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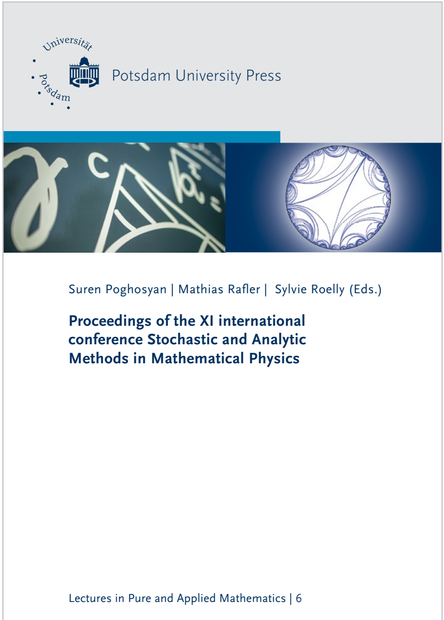

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Activity expansions for Gibbs correlation functions

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Abstract. *We consider Gibbs point processes with non-negative pair potentials. For small activities, a cluster expansion allows us to express the corresponding correlation functions by (multivariate) power series in the activity around zero. We characterise the domain of absolute convergence of those series and derive from this characterisation a new sufficient condition in the setting of abstract polymers improving the known bounds for the convergence radii.*

1 Introduction

Proving convergence conditions for cluster expansions is a classical problem with a long history – see [1, 6] and the references therein. Recent developments include a novel convergence condition by Fernández-Procacci [3] that improves the classical Kotecký-Preiss criterion [5] as well as Dobrushin's criterion [2]. We present a new necessary and sufficient convergence condition that improves on the above-mentioned criteria. The criterion applies to non-negative pair potentials for systems both continuous and discrete.

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After describing the general setting in Section 2, we proceed to introduce a system of integral equations satisfied by the activity expansions ρ, the so-called Kirkwood-Salsburg equations, in Section 3. In Section 4, we consider a sign-flipped version of those equations to prove our main result – Theorem 14.7 – characterising the domain of absolute convergence of ρ; moreover, we are able to use Theorem 14.7 to prove a new sufficient condition for systems of abstract polymers (Proposition 14.8).

2 The setting: Definitions and notations

Let $(\mathbb{X}, \mathscr{X})$ be a measurable space, λ a σ-finite reference measure, and v a non-negative pair potential, i. e., $v : \mathbb{X} \times \mathbb{X} \to \mathbb{R}_+ \cup \{\infty\}$ is measurable and symmetric (in the sense that $v(x,y) = v(y,x)$ for all $x,y \in \mathbb{X}$). Mayer's f function associated with the potential v is given by

$$f(x,y) := \mathrm{e}^{-v(x,y)} - 1.$$

An activity function is a measurable map $z : \mathbb{X} \to \mathbb{R}$. We define the measure λ_z on $\mathscr{X}$ by

$$\lambda_z(B) := \int_B z(x)\lambda(\mathrm{d}x), \qquad B \in \mathscr{X}.$$

The weight of a graph G with vertex set $[n] = \{1,\dots,n\}$ and edge set $E(G)$ is

$$w(G;x_1,\dots,x_n) := \prod_{\{i,j\}\in E(G)} f(x_i,x_j), \qquad x_1,\dots,x_n \in \mathbb{X}.$$

Let $\mathscr{G}_n$ be the set of all graphs with vertex set $[n]$, $\mathscr{C}_n \subset \mathscr{G}_n$ the set of connected graphs and

$$\varphi_n^{\mathsf{T}}(x_1,\dots x_n) := \sum_{G\in\mathscr{C}_n} w(G;x_1,\dots,x_n)$$

the n-th Ursell function. For $k \in \mathbb{N}$ and $1 \leq k \leq n$, let $\mathscr{D}_{k,n} \subset \mathscr{G}_n$ the collection of all graphs G such that every vertex $j \in \{k+1,\dots,n\}$ connects to at least one of the vertices $i \in \{1,\dots,k\}$. We call such graphs multi-rooted graphs on $[n]$ with k roots. Consider the functions

$$\psi_{k,n}(x_1,\dots,x_n) := \sum_{G\in\mathscr{D}_{k,n}} w(G;x_1,\dots,x_n).$$

