processes

Günter Last

(joint work with Sebastian Ziesche)

In a seminal paper Ornstein and Zernike proposed in [7] to split the interaction between molecules in a liquid into a direct and an indirect part. While the resulting spatial convolution equation is of great importance in physics, it seems to be hardly known among mathematicians. The aim of this talk is to bridge this gap and to lay a rigorous mathematical foundation for further studies.

We consider a stationary point process of clusters in $\mathbb{R}^d$. Let η denote the union of all clusters. The direct connectedness function $P(x)$ is the probability that the origin and the point $x \in \mathbb{R}^d$ belong to the same cluster given that both points belong to η, weighted by the pair-correlation function of η. We are interested in the solution Q of the Ornstein-Zernike convolution equation

$$P = Q + \rho Q * P, \tag{1}$$

where ρ denotes the intensity (number density) of η. Let $\mathbb{P}^0_\eta$ denote the Palm probability measures of η (describing η under the condition that the origin 0 belongs to η; see e.g. [4]) and let $C(0)$ be the cluster containing the origin. We consider a subcritical cluster process, that is we assume that

$$\mathbb{E}^0_\eta |C(0)| < \infty, \tag{2}$$

where $\mathbb{E}^0_\eta$ denotes expectation with respect to $\mathbb{P}^0_\eta$. We shall also assume that

$$\mathbb{P}^0_\eta\Big(\sum_{x\in C(0)} e^{\mathbf{i}wx} \neq 0\Big) > 0, \quad w \in \mathbb{R}^d, \tag{3}$$

where wx is the Euclidean scalar product of $x, w \in \mathbb{R}^d$ and $\mathbf{i}$ is the imaginary unit. This is a very weak regularity assumption on the cluster process.

Theorem 1. *Under the assumptions* (2) *and* (3) *there is a unique integrable solution Q of* (1).

The proof of this theorem is based on Palm calculus for stationary point processes (see e.g. [3]) and a classical theorem by Wiener on the inversion of Fourier transforms

In the second part of the talk we discuss a subcritical random connection model based on a stationary Poisson process and a symmetric connection function $\varphi\colon \mathbb{R}^d \to [0,1]$; see e.g. [6]. In this case both P and Q are analytic functions of the intensity. Moreover, for small intensities, P and Q are given by closely related diagram formulae. Such diagram formulae are quite popular in the physics literature (see e.g. [2]) and resemble formulae for the cluster expansion of statistical physics with a pair potential $-\log\varphi$. More details can be found in [5].

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Approaches to modelling classical fluids

Leo Lue

An overview on modelling classical fluids is presented, starting with a review of the grand partition function, its Legendre transform, and their relations to the pair correlation function, the direct correlation function, and the Ornstein-Zernike equation. The representation of these quantities as cluster expansions is reviewed [1]. The development of approximate integral equations based on partial resummations of the cluster expansion (e.g., hypernetted chain and Percus-Yevick equations), their accuracy, and limitations are discussed. These approaches are able to accurately represent the structure and thermodynamics of simple fluids for a broad range of systems and over a wide range of conditions, from gas to liquid densities; they can even be used to describe the vapor-liquid phase transition. However, these approximate theories do have several shortcomings, such as inconsistencies

in the correlation functions and various thermodynamic properties due to these approximations (e.g., the pressure calculated from the virial and compressibility routes). Real solutions to the integral equations may vanish without any apparent physical reason. The main difficulty with this approach, however, is that there is no clear manner to improve the accuracy of the theories without the need for computationally intensive calculations.

An alternate representation of the partition function as a functional integral is introduced, where the focus of the theory is not on the particles themselves, but rather on the interaction fields that they generate [2]. There are a broad range of approximation schemes that can be used to evaluate the functional integral, including cluster expansions and which have fairly clear physical interpretations. An example is the mean field approximation for the development of the Poisson-Boltzmann theory. Approximation schemes that start from the functional integral representation generally work well for describing large wavelength phenomena, however, when short wavelength phenomena become important, it tends to breakdown. The advantages and disadvantages of this approach, as compared to typical "particle-based" approaches are discussed.

Ongoing work on developing an approximation method where these two perspectives are combined is briefly presented [3, 4]. This is motivated by analogy to the Ewald summation method, where the convergence of a slowly converging series is accelerated by splitting it into a series in position space and a series in "Fourier" space. In this approach, the particle view is taken at short length scales and plays the role of the real space summation of the series; the field view is taken at large length scales and plays the role of the Fourier space summation. In this manner, the strengths of both perspectives are combined, leading to a significant improvement of the theory.

