On the Virial Series for a Gas of Particles with Uniformly Repulsive Pairwise Interaction

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Abstract

The pressure of a gas of particles with a uniformly repulsive pair interaction in a finite container is shown to satisfy (exactly as a formal object) a “viscous” Hamilton-Jacobi (H-J) equation whose solution in power series is recursively given by the variation of constants formula. We investigate the solution of the H-J and of its Legendre transform equation by the Cauchy-Majorant method and provide a lower bound to the radius of convergence on the virial series of the gas which goes beyond the threshold established by Lagrange’s inversion formula. A comparison between the behavior of the Mayer and virial coefficients for different regimes of repulsion intensity is also provided.

1 Introduction: Motivations and Results

Context  We shall answer and bring to attention some questions regarding the Kamerlingh Onnes virial series of a system of particles interacting with two–body pairwise repulsive potentials. The model of hard spheres, despite its apparent simplicity and usefulness in modeling fluids, has not been solved except in the limit of infinitely many dimensions ($d = \infty$). In this limit, the equation of state

$$\beta P = \rho + \frac{1}{2} \rho^2$$

(1.1)

truncates at the second virial coefficient and the fact there is no premonitory signs of a phase transition in the fluid phase is attributed to a diminished importance of fluctuations which, according
to the theory of critical phenomena, suggests the presence of phase transition (not manifested by its virial series (1.1) or by its Mayer series, which has no singularity at physical values of activities).

The classical system of hard spheres – as well as the Ford model [UF], that realizes the upper bound for the radius of convergence of its Mayer series – shows, by Padé approximation analysis of its virial series, no pressure maximum [AFLR], indicating the failure of the equation in the fluid phase to supply any information about the freezing phase transition. For a recent discussion on this and other related issues on phase transition of hard-spheres see Clisby-McCoy [CMcC] and references therein.

As early as the study by Riddell and Uhlenbeck [RU], the problem of finding asymptotic behavior of the Mayer and virial coefficients $b_n$ and $B_n$ for high $n$ intended to address the (same) question: *is there (for the gas of hard-spheres) a transition point $\rho^*$ predicted to be smaller by a factor 0.806 than the close-packing density $\rho_{cp}$ (see e.g. [Ro]) by Kirkwood-Monroe [KMon]?* (we refer to Sec. 4 of [CMcC] for a review on numerical studies, approximate equations and sceneries for the position of the leading singularities). This question remains unanswered as far as the present knowledge on the radius of convergence of the Mayer and virial series is concerned (see e.g. [Ru]). Further asymptotic investigation of the $b_n$ and $B_n$, carried by Uhlenbeck and Ford [UF] for the so-called Gaussian model, had not reached any definite answer although the mathematical problems that came out from their study inspired the present investigation.

In the present paper we study a gas of point particles interacting via a uniformly repulsive pairwise potential, in a finite volume $\Lambda$ of size $|\Lambda| = 1/(2\varepsilon)$. We prove, employing a system of equations satisfied by the Ursell functions [BK], that the pressure $p = p(t, \mu)$, as a function of $t$, a parameter (“inverse temperature”) that interpolates the ideal to the real gas, and the chemical potential $\mu$, satisfies (exactly, as a formal object) a “viscous” Hamilton–Jacobi equation

$$p_t + \varepsilon (p_{\mu\mu} - p_{\mu}) + \frac{1}{2} \left(p_{\mu}\right)^2 = 0$$

with $p(0, \mu) = e^\mu$. The repulsive interaction, expressed by the “wrong” sign in front of the Laplacian, avoids the collapse of particles into a single point (equilibrium stability).

We are looking for solutions of (1.2) in the form of a power series in the activity $z = e^\mu$:

$$p(t, \mu) = \sum_{n=1}^{\infty} b_n(t) z^n := \varphi(t, z)$$

which are regular at $\varepsilon = 0$ (infinite volume limit). The so-called Mayer solution exists globally, i.e., for all $t \geq 0$ as a holomorphic function in a neighborhood of $z = 0$, uniformly in $\varepsilon$ (see Theorem D.4 for precise statement, which includes (1.2) among other equations and it is not intended to give optimal estimation on the convergence radius). A refined version, Theorem 4.5, optimizes the estimate on the radius of convergence up to one for which (1.3), being the generating function for labelled enumeration of simply connected Mayer graphs, is majorized by the corresponding sum over labelled trees.
Motivations  The convergence of Mayer series for the class of regular and stable potentials (including nonnegative ones)[Ru, Chapt. 4], is affected by the presence, in its majorant, of a (movable and nonphysical) singularity in the negative real line of the complex $z$–plane (see e.g. [GM] and Appendix B) which would be inherited by the virial series

$$P(t, \rho) = \sum_{n=1}^{\infty} B_n \rho^n$$ (1.4)

whether Lagrange’s inversion formula is applied to estimate the pressure: $\varphi(t, Z(t, \rho))$, where $Z = Z(t, \rho)$ solves $z \varphi_z(t, z) = \rho$ for $z$ (see Appendix B), as in the classic paper by Lebowitz–Penrose [LP].

Alternatively, the virial coefficients $(B_n)_{n \geq 1}$ (or the irreducible cluster integrals $(\beta_n)_{n \geq 1}$, which is related to by

$$B_n = -\frac{n-1}{n} \beta_{n-1}$$ (1.5)

for $n \geq 2$, with $B_1 = 1$) may be obtained from the Helmholtz free energy density (see Proposition A.7):

$$F(t, \rho) = \sup_{\mu} (\mu \rho - p(t, \mu))$$

$$= \rho \log \rho - \rho - \beta(t, \rho),$$

whose derivative $\beta_\rho(t, \rho)$, excluding the free energy of ideal gas $F(0, \rho) = \rho \log \rho - \rho \equiv F_{\text{ideal}}$, generates the labelled “enumeration” (total weight of species) of irreducible (2–connected) Mayer graphs:

$$\varphi(t, \rho) = \sum_{n=1}^{\infty} \beta_n(t) \rho^n .$$ (1.6)

Consequently, with (1.5), the radii of convergence $R_\beta(t)$, $R_P(t)$ and $R_\varphi(t)$ of the power series $\beta(t, \rho)$, $P(t, \rho)$ and $\varphi(t, \rho)$ about $\rho = 0$ are all the same. The Helmholtz free energy (extracted the ideal contribution) $F - F_{\text{ideal}} = -\beta$ has been recently addressed by cluster expansion [PTs] and Morais–Procacci [MoP] have shown, by means of an expression already known by Mayer (see Appendix A for a derivation using Lagrange’s inversion formula), that $R_\beta$ satisfies Lebowitz–Penrose’s lower bound on the radius of convergence of the virial series. It thus seems quite opportune to inquire whether the referred singularity on the Mayer series could somehow be prevented.

The present work has been motivated by the following open problem:

*Is there a system of interacting particles for which $\beta$, $P$ and/or $\varphi$ can be directly assessed, Lagrange’s inversion formula be avoided and Lebowitz-Penrose’s lower bound on $R_P(t)$ be improved?*

Results  We prove (Proposition 2.1.c) that if $p(t, \mu)$ satisfies the initial value problem (1.2) then $\varphi(t, \rho)$ satisfies

$$\varphi_t + \rho + \varepsilon \left( \frac{1 + \rho^2 \varphi_{\rho \rho}}{(1 - \rho \varphi_{\rho})^2} - 1 \right) = 0$$ (1.7)
with $\varphi(0, \rho) = 0$ and an affirmative answer to the “model” described by equation (1.7) has been provided. We establish (Theorem 3.1), via the Cauchy–Majorant method, a lower bound $R_\varphi(t)$ for $R_\rho(t)$, where $\Phi(t, \rho) = \sum_{n \geq 1} \Phi_n(t) \rho^n$ majorizes $\varphi(t, \rho)$ in the sense that $|\beta_n(t)| \leq \Phi_n(t)$ holds for all $n \in \mathbb{N}$ and $t \in \mathbb{R}_+$, uniformly in $\varepsilon$:

$$\lambda R_\varphi(t) \geq \lambda R_\rho(t) = \varepsilon$$

where $\varepsilon = \varepsilon(\eta)$ with $\eta = e^{-2\varepsilon t}$ is given by (3.3) and $\lambda = (1 - \eta) / (2\varepsilon)$ is the $L_1$-norm of the Mayer $f$-function $f = e^{-\varphi} - 1$ with $\varphi$ the uniformly repulsive potential (i.e., $\lambda = 2B_2$). The curve defined by the r.h.s. of (1.8) stays above the Lebowitz-Penrose’s lower bound $R_P(t) > 0.144767 / \lambda$ (eq. (3.11) of [LP] with $u = 1$ and $B = \lambda$) for all $t$ while, for $\varepsilon t \leq 0.00538$, the pre-factor $\varepsilon$ goes beyond the threshold 0.278465, established for nonnegative potentials $R_P(t) > 0.278465 / \lambda$ (see [Ru], Theorem 4.3.2 et seq.). $\varepsilon$ as a function of $\eta$ is plotted in Fig. 2. By (1.8), $R_\varphi(t) > 0$ for all $(t, \varepsilon) \in \mathbb{R}_+ \times \mathbb{R}_+$ and the $t$ and $\varepsilon = 1/(2|\Delta|)$ for which $\varphi$ converges in the domain below the hyperbole $\varepsilon t = 0.00538$ represent the regime of “high temperatures” and/or large volumes. The proof of Theorem 3.1 introduces some novelties with respect to the traditional majorant method and involves technical difficulties (see Proposition E.1).

Stronger results can actually be proven for equation (1.2). It follows from Lieb’s inequalities (see e.g. [Ru], Sect. 4.5, and references therein) that alternating sign property (a.s.p.): $(-1)^{n-1} b_n > 0$ and upper and lower bounds

$$e^{-1} \leq \lambda R_\rho \leq 1$$

on the radius of convergence $R_\rho$ of the Mayer series for the pressure (or density), hold for any nonnegative potential. In Theorem 4.5 we prove, in addition, that (i) $\lambda R_\rho$ is monotone increasing in $t$, (ii) the inequalities (1.9) saturate in both sides at $t = 0$ and $\infty$ and (iii) $\lim_{\varepsilon \to 0} \lambda R_\rho = e^{-1}$ for any $0 < t < \infty$.

Regarding equation (1.7), we rely on few additional results and explicit computation using Mathematica. We prove (Theorem 4.1) that

$$\frac{\beta_n}{\lambda^n} = (-1)^{n+1} \varepsilon t (1 + O(\varepsilon t)),$$

as $\varepsilon t \to 0$ (1.10)

for $n \geq 2$ ($\beta_1 / \lambda \equiv -1$) and, by continuity, the $\beta_n$‘s satisfy both a.s.p. and $\lambda R_\varphi = 1$ if $\varepsilon t$ is sufficiently small. For $\varepsilon t \ll 1$, $\lambda R_\rho = 1$ holds even though, as explained in Appendix D, we have $\lambda R_\rho \geq W(e^{-1}) = 0.278465...$, by Lagrange’s inversion formula. On the other hand, in the limit of $t$ large, $\lim_{t \to \infty} n \beta_n / \lambda^n = -1$ and, as the computer calculations indicate, $\lambda R_\varphi = \lambda R_\rho = 1$ is expected to hold for all $(t, \varepsilon)$.

**Related issues** There are two other issues regarding the virial coefficients of systems with repulsive potentials that can be addressed by the present (mean field) model. The ninth and tenth order
virial coefficients for hard spheres have been calculated (numerically) in dimensions $2 \leq d \leq 8$ by Clisby–McCoy [CMcC]. Collecting and reviewing a great deal of information, the authors found that even coefficients start to be negative when $d \geq 5$ and provided strong evidence that the leading singularity for the virial series lies away from the positive real line. We compute the $\beta_n$ ($= -(n+1)B_{n+1}/n$) from an exact recursion relation satisfied for the “model” (1.7) and show that, as function of $n$, they oscillate about the axis (Fig. 5 depicts $n\beta_n/\lambda$, $n = 1, ..., 17$ for different values of $t$). The calculation indicate that the period increases from 1 (the alternating sign behavior (1.10)) to infinity as $t$ varies from 0 to $\infty$. Each $n\beta_n/\lambda$, as a function of $t$, oscillates wildly, apparently uncorrelated from the others, until it reaches a maximum at $t^*_n$ and from there on it converges rapidly to $-1$ (see Fig. 4), indicating that the leading singularity of the virial series remains away from the positive real line, at least for $t < t^*_\infty = \lim_{n \to \infty} t^*_n$.

The results of our investigation are, to say the least, intriguing and extension of the present analysis will be presented separately. The present paper covers, in addition, some preliminary materials to make it self–contained. We observe that, despite the volume $\Lambda$ is kept finite, the “macroscopic limit” is already realized for a gas of point-like particles. From the point of view of Lee–Yang theory, the partition function $\Xi_{\Lambda} = \Xi_{\Lambda}(z)$ of a gas of hard-spheres is a polynomial in the activity $z$ whose zeros (singularities of the pressure) may accumulate (eventually) at the infinite volume limit. The singularities of the “macroscopic functions” for point–like gas of particles, even at finite $|\Lambda|$, may be seen from the Taylor series of the logarithm of partition function $\varphi = \log \Xi_{\Lambda}/|\Lambda|$ about $z = 0$. According to Jentzsch theorem (see e.g. [1]), each point on the circle of convergence of $\varphi$ is a limit point of zeros of the $n$–th Taylor polynomial $\varphi_n$, $n = 1, 2, \ldots$.

The second issue, concerning with the Mayer and virial series at low temperature, has been addressed recently by Jansen [Ja] for a class of potentials satisfying a $n$–particle ground state geometry condition and some of her results extend to nonnegative potentials as well. We should mention that her results on the radii of convergence of the virial (1.4) and the series of $\varphi \circ Z(\rho)$ in power of $\rho$ (see e.g. Theorem 3.8 of [Ja]) go, however, in the opposite direction of ours for the uniformly repulsive potential. We should warn that, since we are fixing $\beta = 1$ (activity and density are given by $z = e^\mu$ and $\rho = p_\mu$, without $\beta$) the limit $t \to \infty$ does not really mean low temperature limit, although we sometimes abuse of language.

Equation (1.7) has a stationary solution: $\varphi_0(\rho) = \log (1 - \rho/(2\varepsilon))$ (solves (1.7) with $\varphi_t = 0$), from which one obtains the pressure (see eqs. (2.16)-(2.17))

$$ P_0(\rho) = \int_0^\rho (1 - \zeta \varphi'_0(\zeta)) d\zeta = -2\varepsilon \log (1 - \rho/(2\varepsilon)) $$

for the hard core lattice gas or Ford model (B.13) in the low density regime. The lower bound (1.8) on the radius of convergence $R_\varphi$ implies that $\varphi_0(\rho)$ is attained, as $t$ goes to $\infty$, at least inside

\[\text{Other models whose leading singularities are out of the real line include the Gaussian model already mentioned (see [CMcC] and reference therein) and hard–core lattice gases in two–dimensions, particularly the hard–hexagon model whose radius of convergence of the virial series has been determined exactly by Joyce [J] (see eq. (12.30) therein) and is less than the critical density $\rho_c$ of this model.}\]
the domain $|\rho/\lambda| < \kappa_\infty$ where $\kappa_\infty = 3 - 2\sqrt{2} = 0.171573$ (numerically improved to 0.275451, see Remark 4.2). Since the power series $-\sum_{n\geq 1} (\rho/2\varepsilon)^n / n$ of $\varphi_0(\rho)$ converges in a domain $|\rho/\lambda| < 1$ larger than the former, we investigate, in our second paper, the power series solution of (1.7) in exponential time variable $\eta = e^{-2\varepsilon t}$ (transeries, see e.g. [Co]):

$$\varphi(t, \rho) = \varphi_0(\rho) + \sum_{n=1}^\infty \varphi_n(\rho) \eta^n$$

(1.11)

asymptotic to $\varphi_0$ as $t \to \infty$. The results we obtained using a more involved version of the Cauchy–majorant method, which has its own interests, may be summarized as follows:

The $\varphi_n$’s in (1.11) can be written as

$$\varphi_n(\rho) = (k(\rho/2\varepsilon))^{n} Q_n(\rho/2\varepsilon)$$

(1.12)

where $k(\rho)$ is the Kobe function $\rho/(1 - \rho)^2$ and $Q_n(\rho)$ is a polynomial of order $n$ in $\rho$. The series (1.11), written as $\sum_{n\geq 1} Q_n(k\eta)^n$ by (1.12) and with $2\varepsilon = 1$ (w.l.g.), converges uniformly in the domain $\Omega \subset [0, 1) \times D_1$ such that $|\rho| \leq \rho_0 < 1$ and $|\eta| < \eta_0$ where $\eta_0 = \eta_0(\rho_0)$ tends to 0 as $\rho_0$ goes to 1.

These results, together with (1.8) and the global–existence/uniqueness of the initial value problem (1.7), imply that, for large $t$, two solutions of (1.7) coexist in the some domain $|\rho| < \rho_0$, $\rho_0 = \rho_0(t) > 0$ (although (1.11) does not satisfy the (ideal gas) initial value $\varphi(0, \rho) = 0$ and it might not even be seem from the partition function); as long as $\varepsilon > 0$, they belong to different branches, (1.11) corresponding to the “low temperature” solution.

Outline The layout of the present paper is as follows. In Section 2 we introduce our potential model and establish a relationship between macroscopic functions and their corresponding PDE’s. Sections 3 and 4 contain our main contributions: Theorems 3.1 and 4.1 on the Cauchy–majorant and asymptotic methods applied to (1.7); Theorem 4.5 on the radius of convergence of Mayer solution (1.3) of (1.2). Our conclusions and open problems are summarized in Section 4. Four appendices are included to insert our results into the context. In Appendix A we review the theory of imperfect gas due to Mayer. Appendix B provides an overview on the convergence of virial series. Appendix C proves Proposition 2.1a, the derivation of (1.2) for the pressure of a gas of particles interacting via a uniformly repulsive potential, introduced in Section 2. Appendix D establishes global existence and uniqueness of a class of PDEs satisfying initial condition of Mayer type, which includes (1.2), (1.7) and another equation related to irreducible–edges Mayer graphs. Finally, Appendix E contains our technical results: Propositions 4.1 and 4.6 used in the proof of Theorems 3.1 and 4.1 respectively.
2 Thermodynamic Functions and their corresponding PDE’s

Two parameters potential model  We consider an equilibrium system of point-particles in a finite container \( \Lambda \subset \mathbb{R}^d \) interacting via a uniformly repulsive two–body potential

\[
\phi_{ij} \equiv \phi_\Lambda(t; x_i - x_j) = \frac{t}{|\Lambda|} \tag{2.1}
\]

for every \( x_i, x_j \in \Lambda \).

Our interacting potential \( \phi_\Lambda = \phi_\Lambda(t; x) = t/|\Lambda| \) depends on the size \( |\Lambda| \) of the container and on a parameter \( t \) which plays a double role of “time” (evolution) variable and “inverse temperature” or repulsive intensity (so, we set \( \beta = 1 \) in (A.10) and change variable \( \beta \) by \( t \) for all functions defined in Appendix A). Among all features of a reasonable physical potential, \( \phi_\Lambda \) retains only the property of being repulsive (nonnegative). As the so–called Gaussian model, introduced by Montroll et all [MBH] (see [UF]), \( \phi_\Lambda \) is able to isolate the combinatorial problem, arising when thermodynamic functions are represented in power series (see (A.14) and (A.34)), from the integral on the configuration space, which can be easily performed. Because the point-like particles are moving in a continuum space (container \( \Lambda \)), the system is already in the “macroscopic limit”, despite its volume \( |\Lambda| \) is kept finite.

Note that \( \phi_\Lambda \) is positive (\( \phi_\Lambda(t; x) > 0 \)) and of positive-definite type:

\[
\sum_{1 \leq i,j \leq N} z_i \phi_\Lambda(t; x_i - x_j) \bar{z}_j = \frac{t}{|\Lambda|} \left| \sum_{i=1}^N z_i \right|^2 \geq 0,
\]

for any collection of points \( (x_i)_{i=1}^N \) in \( \Lambda \) and complex numbers \( (z_i)_{i=1}^N \), satisfying therefore stability:

\[
\sum_{1 \leq i < j \leq N} \phi_\Lambda(t; x_i - x_j) \geq \frac{-t}{2|\Lambda|} N
\]

and “integrability” (in the \( L_1(\Lambda; d^t x) \)–sense):

\[
\| \phi_\Lambda(t; \cdot) \|_1 = \int_\Lambda \phi_\Lambda(t; y) d^t y = t
\]

and

\[
\| e^{-\phi_\Lambda(t; \cdot)} - 1 \|_1 = \int_\Lambda \left| e^{-\phi_\Lambda(t; y)} - 1 \right| d^t y = |\Lambda| \left( 1 - e^{-t/|\Lambda|} \right) \equiv \lambda(t, |\Lambda|) \tag{2.2}
\]

where \( \lambda(t, |\Lambda|) \) is monotone increasing function of \( t \) and \( |\Lambda| \) such that \( \lambda(\mathbb{R}_+, |\Lambda|) = [0, |\Lambda|] \) and \( \lambda(t, \mathbb{R}_+) = [0, t] \) remain bounded for \( |\Lambda|, t > 0 \).