For $k = 1$, the functions coincide with the standard Ursell functions, i. e., $\psi_{1,n} = \varphi_n^{\mathsf{T}}$. We are interested in the associated series

$$\rho_k(x_1,\dots,x_k;z) := z(x_1)\cdots z(x_k)\Bigg(\psi_{k,k}(x_1,\dots,x_k) + \sum_{n=1}^{\infty}\frac{1}{n!}\int_{\mathbb{X}^n}\psi_{k,k+n}(x_1,\dots,x_k,y_1,\dots,y_n)\lambda_z^{\otimes n}(\mathrm{d}\mathbf{y})\Bigg).$$

The series ρ_k corresponds to the k-point correlation function of a grand-canonical Gibbs measure [8, Eq. (4-7)], see also [4] – it is precisely the expansion of the correlation function in the activity z around zero. Proposition 14.1 provides some intuition for why $\rho = (\rho_k)_{k\in\mathbb{N}}$ is the right candidate for those activity expansions.

We say that the series $\rho_k(x_1,\dots,x_k;z)$ is absolutely convergent if

$$\sum_{n=1}^{\infty}\frac{1}{n!}\int_{\mathbb{X}^n}\Big|\psi_{k,k+n}(x_1,\dots,x_k,y_1,\dots,y_n)z(x_1)\cdots z(x_k)z(y_1)\cdots z(y_n)\Big|\lambda^{\otimes n}(\mathrm{d}\mathbf{y}) < \infty.$$

Our main goal is to provide necessary and sufficient conditions on z ensuring that ρ converges absolutely, i. e., that the series ρ_k converge absolutely on $\mathbb{X}^k$ for all $k \in \mathbb{N}$.

3 Preparations

Some preparations are required before we can state our main results. The following representation of the activity expansions ρ – in the spirit of Equation (2.11) in [1] – turns out to be quite useful for deriving properties of interest (e. g., the signs of the series ρ_k alternating in $k \in \mathbb{N}$ (see Proposition 14.3) or their connection to the k-correlation functions of the corresponding Gibbs point process mentioned in the introduction).

Proposition 14.1 (Exponential representation of ρ) Suppose that all series $\rho_k(z)$ are absolutely convergent on $\mathbb{X}^k$ for some activity function z. Then

$$\rho_k(x_1,\dots,x_k;z) = z(x_1)\cdots z(x_k)\prod_{1\le i<j\le k}\big(1+f(x_i,x_j)\big) \times \exp\Bigg(\sum_{n=1}^{\infty}\frac{1}{n!}\int_{\mathbb{X}^n}\Bigg(\prod_{\substack{1\le i\le k\\ 1\le j\le n}}\big(1+f(x_i,y_j)\big)-1\Bigg)\varphi_n^{\mathsf{T}}(y_1,\dots,y_n)\lambda_z^{\otimes n}(\mathrm{d}\mathbf{y})\Bigg),$$

for all $k \in \mathbb{N}$ and $(x_1,\dots,x_k) \in \mathbb{X}^k$.

Sketch of proof. Under the assumption of the proposition this identity on the level of generating functions can be reduced to the following identity on the level of coefficients given by sums over weighted graphs:

$$\psi_{k,n}(x_1,\dots,x_n) = \prod_{1\le i<j\le k} \big(1+f(x_i,x_j)\big) \times \sum_{\{V_1,\dots,V_r\}} \prod_{\ell=1}^{r} \Bigg(\prod_{\substack{1\le i\le k,\\ j\in V_\ell}} \big(1+f(x_i,x_j)\big) - 1 \Bigg) \varphi^{\mathsf{T}}_{|V_\ell|}\big((x_j)_{j\in V_\ell}\big) \tag{14.1}$$

where the sum runs over all set partitions $\{V_1,\dots,V_r\}$ of non-root vertices $\{k+1,\dots,n\}$.