Finally, the practical importance of the Legendre transform in developing approximate theories for describing phase transitions (e.g., vapor-liquid or isotropic-nematic [5, 6]) is emphasized. The presentation ends with a motivation of the need to develop approximate theories for the second Legendre transform of the grand potential (from the two-body potential to the two-body correlation function) in order to describe the formation of physical clusters in isotropic systems, such as micellar aggregates in aqueous surfactant solutions. This theoretical approach offers a conceptual advantage over conventional approaches [7] in that the formation of aggregates emerge naturally from the theory, rather than needing to presume their presence.

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The Mayer series and the Penrose tree-graph identity

Aldo Procacci
(joint work with Sergio Yuhjtman)

This is an extended abstract of the paper [4].

1. Model and results

We consider a gas of classical pointwise identical particles enclosed in a box $\Lambda \subset \mathbb{R}^d$ with volume $|\Lambda|$. We denotes by $x_i \in \Lambda$ the position vector of the i^{th} particle and $|x_i|$ is its Euclidean norm. Particles interact via a pair potential $v(x_i - x_j)$ with $v(x)$ being a function from $\mathbb{R}^d$ to $\mathbb{R} \cup \{+\infty\}$, such that $v(x) = v(-x)$ and satisfying the following two assumptions.
1. *Stability.* There exists $C \geq 0$ such that, for all $n \in \mathbb{N}$ and all $(x_1, \dots, x_n) \in \mathbb{R}^{dn}$,

$$\sum_{1 \leq i < j \leq n} v(x_i - x_j) \geq -nC \tag{1}$$

2. *Temperedness.* There exists $r_0 \geq 0$ such that $\int_{|x| \geq r_0} |v(x)| dx < \infty$.
The optimal constant in (1) is called *stability constant of* v and denoted ahead by B_v.
The Grand Canonical partition function of the system is given by

$$\Xi_\Lambda(\beta, \lambda) \;=\; 1 + \sum_{n=1}^{\infty} \frac{\lambda^n}{n!} \int_\Lambda dx_1 \cdots \int_\Lambda dx_n \; e^{-\beta \sum_{1 \leq i < j \leq n} v(x_i - x_j)}$$

where $\beta > 0$ is the inverse temperature and $\lambda > 0$ is the activity of the system. Thermodynamics is recovered via the formula

$$\beta P_\Lambda(\beta, \lambda) = \frac{1}{|\Lambda|} \ln \Xi_\Lambda(\beta, \lambda)$$

with $P_\Lambda(\lambda, \beta)$ being the thermodynamical pressure.
It is long known [1] that $\frac{1}{|\Lambda|} \ln \Xi_\Lambda(\beta, \lambda)$ can be written (formally) in terms of a power series of λ, the so called *Mayer series*. Namely,

$$\frac{1}{|\Lambda|} \ln \Xi_\Lambda(\beta, \lambda) \;=\; \lambda + \sum_{n=2}^{\infty} C_n(\beta, \Lambda) \lambda^n \tag{2}$$

with

$$C_n(\beta,\Lambda) \;=\; \frac{1}{n!}\frac{1}{|\Lambda|}\int_\Lambda dx_1\cdots\int_\Lambda dx_n \sum_{g\in G_n}\prod_{\{i,j\}\in E_g}\left[e^{-\beta v(x_i-x_j)}-1\right] \tag{3}$$

where G_n is the set of the connected graphs in $[n]$ and E_g denotes the edge set of $g \in G_n$.

Penrose [2] and Ruelle [5] established in 1963 a celebrated lower bound for the convergence radius of the Mayer series of a classical gas of pointwise particles interacting via a stable and tempered pair potential. Namely, the convergence radius R_v of the Mayer series (2) admits, according to Penrose and Ruelle, the following lower bound

$$R_v \geq R_{PR} \doteq e^{-(2\beta B_v+1)}[C(\beta)]^{-1}$$

where B_v is the stability constant of the potential v and $C(\beta) = \int_{\mathbb{R}^d} dx \;\left|e^{-\beta v(x)}-1\right|$. Here we present the following result which is an improvement of Penrose and Ruelle.

Theorem 1. *Let v be a stable and tempered pair potential with stability constant B_v. Then the n-order Mayer coefficient $C_n(\beta,\Lambda)$ defined in (3) is bounded by*

$$|C_n(\Lambda,\beta)| \leq e^{\beta B_v n} n^{n-2}\frac{[\tilde{C}(\beta)]^{n-1}}{n!} \tag{4}$$

where $\tilde{C}(\beta) = \int_{\mathbb{R}^d} dx \;\left(1-e^{-\beta|v(x)|}\right)$.