We refer to Appendix A for basic properties and formal expressions of the thermodynamic functions pertaining to this section.
**Weight of a connected graph** $G$  

The problem of the evaluation of $B_n$, the $n$–th coefficient \[A.33\] of Kamerlingh Onnes virial series \[A.31\], may be divided into two distinct ones. The combinatorial problem, whose an introductory presentation is given in Appendix \[A\], is independent of the law of interacting forces between any two particles. The second problem for the evaluation of

$$
\beta_n = -(n + 1)B_{n+1}/n
$$

is the integration over the configuration space $\Lambda^n$. For interacting potential \[2.1\], the weight $w_{\Lambda}(G)$ of a irreducible (2–connected) graph $G$ with $n$ vertices and $l = |E(G)|$ edges involved in the sum \[A.34\], satisfies exactly

$$
w_{\Lambda}(G) = \frac{1}{|\Lambda|} \int_{\Lambda^n} \prod_{(ij)\in E(G)} (e^{\phi_{\Lambda}(x_i-x_j)} - 1) dx_1 \cdots dx_n
$$

by \[2.2\], reducing the two problems to a purely combinatorial one – this should be contrasted with the “soft repulsion” Gaussian model whose explicit evaluation,

$w(G) = (-t)^l (\pi/\alpha)^{3(n-1)/2} \gamma^{-3/2}$

depends on the graph complexity $\gamma = \gamma(G)$ of $G$ in addition to the two other dependences, on the number of vertices and edges, already in \[2.3\] (see \[UF\], \[Le\], for definition, evaluation and motivations).

The number of edges $l = |E(G)|$ of a connected graph $G$ with $n$ vertices satisfies

$$
l \geq n - 1 ,
$$

with equality holding only for tree graphs $T$. Since the only 2–connected tree is, by definition, the graph with two vertices connected by a single edge $T_2$, and since for any connected graph $G$, we have, as $|\Lambda|$ goes to infinity,

$$
w^{\infty}(G) = \lim_{|\Lambda| \to \infty} w_{\Lambda}(G) = \begin{cases} (-t)^l & \text{if } G = T \\ 0 & \text{otherwise} \end{cases}
$$

by $\lambda(t, \infty) = t$, the limit weight $w^{\infty}(G)$ vanishes for all irreducible (2–connected) graphs $G$ different from $T_2$. In this limit, the virial series \[A.31\] reads

$$
P^{\infty}(t, \rho) = \rho + \frac{t}{2} \rho^2
$$

by dissymmetry theorem (see e.g. \[BL\]), which agrees with the pressure of a system of hard spheres in $d = \infty$.

Another limit is attained when $t$ tends to $\infty$ (the low temperature limit) with $|\Lambda|$ finite. For this limit, the weight of a 2–connected graph $G$ reads

$$
\lim_{t \to \infty} w_{\Lambda}(G) = (-1)^l |\Lambda|^{n-1}
$$

and, by a subtle cancellation (exactly as in the hard-core lattice gas, for which $f_{ij} = e^{-\phi_{ij}} - 1 = -1$ if $x_i = x_j$ and $f_{ij} = 0$ if $x_i \neq x_j$, except that the sum of a $n$–particle configuration gives $|\Lambda|$ instead
agrees, this time, with the pressure $P_{\Lambda}$ of Ford’s model in the low density regime. Both limit functions will be shown to be attained by our investigation of macroscopic functions (pressure and the Helmholtz free energy) as power series solution of related partial differential equations.

**Partial differential equations** As a consequence of (2.3), we have

**Proposition 2.1**

(a) The pressure $p = p_{\Lambda}(t, \mu)$ of a uniformly repulsive interacting system, as a function of $t$ and the chemical potential $\mu = \log z$, for any fixed $\Lambda$, satisfies a partial differential equation (PDE)

$$p_t + \varepsilon (p_{\mu\mu} - p_{\mu}) + \frac{1}{2} (p_{\mu})^2 = 0,$$

$$\varepsilon = 1/(2|\Lambda|), \text{ with initial condition } p_{\Lambda}(0, \mu) = e^\mu. \tag{2.4}$$

(b) The Helmholtz free energy density $F = F_{\Lambda}(t, \rho)$ defined by the (formal) Legendre transform of $p_{\Lambda}(t, \mu)$ w.r.t. $\mu$ (see Proposition A.7) satisfies

$$F_t - \varepsilon \left( \frac{1}{F_{\rho\rho}} - \rho \right) - \frac{1}{2} \rho^2 = 0 \tag{2.5}$$

with $F_{\Lambda}(0, \rho) = \rho \log \rho - \rho$.

(c) The function $\varphi = \varphi(t, \rho)$, defined by

$$F_{\rho} = \log \rho - \varphi,$$  \tag{2.6}$$

satisfies

$$\varphi_t + \rho + \varepsilon \left( \frac{1 + \rho^2 \varphi_{\rho\rho}}{(1 - \rho \varphi_{\rho})^2} - 1 \right) = 0 \tag{2.7}$$

with $\varphi(0, \rho) = 0$ and generates, by Proposition A.7, the irreducible cluster integrals $\beta_n$, $n = 1, 2, \ldots$, defined by (A.17), i.e., the $\beta_n$’s are the coefficients of a formal power series in $\rho$ (1.6) of $\varphi$.

We defer the proof of item (a) of Proposition 2.1 to Appendix C and anticipate that (2.4) is deduced from the Brydges–Kennedy equations [BK] for the Ursell functions, which are briefly introduced there.
Proof of Proposition 2.1, parts (b) and (c). We follow here [CH]. The Legendre transform of a formal power series \( p(t, \mu) \) in \( e^\mu \), with respect to \( \mu \), is

\[
F(t, \rho) = \rho \mu^* - p(t, \mu^*)
\]  

(2.8)

where \( \mu^* = \mu^*(t, \rho) \) solves (formally)

\[
\rho = p_\mu(t, \mu)
\]

(2.9)

for \( \mu \); the Legendre transform of \( F(t, \rho) \) with respect to \( \rho \) is

\[
p(t, \mu) = \rho^* \mu - F(t, \rho^*)
\]

(2.10)

where \( \rho^* = \rho^*(t, \mu) \) solves (formally)

\[
\mu = F_\rho(t, \rho)
\]

(2.11)

for \( \rho \). Differentiating (2.10) w.r.t. \( \mu \), yields

\[
p_\mu = \rho^* + (\mu - F_\rho) \rho_\mu^* = \rho^*,
\]

(2.12)

by (2.11). Differentiating (2.12) w.r.t. \( \mu \), yields

\[
p_\mu = 2 \rho_\mu^* - (\mu - F_\rho) \rho_\mu^* - F_{\rho \rho} (\rho_\mu^*)^2
\]

\[
= 2 \rho_\mu^* - F_{\rho \rho} (\rho_\mu^*)^2 = \rho_\mu^*,
\]

(2.13)

by (2.11) again. The last equality reads: \( \rho_\mu^* - F_{\rho \rho} (\rho_\mu^*)^2 = 0 \) whose nontrivial solution \( \rho_\mu^* \neq 0 \) satisfies

\[
\rho_\mu^* = \frac{1}{F_{\rho \rho}} = p_{\mu \mu}
\]

(2.14)

by (2.13). We deduce from (2.10), together with (2.11), that

\[
p_t = -F_t.
\]

(2.15)

(2.15), (2.9) and (2.14) substituted into (2.4), yields (2.5) and concludes the proof of part (b).

Differentiating (2.5) w.r.t. \( \rho \) together with (2.6) yields (2.7). We observe that the operations involved in the Legendre transform, together with (2.6), (sum, multiplication, derivatives, inverse, composition, reciprocal, ...) apply over the ring \( \mathbb{C}^1[[z]] \) of formal power series in \( z = e^\mu \) with \( \mathbb{C}^1 \) coefficients \( b_n(t), n \geq 1 \).

For the statement of item (c) after (2.7), we follow Proposition A.7. By differentiating (A.35) w.r.t. \( \rho \), we conclude that \( \varphi \), defined by (2.6) and in Theorem A.4 by (A.19), have the same power series, whose coefficients are the irreducible integrals \( \beta_n \). The proof of Proposition 2.1 is now complete.

□
An alternate proof of the statement (c) starts from (2.8):

\[ F(t, \rho) = \rho \mu^*(t, \rho) - P(t, \rho) \]  

(2.16)

where \( \rho(t, \mu^*(t, \rho)) = P(t, \rho) \). Differentiating (2.16) w.r.t. \( \rho \), together with \( \mu^*(t, \rho) = F_\rho(t, \rho) = \log \rho - \varphi(t, \rho) \), yields

\[ P_\rho(t, \rho) = 1 - \rho \varphi_\rho(t, \rho) . \]

Assuming that \( \varphi \) has a power series (1.6), this equation can be formally integrated, with \( P(t, 0) = 0 \):

\[
P(t, \rho) = \int_0^\rho (1 - \eta \varphi_\rho(t, \eta)) \, d\eta
\]

\[
= \rho - \sum_{n=1}^{\infty} \frac{n}{n+1} \beta_n(t) \rho^{n+1}
\]

(2.17)

from which we conclude that the \( \beta_n \) are the irreducible cluster integrals, by (A.32). The Kamerlingh Onnes virial series (1.4) is thus given by (2.17) so, the power series (1.6) of \( \varphi(t, \rho) \) converges if, and only if, the virial series converges. We address in the following the former convergence to conclude about the latter.

### 3 Convergence of Virial Series: Cauchy–Majorant Method

We shall prove, among other results, the following

**Theorem 3.1** The initial value problem (2.7) admits a unique solution (1.6) in power series of \( \rho \) which converges uniformly in \( \varepsilon \), at least, inside the domain: \( (t, \rho) \in \mathbb{R}_+ \times \mathbb{C} \) such that

\[
|\rho| < \frac{2 + \sqrt{1 - e^{-2\varepsilon t}} - 2 \sqrt{1 - e^{-2\varepsilon t}/2 + \sqrt{1 - e^{-2\varepsilon t}}}}{1 - e^{-4\varepsilon t}} .
\]

(3.1)

**Corollary 3.2** The radius of convergence \( R_P(t) \) of the virial series (2.17) for a system of point particles interacting via the (uniformly repulsive) two–body potential \( \phi_\Lambda \), given by (2.1), satisfies

\[
R_P(t) \geq \frac{1}{\lambda}
\]

(3.2)

where

\[
\lambda = \frac{2 + \sqrt{1 - \eta} - 2 \sqrt{1 - \eta/2 + \sqrt{1 - \eta}}}{1 + \eta}
\]

(3.3)

\( \eta = \eta(t, |\Lambda|) = e^{-t/|\Lambda|} \) and \( \lambda = \lambda(t, |\Lambda|) = |\Lambda| (1 - \eta) \) is the function defined in (2.2).
For fixed $\Lambda$ the prefactor $\kappa$ varies from $1 - 1/\sqrt{2} = 0.292893$ to $3 - 2\sqrt{2} = 0.171573$ as $t$ varies from 0 to $\infty$. Figure 1 plots $\kappa$ as a function of $\eta$ where the two constants are Lebowitz-Penrose’s lower bound ($\kappa = 0.144767$) and the threshold ($\kappa = 0.278465$) established for nonnegative potentials by Lagrange inversion formula (see Sect. D).

The proof of Corollary 3.2 is an immediate consequence of Theorem 3.1 together with the observation after equation (2.17).

Proof of Theorem 3.1. The proof will be divided into two parts. Firstly, the Cauchy-majorant method is applied to (2.7) without preoccupation with the radius of convergence. We then push the method further – not as far it can go, but enough to go beyond the threshold.

Solution of (2.7) in power series. We have introduced in Appendix D a basic majorant method capable of dealing with equation of the form $u_t + \mathcal{A}(t, u_x, u_{xx}) = 0$ (see (D.1)-(D.5)). We observe that for a solution (D.2) of this kind of equation, in power series of $z = e^x$, $\partial/\partial x$ acts over a function of $z$ as $z\partial/\partial z$. In equation (2.7), $\rho$ plays the role of the $z$ variable and we write $\mathcal{A} = \mathcal{A}(\rho, a, b)$ with $a$ and $b$ in the place of $\rho\varphi_\rho$ and $\rho(\rho\varphi_\rho)_\rho$, respectively. Note that (2.7) differs slightly from (D.1) (it has trivial initial condition, $A_0,0 = \mathcal{A}(\rho, 0, 0)$ depends explicitly on $\rho$ and $\mathcal{A}$ doesn’t depend on $t$) and some additional features allow it to be analyzed more carefully.

Since $\rho^2\varphi_{\rho\rho} = \rho(\rho\varphi_\rho)_\rho - \rho\varphi_\rho = b - a$, equation (2.7) can be written in the form of a conservation law:

$$\varphi_t + (\mathcal{J}(\rho, \rho\varphi_\rho))_\rho = 0$$

(3.4)
with
\[
\mathcal{J}(\rho, a) = \frac{\rho^2}{2} + \varepsilon \rho \left( \frac{1}{1-a} - 1 \right)
\]
\[
= \frac{\rho^2}{2} + \varepsilon \rho \sum_{n=1}^{\infty} a^n ,
\]
(i.e., \( \mathcal{A} = \mathcal{J}_\rho + \mathcal{J}_a \cdot (\rho \varphi) \rho = \rho + \varepsilon ((1 + b - a)/(1 - a)^2 - 1) \)) and initial condition \( \varphi(0, \rho) \equiv 0 \). The proof that there exist a unique formal power series solution for equations of the form (3.4) is given in Theorem D.4 or may be concluded from the following calculations. We refer to Appendix D for details.

**Integral equation for the \( \beta_k \)'s** For convenience, we introduce a sequence \( \gamma = (\gamma_k)_{k \geq 1} \), with \( \gamma_k = k \beta_k \), and the convolution product \( \gamma \ast \delta \) of two sequences \( \gamma \) and \( \delta \) is defined by (D.7):
\[
(\gamma \ast \delta)_k = \sum_{j=1}^{k-1} \gamma_{k-j} \delta_j .
\]
The power series (1.6) of \( \varphi \) substituted into the integral (w.r.t. \( \rho \), from 0 to \( \rho \)) of (3.4), together with
\[
\frac{1}{\rho} \int_0^{\rho} \varphi(t, \bar{\rho}) d\bar{\rho} = \sum_{k=1}^{\infty} \frac{1}{k+1} \hat{\beta}_k(t) \rho^k
\]
and the fundamental theorem of calculus, yield a system of first order differential equations
\[
\frac{1}{k(k+1)} J_k + \varepsilon J_k = -h_k(\gamma_1, \ldots, \gamma_{k-1}; t) , \quad k \geq 1
\]
with \( \gamma_k(0) = 0 \), where the \( h_k \)'s are given by \( h_1 = 1/2 \) and, for \( k \geq 2 \),
\[
h_k(\gamma_1, \ldots, \gamma_{k-1}; t) = \varepsilon \sum_{n=2}^{k} \left( \gamma \ast \cdots \ast \gamma \right)_n .
\]
The solution of (3.6) for \( k = 1 \):
\[
\frac{1}{2} \gamma_1 + \varepsilon \gamma_1 = -\frac{1}{2}
\]
with \( \gamma_1(0) = 0 \) is
\[
\gamma_1(t) = e^{-2\varepsilon t} \int_0^t e^{2\varepsilon s} (-1) \, ds
\]
\[
= -\frac{1}{2\varepsilon} (1 - e^{-2\varepsilon t}) = -\lambda
\]
with \( \lambda = \lambda(t, |\Lambda|) \) the function defined by (2.2) (recall \( \varepsilon = 1/(2 |\Lambda|) \)).

By the variation of constants formula, (3.6) is equivalent to a system of integral equations
\[
\gamma_k(t) = -k(k+1) \int_0^{t} e^{-\varepsilon k(k+1)(t-s)} h_k(\gamma_1, \ldots, \gamma_{k-1}; s) ds , \quad k \geq 2
\]
which can be evaluate recursively starting from $\gamma_1(t) = -\lambda$. For the first few $k$’s, e.g., for $k = 2$, $h_2 = \varepsilon \gamma_1^2(t)$ and

$$
\gamma_2(t) = -6\varepsilon e^{-6\varepsilon t} \int_0^t e^{6\varepsilon s} \gamma_1^2(s) ds = -2\varepsilon \lambda^3,
$$

(3.10)

and for certain class of terms the integral (3.9) can be performed by “hand” (see Proposition E.1 and its proof in Appendix E).

An exact equation satisfied by the majorant. To approach equation (2.7) by the Cauchy–Majorant method, we need the following (stronger than usual)

Definition 3.3 A function

$$
\Phi(t, \rho) = \sum_{n=1}^{\infty} \Phi_n(t) \rho^n
$$

(3.11)

is a majorant of $\varphi(t, \rho)$, whose power series in $\rho$ is given by (1.6), if

1. each $\Phi_n(t)$ is positive, continuous and monotone increasing function of $t$;

2. there exist a family of domains $\Omega_t = [0, t) \times \mathbb{D}_{r(t)}$, in which the series (3.11) converges absolutely in $\mathbb{D}_{r(t)}$ and

$$
|\beta_n(s)| \leq \Phi_n(s)
$$

(3.12)

is satisfied for $0 \leq s < t$, uniformly in $\varepsilon$.

We write $\varphi \ll \Phi$ for the majorant relation.

We observe that the majorant relation is preserved by derivative w.r.t. $\rho$, integration in both $t$ and $\rho$, convex combination, multiplication and composition (see e.g. [Ho]).

We start with

$$
|\gamma_1(t)| = \lambda \left( t, (2\varepsilon)^{-1} \right) = \Phi_1(t)
$$

(3.13)

and generate a recursive equation for $(\Phi_k)_{k \geq 1}$ through (3.9). For convenience, we introduce a majorant

$$
\Psi = \rho \Phi_\rho = \sum_{k=1}^{\infty} \Psi_k \rho^k, \quad \Psi_k = k \Phi_k,
$$

(3.14)

of $\rho \varphi_\rho$ and observe that $\varphi \ll \Phi \iff \rho \varphi_\rho \ll \Psi$. In our first attempt of constructing $\Psi$, we shall not push the method to its limit.
Assuming (3.12) holds for $1 \leq n \leq k - 1$, (3.9) can be bounded as

$$|\gamma_k(t)| \leq k(k + 1) \int_0^t e^{-\varepsilon k(k+1)(t-s)} h_k(|\gamma_1|, \ldots, |\gamma_{k-1}|; s) \, ds$$

$$\leq h_k(\Psi_1, \ldots, \Psi_{k-1}; t) k(k + 1) \int_0^t e^{-\varepsilon k(k+1)(t-s)} \, ds$$

$$= \frac{1}{\varepsilon} h_k(\Psi_1, \ldots, \Psi_{k-1}; t) := \Psi_k(t).$$

(3.15)

For $k = 2$, by (3.10), we can do better:

$$|\gamma_2(t)| = 2\varepsilon \lambda^3(t) = \frac{1}{\varepsilon} h_2(\Psi_1; t) - \eta(t) \lambda^2 := \Psi_2(t),$$

(3.16)

where we have used $1 - 2\varepsilon\lambda = e^{-2\varepsilon t} \equiv \eta(t)$.