The latter identity (on the combinatorial level) can be shown simply by exploiting the structure of multi-rooted graphs and their relation to connected graphs. □

Corollary 14.2 (Alternating sign property) We have

$$\psi_{k,n}(x_1,\dots,x_n) = (-1)^{n-k}\big|\psi_{k,n}(x_1,\dots,x_n)\big|$$

for all $n\in\mathbb{N}$, all $k\in\{1,\dots,n\}$, and all $(x_1,\dots,x_n)\in\mathbb{X}^n$.

Sketch of proof. The statement follows directly from the identity (14.1) and the well-known alternating sign property of the Ursell functions φ_n, which holds by a tree-graph equation à la Penrose (e. g., see [3]). □

We use the observation captured by Corollary 14.2 to introduce the sign-flipped version of the activity expansions ρ.

Corollary 14.3 (Introducing $\tilde\rho$) Let z be a non-negative activity function. Then, the series $\rho_k(-z)$ converge for all $k\in\mathbb{N}$ if and only if the series $\rho_k(z)$ converge absolutely for all $k\in\mathbb{N}$. Moreover, define $\tilde\rho(z)$ by setting

$$\tilde\rho_k(x_1,\dots,x_k;z) := (-1)^k\rho_k(x_1,\dots,x_k;-z)$$

for all $k\in\mathbb{N}$ and $(x_1,\dots,x_k)\in\mathbb{N}$. Then

$$\tilde\rho_k(x_1,\dots,x_k;z) = \prod_{i=1}^{k} z(x_i)\sum_{n\ge 0}\frac{1}{n!}\int_{\mathbb{X}^n}\big|\psi_{k,k+n}(x_1,\dots,x_k,y_1,\dots,y_n)\big|\,\lambda_z^{\otimes n}(\mathrm{d}\mathbf{y})$$

holds for all $k \in \mathbb{N}$ and $(x_1,\dots,x_k) \in \mathbb{N}$.

Sketch of proof. The statement follows directly from the alternating sign property given by Corollary 14.2. □

Now we are ready to introduce systems of integral equations satisfied by the activity expansions – the so-called Kirkwood-Salsburg equations. Notice the close relation between those and the GNZ equations (named after Georgii, Nguyen and Zessin; e. g., see [4]), which can serve to define grand-canonical Gibbs measures. In general, the Kirkwood-Salsburg relations for the correlation functions follow from the GNZ equations and even the equivalence holds under additional assumtions (e. g., see [4, Lemma 3.1] and the discussion thereafter.)

Definition 14.4 (Kirkwood-Salsburg operators) Given a fix activity function z, define K_z by the following formal expressions: For $a = (a_p)_{p\in\mathbb{N}}$ such that $a_p : \mathbb{X}^p \to \mathbb{R}$ is measurable for all $p \in \mathbb{N}$, set

$$\begin{aligned}\big(K_z a\big)_{p+1}(x_0,x_1,\dots,x_p) &:= z(x_0)\prod_{i=1}^{p}\big(1+f(x_0,x_i)\big)\\ &\times\left(a_p(x_1,\dots,x_p)+\sum_{k=1}^{\infty}\frac{1}{k!}\int\limits_{\mathbb{X}^k}\prod_{j=1}^{k}f(x_0,y_j)a_{p+k}(x_1,\dots,x_p,y_1,\dots,y_k)\lambda^{\otimes k}(\mathrm{d}\mathbf{y})\right),\end{aligned}$$

where we use the natural convention $a_0 := 0$ for the case $p = 0$.