Therefore the new lower bound for the convergence radius R_v of the Mayer series (2) is

$$R_v \geq R^* \doteq e^{-(\beta B_v+1)}[\tilde{C}(\beta)]^{-1}$$

Note that $R^*/R_{PR} = e^{\beta B_v}[C(\beta)/\tilde{C}(\beta)] \geq 1$ and the equality only holds for non-negative potentials.

2. Sketch of the proof of Theorem 1

The proof of Theorem 1 starts from the so-called Penrose tree-graph identity [3].

Penrose identity. *Let $\boldsymbol{M} : T_n \to G_n$ be a map (partition scheme) such that $G_n = \biguplus_{\tau\in T_n}[\tau,\boldsymbol{M}(\tau)]$ where $\biguplus$ means disjoint union and $[\tau,\boldsymbol{M}(\tau)] = \{g \in G_n : \tau \subseteq g \subseteq \boldsymbol{M}(\tau)\}$, then, given v pair potential and $(x_1,...,x_n) \in \mathbb{R}^{dn}$, the following identity holds.*

$$\sum_{g\in G_n}\prod_{\{i,j\}\in E_g}\left[e^{-\beta v(x_i-x_j)}-1\right] =$$

$$\sum_{\tau\in T_n} e^{-\beta\sum_{\{i,j\}\in E_{\boldsymbol{M}(\tau)}\setminus E_\tau} v(x_i-x_j)}\prod_{\{i,j\}\in E_\tau}\left(e^{-\beta v(x_i-x_j)}-1\right) \tag{5}$$

where T_n denotes the set of all trees with vertex set $[n]$.

Set now $E_\tau^+ = \{\{i,j\} \in E_\tau : v(x_i - x_j) \geq 0\}$, then from (5) one immediately gets

$$\left| \sum_{g \in G_n} \prod_{\{i,j\} \in E_g} \left[e^{-\beta v(x_i - x_j)} - 1 \right] \right| \leq$$

(6)

$$\sum_{\tau \in T_n} e^{-\beta \sum_{\{i,j\} \in E_{\boldsymbol{M}(\tau)} \setminus E_\tau^+} v(x_i - x_j)} \prod_{\{i,j\} \in E_\tau} \left(1 - e^{-\beta |v(x_i - x_j)|} \right)$$

To get this inequality from (5) just observe that, for any $\tau \in T_n$, it holds the identity:
$\prod_{\{i,j\} \in E_\tau} |e^{-v(x_i - x_j)} - 1| = e^{-\sum_{\{i,j\} \in E_\tau \setminus E_\tau^+} v(x_i - x_j)} \prod_{\{i,j\} \in E_\tau} (1 - e^{-|v(x_i - x_j)|})$.

Definition of the partition scheme $\boldsymbol{M}$. For fixed v and $(x_1, \ldots, x_n) \in \mathbb{R}^{dn}$, choose a total order $\succ$ in the set of edges E_n of the complete graph K_n such that $\{i,j\} \succ \{k,l\} \Longrightarrow v(x_i - x_j) \geq v(x_k - x_l)$. Consider the map $\boldsymbol{T} : G_n \to T_n$ that associates to g its unique *minimum spanning tree* $\boldsymbol{T}(g)$, constructed by starting from $\emptyset$ and keeping adding the lowest edge in g that does not create a cycle (this procedure is known as Kruskal algorithm). Then the following lemma holds.

Lemma 2. *Let $\boldsymbol{M} : T_n \to G_n$ be the map that associates to $\tau \in T_n$ the graph $\boldsymbol{M}(\tau) \in G_n$ whose edges are the $\{i,j\} \in E_n$ such that $\{i,j\} \succeq \{k,l\}$ for every edge $\{k,l\} \in E_\tau$ belonging to the path from i to j through τ. Then $\boldsymbol{T}^{-1}(\tau) = \{g \in \mathcal{G}_n : \tau \subset g \subset \boldsymbol{M}(\tau)\}$ and therefore $\boldsymbol{M}$ is a partition scheme in G_n.*

Proof. Let $g \in \boldsymbol{T}^{-1}(\tau)$. We have $\tau = \boldsymbol{T}(g) \subset g$. Now take $\{i,j\} \in E_g$, and let $e \in E_\tau$ be any edge belonging to the path from i to j in τ. Consider the tree τ' obtained from τ after replacing the edge e by $\{i,j\}$. By minimality of τ we must have $\{i,j\} \succ e$, i.e. $\{i,j\} \in E_{\boldsymbol{M}(\tau)}$, whence $g \subset \boldsymbol{M}(\tau)$. Conversely, let $\tau \subset g \subset \boldsymbol{M}(\tau)$. We must show $\boldsymbol{T}(g) = \tau$. By contradiction, take $\{i,j\} \in E_{\boldsymbol{T}(g)} \setminus E_\tau$. Consider the path $p^\tau(\{i,j\})$ in τ joining i with j. Since $\boldsymbol{T}(g) \subset \boldsymbol{M}(\tau)$, $\{i,j\}$ is greater (w.r.t. $\succ$) than any edge in the path $p^\tau(\{i,j\})$. If we remove $\{i,j\}$ from $\boldsymbol{T}(g)$, the tree $\boldsymbol{T}(g)$ splits into two trees. Necessarily, one of the edges in the path $p^\tau(\{i,j\})$ joins a vertex of one tree with a vertex of the other. Thus, by adding this edge we get a new tree which contradicts the minimality of $\boldsymbol{T}(g)$. □

The advantage of this new partition scheme is manifestly clear in the following key lemma.