Summing the above recursive relation for the $\Psi_k$, multiplied by $\rho^k$:

$$\sum_{k \geq 2} \Psi_k \rho^k = \frac{1}{\varepsilon} \sum_{k \geq 2} h_k(\Phi_1, \ldots, \Phi_{k-1}; t) \rho^k - \eta \lambda^2 \rho^2,$$

for $t$ fixed, results

$$\Psi - \Psi_1 \rho = \frac{1}{1 - \Psi} - 1 - \Psi - \eta \lambda^2 \rho^2$$

(3.17)

by (3.14), (3.7), (3.5) and Proposition D.3

We observe that the r.h.s. of (3.17) is the function in (3.5) between parenthesis: $1/(1 - \Psi) - 1$, subtracted by $\Psi + \eta \lambda^2 \rho^2$, and (3.17) is equivalent to a quadratic polynomial equation: $2\Psi^2 - (1 + r - \eta r^2)\Psi + r - \eta r^2 = 0$, with $r = \lambda \rho$, whose solution yields

$$\Psi(t, \rho) = H(\lambda \rho)$$

(3.18)

with

$$H(r) = \frac{1}{4} \left( 1 + r - \eta r^2 - \sqrt{(1 + r - \eta r^2)^2 - 8(r - \eta r^2)} \right).$$

(3.19)

We have chosen the branch of square root in (3.19), for which every coefficient $c_k$ of the power series $\sum_{k \geq 1} c_k r^k$ of $H$ in $r$ remains positive for $0 \leq \eta < 1^2$ Explicitly,

$$H(r) = r + (1 - \eta)r^2 + (3 - 2\eta)r^3 + (11 - 9\eta + \eta^2)r^4 + (45 - 44\eta + 9\eta^2)r^5 +$$

$$(197 - 225\eta + 66\eta^2 - 3\eta^3)r^6 + \cdots$$

$^2$The sign can be checked using (A.25) or Scott’s formula [FLy] for higher order chain rule to the composite function $-\sqrt{p(r)}$, where $p(r)$ is the alternating sign fourth order (discriminant) polynomial in $r$, inside the square root in (3.19).
and we observe that the $c_k$ ’s are monotone decreasing in $\eta$ (monotone increasing in $t$). The fact that (3.18) is a function of $r = \lambda \rho$ is due to the homogeneity of the $h_k$ ’s:

$$h_k(\lambda \delta_1, \ldots, \lambda^{k-1} \delta_{k-1}; t) = \lambda^k h_k(\delta_1, \ldots, \delta_{k-1}; t)$$

(3.20)

for all $k \geq 2$, $\lambda$ and $\delta = (\delta_k)_{k \geq 1}$. Since $\Psi_k(t) = c_k \lambda^k$ and $\lambda(t)$ is (strictly) positive and monotone increasing in $t$, the same may be concluded of the $\Psi_k$’s.

The discriminant polynomial $p(r) = \eta^2 r^4 - 2\eta r^3 + (1 + 6\eta) r^2 - 6r + 1$ of the quadratic equation has four roots:

$$r_{\pm, \pm} = \frac{1 \pm \sqrt{1 - (12 \pm 8\sqrt{2})\eta}}{2\eta}$$

the nearest to the origin $r_{-, -} = r_{-, -}(t, \varepsilon)$, determines the radius of convergence of $H$. So, the power series of $H$ in $r$ converges provided

$$|r| < r_{-, -}(t, \varepsilon).$$

(3.21)

It follows from (3.18) that, the radius of convergence of $\Psi$ (consequently, of $\Phi$ too) is $r_{-, -}/\lambda$. It is clear from definition (3.15), (3.13), (3.16) and property (3.20), that $\Psi_k(t)$ is monotone increasing function of $t$, which, together with the inequality (3.15), proves that $\Psi$ is a majorant of $\rho \varphi_\rho$ in the sense of Definition 3.3 with $r(t) = r_{-, -}(t, \varepsilon)/\lambda(t, 1/2\varepsilon)$. All these properties hold, in addition, uniformly in $\varepsilon \in \mathbb{R}_+$.

As one can see from Fig. 2, the improved definition (3.16) of $\Psi_2$ yields a radius of convergence lying above Lebowitz–Penrose’s lower–bound (eq. (B.10) with $\kappa = 1$: $R \geq 0.144767/\lambda$). If we have used (3.15) also for $k = 2$ (i.e., set $\eta = 0$ from (3.16) to (3.19)), then the root of the second order polynomial $r^2 - 6r + 1$, closest to the origin, $r_{-, -}(\infty, \varepsilon) = 3 - 2\sqrt{2} = 0.17157$. Since $r_{-, -}(t, \varepsilon)$ hasn’t reached the threshold 0.278465 for any $t, \varepsilon \in \mathbb{R}_+$, the improvement, however, isn’t enough.

**Improved majorant equation** We come to the second part of the proof. The $k$–th and $(k - 1)$–th terms of $h_k(\gamma_1, \ldots, \gamma_{k-1}; t)$,

$$l_k(\gamma_1; t) = \varepsilon \left( \frac{\gamma * \cdots * \gamma}{k} \right) = \varepsilon \gamma_1^k$$

$$m_k(\gamma_1, \gamma_2; t) = \varepsilon \left( \frac{\gamma * \cdots * \gamma}{k-1} \right) = \varepsilon (k - 1) \gamma_1^{k-2} \gamma_2$$

(3.22)
depend only on $\gamma_1 = \beta_1 = -\lambda$ and $\gamma_2 = 2\beta_2 = -2\varepsilon\lambda^3$, by (3.8), (3.10) and Definition D.2. They are separated as their integral

$$k(k + 1)\frac{1}{\lambda^k(t)} \int_0^t e^{-\varepsilon k(k+1)(t-s)}(l_k(|\gamma_1|;s) + m_k(|\gamma_1|,|\gamma_2|;s))ds =$$

$$2\varepsilon\lambda(t)\frac{k(k+1)}{2} \frac{1}{\lambda^{k+1}(t)} \int_0^t e^{-\varepsilon k(k+1)(t-s)}\lambda^k(s)(1 + 2\varepsilon\lambda(s)(k-1))ds \equiv \mathcal{F}_k(t) \quad (3.23)$$

will be estimated more accurately than the respective integral for the remaining terms

$$\tilde{h}_k(\gamma_1, \ldots, \gamma_{k-1};t) = h_k(\gamma_1, \ldots, \gamma_{k-1};t) - l_k(\gamma_1;t) - m_k(\gamma_1, \gamma_2; t). \quad (3.24)$$

We refer to (3.15) and its refined procedure (3.16) for $k = 2$. To improve (3.15) for $k \geq 3$, let $\delta = (\delta_k)_{k \geq 1}$ be given by

$$\gamma_k(t) = \lambda^k(t) \delta_k(t), \quad \lambda(t) = \frac{1 - \eta(t)}{2\varepsilon} \text{ and } \eta(t) = e^{-2\varepsilon t}, \quad (3.25)$$

and note that $\sum_{k \geq 1} \delta_k r^k = \rho \varphi_{\rho}(t, \rho)$, $r = \lambda \rho$. By (3.20), (3.9) can be written as $\delta_1 = -1, \delta_2 = -(1-\eta),$

$$\delta_k(t) = -(1 - \eta(t)) \frac{k(k+1)}{2} \frac{1}{\lambda^{k+1}(t)} \int_0^t e^{-\varepsilon k(k+1)(t-s)}\lambda^k(s)\frac{1}{\varepsilon} h_k(\delta_1, \ldots, \delta_{k-1};s)ds, \quad (3.26)$$

for $k \geq 3$, and a majorant $\Psi(t, \rho) = \sum_{k \geq 1} C_k r^k$ of $\rho \varphi_{\rho}(t, \rho)$ will be constructed in the sense of Definition 3.3 for the variable $r$. Supposing that $|\delta_n(s)| \leq C_n(s)$ holds for $1 \leq n \leq k - 1$, equation
\[(3.26)\] can be majorized by
\[
|\delta_k(t)| \leq k(k + 1) \frac{1}{\lambda^k(t)} \int_0^t e^{-\varepsilon k(k+1)(t-s)} \lambda^k(s) \tilde{h}_k(|\delta_1|, \ldots, |\delta_{k-1}|; s) \, ds + \mathcal{S}_k(t)
\]
\[
\leq \frac{1}{\varepsilon} \tilde{h}_k(C_1, \ldots, C_{k-1}; t) + \mathcal{S}_k(t)
\]
\[
\leq \frac{1}{\varepsilon} h_k(C_1, \ldots, C_{k-1}; t) - \mathcal{S}_k(t),
\]
(3.27)
where, by (3.23), (3.24) and (3.25),
\[
\mathcal{S}_k(t) = \mathcal{D}_k(t) + (k-1)(1 - \eta(t)) \mathcal{D}_{k+1}(t)
\]
(3.28)
with
\[
\mathcal{D}_k(t) = 1 - (1 - \eta(t)) \frac{k(k+1)}{2} \frac{1}{\lambda^{k+1}(t)} \int_0^t e^{-\varepsilon k(k+1)(t-s)} \lambda^k(s) \, ds
\]
(3.29)
is such that

**Lemma 3.4** For every \( k \geq 3 \), the function defined by (3.28) and (3.29), as a function of \( \eta \):
\[
\mathcal{S}_k(t) = T_k \circ \eta(t)
\]
(3.30)
is a positive (concave) polynomial of degree \( k(k+1)/2 + 1 \) which satisfies \( T_k(0) = 0 \), \( T_k(1) = 1 \) and
\[
T_k(\eta) > \eta, \quad 0 < \eta < 1.
\]
(3.31)

**Proof.** Lemma 3.4 follows immediately from Proposition E.1 i–iv, whose statements and proof are deferred to Appendix E. A positive polynomial is a polynomial with positive coefficients. The degree and positivity of \( T_k \) follows from items i. and ii. and inequality (3.31) is stated in item iv. \( \square \)

Proposition E.1, the most technical result of the present work, will be useful also in the proof of Theorem 4.1.

**Remark 3.5** \( \mathcal{S}_k(t) \) for \( k = 2 \) differs from the other values of \( k \): \( \mathcal{S}_2(t) = \mathcal{D}_2(t) = \eta(t) \). Note that, by (3.7), \( h_2 \) has exactly one term and the second term in the r.h.s. of (3.28) does not appear for \( k = 2 \). As (E.2) deviates from the linear function \( \eta \) for \( k > 2 \) (see Fig. 3), the majorant sequence (3.32) is susceptible to be improved (see Remark 4.2 below).

Applying Lemma 3.4 to (3.27), the majorant sequence \( (\Psi_k)_{k \geq 1} \), given by (3.15), is redefined for \( k \geq 2 \) as:
\[
|\gamma_k(t)| \leq \frac{1}{\varepsilon} h_k(\Psi_1, \ldots, \Psi_{k-1}; t) - \eta \lambda^k := \Psi_k(t);
\]
(3.32)
summing (3.32) multiplied by $\rho^k$, yields an algebraic equation:

$$\frac{1}{1 - \Psi} - (1 + 2\Psi) + \lambda\rho - \eta \frac{\lambda^2 \rho^2}{1 - \lambda\rho} = 0$$

which is equivalent to a slightly modified quadratic polynomial equation for $\Psi$ (see (3.17) et seq.), whose solution is given by (3.18) with $H(r)$ replaced by

$$H_1(r) = \frac{1}{4} \left( 1 + r - \eta \frac{r^2}{1 - r} - \sqrt{\left( 1 + r - \eta \frac{r^2}{1 - r} \right)^2 - 8 \left( r - \eta \frac{r^2}{1 - r} \right)} \right).$$

As long as $|r| < 1$, the discriminant polynomial $p_1(r) = (1 - r^2 - \eta r^2)^2 - 8(r(1 - r)^2 - \eta r^2(1 - r))$ has four real roots:

$$R_{\sigma,\sigma'}(t, \varepsilon) = \frac{2 - \sigma' \sqrt{1 - \eta} + 2\sigma \sqrt{1 - \eta/2 - \sigma' \sqrt{1 - \eta}}}{1 + \eta}, \quad \sigma, \sigma' \in \{-1, 1\},$$

the smallest one, $R_{--}$, together with the threshold: $r = 0.28952$, has been depicted in Fig. 1 as a function of $\eta = e^{-2\varepsilon t}$.

It follows from (3.32) that $\Psi_k(t)$ is positive and monotone increasing function of $t$, which proves that $\Psi$ is a majorant of $\rho \varphi_{\rho}$ in the sense of Definition 3.3. Moreover, as $H_1|_{\eta=1}(r) = r$ for $0 \leq r \leq 1 - 1/\sqrt{2}$, all coefficients of the series for $\rho \Phi_{\rho}$ em power of $\lambda \rho$, except the first one, vanish in this limit as they are proportional to $(1 - \eta)$.

This concludes the proof of Theorem 3.1.

\[\square\]

4 Convergence of Power Series: Miscellaneous Methods

We summarize the result obtained so far and present some extensions, conclusions and comparisons.
1. The radius of convergence $R_\Phi(t)$ for the majorant $\Phi$ of $\varphi$ (r.h.s. of (3.1)) varies monotonously from $\infty = (1 - 1/\sqrt{2}) / \lim_{t \to 0} \lambda(t)$ to $2\varepsilon \cdot 0.171573 = (3/2 - \sqrt{2}) / \lim_{t \to \infty} \lambda(t)$ as $t$ varies from 0 to $\infty$. We recall that $\lambda = 2B_2$, where $B_2$ is the second virial coefficient.

2. The radius of convergence for the pressure $P(t, \rho)$, the Helmholtz free energy $F(t, \rho) - F_{\text{ideal}}(\rho) = -\beta(t, \rho)$ and the generating function $\varphi(t, \rho)$ satisfy

\[ R_P(t) = R_\beta(t) = R_\varphi(t) \geq R_\Phi(t) \]

by (2.17), Proposition 2.1 and (3.12). Inequality (3.2) in Corollary 3.2 improves Lebowitz–Penrose lower bound (B.10) for nonnegative potentials (put $\kappa = 1$ and $B = \lambda$ there) and surpass the threshold $0.278465/\lambda$ (see (B.4)), attainable via Mayer series (Theorem 4.3.2 of [Ru] et. seq.) for $\eta \geq 0$.

Asymptotic solution as $\varepsilon t$ tends to 0

As observed in Remark 3.5, the majorant sequence (3.32) may be modified to improve (3.2) further but we shall not follows this route. Instead, we re–address equations (3.25) et seq., satisfied by the coefficients $\delta_k = k\beta_n/\lambda^k$ of the power series of $\rho \varphi_\rho$ in the variable $r$, in order to obtain their asymptotic limit as $\varepsilon t$ tends to 0.

Our third conclusion, due to Theorem 4.1 below, together with (B.2)-(B.4), is

3. For $t\varepsilon \ll 1$, $\lambda R_P = 1$ holds even though $\lambda R_P \geq W(e^{-1}) = 0.278465...$, by Lagrange’s inversion formula.

**Theorem 4.1** Let (1.6) be the solution to the initial value problem (2.7) in power series of $\rho$ and write $\delta_k = k\beta_n/\lambda^k$, where $\lambda$ is given by (2.2). Then, $\delta_1(t) = -1$ and, for $k \geq 2$, $\delta_k(t)$ is $C^1$ with

\[ \lim_{t \to 0} \frac{\delta_k(t)}{t} = \dot{\delta}_k(0) = (-1)^{k+1}k\varepsilon . \]

(4.1)

The irreducible cluster integrals is thus given by $\beta_1 = -\lambda$ and

\[ \beta_k(t) = (-1)^{k+1}\lambda^k(t)\varepsilon t(1 + O(\varepsilon t)) , \quad k \geq 2 , \quad \varepsilon t \to 0 \]

(4.2)

where the $O(\varepsilon t)$ term has negative sign and

\[ \varphi(t, \rho) \sim -t\rho - \frac{t^2\rho^2}{1 + t\rho} \varepsilon t \]

(4.3)

is analytic in the domain $t |\rho| < 1$, as $\varepsilon t$ tends to 0.

**Proof.** Let $\delta = (\delta_k)_{k \geq 1}$ be the sequence of coefficients defined by (3.25)-(3.26). The derivative of (3.26), reads

\[ \dot{\delta}_k = -k(k + 1)h_k - \varepsilon k(k + 1)\delta_k + k\frac{\dot{\lambda}}{\lambda} \delta_k . \]

(4.4)
We observe that \( \lambda = (1 - \eta) / 2 \varepsilon \sim t \), \( \dot{\lambda} = \eta / \varepsilon \sim 1 \) and, with \( \delta_1 = -1 \) and \( \lim_{t \to 0} \delta_k = 0 \), for \( k \geq 2 \), (which will be proven by induction),

\[
\frac{h_k}{\varepsilon} \sim \left( \delta \ast \cdots \ast \delta \right)_k = (-1)^k .
\tag{4.5}
\]

These, together with \( (3.26) \), imply

\[
\lim_{t \to 0} \frac{1}{1 - \eta} \delta_k = -\frac{k(k + 1)}{2} \int_0^t (-1)^k s^k ds = (-1)^k \frac{k}{2} .
\tag{4.6}
\]

Substituting \( (4.5) \) and \( (4.6) \) into \( (4.4) \) gives \( (4.1) \).

Now, we prove that \( (4.2) \), for \( k \geq 2 \), hold by induction. For \( k = 2 \), \( \delta_2 = (1 - \eta) = -2 \varepsilon t + O((\varepsilon t)^2) \). Let us assume that \( \delta_j(t) \) is a \( C^1 \) function satisfying

\[
\delta_j(t) = (-1)^{j+1} \varepsilon t (1 + O(\varepsilon t)) , \quad j = 2, \ldots, k - 1 .
\tag{4.7}
\]

Since

\[
\left( \delta \ast \cdots \ast \delta \right)_k = (-1)^{k+1} j(k + j + 1) \varepsilon t + O((\varepsilon t)^2) , \quad j = 2, \ldots, k - 1
\tag{4.8}
\]

we have, by \( (3.7) \), together with \( (4.5) \),

\[ h_k(\delta_1, \ldots, \delta_{k-1}; s) = (-1)^k \varepsilon (1 + O(\varepsilon s)) \]

is \( C^1 \) and, by \( (3.26) \),

\[
\delta_k(t) = -2 \varepsilon t k(k + 1) \frac{1}{t^{k+1}} \int_0^t (-1)^k s^k (1 + O(\varepsilon s)) ds
\]

\[
= (-1)^{k+1} k \varepsilon t (1 + O(\varepsilon t))
\]

proving \( (4.7) \) for \( j = k \). Observe that the error term depends algebraically on \( k \), has negative sign, and \( \lim_{t \to 0} \delta_k(t) = 0 \) holds for any \( k \) fixed. Consequently, with \( r = \lambda \rho < 1 \),

\[
\sum_{k=1}^\infty \beta_k(t) r^k = -r - \sum_{k=2}^\infty (-1)^k r^k \varepsilon t (1 + O(\varepsilon t))
\]

\[
= -r - \frac{r^2}{1-r} \varepsilon t (1 + O(\varepsilon t))
\]

proving \( (4.3) \).
The stationary solution $\varphi_0$ of (2.7): upper bound for $\mathcal{R}_\varphi(\infty)$ We compare $\mathcal{R}_\varphi(\infty) = 2\varepsilon \times 0.171573$ with the radius of convergence $\mathcal{R}_\psi_0$ of the power series $\psi_0(\rho) = \sum_{k \geq 1} \tilde{\gamma}_n \rho^k$ whose coefficients $\tilde{\gamma}_k$’s solve the system of integral equations (3.9) in the limit as $t$ goes to $\infty$. Although the (limit) system of integral equations can be solved explicitly, the limit in $\rho \varphi_0(\infty, \rho) = \lim_{t \to \infty} \sum_{k \geq 1} \gamma_n \rho^k$ can be passed inside the sum in the domain $|\rho| < \mathcal{R}_\varphi(\infty)$, for which (1.6) is known to be uniformly convergent, by Definition 3.3. Consequently,

$$\mathcal{R}_\varphi(\infty) \leq \mathcal{R}_\varphi(\infty) \leq \mathcal{R}_\psi_0$$

with equality $\mathcal{R}_\varphi(\infty) = \mathcal{R}_\psi_0$ being satisfied if, and only if, the limit and sum in $\rho \varphi_0(\infty, \rho)$ can be interchanged.

The $\tilde{\gamma}_k$’s are shown in Proposition 4.3 below to be the coefficients of $\rho \varphi_0'(\rho)$ in power series of $\rho$, with $\varphi_0$ the stationary solution (4.14) of (2.7). We shall first calculate $\psi_0 = \rho \varphi_0'$. Setting $\varphi_t = 0$ in (3.4): $J(\rho, \rho \varphi_0') = 0$ where $J$ is given by (3.5), yields

$$\rho + \varepsilon \frac{\psi_0}{1 - \psi_0} = 0 \quad (4.9)$$

whose solution

$$\psi_0(\rho) = -\frac{\rho}{2\varepsilon \left( 1 - \rho/(2\varepsilon) \right)} \quad (4.10)$$

implies $\mathcal{R}_\psi_0 = 2\varepsilon = 1/\lambda(\infty)$. In view of (4.15), we have

$$0.171573 \leq \lim_{t \to \infty} \lambda(t) \mathcal{R}_P(t) \leq 1 \quad (4.11)$$

holds In the “low–temperature” limit ($t \to \infty$).