Similarly, define $\tilde{K}_z$ by

$$\begin{aligned}\big(\tilde{K}_z a\big)_{p+1}(x_0,x_1,\dots,x_p) &:= z(x_0)\prod_{i=1}^{p}\big(1+f(x_0,x_i)\big)\\ &\times\left(a_p(x_1,\dots,x_p)+\sum_{k=1}^{\infty}\frac{1}{k!}\int\limits_{\mathbb{X}^k}\prod_{j=1}^{k}\big|f(x_0,y_j)\big|\,a_{p+k}(x_1,\dots,x_p,y_1,\dots,y_k)\lambda^{\otimes k}(\mathrm{d}\mathbf{y})\right).\end{aligned}$$

Furthermore, for all $(x_1,\dots,x_p) \in \mathbb{X}^p$ set $\big(e_z\big)_1(x_1) := z(x_1)$ and $\big(e_z\big)_p(x_1,\dots,x_p) := 0$ for $p \geq 2$.

Proposition 14.5 (Kirkwood-Salsburg equations for ρ) Assume that $\rho(z)$ converges absolutely for some activity function z (i. e., the series $\rho_p(x_1,\dots,x_p;z)$ are absolutely convergent for all $p \in \mathbb{N}$ and all $(x_1,\dots,x_p) \in \mathbb{X}^p$), then

$$\rho(z) = K_z\rho(z) + e_z, \tag{14.2}$$

in the sense that $\rho_p(x_1,\dots,x_p;z) = \big(K_z\rho(z) + e_z\big)_p(x_1,\dots,x_p)$ for all $p \in \mathbb{N}$ and all $(x_1,\dots,x_p) \in \mathbb{X}^p$.

Sketch of proof. Following the proof by Jansen in [4], one uses the structure of multi-rooted graphs to show that $\rho(z)$ is given (pointwise) by the limit of the Picard iterates of the map $a \mapsto K_z a + e_z$, which by a slight abuse of notation we denote $K_z + e_z$, starting in e_z (i. e. $\rho(z) = \lim_{n\to\infty}(K_z + e_z)^n e_z$, where $(K_z + e_z)^n$ denotes the n-fold composition of $K_z + e_z$ with itself). □

Furthermore, for the sign-flipped functions $\tilde{\rho}_k(z)$, a system of integral equations in terms of the sign-flipped operator $\tilde{K}_z$ can be derived from the original Kirkwood-Salsburg equations for $\rho_k(z)$.

Proposition 14.6 (Kirkwood-Salsburg equations for $\tilde{\rho}$) Assume that $\tilde{\rho}(z)$ converges for some non-negative activity function z (i. e., the series $\tilde{\rho}_p(x_1,\dots,x_p;z)$ are convergent for all $p \in \mathbb{N}$ and all $(x_1,\dots,x_p) \in \mathbb{X}^p$), then

$$\tilde{\rho}(z) = \tilde{K}_z\tilde{\rho}(z) + e_z, \tag{14.3}$$

in the sense that $\tilde{\rho}_p(x_1,\dots,x_p;z) = \big(\tilde{K}_z\tilde{\rho}(z) + e_z\big)_p(x_1,\dots,x_p)$ for all $p \in \mathbb{N}$ and all $(x_1,\dots,x_p) \in \mathbb{X}^p$.

Sketch of proof. The statement follows directly from Proposition 14.5 by the definition of $\tilde{\rho}(z)$ and the alternating sign property from Corollary 14.2. □

4 Main results

Now we are ready to state our main result – a condition both necessary and sufficient for absolute convergence of $\rho(z)$ – inspired by the extended Gruber-Kunz approach as introduced by Bissacot et al. in [1].

Theorem 14.7 Let z be a non-negative activity function. Then the following statements are equivalent:

1) $\tilde{\rho}(z)$ converges.