Lemma 3. *Let v be stable with stability constant B_v, and let $\tau \in T_n$. Let $(x_1, ..., x_n) \in \mathbb{R}^{dn}$ and let $\boldsymbol{M}$ be the partition scheme given in Lemma 2, then*

$$\sum_{\{i,j\} \in \boldsymbol{E}_{M(\tau)} \setminus E_\tau^+} v(x_i - x_j) \geq -Bn \tag{7}$$

Proof. The set of edges $E_\tau \setminus E_\tau^+$ forms the forest $\{\tau_1, ..., \tau_k\}$. Let us denote V_{τ_s} the vertex set of the tree τ_s of the forest. Assume $i \in V_{\tau_a}$, $j \in V_{\tau_b}$. If $a \neq b$, the path from i to j through τ involves an edge $\{k,l\}$ in E_τ^+. Thus, if in addition

$\{i.j\} \in E_{\boldsymbol{M}(\tau)}$, we have $\{i,j\} \succeq \{k,l\}$ and therefore $v(x_i - x_j) \geq v(x_k - x_l) \geq 0$. If $a = b$, the path from i to j through τ is contained in τ_a. Thus, if in addition $\{i,j\} \notin E_{\boldsymbol{M}(\tau)}$, there must be at least one edge $\{r,s\}$ in that path such that $\{i,j\} \prec \{r,s\}$ and therefore $v(x_i - x_j) \leq v(x_r - x_s) < 0$. This allows to bound:

$$\sum_{\{i,j\} \in E_{\boldsymbol{M}(\tau)} \setminus E_\tau^+} v(x_i - x_j) \geq \sum_{s=1}^{k} \sum_{\{i,j\} \subset V_{\tau_s}} v(x_i - x_j) \geq \sum_{s=1}^{k} -|V_{\tau_s}| B_v \geq -nB_v \ \square$$

From Lemma 3, inserting (7) into (6), one gets the following decisive Lemma.

Lemma 4. *Let v be a stable pair potential with stability constant B_v. Then, for any $n \geq 2$ and any $(x_1, \ldots, x_n) \in \mathbb{R}^{dn}$, the following inequality holds*

$$(8) \quad \Big| \sum_{g \in G_n} \prod_{\{i,j\} \in E_g} (e^{-\beta v(x_i - x_j)} - 1) \Big| \ \leq \ e^{\beta B_v n} \sum_{\tau \in T_n} \prod_{\{i,j\} \in E_\tau} (1 - e^{-\beta |v(x_i - x_j)|})$$

Now Theorem 1 follows easily from Lemma 4 and the observation that, for any $\tau \in T_n$, it holds

$$(9) \qquad \int_\Lambda dx_1 \cdots \int_\Lambda dx_n \prod_{\{i,j\} \in E_\tau} \Big(1 - e^{-\beta |v(x_i - x_j)|}\Big) \leq |\Lambda| \left[\tilde{C}(\beta)\right]^{n-1}$$

Indeed, using first (8) and subsequently (9) we get

$$|C_n(\Lambda, \beta)| \ \leq \ \frac{1}{n!} \frac{1}{|\Lambda|} \int_\Lambda dx_1 \cdots \int_\Lambda dx_n \Big| \sum_{g \in G_n} \prod_{\{i,j\} \in E_g} \Big[e^{-\beta v(x_i - x_j)} - 1\Big] \Big| \ \leq$$

$$\leq \ \frac{e^{\beta B_v n}}{n!} \frac{1}{|\Lambda|} \sum_{\tau \in T_n} \int_\Lambda dx_1 \cdots \int_\Lambda dx_n \prod_{\{i,j\} \in E_\tau} \Big(1 - e^{-\beta |v(x_i - x_j)|}\Big) \ \leq$$

$$\leq \ \frac{e^{\beta B_v n}}{n!} \left[\tilde{C}(\beta)\right]^{n-1} \sum_{\tau \in T_n} 1 \ = \frac{e^{\beta B_v n}}{n!} \left[\tilde{C}(\beta)\right]^{n-1} n^{n-2} \ \square$$

which is the bound (4).