**Remark 4.2** Substituting in (3.27) the inequality $T_k(\eta) \geq \frac{6^k \varepsilon^k}{4^k \varepsilon^k},$ valid for $k \geq 3$ as $\eta \to 0$ (see Fig. 3), the lower bound 0.171573 in (1.11) can be replaced by 0.275451, still far from 1 (the upper bound). Since $\varphi_0(\rho)$ converges in a domain $|\rho/(2\varepsilon)| < 1$ so large as the domain $|\rho \lambda(t)| < 1$ of convergence of $\varphi$ for $\varepsilon$ small enough, in our second paper we investigate the power series solution (1.11) of (2.7) in exponential time variable $\eta = e^{-\varepsilon t}$ (transeries, see e.g. [Co]), asymptotic to $\varphi_0$ as $\varepsilon t \to \infty$, but we have found that solution belongs to a branch different from the one obtained by solving (3.9) for $t < \infty$.

**Proposition 4.3** Let the $\tilde{\gamma}_k$’s be recursively defined by

$$\tilde{\gamma}_k = -k(k + 1) \lim_{t \to \infty} e^{-\varepsilon k(k+1) t} \int_0^t e^{\varepsilon k(k+1)s} h_k(\tilde{\gamma}_1, \ldots, \tilde{\gamma}_{k-1}; s) \, ds, \quad k \geq 2 \quad (4.12)$$

with $\tilde{\gamma}_1 = -1/(2\varepsilon)$. Then, the system of integral equations is equivalent to

$$\tilde{\gamma}_k = -\frac{1}{\varepsilon} h_k(\tilde{\gamma}_1, \ldots, \tilde{\gamma}_{k-1}), \quad k \geq 2 \quad (4.13)$$
with \( \tilde{\gamma}_1 = -1/(2\varepsilon) \), whose solution

\[
\tilde{\gamma}_k = -\left(\frac{1}{2\varepsilon}\right)^k, \quad k \geq 1,
\]

are the coefficients of (4.10) in power series of \( \rho \).

Proof. The equivalence between (4.12) and (4.13) is shown by induction. Since \( \tilde{\gamma}_1 \) is constant, \( h_2(\tilde{\gamma}_1; s) = \tilde{\gamma}_1^2 \) does not depend on \( s \) and (4.12) reads

\[
\tilde{\gamma}_2 = -h_2(\tilde{\gamma}_1) \lim_{t \to \infty} 6e^{-6\varepsilon t} \int_0^t e^{6\varepsilon s} ds = -\frac{1}{\varepsilon} h_2(\tilde{\gamma}_1) \lim_{t \to \infty} (1 - e^{-6\varepsilon t}) = -\frac{1}{\varepsilon} h_2(\tilde{\gamma}_1)
\]

proving (4.13) for \( k = 2 \). Assuming that \( \tilde{\gamma}_1, \ldots, \tilde{\gamma}_{n-1} \) has been obtained by equation (4.13), then \( h_n(\tilde{\gamma}_1, \ldots, \tilde{\gamma}_{n-1}; s) \) does not depend on \( s \), and

\[
\tilde{\gamma}_n = -n(n+1) \lim_{t \to \infty} e^{-\varepsilon n(n+1)t} \int_0^t e^{\varepsilon n(n+1)s} h_n(\tilde{\gamma}_1, \ldots, \tilde{\gamma}_{n-1}; s) ds
\]

\[
= -\frac{1}{\varepsilon} h_n(\tilde{\gamma}_1, \ldots, \tilde{\gamma}_{n-1}) \lim_{t \to \infty} (1 - e^{-\varepsilon n(n+1)t})
\]

which proves (4.13) for \( k = n \) and concludes the induction. For the second part, multiplying by \( \rho^k \) and summing over \( k \geq 2 \) both sides of (4.13), yields

\[
\psi_0 + \frac{\rho}{2\varepsilon} = -\frac{\psi_0^2}{1 - \psi_0},
\]

by \( \tilde{\gamma}_1 = -1/(2\varepsilon) \), which is equivalent to (4.9), concluding the proof.

\[\square\]

Since \( \varphi_0'(\rho) = \psi_0(\rho)/\rho = (\log(1 - \rho/2\varepsilon))' \) and \( \varphi_0(0) = 0 \), we have

\[
\varphi_0(\rho) = \log \left(1 - \frac{\rho}{2\varepsilon}\right) \quad (4.14)
\]

Replacing \( \varphi_0'(\rho) \) into the first line of (2.17), taking into account that

\[
\psi_0(\rho) = 1 - \frac{1}{1 - \rho/(2\varepsilon)} = (\rho + 2\varepsilon \log (1 - \rho/(2\varepsilon)))'
\]

yields, for fixed \( \varepsilon > 0 \), the pressure at the stationary (ground) state

\[
P_0(\rho) = -2\varepsilon \log \left(1 - \frac{\rho}{2\varepsilon}\right) \quad (4.15)
\]

Note that the singularity at \( \rho = 2\varepsilon \) of \( P_0(\rho) \) is on the (positive) real line and its is of the same type as the one in Ford’s model (B.13). Summarizing the conclusions of the last two paragraphs,
we distinguish three different limits for the pressure of our simple particle system:

\[
\begin{align*}
\lim_{t \to 0} P(t, \rho) &= \rho \\
\lim_{\varepsilon \to 0} P(t, \rho) &= \rho + \frac{t}{2} \rho^2 \\
\lim_{t \to \infty} P(t, \rho) &= -2 \varepsilon \log \left(1 - \frac{\rho}{2 \varepsilon}\right)
\end{align*}
\]

attained for \(\rho\) on the domain of convergence (see items 3. and 4. above).

Remark 4.4

1. Mayer coefficients (4.14) satisfy \((-1)^{n-1}b_n \geq 0\) (see e.g. Theorem 4.5.3 of [Ru]) for any nonnegative potential (the uniformly repulsive in consideration, in particular) which means that the first (leading) singularity of \(\varphi(z)\) is at the negative real axis for all \(t > 0\). Theorem 4.1 shows that \((-1)^{n-1}\beta_n \geq 0\) holds in the limit as \(\varepsilon t\) goes to 0 whereas (4.15), the pressure as \(t\) goes to \(\infty\), is singular at \(\rho = 2 \varepsilon > 0\). The explicit computation of few coefficients \(\delta_n = \gamma_n/\lambda^n = n\beta_n/\lambda^n, n = 1, \ldots, 29\), in Fig. 4 of the power series of \(\rho \varphi_\rho\) in \(r\), reveals the interpolation of these two distinct behaviors: the \(\delta_n\)’s, as a function of \(t\), oscillates very much for \(t\) small but becomes more like each other as \(t\) increases. They will eventually converges to \(-1\) (the coefficients of \(\psi_0 = \rho \varphi'_0\) – see (4.10)). The time \(t^*_n\) for which \(\delta_n\) starts to converge from its maximum to \(-1\) depends on \(n\) and the convergence is very fast. Oscillations and change of signs of the \(\delta_n\)’s, as function of \(n\), are shown in Fig. 5 for different fixed values of \(t\). Sinusoidal oscillations occurs for most \(t\) (excluding special values), the period of which increasing with \(t\).

2. (4.15) can be rescaled to become independent of \(\varepsilon\). As a matter of fact,

\[
P_\varepsilon(t, \rho) = \varepsilon P_1 \left(\varepsilon t, \frac{\rho}{\varepsilon}\right)
\]

holds for any \((t, \rho) \in \mathbb{R}_+ \times \mathbb{C}\) by (2.7) and (2.17). We shall call (4.15) equation of state of Ford’s type as it is similar to equation (B.13), for \(|\rho| < 1/2\), and to the equation of state of a hard–core lattice gas.

Comparison with the Mayer series

Equations (2.4) and (1.7) have seen to be related to a combinatorial problem involving the sum of weights (E.20) over simply and two-connected, respectively, Mayer graphs. Our aim is to investigate how the reduction from simply to two-connected Mayer graphs affects the convergence of their generating functions and characterize, as much as possible, the nature of their leading singularities. In this investigation we are not concerned with the Lagrange’s inversion formula – we just compare both solutions, of (2.4) and (1.7), as a power series in \(z = e^\mu\) and \(\rho\), respectively.
Figure 4: The first 29 coefficients of the power series of $\rho \varphi$ in $r = \lambda \rho$, as $t$ varies in $[0, 0.5]$ (top) and $[0, 3]$ (bottom).
Figure 5: The value of the first 15 coefficients of the power series of $\rho \varphi$ in $r$ for $t = 0.17, 0.33$ and 0.75.
Restricting our attention to (2.4), we shall write a majorant series whose radius of convergence attains the best known lower bound for $R_{\wp}(t)$. We prove, in addition, that the radii of convergence of both, the majorant and the Mayer series for equation (2.4), are exactly the same in the limit as $\varepsilon t$ tends to 0.

**Theorem 4.5** The (normalized) radius of convergence $\lambda(t)R_{\wp}(t)$ of the Mayer series for the pressure (or density) of a system of point–particles with uniformly repulsive pairwise potential is a (strictly) monotone increasing function of $t \in \mathbb{R}_+$ and satisfies

$$\frac{1}{e} \leq \lambda(t) \leq 1$$

with equalities at the two extreme points $t = 0$ and $\infty$. Moreover, $\lim_{\varepsilon \to 0} e \lambda R_{\wp} = 1$ for any $0 < t < \infty$.

We thus conclude:

5. As $\varepsilon t$ tends to 0, an expressive gain of equation (1.7) is seen by Theorem 4.1 as

$$e^{-1} \leq \lambda(t) R_{\wp}(t) < \lambda(t) R_{\wp}(t) = 1.$$ In this limit, the radius of convergence of the generator function of two-connected Mayer graphs is 2.7 times larger than the radius of convergence of the generator function of simply-connected ones.

**Proof of Theorem 4.5** Writing $q(t,z) = \wp_z(t,z) = \sum_{k=0}^{\infty} q_k z^k$, by (1.3), we have

$$q_k = (k + 1)b_{k+1}$$

and equality of radii of convergences: $R_{\wp}(t) = R_q(t)$. The relation of the $q$–function to the density is $\rho(t,z) = z\wp_z(t,z) = zq(t,z)$ and equation (2.4) can be written in the form of a conservation law

$$q_t + \left(\varepsilon z^2 q_z + \frac{1}{2} z^2 q^2\right)_z = 0$$

with $q(0,z) = 1$. The sequence $(q_k)_{k \geq 0}$ of coefficients of its power series, denoted by $q$, satisfies

$$\dot{q}_0 = 0$$

$$\frac{1}{k+1} \dot{q}_k + \varepsilon k q_k = -\frac{1}{2} (q * q)_{k-1}, \quad k \geq 1$$

with $q_0 = 1$ and $q_k = 0$, $k \geq 1$. Here, the convolution product $(q * q)_m = \sum_{j=0}^{m} q_j q_{m-j}$, in contrast with (D.7), is defined for $m \geq 0$. By the variation of constants formula, (4.19) are analogous to

$$q_0(t) = 1$$
and
\[ q_k(t) = -\frac{1}{2} (k + 1) \int_0^t e^{-\varepsilon k (k+1)(t-s)} (q(s) * q(s))_{k-1} \, ds, \quad k \geq 1. \] (4.20)

For \( k = 1 \), we have
\[ q_1(t) = -\frac{1}{2\varepsilon} (1 - e^{-2\varepsilon t}) = -\lambda \]
where \( \lambda = \lambda(t, 1/(2\varepsilon)) \) is given by (2.2). By convenience, we write \( \lambda = (1 - \eta)/(2\varepsilon) \), \( \eta(t) = e^{-2\varepsilon t} \), and introduce \( \tilde{q} = (\tilde{q}_k)_{k \geq 0} \) with \( \tilde{q}_k = q_k/\eta^k \), so (4.20) can be written as
\[ \tilde{q}_k(t) = -\frac{1}{2} (k + 1) \int_0^t e^{-\varepsilon k (k-1)(t-s)} \frac{1}{\eta(s)} (\tilde{q}(s) * \tilde{q}(s))_{k-1} \, ds. \] (4.21)

A sequence \( \tilde{Q} = (\tilde{Q}_k)_{k \geq 0} \) that majorizes \( \tilde{q} = (\tilde{q}_k)_{k \geq 0} \) (putting \( \tilde{Q}_k = Q_k/\eta^k \), \( (q_k)_{k \geq 0} \) is majorized by \( (Q_k)_{k \geq 0} \)), in the sense of Definition (3.3), is obtained as follows:
\[ \tilde{q}_0(t) = \tilde{Q}_0(\tau) = 1 \]
and
\[ |\tilde{q}_k(t)| \leq \frac{1}{2} (k + 1) \int_0^t e^{-\varepsilon k (k-1)(t-s)} \frac{1}{\eta(s)} (|\tilde{q}(s)| * |\tilde{q}(s)|)_{k-1} \, ds \]
\[ \leq \frac{1}{2} (k + 1) \int_0^t \frac{1}{\eta(s)} (|\tilde{q}(s)| * |\tilde{q}(s)|)_{k-1} \, ds \]
\[ \leq \frac{1}{2} (k + 1) \int_\tau^t \tilde{Q}(\tau') * \tilde{Q}(\tau')_{k-1} \, d\tau' := \tilde{Q}_k(\tau). \] (4.22)

where \( \tau = \tau(t) = \int_0^t (1/\eta(s)) \, ds = \lambda(t)/\eta(t) \) is strictly increasing. Writing \( \omega = \eta(t)z \), we have
\[ Q(t, z) := \sum_{k=0}^\infty Q_k(t)z^k = \sum_{k=0}^\infty \tilde{Q}_k(\tau)\omega^k := \tilde{Q}(\tau, \omega) \] (4.23)
and the system of equations for \( (\tilde{Q}_k)_{k \geq 1} \), going backward through the steps (4.19)-(4.20), is equivalent to the following PDE (compare with (4.18))
\[ \tilde{Q}_\tau - \frac{1}{2} (\omega^2 \tilde{Q}^2)_{\omega} = 0 \] (4.24)
with \( \tilde{Q}(0, \omega) = 1 \), whose solution can be explicitly written in terms of the Lambert \( W \)-function (see Subsection 5.1 of [GM])
\[ Q(t, z) = \tilde{Q}(\tau, \omega) = -\frac{1}{\tau \omega} W(-\tau \omega) = -\frac{1}{\lambda z} W(-\lambda z) \] (4.25)
(i.e., \( W(x) \) is the principal branch of the inverse of \( f(W) = W e^W \), regular at origin \([\text{C-K}]\)). As a consequence (see Appendix \([\text{B}]\), (4.23) converges provided

\[
e^\tau |\omega| = e\lambda |z| < 1 \quad (4.26)
\]

which, together with (4.22), establishes the first inequality of (4.16): \( e\lambda R_\varphi \geq e\lambda R_Q \geq 1 \). Note that the majorant relation (4.22) (denoted by \( q \ll Q \)) is preserved by derivation, anti–derivation integration w.r.t. \( t \) and composition.

To prove equality, we introduce another sequence \( c = (c_k)_{k \geq 0} \) with \( c_k = (-1)^k q_k / \lambda^k \). As one can see from (4.20), the factor \((-1)^n\) compensates the alternating sign of \((q_k)_{k \geq 0}\) (see Theorem 4.5.3 of \([\text{Ru}]\)) so \( c_k \geq 0 \) holds for every \( k \). It also follows from (4.20) that

\[
c_k(t) = \frac{k + 1}{2} \frac{1}{\lambda^k(t)} \int_0^t e^{-\varepsilon k (k+1)(t-s)} \lambda^{k-1}(s) (c(s) * c(s))_{k-1} \, ds , \quad k \geq 1 \quad (4.27)
\]

with \( c_0(t) \equiv 1 \). The asymptotic \( \lambda(t) \sim t \), as \( t \) tends to 0, together with right continuity of \( c_k(t) \) at \( t = 0 \) yield

\[
c_k(0) = \frac{k + 1}{2k} (c(0) * c(0))_{k-1} , \quad k \geq 1 \quad (4.28)
\]

with \( c_0 = 1 \), whose solution is well known (see Lemma \([\text{E.3}]\) in Appendix \([\text{E}]\)):

\[
c_k(0) = \frac{(k + 1)^k}{(k + 1)!} . \quad (4.29)
\]

Note that, by (4.17), \((-1)^{n-1} c_{n-1}(0) = nb/n! = (-n)^{n-1}/n!\) coincide with the coefficients of the Mayer series \([\text{B.3}]\) for the (conveniently normalized) density of a hard sphere gas in \( d = \infty \) and also (in absolute value) with the coefficients of the majorant function (4.25), proving the equality \( \lim_{t \to 0} e\lambda (t) R_\varphi(t) = 1 \). The same is true as \( \varepsilon \) tends to 0 for any \( t \in \mathbb{R}_+ \), as one can see by taking \( \varepsilon = 0 \) in (4.18) (or indirectly from (4.20)), whose solution is given by (4.25) with \( z \) replaced by \(-z\), by which the sign of the nonlinear term in (4.24) changes from minus to plus.

Differentiating (4.27) w.r.t. \( t \), gives

\[
\dot{c}_k = -\varepsilon k (k + 1) c_k - \frac{1}{2\lambda} (2\eta k c_k - (k + 1) (c * c)_{k-1}) , \quad k \geq 2 \quad (4.30)
\]

with \( \dot{c}_0 = \dot{c}_1 \equiv 0 \) and, to prove Theorem 4.5, we need to show that \( \dot{c}_k(t) \) remains negative for all \( t \in \mathbb{R}_+ \). We also need \( \lim_{t \to \infty} c_k(t) = 1 \) for the upper bound in (4.16) – see computer evaluation of \( q_k(t) / \lambda^k(t) \), \( k = 0, \ldots, 13 \), in Fig. 6. We formulate these statements in the following proposition, whose proof (considerably more technical) is deferred to Appendix \([\text{E}]\).

**Proposition 4.6** Let \( (c_k(t))_{k \geq 0} \) be given by \( c_k = (-1)^k q_k / \lambda^k \) with \( (q_k)_{k \geq 0} \) the solution of (4.20) with \( q_0(t) \equiv 1 \). Then, for every \( k \), \( c_k(t) \) is monotone decreasing in \( t \), \( c_k(0) = \lim_{t \to 0} c_k(t) \) satisfies (4.29) and \( \lim_{t \to \infty} c_k(t) = 1 \).
This concludes the proof of Theorem 4.5.

**Remark 4.7** As $t$ tends to $\infty$, $\lambda \to 1/(2\varepsilon)$, $q \to \sum_{k \geq 0} (-z/2\varepsilon)^k = 1/(1 + z/2\varepsilon)$ and $\rho = zq \to z/(1 + z/2\varepsilon)$ can be inverted $Z(\rho) = \rho/(1 - \rho/2\varepsilon)$. The pressure $\varphi_0 = 2\varepsilon \sum_{k \geq 1} (-z/2\varepsilon)^k / k$ composed with $Z(\rho)$:

$$P_0(\rho) = \varphi_0 \circ Z(\rho) = 2\varepsilon \log \left( 1 + \frac{\rho/2\varepsilon}{1 - \rho/2\varepsilon} \right),$$

agrees with the limit pressure (4.15). In this limit, $Z(\rho)$ and its inverse $\rho(z)$ are single–valued inside the disc $D_{2\varepsilon}$, the same disc for which the power series of $Z(\rho)$ and $P_0(\rho)$ converge. However, $D_\varepsilon$ is the largest disc such that $Z(D_\varepsilon) \subset D_{2\varepsilon}$ and we can only conclude with this information that $P_0(\rho) = \varphi_0 \circ Z(\rho)$ converges, at least, in $D_\varepsilon$.

# A Irreducible Cluster Integrals and their Relation to the Virial Coefficients

The grand–canonical ensemble of interacting particles in a container $\Lambda$, i.e. a regular domain in $\mathbb{R}^d$ of volume $V = |\Lambda|$, with activity (fugacity) $z$ at the inverse temperature $\beta = 1/(kT)$ has a
partition function
\[ \Xi_\Lambda(\beta, z) = \sum_{n=0}^{\infty} z^n Q_{\Lambda,n}(\beta) \] (A.1)

where \((Q_{\Lambda,0} = 1)\)

\[ Q_{\Lambda,n}(\beta) = \frac{1}{n!} \int_{\Lambda^n} e^{-\beta U(x)} d^{dn}x \] (A.2)
is the canonical partition function and \(U = U(x)\) is the pairwise interacting energy of a configuration \(x = (x_1, \ldots, x_n) \in \Lambda^n = \Lambda \times \cdots \times \Lambda\) of \(n\) particles.