2) There exists a sequence of non-negative measurable functions a, such that

$$\tilde{K}_z a + e_z \leq a. \tag{14.4}$$

Sketch of proof. The implication $1) \Rightarrow 2)$ is given by Proposition 14.6. For the converse, we notice that $\tilde{\rho}(z)$ is – if convergent – equal to the Neumann series $\sum_{n=0}^{\infty} \tilde{K}_z^n e_z$, since the latter is also given by the unique limit of the Picard iterates of $\tilde{K}_z + e_z$ starting in e_z, i. e., $\sum_{n=0}^{\infty} \tilde{K}_z^n e_z = \lim_{n\to\infty}(\tilde{K}_z + e_z)^n e_z = \tilde{\rho}(z)$. Following a proof by Fernández and Procacci (see [1]) one can exploit certain positivity and monotonicity properties of $\tilde{K}_z$ to show that $2)$ implies the convergence of the Neumann series $\sum_{n=0}^{\infty} \tilde{K}_z^n e_z$. □

Given Theorem 14.7, proving sufficient conditions for absolute convergence of the activity expansions can be reduced to finding appropriate ansatz functions a satisfying the system of Kirkwood-Salsburg inequalities (14.4). We demonstrate how this can be done by considering the classical criteria:

1) Kotecký-Preiss criterion: First introduced by Kotecký and Preiss in [5] for abstract polymers, the criterion was generalised for the setup of repulsive pair interactions by Ueltschi in [9]; its generalised version can be formulated as: If there exists $\mu : \mathbb{X} \to [0,\infty)$, such that for all $x_0 \in \mathbb{X}$

$$z(x_0)e^{\int |f(x_0,y)|\mu(y)\lambda(\mathrm{d}y)} \leq \mu(x_0), \tag{14.5}$$

   then the activity expansions $\rho(z)$ converge absolutely.

   In this case, choose $a = (a_p)_{p\in\mathbb{N}}$ to be given by $a_p(x_1,\dots,x_p) := \prod_{i=1}^{p} \mu(x_i)$ for some $\mu \geq 0$ satisfying condition (14.5). Just by using the uniform bound $|1+f| \leq 1$ (repulsive interactions) one immediately confirms that this choice of a satisfies the inequalities (14.4).

2) Fernández-Procacci criterion: First introduced by Fernández and Procacci in [3] for abstract polymers, the criterion was generalised for the setup of repulsive pair

interactions by Jansen in [4]; its generalised version can be formulated as: If there exists $\mu : \mathbb{X} \to [0,\infty)$, such that for all $x_0 \in \mathbb{X}$

$$z(x_0)\left(1+\sum_{k=1}^{\infty}\frac{1}{k!}\int_{\mathbb{X}^k}\prod_{j=1}^{k}\left|f(x_0,y_j)\right|\prod_{1\le i<j\le k}\big(1+f(y_i,y_j)\big)\prod_{j=1}^{k}\mu(y_j)\lambda^{\otimes k}(\mathrm{d}\mathbf{y})\right) \le \mu(x_0), \quad (14.6)$$

then the activity expansions $\rho(z)$ converge absolutely.

Here we define $a=(a_p)_{p\in\mathbb{N}}$ by $a_p(x_1,\dots,x_p) := \prod_{1\le i<j\le p}\big(1+f(x_i,x_j)\big)\prod_{i=1}^{p}\mu(x_i)$ for some $\mu \ge 0$ satisfying condition (14.6). Again, the uniform bound $|1+f|\le 1$ immediately yields the inequalities (14.4) for our choice of a.

But not only can the classical convergence criteria be reconstructed by the approach given by Theorem 14.7, also new results improving on the known bounds for the convergence radii can be proven by choosing "less multiplicative" ansatz functions (notice that all the ansatz functions a considered are submultiplicative – in the sense that $a_{p+k}(x_1,\dots,x_p,x_{p+1},\dots,x_{p+k}) \le a_p(x_1,\dots,x_p)\,a_k(x_{p+1},\dots,x_{p+k})$ for all $p,k\in\mathbb{N}$ and all $(x_1,\dots,x_p,x_{p+1},\dots,x_{p+k})\in\mathbb{X}^{p+k}$). In the following we consider the setup of abstract polymers, in which the two classical conditions above were first introduced.