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Cluster expansion for the LMP - hard spheres model

Elena Pulvirenti
(joint work with Dimitrios Tsagkarogiannis)

In a paper by Lebowitz, Mazel and Presutti [1], the existence of a phase transition in $d \geq 2$ has been proven for a continuum model with long range Kac interaction. In this talk a generalization of the LMP model is considered, where a small short range repulsive interaction (for instance hard-core) is added to the already existing Kac potential. We show that, choosing the radius of the hard-core small enough, the behaviour of the LMP model persists in the region where the liquid-vapor transition is present. In particular, using a perturbative argument, we show that for β larger than some β_c we still get two equilibrium measures with two different values of the density, which are close to those for the LMP model. This is the content of a paper in preparation [2].

Our proof will follow Pirogov-Sinai theory in the version proposed by Zahradník, [5]. The analysis requires first of all the notions of *coarse-graining* and *contour model* in the continuum and subsequently, with an argument á la Peierls, one has to prove that contours are improbable. In this scenario we are able to compute the effective Hamiltonian for the coarse-grained system with a multi-canonical constraint (given by the fixed density in each cell). This computation involves an integration over the positions of the particles in each cell leading to a new measure on the density at the cells. The computations which lead to the effective Hamiltonian are in general very complicated, nevertheless due to the choice of the interaction they can be carried out. The crucial point here is to show convergence of a cluster expansion in the canonical ensemble with hard-core, Kac 2 and 4 body interaction and contour weights.

In the first step we show the convergence of the cluster expansion for the hard spheres gas in the canonical ensemble when the density is small. This is the content of a paper written in collaboration with D. Tsagkarogiannis [3], in which we prove the cluster expansion in the canonical ensemble in the more general case of stable and tempered potentials. Another crucial step relies on the possibility to control the difference between the finite-volume and infinite-volume free energy. This is addressed in another paper written in collaboration with D. Tsagkarogiannis [4].

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An improved tree-graph bound

Daniel Ueltschi

The day before my talk, Aldo Procacci told us about the beautiful new bound for the convergence of the cluster expansion, which he obtained recently with S. Yuhjtman [5]. This suggested a way to improve the tree-graph bounds stated in [3]. Additional comments by David Brydges and Tyler Helmuth during Procacci's talk were illuminating; they noticed in particular the relevance of Kruskal's algorithm.

The goals of my talk were to turn the result of [5] as an explicit tree-graph bound, and to provide a simplified, streamlined proof. It turns out that the result is immediately useful for the work of another participant, Martin Hanke [2] (who suggested the extension to complex numbers).

The difficulty with the convergence of cluster expansions is to estimate a sum over connected graphs of arbitrary sizes. One needs to use cancellations in order to make it convergent. It turns out that the sum over connected graphs can be reduced to a sum over spanning trees; this sum is considerably smaller.

Here, we state the result with minimal setting. $\mathcal{C}_n$ and $\mathcal{T}_n$ denote the sets of connected graphs and of trees with n vertices.

Theorem 1. *Let $u_{i,j} \in \mathbb{R}$ and $b_i \in [0,\infty)$, $1 \le i,j \le n$, be numbers such that for all subsets $I \subset \{1,\dots,n\}$, we have the "stability condition"*

$$\sum_{i,j\in I, i<j} u_{i,j} \ge -\sum_{i\in I} b_i. \tag{1}$$

Then

$$\Big|\sum_{g\in\mathcal{C}_n}\prod_{ij\in g}\big(\mathrm{e}^{-u_{i,j}}-1\big)\Big| \le \mathrm{e}^{\sum_{i=1}^n b_i}\sum_{t\in\mathcal{T}_n}\prod_{ij\in t}\big(1-\mathrm{e}^{-|u_{i,j}|}\big). \tag{2}$$

A similar theorem can be found in [3] with two different upper bounds. The first one follows Ruelle's algebraic method. The second one is motivated by the tree-graph identity of Brydges and Federbush [1], combined with an extension of Procacci [4]. The two bounds in [3] are strictly larger than the one above, so this constitutes an improvement indeed.

In the case of complex numbers, $u_{i,j} \in \mathbb{C}$, the stability assumption (1) is replaced by $\sum \mathrm{Re}\, u_{i,j} \ge -\sum_{i\in I} b_i$. One can generalise the tree-graph bound as

$$\Big|\sum_{g\in\mathcal{C}_n}\prod_{ij\in g}\big(\mathrm{e}^{-u_{i,j}}-1\big)\Big| \le \mathrm{e}^{\sum_{i=1}^n b_i}\sum_{t\in\mathcal{T}_n}\prod_{ij\in t}\big|1-\mathrm{e}^{-|\mathrm{Re}\, u_{i,j}|+\mathrm{i}\,\mathrm{Im}\, u_{i,j}}\big|. \tag{3}$$

Notice that the last term is smaller than $|1-\mathrm{e}^{-u_{i,j}}|$. We now give a proof of Theorem 1.