Let \(\Lambda^\sharp = \bigcup_{n=0}^{\infty} \Lambda^n\) be the space of all (finite) \(n\)-tuple \(x = (x_1, \ldots, x_n) \in \Lambda^n\) (\(\Lambda^0\) is a set of a single point; the integral over \(\Lambda^0\) in (A.2) is 1, by convention) and let

\[ N : \Lambda^\sharp \rightarrow \{0, 1, \ldots\} \equiv \mathbb{Z}_+ \] (A.3)

be a function that assigns the number of particles (components) to each state \(x = (x_1, \ldots, x_n)\) in \(\Lambda^\sharp: N(x) = n\). The equilibrium measure in \(\Lambda^\sharp\) can thus be written as

\[ \mu_{\Lambda,\beta,z}(d^\#x) = \frac{1}{\Xi_\Lambda(\beta, z) N(x)!} z^{N(x)} e^{-\beta U(x)} d^\#x \] (A.4)

where, for each \(n = 0, 1, \ldots\), the restriction of \(d^\#x\) to \(\Lambda^n\) is the Lebesgue measure.

**Proposition A.1** The formal pressure \(p = p_\Lambda(\beta, \mu)\) and mean density \(\rho = \rho_\Lambda(\beta, z)\), defined by\(^3\)

\[ \beta p_\Lambda(\beta, \mu) = \frac{1}{|\Lambda|} \log \Xi_\Lambda(\beta, e^\mu) \] (A.5)

and

\[ \rho_\Lambda(\beta, z) = \beta \frac{\partial p_\Lambda}{\partial \mu}(\beta, \mu) \] (A.6)

are, respectively, convex and monotone non-decreasing function of \(\mu = \log z\).

**Proof.**

\[ \beta \frac{\partial^2 p_\Lambda}{\partial \mu^2} = \frac{1}{|\Lambda|} \left( \mathbb{E} N^2 - (\mathbb{E} N)^2 \right) = \frac{1}{|\Lambda|} \text{Var} N \geq 0 \]

\[ \beta \frac{\partial p_\Lambda}{\partial \mu} = \frac{1}{|\Lambda|} \mathbb{E} N \geq 0 \]

where \(\mathbb{E}(\cdot)\) means expectation with respect to (A.4).

\(\square\)

\(^3\)We denote by \(p\) and \(\rho\) the pressure as a function of the chemical potential \(\mu\) and activity \(z = e^\mu\), respectively. The derivative of the pressure with respect to \(\mu\) and \(z\) are related by \(\partial p/\partial \mu = z \partial \rho/\partial z\). The capital letter \(P\) is reserved to the pressure as a function of the density \(\rho\).
Ideal gas equation of state  For an ideal gas, we set $U \equiv 0$ in (A.4). By (A.5) and (A.6), we have
\[ \beta \varphi = z \quad \text{and} \quad \rho = z ; \] (A.7)
therefore, the equation of state $P(\rho) = \varphi \circ Z(\rho)$ ($Z$ is the inverse of $\rho(z)$) for an ideal gas reads
\[ \beta P = \rho , \]
for all $\Lambda$.

Mayer series  For a real (non–ideal) gas of particles interacting via a two–body potential
\[ \phi(x_i - x_j) \equiv \phi_{ij} \] (A.8)
invariant under translations and rotations in $\mathbb{R}^d$, we have
\[ U(x) = \sum_{1 \leq i < j \leq N(x)} \phi_{ij} . \]
We define
\[ f_{ij} = e^{-\phi_{ij}} - 1 \] (A.9)
and write the Boltzmann factor as a sum over the set $\mathcal{M}$ of Mayer graphs $G$ (i.e., simple linear graphs) in the set \{1, 2, \ldots, $N(x)$\} of labelled vertices:
\[ e^{-\beta U(x)} = \prod_{1 \leq i < j \leq N(x)} (1 + f_{ij}) = \sum_{G \in \mathcal{M}} \prod_{(ij) \in E} f_{ij} \] (A.10)
where the product runs over the $(ij)$ in the set of edges $E = E(G)$ of $G$.

We define for every Mayer graph $G$ a weight
\[ W(G) = \int_{\Lambda^N} \prod_{(ij) \in E(G)} f_{ij}(x) d^d x , \] (A.11)
($N = N(G)$ being, by definition, the number of vertices in $G$) and write the grand–partition function as
\[ \Xi_{\Lambda}(z) = \sum_{G \in \mathcal{M}} \frac{z^N}{N!} W(G) . \]
The first Mayer theorem reads (see Theorem I of [UF])

**Theorem A.2**
\[ \log \Xi_{\Lambda}(z) = \sum_{G \in \mathcal{M} : G \text{ connected}} \frac{z^N}{N!} W(G) \] (A.12)
Proof. We observe that the weight function \( \text{(A.11)} \) is independent of the labelling of the \( N \) vertices and, for any Mayer graph \( G \) whose connected parts are \( G_1, \ldots, G_k \), we have \( W(G) = W(G_1) \cdots W(G_k) \). These are the ingredients behind its proof, which we refer to [Ru, B].

By Theorem A.2, the pressure \( \text{(A.5)} \) can be written as a formal power series

\[
\beta \varphi_{\Lambda}(\beta; z) = \frac{1}{|\Lambda|} \sum_{G \in \mathcal{G}: G \text{ connected}} \frac{z^N}{N!} W(G)
\]

\[
= \sum_{n=1}^{\infty} b_{\Lambda,n} z^n := \chi_{\Lambda}(z)
\]

where, for \( n \geq 1 \),

\[
b_{\Lambda,n} = \frac{1}{n!} \sum_{G \in \mathcal{G}: G \text{ connected}, N(G) = n} \frac{1}{|\Lambda|} \int_{\Lambda^n} \prod_{(ij) \in E(G)} f_{ij}(x) d^d x
\]

are the Mayer coefficients. From now on we omit the dependence on the inverse temperature \( \beta \) to avoid notational conflict.

**Irreducible cluster integrals** Referring to \( \text{(A.11)} \) with \( G \) connected, we define \( w(G) \) by holding one vertex, let us say \( x_1 \), fixed at origin while \( x = (x_1, \ldots, x_N) \) is integrated over \( \Lambda^{N-1} \)

\[
w(G) = \int_{\Lambda^{N-1}} \prod_{(ij) \in E(G)} f_{ij}(x) d^d x.
\]

By translational invariance of \( \phi_{ij} \), in the thermodynamic limit, \( w(G) \) is independent of the vertex to be fixed. Assuming \( f_{ij} \in L^1(\mathbb{R}^d) \), the limit of \( W(G)/|\Lambda| \) and \( w(G) \) exist along any sequence \( (\Lambda_m)_{m \geq 1} \) of regular domains tending to \( \mathbb{R}^N \) (see e.g. [Ru]), and for any connected graph \( G \), we have

\[
\lim_{m \to \infty} \frac{1}{|\Lambda_m|} W_m(G) = \lim_{m \to \infty} w_m(G) = w_{\infty}(G).
\]

**Definition A.3** A vertex \( i_0 \) is said to be an articulation point of a connected Mayer graph \( G \) if \( G \) becomes disconnected after its removal. A graph \( G \) with no articulation points is called a block or a irreducible graph.

A weight function \( w \) is said to be block–multiplicative if for any connected Mayer graph \( G \), whose blocks are \( G_1, \ldots, G_k \), we have

\[
w(G) = w(G_1) \cdots w(G_k).
\]

We define the Mayer graph consisting of a single vertex to be not a block. The simplest block (2–block) consists of a single edge together with two end points. The next simplest one (3–block) has three vertices and three edges cyclically connected.
Referring to (A.12), with connected Mayer graphs $G$ replaced by blocks, we define

$$B(\Lambda) = \sum_{G\in \mathcal{M}: G \text{ is a block}} \frac{\rho^N}{N!} W(G)$$

and, analogously,

$$\beta(\Lambda) = \sum_{G\in \mathcal{M}: G \text{ is a block}} \frac{\rho^N}{N!} w(G) = \sum_{n=1}^{\infty} \frac{1}{n+1} \beta_n \rho^{n+1}$$

where (A.17) defines the $\beta_{n-1}$, which are called (irreducible) cluster integrals of order $n$. The second Mayer theorem may be stated as (see Theorem II of [UF] for a proof)

**Theorem A.4** The thermodynamic limits $\rho(z) = \lim_{n\to\infty} \rho_{\Lambda_n}(z)$ and $\beta(\rho) = \lim_{n\to\infty} \beta_{\Lambda_n}(\rho)$, satisfy a functional equation

$$\rho(z) = ze^{\beta' \circ \rho(z)} .$$

A simpler proof which holds for formal power series is provided in Leroux’s article on combinatorial species [Le], Theorem 1.3. The key ingredient is the block–multiplicative property of the weight function (A.15) in the thermodynamic limit (see Proposition 2.2 of [Le]).

Theorem A.4 also holds for finite $\Lambda$ provided the limit is taken over $\Lambda_m = [k_m, k_m^d]$, for an strictly increasing sequence of positive numbers $(k_m)_{m\geq 1}$, with $\phi = \phi(x)$ satisfying periodic boundary conditions: $\phi(x) = \phi(x + k_m e_j)$ for each direction $e_j$ of $\mathbb{R}^d$. In this case $w_m(G)$ for any finite volume $\Lambda_m$ is block–multiplicative (see Lemma 2 of [PTS]). We gave in (2.1) another example of pair potential in which block–multiplicativity (A.16) holds for any $\Lambda \subset \mathbb{R}^d$, with $w(G)$ depending only on its volume $|\Lambda|$. From here on, we deal with the formal power series (A.13) and (A.17). For notational simplicity, we drop the index $\Lambda$ everywhere, independently of whether the thermodynamic limit has already been taken.

**Reduction of cluster integrals** The relation between the cluster integrals $(b_l)_{l\geq 1}$ (Mayer coefficients) and the irreducible cluster integrals $(\beta_l)_{l\geq 1}$ (related to virial coefficients) is obtained as follows. By definitions (A.17),

$$\beta'(\rho) = \sum_{n=1}^{\infty} \beta_n \rho^n := \varphi(\rho)$$

and the equation (A.18) can be written as

$$z = \rho(z) e^{-\varphi \circ \rho(z)} .$$
Taking the derivative in both sides

\[ 1 = (1 - \rho(z)(\varphi' \circ \rho)(z)) e^{-\varphi(\rho)} \rho'(z) \]

yields, assuming provisionally that the series (A.19) converges absolutely in a disc \( D \) centered at \( \rho = 0 \),

\[ z\rho'(z) = \frac{\rho(z)}{1 - \rho(z)(\varphi' \circ \rho)(z)} \quad (A.21) \]

by the residue theorem (see Theorem 9.1.1 of [Hi] et seq.), with the integral over a contour \( C \) in \( D \) containing the origin in its interior. Note that, by the implicit function theorem (see e.g. Theorem 9.4.4 of [Hi])

\[ \rho - ze^{\varphi(\rho)} = 0 \quad (A.23) \]

has a unique holomorphic solution \( \rho^* = \rho^*(z) \) for \( z \) in a disc \( D' \) centered at \( z = 0 \) with \( \rho^*(0) = 0 \) and \( \rho''(0) = 1 \) and \( C \) can be chosen so that \( \rho^*(z) \) remains inside \( C \) for every \( z \in D' \). By Rouché’s theorem, [Hi] that condition is expressed by

\[ \left| \frac{z}{\rho} e^{\varphi(\rho)} \right| < 1, \quad \rho \in C, \quad (A.24) \]

and (A.22) can be written as

\[ z\rho'(z) = \frac{1}{2\pi i} \int_C \sum_{l=1}^{\infty} \frac{z^l e^{l\varphi(\rho)}}{\rho^l} d\rho \]

\[ = \sum_{l=1}^{\infty} \left( \frac{1}{2\pi i} \int_C \frac{e^{l\varphi(\rho)}}{\rho^l} d\rho \right) z^l \]

which, when compared to the series (the second derivative of (A.13) times \( z^2 \)):

\[ z\rho'(z) = \sum_{l=1}^{\infty} l^2 b_l z^l, \]

together with Cauchy theorem, gives \( b_1 = 1 \) and

\[ b_l = \frac{1}{l^2} \left( e^{l\varphi(\rho)} \right)^{(l-1)}(0) \]

for every \( l \geq 2 \) (from here on, \( h^{[l]}(\rho_0) = h^{(l)}(\rho_0)/l! \) denotes \( l \)–th derivative of \( h(\rho) \), divided by \( l! \), at the point \( \rho_0 \)).
Applying Faà di Bruno formula (see e.g. \[FLy\])

\[
(f \circ g)^{(l)}(\rho) = \sum_{n_1, \ldots, n_l \geq 0; \ n_1 + 2n_2 + \cdots + l n_l = l} \frac{1}{n_1! \cdots n_l!} \cdot g^{[1]}(\rho)^{n_1} \cdots g^{[l]}(\rho)^{n_l} \cdot (f^{(n_1 + \cdots + n_l)} \circ g)(\rho)
\]  

(A.25)

for high order chain with \(f(y) = e^y\) and \(g(\rho) = l\varphi(\rho) = l\beta'(\rho)\) at \(\rho = 0\), yields the desired reduction of cluster integrals in terms of the irreducible ones:

\[
b_l = \frac{1}{l^2} \sum_{n_1, \ldots, n_{l-1} \geq 0; \ n_1 + 2n_2 + \cdots + (l-1)n_{l-1} = l-1} \frac{1}{n_1! \cdots n_l!} \cdot \prod_{i=1}^{l-1} (l\beta_i)^{n_i}.
\]  

(A.26)

\[\square\]

**Remark A.5** We have applied the analytic function method (Lagrange’s inversion formula) proposed in \[UK\] and developed in \[BF\] backward, i.e., starting from the functional equation \(\rho(\varphi) = \rho\). A combinatorial interpretation of \(\text{(A.26)}\) is possible in terms of Husimi graphs \(G\) with \(N(G) = l\), labelled by \(\{1, \ldots, l\}\), all of whose blocks \(K_{n_j}, j = 1, \ldots, k\), are complete graphs of size \(n_j\) (see eq. (36) and Theorem 3.2 of \[Le\]).

**Remark A.6** The very same equations hold as a formal power series if, instead of \(\text{(A.22)}\), Lagrange –Bürmann formula \[He\]

\[
R \circ \rho(z) = \sum_{n=1}^{\infty} \frac{1}{n} \cdot \text{Res} \left( R' Z^{-n} \right) z^n
\]  

is applied to \(\text{(A.21)}\). Here \(Z \circ \rho(z) = z\), i.e., \(Z(\rho) = \sum_{n \geq 1} c_n \rho^n\) is the formal inverse of \(\rho(z)\)

\[
R(\rho) = \frac{\rho}{1 - \rho \varphi'(\rho)} = \sum_{n=1}^{\infty} a_n \rho^n
\]

and, for \(m \in \mathbb{Z}\),

\[
Z^m(\rho) = \sum_{n=-\infty}^{\infty} c_n^{(m)} \rho^n
\]

is the \(m\)-th power (not necessarily positive) of \(Z\), defined on the ring of formal Laurent series with finitely many negative subscripts different from zero; \(\text{Res}(F)\) in \(\text{(A.27)}\) means the \(a_{-1}\) coefficient of \(F\).

The inverse of \(\text{(A.26)}\),

\[
\beta_k = \sum_{n_1, \ldots, n_{k+1} \geq 0; \ n_2 + 2n_3 + \cdots + kn_{k+1} = k} (-1)^{n_2 + \cdots + n_{k+1} - 1} \frac{(k + n_2 + \cdots + n_{k+1} - 1)!}{k!} \prod_{i=2}^{k+1} \frac{(ib_i)^{n_i}}{n_i!}
\]  

(A.28)
can be obtained analogously (see eq. (49) of [M] and eqs. (2.1)-(2.5) of [LP]). Let (A.18) be written as

\[ \rho = Z(\rho)e^{\varphi(\rho)}, \]

where \( Z(\rho) \) is the inverse of \( \rho(z) \). Differentiating both sides w.r.t. \( \rho \) and using the fact that the condition \( (A.24) \), expressed by Rouché’s theorem, is equivalent to \( |\rho/\rho(z)| < 1 \) for \( z \in C' = Z(C) \) where \( C \) is the contour chosen in \( (A.22) \), we have

\[
\rho \varphi'(\rho) = 1 - \frac{\rho}{Z(\rho)} \frac{1}{\rho' \circ Z(\rho)} \int_{C'} \frac{1}{z} \left( 1 - \frac{\rho(z)}{\rho(z) - \rho} \right) dz
\]

\[
= -\frac{1}{2\pi i} \oint_{C'} \frac{1}{z} \frac{\rho/\rho(z)}{1 - \rho/\rho(z)} dz
\]

\[
= \sum_{k=1}^{\infty} \left( -\frac{1}{2\pi i} \oint_{C'} \frac{1}{z} \left( \frac{\rho(z)}{z} \right)^k \frac{1}{z^{k+1}} dz \right) \rho^k
\]

which implies

\[ k\beta_k = -((\rho(z)/z)^{-k})^{[k]}(0), \]

by Cauchy formula, and \( (A.28) \) by applying Faà di Bruno formula \( (A.25) \) – the argument \( \rho \) changed to \( z \) – with \( f(y) = y^{-k} \) and \( g(z) = \rho(z)/z = 1 + \sum_{n \geq 2} n b_n z^{n-1} \) at \( z = 0 \).

**Kamerlingh Onnes virial series**  Equation \( (A.21) \) together with \( (A.6) \) yields (with \( P(\rho) = \varphi \circ Z(\rho) \))

\[
\beta P'(\rho) = \frac{\beta \varphi'(\rho)}{\rho'}
\]

\[
= 1 - \rho \varphi'(\rho)
\]

\[ (A.29) \]

\[
= 1 - \sum_{l=1}^{\infty} l \beta_l \rho^l.
\]

\[ (A.30) \]

The Kamerlingh Onnes virial series

\[
\beta P(\rho) = \sum_{n=1}^{\infty} B_n \rho^n
\]

is thus obtained by integrating term–by–term \( (A.30) \):

\[
\beta P(\rho) = \rho \left( 1 - \sum_{l=1}^{\infty} \frac{l}{l+1} \beta_l \rho^l \right)
\]

\[ (A.32) \]
which gives, by (A.17),

\[ B_n = -\frac{n-1}{n} \beta_{n-1} \]  \hspace{1cm} (A.33)

with

\[ \beta_{n-1} = \frac{1}{(n-1)!} \sum_{G: G \text{ is a block of order } n} \frac{1}{|\Lambda|} \int_{\Lambda^n} \prod_{(ij) \in E(G)} f_{ij}(x) d^2 x . \]  \hspace{1cm} (A.34)

**The Helmholtz Free–Energy** Alternatively, we may follow another direction already known by Mayer (see e.g. [MM], eqs. (13.47)-(13.50))

**Proposition A.7** The Helmholtz free energy density \( F(\rho) = -(1/|\Lambda|) \log Q_{\Lambda,N} \), with \( \rho = N/|\Lambda| \) finite, in the thermodynamic limit, is formally given by the Legendre transform

\[ F(\rho) = \sup_{\mu} (\mu \rho - \beta \varphi(e^{\mu})) = \rho \log \rho - \rho - \beta(\rho) \]  \hspace{1cm} (A.35)

where \( \beta(\rho) \) is defined by (A.17). Hence, by (A.19), \( \varphi(\rho) = \beta'(\rho) = -F'(\rho) + \log \rho \) generates the irreducible cluster integrals \( \beta_n, n = 1, 2, \ldots \).

**Proof.** As a formal power series, \( \mu^* = \mu^*(\rho) \) solves the equation \( \rho = \beta \varphi'(e^{\mu}) \cdot e^{\mu} \) for \( \mu \), and \( P(\rho) = \varphi \circ e^{\mu^*}(\rho) \) is, by definition, the pressure (as a function of \( \rho \)) where \( p(\mu) = \varphi(e^{\mu}) \) is a convex function of \( \mu \in \mathbb{R} \), by Proposition A.1. This implies that \( F \) is a convex function of \( \rho \in \mathbb{R}_+ \) and

\[ \beta p(\mu) = \sup_{\rho} (\mu \rho - F(\rho)) . \]

The two first terms in the r.h.s. of (A.35) are ideal gas contributions to the Legendre transform: by (A.7), \( F_{\text{ideal}}(\rho) = \sup_{\mu} (\mu \rho - e^{\mu}) = \mu^* \rho - e^{\mu^*} = \rho \log \rho - \rho \). The last term of (A.35) is obtained by solving (A.20) with \( z = e^{\mu} \) and \( \varphi \) given by (A.19) for \( \mu \):

\[ \mu^* = \mu^*(\rho) = \log \rho - \sum_{n=1}^{\infty} \beta_n \rho^n \]  \hspace{1cm} (A.36)

Replacing \( \mu^* \) into \( F(\rho) = \mu^* \rho - \beta \varphi(e^{\mu^*}) = \mu^* \rho - \beta P(\rho) \), together with (A.32) and (A.17), yields (A.35).

\[ \square \]

**B Convergence of Virial Series: Overview and Previous Results**

The first convergence proof of virial series by Lebowitz–Penrose [LP] (see Ruelle [Ru], Theorem 4.3.2, commentary on p. 86 for non–negative potentials and review MR0226924 by O. Penrose)
estimates $R_P$ from an estimate on the convergence of the Mayer series (A.13). Lebowitz–Penrose’s method provides a lower bound for $R_P$ which inherits a limitation coming from a (nonphysical) singularity, of combinatorial origin, that prevents the Mayer series to be convergent beyond that point. We shall explain how this limitation has been circumvented by our method.