Let $\mathbb{X}$ be a countable set (the set of polymers), let $\mathscr{X}$ be the powerset of $\mathbb{X}$ and let λ simply be given by the counting measure. Moreover, let $R\subset\mathbb{X}\times\mathbb{X}$ be a symmetric and reflexive relation. We write $x \nsim y$ for $(x,y)\in R$ and $x\sim y$ for $(x,y)\notin R$. We set $\Gamma(x) := \{y\in\mathbb{X}|\ y\nsim x\}$ for any $x\in\mathbb{X}$ and extend this notation to $\Gamma(X) := \cup_{x\in X}\{y\in\mathbb{X}|\ y\nsim x\}$ for any $X\subset\mathbb{X}$. Notice that we do not require $\Gamma(x)$ to be finite sets and that $x\in\Gamma(x)$ for every $x\in\mathbb{X}$. Finally, we consider hard-core interactions given by $f(x,y) := -\mathbb{1}_{\{x\nsim y\}}$.

In this setting we prove the following new sufficient condition:

Proposition 14.8 Let z be a non-negative activity function. If there exists $\mu:\mathbb{X}\to[0,\infty)$, such that for all $x_0\in\mathbb{X}$

$$z(x_0)\left(1+\sum_{k\ge 1}\sum_{\substack{Y=\{y_1,\dots,y_k\}\\ y_i\nsim x_0,\ y_i\sim y_j}}\prod_{i=1}^{k}\mu(y_i)\prod_{w\in\Gamma(Y)}e^{\mu(w)}\right) \le \mu(x_0)\prod_{w\in\Gamma(x_0)}e^{\mu(w)}, \quad (14.7)$$

then the activity expansions $\rho(z)$ converge absolutely.

Sketch of proof. One shows that – under the assumption of the the proposition – the ansatz functions $a = (a_p)_{p\in\mathbb{N}}$, $a_p : \mathbb{X} \to [0,\infty)$, given by setting

$$a_p(x_1,\ldots,x_p) := \prod_{1\le i<j\le p} \mathbb{1}_{\{x_i\sim x_j\}} \prod_{i=1}^{p} \mu(x_i) \prod_{w\in\Gamma(X)} e^{\mu(w)}$$

for some μ satisfying (14.7), any $p \in \mathbb{N}$ and every $(x_1,\ldots,x_p) \in \mathbb{X}^p$, satisfy the system of Kirkwood-Salsburg inequalities (14.4). □

Notice how the sufficient conditions are successively improved by having the corresponding ansatz functions a capture more of the structure of the expansion from Proposition 14.1 (for a modified activity $\mu \ge z$, where the inequality is understood to hold pointwise). To illustrate the improvement we consider the following somewhat typical case of an abstract polymer model given by subset polymers, i. e. the polymers are given by finite subsets of the regular lattice $\mathbb{Z}^d$ and the relation R on the set of polymers is given by having non-empty intersection.

Example 14.9 Consider non-overlapping (hard-core-interactions) cubes on $\mathbb{Z}^2$ of side-length 2 with translation-invariant activity z. The sufficient condition on z for the absolute convergence of $\rho(z)$ given by the Fernández-Procacci criterion provides the bound

$$z \le \max_{\mu\ge 0} \frac{\mu}{1+9\mu+16\mu^2+8\mu^3+\mu^4} \approx 0.057271,$$

while our condition from Proposition 14.8 provides

$$z \le \max_{\mu\ge 0} \frac{\mu e^{9\mu}}{1+9e^{9\mu}\mu+(6e^{15\mu}+8e^{16\mu}+2e^{17\mu})\mu^2+8e^{21\mu}\mu^3+e^{25\mu}\mu^4} \approx 0.060833.$$

This corresponds to an improvement of approximately 6 percent.

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