Recall that a *partition scheme* is given by a map $T : \mathcal{C}_n \to \mathcal{T}_n$ with the property that, for each $t \in \mathcal{T}_n$, there corresponds a set of edges $E(t)$ such that

$$T^{-1}(t) = \big\{g \in \mathcal{C}_n : t \subset g \subset t \cup E(t)\big\}. \tag{4}$$

(We suppose that $E(t) \cap t = \emptyset$.)

Kruskal's algorithm provides just such a partition scheme. One is given an arbitrary order on all edges of the complete graph of n vertices. Given $g \in \mathcal{C}_n$, we define a spanning tree by adding edges in increasing order, provided the new edge does not form a loop (if it does, we ignore the new edge). For $t \in \mathcal{T}_n$, the set $E(t)$ contains exactly all edges $ij \notin t$ such that ij is bigger than all the edges in the path from i to j in t. This characterisation of the set $E(t)$ is important.

Given $(u_{i,j})$, we choose an order on edges such that $u_{i,j}$ is nondecreasing. Using Hamlet's lemma (*to be or not to be, this is the expansion*), we have

$$\begin{aligned} \sum_{g\in\mathcal{C}_n}\prod_{ij\in g}\bigl(\mathrm{e}^{-u_{i,j}}-1\bigr) &= \sum_{t\in\mathcal{T}_n}\prod_{ij\in t}\bigl(\mathrm{e}^{-u_{i,j}}-1\bigr)\prod_{ij\in E(t)}\mathrm{e}^{-u_{i,j}}, \\ \Bigl|\qquad\qquad\qquad\Bigr| &\le \sum_{t\in\mathcal{T}_n}\prod_{ij\in t}\bigl|\mathrm{e}^{-u_{i,j}}-1\bigr|\prod_{ij\in E(t)}\mathrm{e}^{-u_{i,j}}. \end{aligned} \tag{5}$$

A key trick in [5] is to use the identity

$$\bigl|\mathrm{e}^{-u_{i,j}}-1\bigr| = \mathrm{e}^{(u_{i,j})_-}\bigl(1-\mathrm{e}^{-|u_{i,j}|}\bigr). \tag{6}$$

The upper bound in Eq. (5) becomes

$$\prod_{ij\in t}\bigl|\mathrm{e}^{-u_{i,j}}-1\bigr|\prod_{ij\in E(t)}\mathrm{e}^{-u_{i,j}} = \prod_{ij\in t}\bigl(1-\mathrm{e}^{-|u_{i,j}|}\bigr)\exp\Bigl\{-\sum_{ij\in t_-}u_{i,j}-\sum_{ij\in E(t)}u_{i,j}\Bigr\}. \tag{7}$$

Here, t_- denotes the set of edges of t where $u_{i,j}<0$. This subgraph is a forest and is illustrated in Fig. 1. Let us denote the forest $\{t_1,\dots,t_k\}$, with t_m, $m=1,\dots,k$,

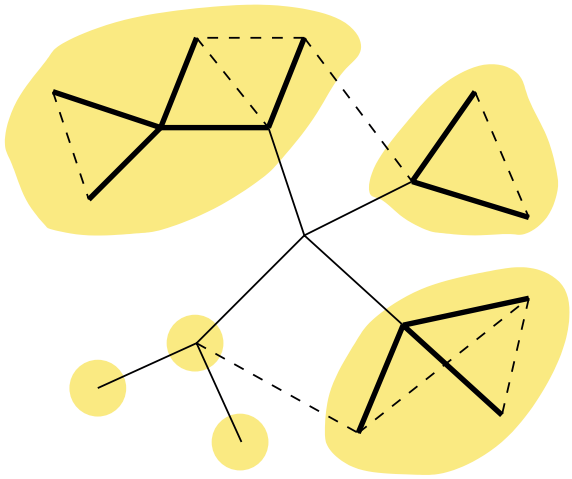

FIGURE 1. The tree t with bold edges when $u_{i,j}<0$ and light edges when $u_{i,j}\ge 0$. Edges of $E(t)$ are shown with dashed lines.

being the subtrees. With $K(t_m)$ the complete graph on the vertices of t_m, we have the lower bound (which we justify below)

$$\sum_{ij\in t_-}u_{i,j}+\sum_{ij\in E(t)}u_{i,j} \ge \sum_{m=1}^{k}\sum_{ij\in K(t_m)}u_{i,j}; \tag{8}$$

this is larger than $-\sum_{i=1}^{n} b_i$ by the stability condition. The claim of the theorem follows immediately.