**Gas of hard spheres in $d = \infty$: virial series** We begin by examining (A.23) for a gas of hard spheres in infinitely many dimensions. In this limit, since all $n$–blocks with $n > 2$ give no contributions, we have (see eq. (6) of \[FRW\])

$$\varphi(\rho) = \rho \; . \quad (B.1)$$

We look at (A.20) as a map from the complex $\rho$–plane to the complex $z$–plane:

$$\rho \in \mathbb{C} \mapsto \rightarrow Z(\rho) \in \mathbb{C} \quad \text{where} \quad Z(\rho) = \rho e^\rho \; . \quad (B.2)$$

Figure 7 depicts circles images $Z(\rho)$, $|\rho| = \text{const.}$, in the complex $\rho$–plane. Note the formation of a cusp at $-e^{-1}$ as a consequence of the fact that $Z'(\rho) = (1 + \rho) e^\rho$ vanishes at $\rho = -1$. Recall that an analytic function $f : D \to \mathbb{C}$ is univalent in an open domain $D$ if $f(\rho_1) \neq f(\rho_2)$ for all $\rho_1, \rho_2 \in D$ with $\rho_1 \neq \rho_2$. Hence, $Z(\rho)$ is univalent in any disc $D_\tau$ centered at origin with radius $\tau \leq 1$.

The inverse $\rho(z)$ of $Z(\rho)$ is the Lambert $W$–function $W(z)$, a multivalued function whose principal branch is defined in the slit domain $\mathbb{C}\setminus(-\infty, e^{-1}]$ (see e.g. \[C-K\]).

The Mayer series $\rho(z) = \sum_{n \geq 1} nb_n z^n$ for the hard-sphere density function is, in this limit, a sum of free diagrams which may be evaluated from $\rho(z) = W(z)$ by the Lagrange method:

$$nb_n = \frac{(-n)^{n-1}}{n!} \; ; \quad (B.3)$$

its radius of convergence is thus $r = e^{-1}$. To recover the virial series, $P(\rho) = \varphi \circ Z(\rho)$ is defined in a disc $D_{r'}$ of radius $r'$ in the $\rho$–plane such for $|Z(\rho)| < e^{-1}$ for every $\rho \in D_{r'}$, i.e., $Z(D_{r'}) \subset D_{e^{-1}}$. Since $|Z(\rho)| \leq |\rho| e^{|\rho|}$ holds as equality for $\rho \geq 0$ (with no absolute values), by inverting $Z$ on the semi-line, we have

$$r' = W(e^{-1}) = 0.278465 \quad (B.4)$$

(in Figure 7 the image of two (almost three) circles of radius $i/10$, $i = 1, 2, \ldots, 10$, are inside the disc $D_{e^{-1}}$) despite of $Z(\rho)$ has a radius of univalence $\tau = 1$.

We can, however, obtain the virial series directly from (B.2). By (A.29), (B.1) and $P(0) = 0$

$$\beta P(\rho) = \int_0^\rho (1 - \tilde{\rho} \varphi'(\tilde{\rho})) d\tilde{\rho} = \rho + \frac{1}{2} \rho^2$$

\[\text{We need to multiply } p, \rho \text{ and } z \text{ by its proper natural scale } v_0, \text{ the volume of a } d \text{–dimensional sphere with radius } a, \text{ prior the limit of } d \text{ to infinity.}\]
Figure 7: Image of circles under $\rho \mapsto Z(\rho)$

which is the equation of state (1.1). We observe that the image $P(D_\tau)$ of a disc $D_\tau$ of radius $\tau$, is a cardioid domain and the radius of univalence of $P(\rho)$ is also $\tau = 1$. If, on the other hand, we have applied Faà di Bruno (or Scott’s) formula (A.25), together with the Lagrange–Bürmann formula (A.27), to the formal power series $\wp(z)$ and $\rho(z) = \beta z \wp'(z)$, we would see the cancellation of all terms of order larger than 2: $\wp \circ Z(\rho) = \rho + \rho^2 / 2$.

**Lebowitz–Penrose lower bound**  The Lambert $W$–function plays an important rule for a system of particles interacting via a pair potential $\phi$ satisfying (i) (stability) there exists $\Phi \geq 0$ such that

$$\exists \Phi \geq 0 : \sum_{1 \leq i < j \leq n} \phi(x_i - x_j) \geq -n\Phi \tag{B.5}$$

for every $n \geq 2$ and $(x_1, \ldots, x_n) \in \mathbb{R}^d$; and (ii)

$$\|e^{-\beta \phi} - 1\|_1 = B(\beta) < \infty, \tag{B.6}$$

with $\|f\|_1 = \int_{\mathbb{R}^d} |f(x)| \, dx$ the $L^1$–norm in $\mathbb{R}^d$. A $\phi$ satisfying (i) and (ii) is called regular potential; note that (i) implies that $\phi$ is bounded from below. For systems with regular potentials, Penrose’s estimate \cite{P} yields

$$|\rho_\Lambda(z) - z| \leq \frac{-1}{\kappa^2 B} W(-\kappa B |z|) - \frac{|z|}{\kappa} \tag{B.7}$$
where $\kappa = \exp(2\beta \Phi) \geq 1$, uniformly in $\Lambda$, provided

$$we^{-w} \equiv \kappa B |z| < e^{-1}. \quad (B.8)$$

Note that $0 \leq w < 1$ preserves this inequality. \[B.7\] together with $W(-we^{-w}) = -w$, by definition of $W(z)$, imply

$$|\rho_\Lambda(z)| \geq (1 + \frac{1}{\kappa}) |z| + \frac{1}{\kappa^2 B} W(-\kappa B |z|)$$

$$= ((1 + \kappa) e^{-w} - 1) \frac{w}{\kappa^2 B} \quad (B.9)$$

which, by maximizing in $w$ satisfying \[B.8\], yields

$$|\rho_\Lambda(z)| \geq 0.28952 \frac{1}{(1 + \kappa)B} \equiv R_0. \quad (B.10)$$

Applying Lagrange–Bürmann formula \[A.27\] on the other way around, i.e., replacing $R$ by $\beta \varphi(z)$ and $\rho(z)$ by its inverse $Z = Z(\rho)$, together with $\beta z \varphi'(z) = \rho(z)$, the coefficients of virial series \[A.31\] reads

$$B_n = \frac{1}{n} \text{Res} \left( \beta \varphi' \rho^{-n} \right) = \frac{1}{n} \text{Res} \left( z^{-1} \rho^{-n+1} \right) = \frac{1}{n} \frac{1}{2\pi i} \oint_{|z|=\delta_0} \rho^{-n+1}(z) \frac{dz}{z} \leq n^{-1} R_0^{-n+1}, \quad (B.11a)$$

or, equivalently,

$$\beta_n \leq n^{-1} R_0^{-n}$$

by \[A.33\].

The integral representation of $B_n$ (third equality in \[B.11a\]) has been derived by Lebowitz–Penrose (see eq. (2.5) in \[LP\]) using Lagrange’s theorem. By the ratio test, $R_0$ is thus a lower bound for the radius of convergence $R_P$ of the virial series. Recently, Morais–Procacci\[MoP\], using the cluster expansion proposed by \[PTs\] for dealing with the canonical partition function, together with Penrose’s estimate on the Mayer coefficients, have (surprisingly) produced the same lower bound on the radius of convergence of the series of Helmholtz free energy in powers of the density $\rho = N/|\Lambda|$ (see Theorem 1 and Remark 2 and 4 therein. Their expansion also yields \[A.28\] in the limit as $|\Lambda|$ goes to $\infty$).

Apart from the factor $1 + \kappa \geq 2$, which came into \[B.9\] in view of the estimation \[B.7\] by the majorant sum, the constant 0.28952 appearing in both estimates is very near to $r'$ defined by \[B.4\]. If Lagrange’s theorem is applied to hard spheres in infinitely dimensions, whose density is exactly given by $\rho(z) = W(z)$, the same estimate $r'$ on radius of convergence of its virial series is obtained (see eq. (3.1) of \[LP\]):

$$R^{h.s.}_P \geq \mu \equiv \min_{z \in C} |\rho(z)| = W(e^{-1}) \equiv r'.$$

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where the contour $C = \{e^{it-1}, 0 \leq t < 2\pi\}$ has been chosen on the domain $e |z| \leq 1$ such that the minimum value on $C$ is the largest possible (see Fig. 8). However, repeating the same steps (B.7)-(B.10),

$$|\rho_\Lambda(z) - z| \leq -W(-|z|) - |z|$$

with $C = \{z = re^{it}, 0 \leq t < 2\pi\}$ and $we^{-w} \equiv r < e^{-1}$, yields an estimate $0.52 \times r'$ (instead $0.5 \times r'$)

$$|\rho_\Lambda(z)| \geq \max_{0 \leq r < e^{-1}} (2r + W(-r)) = \max_{w \geq 0} (2e^{-w} - 1)w \simeq 0.14476 = \frac{0.28952}{2}$$

The slightly increasing on the numerical factor, in comparison to $r'$, is intrinsic to the majorant method employed: the curve $C$ in the Lagrange’s theorem is chosen to minimize the amount lost by replacing the coefficients of $\rho_\Lambda(z) - z$ by their absolute values. We have done something similar in our majorant method in Section 3 when (3.15) is replaced by (3.32) in order the estimate on $R_\phi(t)$ exceeds the threshold $r'$. This and the fact that our lower bound on $R_P(t)$ goes beyond Lebowitz-Penrose’s for nonnegative potentials are manifestations that our approach circumvents the (nonphysical) singularity of the Lambert $W$–function.

**Example of an equation of state presenting a plateau**  
The purpose here is review an explicit example in which the condensation phenomenon is not determined by the singularities present on $P(\rho)$.

Lee–Yang’s theory[YL] is capable to explain condensation directly from the partition function (A.1). To illustrate how this phenomenon takes place, Uhlenbeck and Ford (see Section III.4 of [UF]) have devised an artificial example in which the grand–canonical partition function is given
by $^{5}$

$$\Xi_\Lambda(z) = (1 + z)^{|\Lambda|} \frac{1 - z^{|\Lambda|}}{1 - z}$$

$$= \exp \left| \Lambda \right| \log (1 + z) + \sum_{n=0}^{\left| \Lambda \right|-1} \log \left( 1 - z e^{-2\pi i n/|\Lambda|} \right) - \log (1 - z) .$$

One sees that (see e.g. Example 5.7 in Chap. 0 of [$ST$])

$$\wp(z) = \lim_{|\Lambda| \to \infty} \frac{1}{|\Lambda|} \log \Xi_\Lambda(z) = \begin{cases} \log (1 + z) & \text{if } \left| z \right| \leq 1 \\ \log (1 + z) + \log z & \text{if } \left| z \right| > 1 \end{cases}$$

(B.12)

is the logarithmic potential due to one unit of charge at $z = -1$ and one unit of charge uniformly distributed on the unit circle. The pressure $P(\rho) = \wp \circ (z \wp')^{-1}(\rho)$ in the so called Ford model does present a plateau

$$P(\rho) = \begin{cases} \log(1/(1 - \rho)) & \text{if } 0 \leq \rho < 1/2 \\ \log 2 & \text{if } 1/2 \leq \rho < 3/2 \\ \log(\rho - 1)/(2 - \rho)^2 & \text{if } 3/2 \leq \rho < 2 \end{cases}$$

(B.13)

although Padé approximation is unable to detect the singularity on its virial expansion because is not of algebraic type and it is beyond the critical saturation point $\rho_{sat.} = 1/2$.

Although the power series of $P_1(\rho) = \log(1/(1 - \rho))$ converges for $|\rho| < 1$, the image of $\Re \rho > 1/2$ by $Z_1(\rho) = (z \wp')^{-1}(\rho) = \rho/(1 - \rho)$ is on the complement $\mathbb{C} \setminus D_1$ of the unit disk $D_1$, where $\wp_1(z) = \log (1 + z)$ is defined ($P(\rho)$ is, indeed, not defined at any point $\rho$ of the forbidden domain $1/2 < \Re \rho < 3/2$). The presence of plateau results from the convex envelop of the Helmholtz free energy, defined by (A.35) in each of the two branches:

$$F(\rho) = \begin{cases} \rho \log \rho + (1 - \rho) \log(1 - \rho) & \text{if } 0 \leq \rho < 1/2 \\ - \log 2 & \text{if } 1/2 \leq \rho < 3/2 \\ (\rho - 1) \log(\rho - 1) + (2 - \rho) \log(2 - \rho) & \text{if } 3/2 \leq \rho < 2 \end{cases}$$

with the horizontal line being tangent to both curves $(\rho, F_i(\rho)), i = 1, 2$, the first at $\rho = 1/2$ and the second at $\rho = 3/2$.

C Hamilton-Jacobi Equation

We shall show that the pressure $p = p(t, z)$, for a gas of interacting point–particles with uniformly repulsive pair potential, satisfies (exactly) a “viscous” Hamilton–Jacobi equation (2.4) with

$^{5}$Although no potential system has been assigned, so far, to this model, there is, beside the hard-core hypothesis (to make $\Xi_\Lambda$ a polynomial in $z$), an “attractive sign” behind the assumption on the distribution of zeros over the unit circle.
\[ \mu = \log z \] the chemical potential, \( \varepsilon = 1/(2|\Lambda|) \) the inverse volume, proving Proposition 2.1 part (a); \( t \) represents both, the “inverse temperature” (repulsive intensity) and the “time evolution” (interpolating) parameter starting at \( t = 0 \) from the ideal gas \( p(0, z) = z \). The repulsive (positive) interaction, expressed by the “wrong” sign in front of the Laplacian, is responsible for the equilibrium stability (i.e., avoids the collapse of a large number of particles into a point).

Brydges–Kennedy’s system of equations for the Ursell functions We modify slightly and extend some of the notions introduced in Appendix A. For a \( n \)-tuple \( x = (x_1, \ldots, x_n) \) of points in \( \mathbb{R}^d \), let \( x_I = (x_{i_1}, \ldots, x_{i_s}) \) denote the \( s \)-tuple, \( s \leq n \), of points indexed by \( I = \{i_1, \ldots, i_s\} \subseteq \{1, \ldots, n\} \). We denote by \( |I| \) the cardinality of \( I \).

Boltzmann \( \psi(t, x) \) and Ursell \( \psi^c(t, x) \) functions are assigned to each \( t \in \mathbb{R}_+ \) and \( x \in \mathbb{R}^# \) as follows. Given the total energy of a configuration \( x \) at \( t \):

\[ U(t, x) = \sum_{1 \leq i < j \leq N(x)} \phi(t; x_i - x_j), \]

with \( \phi(t; x) \) satisfying the assumptions stated in Appendix A we write (with \( \beta = 1 \))

\[ \psi(t, x) = e^{-U(t, x)}. \] (C.1)

**Definition C.1** Let \( \circ \) denote the (algebraic) convolution product:

\[ f \circ g(x) = \sum_{I, J: I \cap J = \emptyset, \ I \cup J = \{1, \ldots, n\}} f(x_I)g(x_J) \]

for any pair of state functions \( f \) and \( g \) on \( \mathbb{R}^# \). The (algebraic) exponential function \( \text{Exp}(f) \) of \( f \) is (formally) given by

\[ \text{Exp}(f)(x) = 1(x) + f(x) + \frac{1}{2}(f \circ f)(x) + \cdots \] (C.2)

where \( 1(x) = 1 \) if \( x = 0 \) (i.e., \( x \in \mathbb{R}^0 = \{0\} \)) and \( = 0 \) otherwise.

We define a inner product \( \langle \cdot, \cdot \rangle(z) \) as a (positive) bilinear form

\[ \langle f, g \rangle(z) = \sum_{n=0}^{\infty} \frac{z^n}{n!} \int_{\mathbb{R}^d} f(x)g(x)d^#x \] (C.3)

over any two state functions \( f \) and \( g \) on \( \mathbb{R}^# \) and \( z \in \mathbb{R}_+ \).

We define the Ursell function recursively (in \( n = N(x), n = 1, 2, \ldots \)) by the equation

\[ \psi(t, x) = \text{Exp}(\psi^c)(t, x) \] (C.4)

and write the indicator function of a state in \( \Lambda^2 \) as

\[ \chi_{\Lambda}(x) = \begin{cases} 1 & \text{if } x \in \Lambda^2 \\ 0 & \text{otherwise} \end{cases}. \] (C.5)

With these notations and definitions, we have
**Proposition C.2** The formal pressure (A.5) may be written as

\[ p_\Lambda(t, \mu) = \frac{1}{|\Lambda|} \langle \chi_\Lambda, \psi^\Lambda \rangle \left( e^\mu \right) . \]  

(C.6)

We need the following

**Lemma C.3**

\[ \langle \chi_\Lambda, f \circ g \rangle = \langle \chi_\Lambda, f \rangle \langle \chi_\Lambda, g \rangle \]

**Proof.** Write \( x = (x_1, \ldots, x_n) = (x_I, x_J) \) for any \( I, J \) such that \( I \cap J = \emptyset \) and \( I \cup J = \{1, \ldots, n\} \). Then, by (C.5) and Definitions C.1 we have

\[ \chi_\Lambda(x) = \chi_\Lambda(x_I) \chi_\Lambda(x_J) \]

and

\[ \langle \chi_\Lambda, f \circ g \rangle(z) = \sum_{n=0}^\infty \frac{z^n}{n!} \sum_{I,J: I \cap J = \emptyset, I \cup J = \{1,\ldots,n\}} \int_{\Lambda^I} f(x_I) d^# x \int_{\Lambda^J} g(x_J) d^# x \]

\[ = \sum_{n=0}^\infty \frac{z^n}{n!} \sum_{s=0}^n \binom{n}{s} \int_{\Lambda^s} f(x) d^# x \int_{\Lambda^{n-s}} g(y) d^# y \]

\[ = \sum_{s=0}^\infty \frac{z^s}{s!} \int_{\Lambda^s} f(x) d^# x \sum_{n=s}^\infty \frac{z^{n-s}}{(n-s)!} \int_{\Lambda^{n-s}} g(y) d^# y \]

\[ = \langle \chi_\Lambda, f \rangle(z) \cdot \langle \chi_\Lambda, g \rangle(z) . \]



**Proof of Proposition C.2** By (A.5), (A.1), (C.3) and (C.5), we have

\[ p_\Lambda(t, \mu) = \frac{1}{|\Lambda|} \log \left( \langle \chi_\Lambda, \psi \rangle \left( e^\mu \right) \right) \]

\[ = \frac{1}{|\Lambda|} \log \left( \langle \chi_\Lambda, \operatorname{Exp}(\psi^c) \rangle \left( e^\mu \right) \right) \]

\[ = \frac{1}{|\Lambda|} \langle \chi_\Lambda, \psi^c \rangle \left( e^\mu \right) . \]

in view of (C.2) and Lemma C.3



The following is our main result in this paragraph. We refer to Lemma 3.3 of [BK] for a proof.
Proposition C.4 If $\phi(t; x)$ is differentiable w.r.t. $t$ and satisfies $\phi(0; x) \equiv 0$, then the Brydges–Kennedy system of equations
\[
f_t(t, x) + U(t, x) f(t, x) + \frac{1}{2} \sum_{I,J: I \cap J = \emptyset, I \cup J = \{1, \ldots, n\}} U(t, x_I, x_J) f(t, x_I) f(t, x_J) = 0, \quad t > 0
\] (C.7)
for all $x \in \mathbb{R}^n$, $N(x) = n$ and $n = 1, 2, \ldots$, together with the initial condition
\[
f(0, x) = \begin{cases} 1 & \text{if } N(x) = 1 \\ 0 & \text{if } N(x) > 1 \end{cases}
\]
has a unique solution given by the Ursell functions: $f = \psi^c$. Here $U_t$ means derivative of $U$ w.r.t. $t$ and
\[
U_t(t, x_I, x_J) = \sum_{i \in I, j \in J} \phi_t(t, |x_i - x_j|).
\]

We apply Proposition C.4 to our system of point–particles with uniformly repulsive pair–interacting potential (2.1).