The lower bound (8) is the clever observation of [5]. It follows quite easily from the partition scheme of Kruskal's algorithm, because

- If ij is an edge between distinct subtrees, we necessarily have $u_{i,j} \geq 0$, since it is bigger than at least one nonnegative edge; we neglect them in the lower bound.
- All positive edges within $K(t_m)$ belong to $E(t)$; indeed, they are bigger than all edges in the path between i and j, which are all negative. Thus no extra positive $u_{i,j}$ have been added in the right side.
- We have perhaps added a few negative $u_{i,j}$ in the right side, which can only make it smaller.

This is illustrated in Fig. 1; this completes the proof of Theorem 1.

In the case of complex numbers, we can order the edges according to Re $u_{i,j}$; we use $|\,\mathrm{e}^{-u_{i,j}} - 1| = \mathrm{e}^{-\mathrm{Re}\, u_{i,j}}\, |1 - \mathrm{e}^{\mathrm{Re}\, u_{i,j} + \mathrm{i}\,\mathrm{Im}\, u_{i,j}}\,|$ for $ij \in t_-$; then we prove the inequality (8) with Re $u_{i,j}$ instead of $u_{i,j}$, and we get (3).

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Toward Onsager density functional via Penrose's tree identity

Epifanio G. Virga

(joint work with P. Palffy-Muhoray, X. Zheng)

Onsager's celebrated theory for liquid crystals, put forward between the years 1942 and 1949 [8, 9], showed that purely steric, repulsive interactions between molecules can explain the ordering transition that underpins the formation of the nematic phase. Often Onsager's theory is considered as the first successful instance of modern density functional theory. It was however a theory rooted in its time, in the theory that Mayer had proposed in the late 1930's with the aim of explaining condensation of real gases [3, 5, 6, 2, 4, 12].

Despite its undeniable success, Onsager's theory lacks rigour at its onset, as no convincing justification is given for the truncation at the first order in the number density ρ_0 of the Helmholtz free energy of a system of slender cylindrical rods in solution [15]. Not much justice is done either to it by the cursory accounts that

most statistical mechanics textbooks give of the same approximation for Mayer's expansion (see, for example, pp. 224–225 of [7][1]).

Onsager's theory of lyotropic liquid crystals is based on the following form of the Helmholtz free energy:

$$\mathscr{F}_{\mathrm{O}}[\varrho] := \int_{\mathbb{S}^2} \varrho(\omega) \ln \varrho(\omega) \mathrm{d}\omega + \frac{1}{2}\rho_0 \int_{\mathbb{S}^2 \times \mathbb{S}^2} \beta_1(\omega, \omega') \varrho(\omega) \varrho(\omega') \mathrm{d}\omega \mathrm{d}\omega', \tag{1}$$

where $\varrho : \mathbb{S}^2 \to \mathbb{R}^+$, which is subject to the constraint

$$\int_{\mathbb{S}^2} \varrho(\omega) \mathrm{d}\omega = 1, \tag{2}$$

represents the probability distribution of rods with orientation $\omega \in \mathbb{S}^2$, and $\beta_1(\omega, \omega')$ is the excluded volume of two rods with orientations ω and ω'.

The offered justification of (1) requires embracing the ingenious *multi-spiecies* argument put forward by Onsager [9], an argument that regards particles distributed in their orientation as if they were belonging to different species [14]. As questionable as this argument may be, the first-principle foundation of(1) relies on proving under what assumptions the free energy F_N of a system of N particles in the *canonical ensemble* can be given the following form,

$$\lim_{N\to\infty} \frac{F_N}{N} = kT \left(\ln \rho_0 - 1 + \frac{1}{2}\rho_0 \beta_1 \right), \tag{3}$$

in the thermodynamic limit where the *number density* $\rho_0 = \frac{N}{V}$ is kept fixed.

It is proved in [10] that, under certain circumstances, (3) follows from the general expression for F_N,

$$F_N = -kT \ln \left(\frac{1}{N!} G_N \right), \tag{4}$$

where the total number of states G_N is given by the intergral

$$G_N = \int_{\mathscr{B}^N} \sum_{\mathsf{G} \in \mathscr{G}_N} \prod_{(i,j)\in \mathsf{G}} \Phi_{ij} \mathrm{d}q_1 \ldots \mathrm{d}q_N, \tag{5}$$

$\mathscr{B}$ is the region in space (of volume V) occupied by the particles, Φ_{ij} is the Mayer function associated with the hard-core repulsion potential between particles with coordinates q_i and q_j, $\mathscr{G}_N$ is the collection of all graphs on N vertices, of which (i, j) denotes an edge [14]. If in (5) only the forests of trees obtained through Penroses's partition scheme [11] are retained, which amounts to disregard all more highly connected cyclic graphs, a result of Britikov [1] and an estimate of Temme

[1]There it is suggested to expand the exponential in the grand canonical partition function $\Xi = \mathrm{e}^{pV/kT}$ (where p is the pressure, V is the volume, T is the temperature, and k is Boltzmann constant), failing to realise that the exponent is expected to be proportional to the number of particles N, which is very large.