Proof of Proposition 2.1, part (a) For $\phi_A(t; x)$ given by (2.1), write
\[
U(t, x) = \sum_{1 \leq i < j \leq N(x)} \phi_A(t; x_i - x_j)
\]
and let $\psi(t, x)$ and $\psi^c(t, x)$ be given by (C.1) and (C.4). Then,
\[
U(t, x) = \frac{N(x)(N(x) - 1)}{2} \frac{t}{|\Lambda|}
\]
holds for any state $x \in \Lambda^\#$ and Brydges-Kennedy’s system (C.7) reads
\[
\psi^c_t(t, x) + \frac{1}{2|\Lambda|}(n^2 - n) \psi^c(t, x) + \frac{1}{2|\Lambda|} \sum_{I,J: I \cap J = \emptyset, I \cup J = \{1, \ldots, n\}} |I| \psi^c(t, x_I) |J| \psi^c(t, x_J) = 0.
\] (C.8)

By (A.3) and Definition C.1 they can be written, more compactly, as
\[
\psi_t^c + \frac{1}{2|\Lambda|}(N^2 - N) \psi^c + \frac{1}{2|\Lambda|} (N \psi^c \circ N \psi^c) = 0.
\] (C.8)

Applying $\frac{1}{|\Lambda|} \langle \chi_\Lambda, \cdot \rangle (e^\mu)$ to equation (C.8) together with the following

Lemma C.5
\[
\frac{1}{|\Lambda|} \langle \chi_\Lambda, N^k \psi^c \rangle (e^\mu) = \frac{\partial^k p_\Lambda}{\partial \mu^k}(t, \mu), \quad k = 1, 2
\] (C.9)
\[
\frac{1}{|\Lambda|^2} \langle \chi_\Lambda, N \psi^c \circ N \psi^c \rangle (e^\mu) = \left( \frac{\partial p_\Lambda}{\partial \mu} \right)^2(t, \mu);
\] (C.10)
we arrive to desired PDE equation:

\[ p_t + \varepsilon (p_{\mu\mu} - p_\mu) + \frac{1}{2} (p_\mu)^2 = 0 \]

with \( \varepsilon = 1/(2 \, |\Lambda|) \), reducing the proof of Proposition 2.1 part (a), to the proof of Lemma C.5.

**Proof of Lemma C.5.** By (C.5) and Definitions C.1 we have

\[
\frac{1}{|\Lambda|} \langle \chi_\Lambda, N^k \psi^c \rangle (e^\mu) = \sum_{n=0}^{\infty} \frac{n^k e^{n\mu}}{n!} \int_{\Lambda^n} \psi^c(t,x) d^\# x
\]

\[
= \frac{\partial^k}{\partial \mu^k} \sum_{n=0}^{\infty} \frac{e^{n\mu}}{n!} \int_{\Lambda^n} \psi^c(t,x) d^\# x
\]

\[
= \frac{\partial^k}{\partial \mu^k} \langle \chi_\Lambda, \psi^c \rangle (e^\mu),
\]

by formal manipulation of derivatives, and (C.9) follows by Proposition C.2. The proof of (C.10) is analogous. By Proposition C.3

\[
\frac{1}{|\Lambda|^2} \langle \chi_\Lambda, N\psi^c \circ N\psi^c \rangle (e^\mu) = \frac{1}{|\Lambda|} \langle \chi_\Lambda, N\psi^c \rangle (e^\mu) \cdot \frac{1}{|\Lambda|} \langle \chi_\Lambda, N\psi^c \rangle (e^\mu)
\]

which, in view of (C.9), proves (C.10).

\[ \Box \]

**Hopf-Lax-Oleinik formula.** We have devised also a way of deriving, from (1.2), another equation directly related to the virial series. Assuming that (1.2) can be solved by Hopf-Lax-Oleinik (HLO) formula\(^6\)

\[ p(t, x) = \min_y \left( g_\varepsilon(t, y) + \frac{1}{2t} (x - y)^2 \right), \quad (C.11) \]

\( g_\varepsilon(t, x) \) satisfies the following initial value problem

\[ g_t + \varepsilon \left( \frac{g_{xx}}{1 + tg_{xx}} - g_x \right) = 0 \quad (C.12) \]

with \( g(0, x) = e^x \). The formal series solution of (C.12), in powers of \( z = e^x \), is related with edge–irreducible graphs, i.e., connected graphs \( G \) whose removal of an edge \( e \in E(G) \) remain connected. We prove in Appendix D a general convergence theorem which implies, in particular, convergence of the (Mayer) power series solution of (C.12).

\(^6\)With the Inf-convolution transformation in the formal sense: \( p(t, x) = g_\varepsilon(t, y^*) + \frac{1}{2t} (x - y^*)^2 \) where \( y^* = y^*(t, x) \) solves (formally) the equation \( g'_\varepsilon(y) - (x - y)/t = 0 \) for \( y \).
Global existence and uniqueness of Mayer type solution

Power series solutions: General result

This section is devoted to the investigation of partial differential equations of the form

$$u_t + \mathcal{A}(t, u, u_x, u_{xx}) = 0 \quad (D.1)$$

for some function $\mathcal{A} : \mathbb{R}_+ \times U \times V \rightarrow \mathbb{C}$ smooth in the variable $t$ and holomorphic in both domains $U, V \subset \mathbb{C}$ containing the origin.

**Definition D.1** A solution of (D.1) is said to be of Mayer type if may be represented by a (formal) power series of $z = e^x$:

$$u(t, x) = \sum_{n=1}^{\infty} u_n(t) e^{nx} \quad (D.2)$$

We are interested in the (ideal gas) initial condition

$$u(0, x) = e^x \quad (D.3)$$

The solution of (D.1) starting from (D.3), or any other initial conditions of (Mayer) power series type, preserve the form (D.2). For simplicity, we restrict ourselves to (D.3).

Equations (2.4) and (C.12) are examples of (D.1) with $\mathcal{A}(t, a, b) = \frac{1}{2} a^2 + \varepsilon (b - a)$ and $\mathcal{A}(t, a, b) = \varepsilon \left( \frac{b}{1 + tb} - a \right)$, respectively, satisfying the initial condition (D.3). The other equation (2.5) for the free energy $F$ cannot be handled directly but equation (2.7) for $\varphi(t, \rho) = F(\rho(t, \rho)) - \log \rho$, can also be dealt by the following procedure (the initial condition is trivial but $A_{0,0}$ in (D.4) depends on $\rho$).

Our aim is to prove that (D.2) converges uniformly in $t \in [0, T]$, for all $T > 0$, and $z = e^x$ in a domain $D_t = \mathbb{D}_{r(t)}$ where $\mathbb{D}_r$ is an open disc in $\mathbb{C}$ centered at origin with radius $r$, provided it solves (D.1) with

$$\mathcal{A}(t, a, b) = \sum_{\substack{n, m=0; \ n+m \neq 0}}^{\infty} A_{n,m}(t)a^n b^m \quad (D.4)$$

satisfying the assumptions:

1. $A_{1,0} = \varepsilon \alpha$, $A_{0,1} = \varepsilon$ and $A_{2,0} = \gamma$, are constant in $t$, for some $\varepsilon, \gamma > 0$ and $\alpha \geq -1$;
2. if $n + m > 1$ and $(n, m) \neq (2, 0)$,

$$|A_{n,m}(t)| \leq C (tn)\eta^{n+m-1} \quad (D.5)$$

holds for some positive constants $C$ and $\eta$.

Equations (2.4) and (C.12) satisfy the assumptions: $\alpha = -1, \gamma = 1/2$ and $C = 0$ for the former; $\alpha = -1, \gamma = 0, A_{n,m} = 0$ if $n \geq 2, C = \varepsilon$ and $\eta = 1$ for the latter.
Definition D.2 For any two sequences $\alpha = (\alpha_n)_{n \geq 1}$ and $\beta = (\beta_n)_{n \geq 1}$, their product $\alpha \cdot \beta = ((\alpha \cdot \beta)_k)_{k \geq 1}$ and convolution product $\alpha \ast \beta = ((\alpha \ast \beta)_k)_{k \geq 1}$ are sequences defined, respectively, by

$$(\alpha \cdot \beta)_k = \alpha_k \beta_k \quad \text{(D.6)}$$

and by $$(\alpha \ast \beta)_k = \sum_{l=1}^{k-1} \alpha_l \beta_{k-l} \quad \text{(D.7)}$$

Proposition D.3 If $f(z) = \sum_{n \geq 1} \alpha_n z^n$ and $g(z) = \sum_{n \geq 1} \beta_n z^n$ are two formal series, then

$$(fg)(z) = \sum_{k \geq 1} (\alpha \ast \beta)_k z^k \quad \text{(D.8)}$$

Proof. Proposition D.3 is proved by rearranging the double sum

$$(fg)(z) = \sum_{n \geq 1} \sum_{m \geq 1} \alpha_n \beta_m z^{n+m} = \sum_{k \geq 1} \sum_{n,m \geq 1: n+m=k} \alpha_n \beta_m z^k$$

with the sum between parenthesis equivalent to the r.h.s. of (D.7).

Formal derivatives of (D.2) with respect to $t$ and $x$, i.e., term by term, lead to a formal power series of the same type with coefficients of $u_t$, $u_x$ and $u_{xx}$ given by $\dot{u}_n$, $nu_n \equiv v_n$ and $n^2u_n \equiv w_n$, respectively. Plugging the expansion of these functions into (D.1) yields for the $k$–th coefficient of the equation, $k \geq 1$,

$$\ddot{u}_k + \sum_{n,m: 1 \leq n+m \leq k} A_{n,m}(t) \left( \underbrace{v \ast \cdots \ast v}_{n} \ast \underbrace{w \ast \cdots \ast w}_{m} \right)_k = 0 \quad \text{(D.8)}$$

The restriction $n + m \leq k$ in (D.8) results from the fact that our sequence $u = (u_n)_{n \geq 1}$ starts with $n = 1$ and a convolution involving $n + m$ sequences cannot have nonvanishing component $k$ if $k > n + m$. Consequently, for any $K \in \mathbb{N}$, with $1 \leq k \leq K$, form a closed system of $K$ (first order) differential equations, involving $K$ unknown functions: $u_1(t), \ldots, u_K(t)$ satisfying the initial condition

$$u_k(0) = \begin{cases} 1 & \text{if } k = 1 \\ 0 & \text{otherwise} \end{cases} \quad \text{(D.9)}$$
Theorem D.4 There exists an unique formal series of the form (D.2) that solves (D.1) with the initial condition (D.3). Under assumptions 1. and 2. on the coefficients \( A_{n,m} \) of \( \mathcal{A} \) one can find a power series \( U(t,x) \) of the form

\[
U(t,x) = \sum_{n=1}^{\infty} P_n(t)e^{-(1+a)nt}e^{nx}
\]

where \( P_n(t) = \sum_{l=1}^{n} C_{n,l} t^{l-1} \) is a polynomial of order \( n-1 \) with (positive) coefficients such that \( U(t,x) \) majorizes (D.2): \( u(t,x) \ll U(t,x) \) in the sense that

\[
|u_n(t)| \leq P_n(t)e^{-(1+a)nt}
\]

holds for any \( n \geq 1 \) and \( t \in \mathbb{R}_+ \). Moreover,

\[
C_{n,l} \leq \delta A^2 \frac{B^n}{n!} \frac{1}{l^2}
\]

with \( B = (\delta A^2)^{-1} \), \( A = 3/(2\pi^2) \) and \( \delta = 1/\eta + C/\varepsilon - \sqrt{2/\eta + C^2/\varepsilon^2} \), and the series (D.2) converges uniformly for \( t \) and \( z = e^z \) in the domain \( \Omega \subset \mathbb{R}_+ \times \mathbb{C} \) defined by

\[
B \max(1,t)e^{-(1+a)t} |z| < 1 ,
\]

representing therein the unique solution of the initial value problem.

Proof of Theorem D.4 The formal series solution of (D.1) is obtained by integrating the system of first order differential equations (D.8). Isolating its linear term, equation (D.8) reads

\[
\dot{u}_k + \varepsilon (k^2 + ak)u_k = f_k (u_1, \ldots, u_{k-1};t)
\]

where, by definition (D.7),

\[
f_k (u_1, \ldots, u_{k-1};t) = - \sum_{2 \leq n+m \leq k} A_{n,m}(t) \left( \underbrace{v \ast \cdots \ast v}_{n} \ast \underbrace{w \ast \cdots \ast w}_{m} \right)_k
\]

does not depend on \( u_n \) with \( n \geq k \).

The solution of (D.13) for \( k = 1 \):

\[
\dot{u}_1 + \varepsilon (1+a) u_1 = 0
\]

with \( u_1(0) = 1 \) is

\[
u_1(t) = e^{-\varepsilon(1+a)t}.
\]

Given that we have already solved for \( u_1(t), \ldots, u_{k-1}(t) \), we solve equation (D.13) with \( u_k(0) = 0 \):
\[ u_k(t) = e^{-\varepsilon(k^2+ak)t} \int_0^t e^{\varepsilon(k^2+ak)s} f_k(u_1, \ldots, u_{k-1}; s) \, ds \]  

(D.16)

uniquely defines the coefficient of the formal series, proving the first statement of Theorem D.4.

To prove the existence of a majorant series of the form (D.10), we show that the sequence \((U_n(t))_{n \geq 1}\) with \(U_n(t) = P_n(t)e^{-\varepsilon(1+a)t}\) satisfies (D.16), with \(-A_{n,m}\) in (D.14) replaced by the upper bound of \(|A_{n,m}|\), as an equality. We then find \(\delta > 0\) and \(B > 1\) such that (D.11) holds for every \(n \geq 1\) and \(1 \leq l \leq n\), by induction. For this, we need

**Lemma D.5** Let \(c = (c_i)_{i \geq 1}\) be a sequence of positive numbers defined by

\[ c_i = A \frac{1}{i^2} d^i \]  

(D.17)

for some \(d > 0\) and \(A = 3/(2\pi^2) = 0.1519\ldots\) as in Theorem D.4. Then the sequence formed by convolution of \(c\) with itself is dominated by the sequence \(c\), i.e.,

\[ (c * c)_n \leq c_n \]

holds for any \(n \geq 1\).

**Proof.** By definition (D.7) together with (D.17), we have

\[
\frac{1}{c_n} \sum_{i=1}^{n-1} c_i c_{n-1} = A \sum_{i=1}^{n-1} \frac{n^2}{i^2(n-i)^2} = A \sum_{i=1}^{n-1} \left( \frac{1}{i} + \frac{1}{n-i} \right)^2 \leq 2A \sum_{i=1}^{n-1} \left( \frac{1}{i^2} + \frac{1}{(n-i)^2} \right) \leq \frac{2\pi^2}{3} A = 1.
\]

For the two inequalities, we have used

\[ 0 \leq (a-b)^2 = 2(a^2 + b^2) - (a+b)^2 \implies (a+b)^2 \leq 2(a^2 + b^2) \]

with \(a = 1/i\) and \(b = 1/(n-i)\) and \(\sum_{i \geq 1} 1/i^2 = \pi^2/6\). This concludes the proof of Lemma D.5. \(\square\)

We also need

**Lemma D.6**

\[ \int_0^T s^{r-1} e^s ds \leq T^{r-1} e^T \]  

(D.18)

holds for any integer \(r \geq 1\) and \(0 \leq T < \infty\).
Proof. For \( r = 1 \), \([D.18]\) is easily true. For \( r \geq 2 \), by integration by parts, we have
\[
\int_0^T s^{r-1} e^s \, ds = T^{r-1} e^T - (r-1) \int_0^T s^{r-2} e^s \, ds
\]
from which the proof is concluded.

\( \square \)

Convolutions appears not only in the product of power series but also due to products of polynomials when two or more majorant solutions are multiplied together. If \( P_n(t) \) and \( P_m(t) \) are two polynomials as in the statement of Theorem \([D.4]\), then
\[
t P_n(t) P_m(t) = \sum_{r=1}^{n+m-1} \left( \sum_{1 \leq l_1 \leq n, 1 \leq l_2 \leq m: \frac{l_1 + l_2}{l_1 + l_2} = r} C_{n,l_1} C_{m,l_2} \right) t^{r-1}
\]
is a polynomial of order \( n + m - 1 \). In order to write the sum between parenthesis as \((C_n * C_m)_r\), we extend the coefficients \( C_{n,l} \), \( 1 \leq l \leq n \), as an infinite sequence \( C_n = (C_{n,l})_{l \geq 1} \) with \( C_{n,l} = 0 \) for \( l > n \). To make our expressions shorter, we introduce a double (weighted) convolution product of two sequences \((C_n,l)\) and \((D_{n,l})\) as a sequence \((C \otimes D)_{n,r}\) defined by
\[
(C \otimes D)_{n,r} = \sum_{n_1,n_2 \geq 1: n_1 + n_2 = n} \sum_{1 \leq l_1 \leq n_1, 1 \leq l_2 \leq n_2: \frac{l_1 + l_2}{l_1 + l_2} = r} C_{n_1,l_1} D_{n_2,l_2}
\]
(D.19)

Now, by induction, we construct an equation for the majorant polynomials \( P_n(t) \). Suppose we have already had \( k-1 \) polynomials \( P_1(t), \ldots P_{k-1}(t) \), with \( P_j \) of order \( j-1 \), whose coefficients are positive. Then, writing
\[
V_n = n U_n
\]
\[
W_n = n^2 U_n
\]
\[
U_n(t) = e^{-\varepsilon (1+\alpha) n t} P_n(t)
\]
and using \( k \leq k^2 \) and \( |A_{n,m}| \leq C (\eta)^{n+m-1} \) on the r.h.s of \([D.14]\), we have
\[
|A_{n,m}| (s) \left( V_1 \ast \cdots \ast V_n \ast W_1 \ast \cdots \ast W_m \right) (s) \leq C \eta^{n+m} e^{-\varepsilon (1+\alpha) k s} s^{n+m-1}
\]
\[
\times \sum_{k_1, \ldots, k_{n+m} \geq 1} \sum_{k_1 + \cdots + k_{n+m} = k} k_1^2 P_{k_1} \cdots k_{n+m}^2 P_{k_{n+m}}
\]
(D.20)

where
\[
s^{n+m-1} P_{k_1} \cdots P_{k_{n+m}} = \sum_{r=1}^{k} \left( C_{k_1} \ast \cdots \ast C_{k_{n+m}} \right)_r s^{r-1}
\]
(D.21)
is a polynomial of order \( k - 1 \) whose coefficients are positive. The integration needed to be performed to each term of (D.16) is of the form
\[
e^{-\varepsilon(k^2 + ak)t} \int_0^t s^{r-1} e^{\varepsilon(k^2 - k)s} ds = e^{-\varepsilon(k^2 + ak)t} \frac{1}{\varepsilon^r(k^2 - k)^r} \int_0^{\varepsilon(k^2 - k)t} s^{r-1} e^s ds
\]
\[
\leq \frac{1}{\varepsilon k(k - 1)} e^{-\varepsilon(1+a)kt} t^{r-1} ,
\]
by (D.18).

The result of summing (D.20) over \( 2 \leq n, m \leq k \), together with (D.21) and (D.22), is bounded by a polynomial of order \( k - 1 \), denoted by \( P_k(t) \), whose coefficients are positive. Defining \( U_k(t) = e^{-\varepsilon(1+a)kt} P_k(t) \) together with (D.19), the coefficients \( C_{k,l} \) of \( P_k \) satisfy the recursion relation
\[
C_{k,l} = \frac{C}{\varepsilon k(k - 1)} \sum_{2 \leq n,m \leq k} \eta^{n+m} \left( C \otimes \cdots \otimes C \right)_{n+m}^{k,l}
\]
(D.23)

For \( k = 1 \), we have
\[
u_1(t) = e^{-\varepsilon(1+a)t} = U_1(t)
\]
with \( P_1 \equiv 1 \). Suppose that
\[
|u_n(t)| \leq U_n(t)
\]
(D.24)
holds for \( 1 \leq n \leq k - 1 \) and \( t \in \mathbb{R}_+ \) and let \( \tilde{f}_k \) be defined by (D.14) with \( -A_{n,m} \) replaced by \( |A_{n,m}| \). Then,
\[
|u_k(t)| \leq e^{-\varepsilon(k^2 + ak)t} \int_0^t e^{\varepsilon(k^2 + ak)s} \tilde{f}_k(U_1, \ldots, U_{k-1}; s) ds
\]
\[
\leq e^{-\varepsilon(k^2 + ak)t} \frac{C}{\varepsilon k(k - 1)} \sum_{2 \leq n,m \leq k; 1 \leq i \leq k} \eta^{n+m} \left( C \otimes \cdots \otimes C \right)_{n+m}^{k,i} t^{i-1} = U_k(t)
\]
which establishes the second statement.

To conclude the proof of Theorem D.4, we note that estimate (D.11) can be written as
\[
C_{n,l} \leq \frac{1}{n^2} c_n \tilde{c}_l \equiv \tilde{C}_{n,l}
\]
(D.25)
where \( c_n = AB^n/n^2 \) and \( \tilde{c}_l = A/l^2 \) are sequences satisfying the hypothesis of Lemma D.5. Clearly (D.25) holds for \( n = l = 1 \)
\[C_{1,1} = 1 \leq \delta c_1 \tilde{c}_1 = \delta A^2 B \]
provided \( B = (\delta A^2)^{-1} \). Assuming that (D.25) holds for \( 1 \leq n \leq k - 1 \) and \( 0 \leq l \leq n \) with \( k \geq 2 \), then plugging (D.25) into (D.23) together with Lemma D.5 yields
\[
C_{k,l} \leq \frac{C}{\varepsilon k(k - 1)} \frac{\delta^2 \eta^2}{(1 - \delta \eta)^2} c_k \tilde{c}_l \leq \frac{1}{k^2} c_k \tilde{c}_l
\]
(D.26)
provided \( \delta \) is chosen to be the smaller solution, \( \delta = 1/\eta + C/\varepsilon - \sqrt{2/\eta + C^2/\varepsilon^2} \), of

\[
\frac{2\delta^2 C}{\varepsilon (1 - \delta \eta)^2} = 1.
\]

The power series solution converges if

\[
\lim_{n \to \infty} \frac{\tilde{P}_{n+1}(t)}{P_n(t)} e^{-\varepsilon(1+a)t} |z| < 1
\]

where \( \tilde{P}_n \) is the polynomial whose coefficients \( \tilde{C}_{n,l} \) are given by r.h.s. of (D.11), concluding the proof.

\[\square\]

## E Polynomials with Positive Coefficients

We devote this appendix to the proof of Lemma \[\text{3.4}\] and Proposition \[\text{4.6}\].

Lemma \[\text{3.4}\] is consequence of the following

**Proposition E.1** For any \( k \geq 2 \), let \( \mathcal{D}_k(t) \) be given by (3.29)

\[
\mathcal{D}_k(t) = (Q_k \circ \eta)(t), \quad \eta(t) = e^{-2\varepsilon t}
\]

\[
Q_k(\eta) = 1 - (1 - \eta)P_k(\eta)
\]

is such that

i. \( P_k(\eta) = 1 + \sum_{n=1}^{D_k} p_{k,n} \eta^n \), is a polynomial in \( \eta \) of order \( D_k = (k - 2)(k + 1)/2 \) whose the coefficients \( p_{k,n} \) are positive and satisfy

\[
p_{k,n-1} - p_{k,n} > 0 , \quad 1 \leq n \leq D_k
\]

ii. \( Q_k(\eta) = \sum_{n=1}^{D_k+1} q_{k,n} \eta^n \), is a polynomial in \( \eta \) of order \( D_k+1 \) with \( q_{k,n} = p_{k,n-1} - p_{k,n} \) if \( 1 \leq n \leq D_k \) and \( p_{k,D_k+1} = p_{k,D_k} \) positive, by i., satisfying (with \( p_{k,D_k+1} = 0 \))

\[
q_{k,n} - q_{k,n+1} = p_{k,n-1} + p_{k,n+1} - 2p_{k,n} > 0 , \quad 1 \leq n \leq D_k
\]

iii. It follows by i. and ii. that \( Q_k(\eta) \) is a convex function such that \( Q_k(0) = 0, Q_k(1) = 1 \) and

\[
\lim_{k \to \infty} Q_k(\eta) = 0 \quad \text{if} \quad 0 \leq \eta < 1
\]
iv.

\[ T_k(\eta) := Q_k(\eta) + (k-1)(1-\eta)Q_{k+1}(\eta) \geq \eta \]  
(E.2)

holds for every \( k \geq 2 \) and \( 0 \leq \eta \leq 1 \) (equality only for \( \eta = 0 \) and \( 1 \)).

**Proof.** It follows by (3.29), (E.1) and \( \eta = 1 - 2\varepsilon \lambda \) that

\[ P_k(\eta) = \frac{k(k+1)}{2} \frac{\eta^{k(k+1)/2}}{(1-\eta)^{k+1}} \int_0^1 \xi^{-k(k+1)/2} (1-\xi) \frac{d\xi}{\xi} . \]

Note that \( N_k = k(k+1)/2 \) is an integer for any \( k \in \mathbb{N} \) and, as shown in the calculation performed below, \( P_k \) is a polynomial whose degree \( D_k = k(k-1)/2 - 1 = (k-2)(k+1)/2 \) is non-negative for all \( k \geq 2 \). Observe that

\[ N_k = D_k + k + 1 \]  
(E.3)

We change variable \( y = (1-\xi)/\xi \) so

\[ P_k(\eta) = \frac{k(k+1)}{2} \frac{\eta^{k(k+1)/2}}{(1-\eta)^{k+1}} \int_0^{(1-\eta)/\eta} y^k (1+y)^{k(k-1)/2-1} dy , \]

by the binomial theorem and explicit integration can be written as

\[ P_k(\eta) = \sum_{l=0}^{D_k} \frac{N_k}{k+l+1} \binom{D_k}{l} 
\eta^{D_k-l} (1-\eta)^l . \]

Applying the binomial theorem once again, we have

\[ P_k(\eta) = \sum_{m=0}^{D_k} \left( \sum_{l=0}^{D_k-m} (-1)^{l-m} \binom{l}{m} \frac{N_k}{k+l+1} \binom{D_k}{l} \eta^{D_k-m} \right) \]

\[ = \sum_{m=0}^{D_k} \binom{D_k}{m} \left( \sum_{l=0}^{D_k-m} (-1)^l \binom{D_k-m}{l} \frac{N_k}{k+l+m+1} \right) \eta^{D_k-m} \]

which, by inserting the identity

\[ \frac{1}{k+l+m+1} = \int_0^\infty e^{-(k+l+m+1)s} ds \]

together with the binomial theorem and (E.3), yields

\[ P_k(\eta) = \sum_{m=0}^{D_k} \binom{D_k}{m} \left( N_k \int_0^\infty e^{-(k+m+1)s} (1-e^{-s})^{D_k-m} ds \right) \eta^{D_k-m} \]

\[ = \sum_{n=0}^{D_k} \binom{D_k}{n} \left( N_k \int_0^\infty e^{-N_k s} (e^{s} - 1)^n ds \right) \eta^n \]

\[ \equiv 1 + \sum_{n=1}^{D_k} p_{k,n} \eta^n \]  
(E.4)
establishing the first part of the statement i.: \( p_{k,n} > 0 \).

Successive partial integrations on

\[
I_{k,n} = N_k \int_0^\infty e^{-N_k s} (e^s - 1)^n ds
\]

\[
= N_k \frac{n}{N_k} \int_0^\infty e^{-(N_k-1) s} (e^s - 1)^{n-1} ds
\]

\[
= \cdots
\]

\[
= \frac{n}{N_k - 1} \frac{n - 1}{N_k - 2} \cdots \frac{2}{N_k - n + 1} \frac{1}{N_k - n}
\]

(E.5)

yields

\[
p_{k,n} = \left( \frac{D_k}{n} \right) I_{k,n} = \frac{D_k}{N_k - 1} \frac{D_k - 1}{N_k - 2} \cdots \frac{D_k - n + 1}{N_k - n}
\]

(E.6)

and thus (with \( p_{k,0} = 1 \))

\[
(-\nabla p_k)_n = p_{k,n} - p_{k,n+1}
\]

\[
= p_{k,n} \left( 1 - \frac{D_k - n}{N_k - n - 1} \right) > 0
\]

(E.7)

for \( n = 0, \ldots, D_k - 1, k > 2 \), by (E.3). This concludes the proof of item i.. Now, since

\[
Q_k(\eta) = 1 - (1 - \eta) P_k(\eta) = \sum_{n=1}^{D_k} (p_{k,n-1} - p_{k,n}) \eta^n + p_{k,D_k} \eta^{D_k+1}
\]

and \( Q_k(\eta) = \sum_{n=1}^{D_k+1} q_{k,n} \eta^n \), equations (E.4) and (E.7) imply the first part of statement ii.. By (E.5), we have

\[
(\nabla^* q_k)_n = q_{k,n} - q_{k,n+1}
\]

\[
= p_{k,n-1} + p_{k,n+1} - 2p_{k,n}
\]

\[
= p_{k,n} \left( \frac{N_k - n}{D_k - n + 1} + \frac{D_k - n}{N_k - n - 1} - 2 \right)
\]

\[
= p_{k,n} \left( \frac{k (k - 1)}{(N_k - n - 1) (D_k - n + 1)} \right) > 0
\]

(E.8)

for \( 1 \leq n \leq D_k \) and \( k > 2 \) (for \( k = 2, D_2 = 0 \) and \( Q_2 = p_{2,0} = \eta \)), establishing item ii..
Clearly, $Q_k(0) = 0$,

$$Q_k(1) = \sum_{n=1}^{D_k} (p_{k,n-1} - p_{k,n}) + p_{k,D_k} = p_{k,0} = 1$$

and, as $q_{k,n} > 0$, $Q''_k(\eta) > 0$ for $0 < \eta < 1$, verifying the first statements of iii.

Finally, (E.2) is consequence of the following

**Claim E.2** For any $k \geq 2$, the numerical sequence $(t_{k,n})_{1 \leq n \leq D_k}$ defined by

$$T_k(\eta) = Q_k(\eta) + (k-1)(1-\eta)Q_k+1(\eta) = t_{k,1}\eta - \sum_{n=2}^{D_k+1} t_{k,n}\eta^n$$

satisfies

$$t_{k,1} > 1$$

$$t_{k,n} > 0 \quad \text{for } 2 \leq n \leq D_k + 1.$$  

Since $T_k(1) = Q_k(1) = 1$, it follows by Claim E.2 together with $\eta^n \leq \eta$ for $0 \leq \eta \leq 1$, that

$$T_k(\eta) \geq T_k(1)\eta = \eta$$

which is exactly the statement (E.2), concluding the proof of Proposition E.1. □

**Proof of Claim E.2** The coefficients of terms in

$$(1-\eta)Q_{k+1}(\eta) = q_{k+1,1}\eta - \sum_{n=1}^{D_{k+1}-1} (\nabla^\ast q_{k+1,\ast}.)_n \eta^{n+1} - p_{k+1,D_k+1}\eta^{D_{k+1}}$$

with degree larger than 2 are all negative in view of (E.6) and (E.8). Since $Q_k(\eta)$ has degree $D_k + 1$, this implies $t_{k,n+1} > 0$ for $D_k + 1 \leq n \leq D_k + 1$ and we thus need to prove: (a)

$$t_{k,1} = q_{k,1} - (k-1)q_{k+1,1}$$

$$= 1 - p_{k,1} + (k-1)(1-p_{k+1,1})$$

$$= k - \left( \frac{D_k}{N_k - 1} + (k-1) \frac{D_{k+1}}{N_{k+1} - 1} \right) > 1$$

and (b)

$$t_{k,n+1} = -(p_{k,n} - p_{k,n+1}) + (k-1)(p_{k+1,n-1} + p_{k+1,n+1} - 2p_{k+1,n}) > 0$$

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for \( k \geq 3 \) and \( 1 \leq n \leq D_k \). Note that, since \( Q_2(\eta) = \eta \) has degree 1, \( t_{2,n+1} > 0, 1 \leq n \leq 2 \) follows from (E.10).

By (E.3),
\[
\frac{D_{k+1} - N_{k+1}}{N_{k+1}} - \frac{D_k - N_k}{N_k} = \left(1 - \frac{1}{k}\right) \left(1 - \frac{1}{k+3}\right) - \left(1 - \frac{1}{k-1}\right) \left(1 - \frac{1}{k+2}\right) > 0
\]
which, together with (E.11), yields
\[
t_{k,1} > k \left(1 - \frac{D_{k+1}}{N_{k+1}}\right)
\]
\[
= k \left(1 - \left(1 - \frac{1}{k}\right) \left(1 - \frac{1}{k+3}\right)\right) = 1 + \frac{k-1}{k+3}
\]
proving (a).

Each factor \( \frac{D_k - m + 1}{N_k - m} = \frac{k(k-1) - 2m}{k(k+1) - 2m} \) involved in \( p_{k,n} \) (see (E.6)) is an increasing function of \( k \) and decreasing function of \( m \). For this, let \( f(x, y) = \frac{x^2 - x - 2y}{x^2 + x - 2y} \) and note that \( f_x = \frac{2(x^2 + y)}{(x^2 + x - 2y)^2} > 0 \) and \( f_y = -\frac{4}{(x^2 + x - 2y)^2} < 0 \). This implies, in particular, that \( p_{k,n} \) is monotone increasing function of \( k \) and
\[
\frac{p_{k+1,n}}{p_{k,n}} > \frac{D_{k+1} - N_{k+1}}{N_{k+1}} - \frac{D_k - N_k}{D_k} = \frac{(k^2 + k - 2)^2}{k(k+1)(k^2 + k - 6)} > 1 \tag{E.13}
\]
for \( k \geq 3 \). By (E.7), (E.8) and (E.13), (E.12) can be estimated by
\[
t_{k,n+1} \geq \frac{p_{k+1,n}}{(N_k - n - 1)(N_{k+1} - n - 1)(D_{k+1} - n + 1) k^2 + k - 6} h_{k,n}
\]
where
\[
h_{k,n} = -k(k^2 + k - 6)(N_{k+1} - n - 1)(D_{k+1} - n + 1) + (k - 1) \left(k^2 + k - 2\right)^2 (N_k - n - 1)
\]
\[
= -\frac{1}{4} k \left(k^2 + k - 6\right) \left(k^2 + 3k - 2n\right) \left(k^2 + k - 2n\right) + \frac{1}{2} (k - 1)^3 (k + 2)^2 \left(k^2 + k - 2(n + 1)\right)
\]
for \( k \geq 3 \) and \( 1 \leq n \leq D_k \), satisfies
\[
h_{k,n} \geq \min (h_{k,1}, h_{k,D_k}) \geq h_{3,1} = 80
\]
proves (b) and concludes the proof of Claim E.2.

\[\square\]

**Proof of Proposition 4.6.** The limit of \( c_k(t) \) as \( t \) goes to 0 exists by continuity, is finite by (4.26) and satisfies equation (4.28) whose solution is uniquely determined by the recursive equation (4.28):
\[
c_0(0) = 1, \ c_1(0) = c_2(0) = 1, \ c_2(0) = 3c_0(0)c_1(0)/2 = 3/2, \ c_3(0) = 8/3, \ c_4(0) = 125/24 \text{ and so on.}
\]
The solution’s explicit form (4.29) is a consequence of the following
Lemma E.3

\[
\frac{1}{2} \sum_{j=1}^{n-1} \binom{n}{j} j^{j-1} (n-j)^{n-j-1} = (n-1)n^{n-2} \tag{E.14}
\]

Proof. See Lemma 4.2 of [BK]. □

Setting \( k = n - 1 \) and \( l = j - 1 \), equation \((E.14)\) can be written as

\[
\frac{k+1}{2k} \sum_{l=0}^{k-1} \frac{(l+1)^j}{(l+1)!} (n-l-1)^{n-l} = \frac{(k+1)^k}{(k+1)!}
\]

which, together with the definition of convolution product, proves that \((4.29)\) solves \((4.28)\).

Let us now suppose that \( t_0 \) is the largest “time” for which \( c_k(t) < c_k(t') \) is satisfied for \( 0 \leq t < t' \leq t_0 \) and \( k \geq 2 \). Then, for all \( t \leq t_0 \),

\[
c_k(t) > \mathcal{R}_k(t) \frac{1}{k} (c(t) * c(t))_{k-1}, \tag{E.15}
\]

where

\[
\mathcal{R}_k(t) = \frac{k+1}{2k} \frac{1}{\lambda^k} \int_0^t e^{-\varepsilon k(k+1)(1-s)} \lambda^{k-1} \lambda^s ds \equiv (R_k \circ \eta)(t)
\]

and, with \( N_k = k(k+1)/2 \) and \( D_k = k(k-1)/2 \),

\[
R_k(\eta) = \sum_{n=0}^{D_k} \binom{D_k}{k+1} \binom{D_k}{l} \eta^{p_{k-1}} (1-\eta)^l \equiv 1 + \sum_{n=1}^{D_k} p_{k,n} \eta^n \tag{E.16}
\]

is a polynomial of degree \( D_k \) in \( \eta \), with \( p_{k,n} > 0 \) given by \((E.6)\), satisfying

\[
1 \leq R_k(\eta) \leq \frac{k+1}{2}. \tag{E.17}
\]

Equation \((E.15)\) together with \((4.30)\) and \( 2\varepsilon \lambda = 1 - \eta \), yields

\[
\dot{c}_k = \frac{-k(k+1)}{2\lambda} \left( (1-\eta)c_k + \frac{2\eta}{1+k} c_k - \frac{1}{k} (c \ast c)_{k-1} \right)
\]

\[
< \frac{-k(k+1)}{2\lambda} L_k(\eta) \mathcal{R}_k(\eta)c_k \tag{E.18}
\]

where

\[
L_k(\eta) = \sum_{n=1}^{D_k+1} l_{k,n} \eta^n = \left( 1 - \frac{k-1}{k+1} \right) R_k(\eta) - 1, \tag{E.19}
\]

is a polynomial in \( \eta \) of degree \( D_k + 1 \) whose coefficients (with \( p_{k,D_k+1} = 0 \))

\[
l_{k,n} = p_{k,n} - \frac{k-1}{k+1} p_{k,n-1}, \tag{E.20}
\]

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Figure 9: $L_k$ as a function of $\eta$ for several $k$’s.

the first few of them are positive. By (E.6),

$$p_{k,n} - \frac{k-1}{k+1} p_{k,n-1} = \left(1 - \frac{k-1}{k+1} \frac{N_k - n}{D_k - n + 1}\right) p_{k,n}$$

$$= 2 \left(k + 1 - 2n\right) \frac{1}{k+1} \frac{p_{k,n}}{D_k - n + 1} > 0$$

iff $n < (k + 1)/2$, which is not an empty set for $k > 2$ as one can see for $k = 3$ ($L_3(\eta)$ has degree $D_3 + 1 = 4$): $l_{3,1}$ is strictly positive, $l_{3,2} = 0$ and $l_{3,3}$, $l_{3,4} < 0$.

By (E.19), (E.17) and since $R_k$ attains its minimum and maximum values at $\eta = 0$ and $\eta = 1$, resp., we have

$$L_k(0) = L_k(1) = 0.$$ (E.21)

which, together with and $\eta^{n'} < \eta^n$ if $n < n'$, imply that

$$L_k(\eta) > 0, \quad \text{for } 0 < \eta < 1.$$ (E.22)

(E.18) and (E.22) together imply that $c_k(t)$, for each $k \geq 2$, is monotone decreasing in $t$; (E.21) and (E.22) are not faithful for large $\eta$ and can be improved from equation (E.18) in the limit $t \to 0$. In Fig. 9 we plot $L_k(\eta)$ for several values of $k$.

So far $c_k(t) < c_k(t')$ has been established for $0 \leq t < t' \leq t_0$ and $k \geq 2$ where $t_0$ is arbitrarily large. As $t$ goes to $\infty$, $\eta \to 1$, $\lambda \to (2\varepsilon)^{-1}$ and equation (4.30), reads

$$\dot{c}_k(\infty) = -\varepsilon (k+1) \left(kc_k(\infty) - (c(\infty) \ast c(\infty))_{k-1}\right).$$

The sequence $\dot{c}(\infty) = (\dot{c}_k(\infty))_{k \geq 0}$ vanishes iff

$$c_k(\infty) = \frac{1}{k} (c(\infty) \ast c(\infty))_{k-1} = \frac{1}{k} \sum_{j=0}^{k-1} c_j(\infty)c_{n-1-j}(\infty), \quad k \geq 0$$
and this holds only for $c(\infty) \equiv 1$. Estimate (E.15) is, however, sharp enough for $t$ close to $\infty$; Equations (E.18), (E.22) imply that $\dot{c}_k(t) < 0$ for all $t \geq 0$ and, as $c_k(t)$ is bounded from below, $\lim_{t\to\infty} c_k(t) = 1$, concluding the proof of Proposition 4.6.

□

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