[13] lead us to (3). However, the function that expresses G_N under this assumption of limited connectivity is positive only if ρ_0 satisfies the inequality

$$\rho_0 \beta_1 < W\left(\frac{1}{\mathrm{e}}\right) \doteq 0.2785, \tag{6}$$

where W is the Lambert function. This inequality makes quantitative the claim often made in the literature on density functional theory [15] that Onsager's theory is only suitable in the *dilute* limit.

When (6) is violated, more highly connected graphs (all of which including cycles) must be accounted for in (5) to compute correctly G_N. How to achieve this is at the moment unclear. However, there is no reason why adding more connected graphs in (5) should lead to higher power corrections in ρ_0 to (3), as nowhere was in our development the assumption that the free energy per particle should be a *power series* in ρ_0. Devising an estimate of (5) based on cycles might deliver a form of $\mathscr{F}_{\mathrm{O}}$ better suited than (1) to tackle denser systems.

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Statistical physics of exponential random graphs

Mei Yin
(joint work with Charles Radin)

Exponential random graphs form one of the most prominent class of probability models for networks, but also one for which the issue of lack of insight into their fundamental characteristics is particularly pressing. Their popularity lies in the fact that they capture a wide variety of common network tendencies by representing a complex global structure through a set of tractable local features. We aim at establishing a quantitative theory of "phase transitions" in large exponential random graphs. The main techniques that we use are variants of statistical physics, such as cluster expansion methods and large deviation techniques, but the exciting new theory of graph limits [6], which has rich ties to many parts of mathematics and beyond, also plays an important role in the interdisciplinary inquiry.

In the statistical physics literature, phase transition is often associated with loss of analyticity in the limiting normalization constant (free energy), which gives rise to discontinuities in the observed statistics [9, 10]. In the vicinity of a phase transition, even a tiny change in some local characteristic can result in a dramatic change of the entire system. An explicit criterion for such an asymptotic phase transition was given in Chatterjee and Diaconis [3], and has since then led to exponentially growing interest in exponential models and their variations [1, 2, 4, 7, 8]. In "A cluster expansion approach to exponential random graph models" (2012) [14], we viewed exponential random graphs from an Ising perspective, making the model treatable by cluster expansion techniques from statistical physics. We showed that any k-parameter exponential random graph may alternatively be viewed as a lattice gas system with a finite Banach space norm and derived a convergent power series expansion for the limiting normalization constant in the case of small parameters. In "Critical phenomena in exponential random graphs" (2013) [15], we derived the full phase diagram for a large family of 3-parameter exponential random graph models with attraction through a detailed analysis of a maximization problem for the normalization constant. This extends an earlier work "Phase transitions in exponential random graphs" (with Charles Radin, 2013) [11] which dealt with the 2-parameter framework and may be further extended to a general k-parameter setting. The parameter space comprises a single phase with first order phase transitions across one or more hypersurfaces and second order phase

transitions along their boundaries. The transition lies within the replica symmetric phase and is between graphs of similar characters but different densities and corresponds to the gas/liquid transition in equilibrium materials.

Despite their flexibility, conventionally used exponential random graphs admittedly have one shortcoming. They cannot directly model weighted networks as the underlying probability space consists of simple graphs only, i.e., edges are either present or absent. Since many substantively important networks are weighted, this limitation is especially problematic. The need to enrich the existing exponential framework is thus justified, and several generalizations have been proposed [5, 12, 13]. An alternative interpretation for simple graphs is such that the edge weights are iid and satisfy a Bernoulli distribution. In "Phase transitions in edge-weighted exponential random graphs" (2016) [16], we extended the existing exponential framework for simple graphs by proposing a generic common distribution for the edge weights. The general results regarding the associated phase transitions and critical phenomena were employed to get concrete answers in exponential random graph models where the edge weights are uniformly distributed. Currently, my students (Danielle Larcomb and Ryan DeMuse) and I are making progress towards recognizing the essential properties related to universality in generic edge-weighted exponential random graphs. Though the near degenerate graph structures depend on the specific form of the edge-weights distribution, surprisingly (or not), we found that the asymptotics in the dual space constructed via Legendre duality remain the same.

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