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The Analyticity Region of the Hard Sphere Gas. Improved Bounds

Roberto Fernández · Aldo Procacci · Benedetto Scoppola

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Abstract We find an improved estimate of the radius of analyticity of the pressure of the hard-sphere gas in d dimensions. The estimates are determined by the volume of multidimensional regions that can be numerically computed. For $d = 2$, for instance, our estimate is about 40% larger than the classical one.

In a recent paper [4] two of us have shown that it is possible to improve the radius of convergence of the cluster expansion using a tree graph identity due to Penrose [2], see also [5, Sect. 3]. In this short letter we use the same idea to improve the estimates of the radius of analyticity of the pressure of the hard-sphere gas.

The grand partition function $\Xi(z, \Lambda)$ of a gas of hard spheres of diameter R enclosed in a volume $\Lambda \subset \mathbb{R}$ is given by

$$\Xi(z,\Lambda) = \sum_{n=0}^{\infty} \frac{z^n}{n!} \int_{\Lambda^n} dx_1 \cdots dx_n \exp\left\{- \sum_{1\le i<j\le n} U(x_i - x_j)\right\}$$

with

$$U(x-y) = \begin{cases} 0 & \text{if } |x-y| > R, \\ +\infty & \text{if } |x-y| \le R \end{cases}$$

R. Fernández
Laboratoire de Mathematiques Raphael Salem, UMR 6085 CNRS-Universite de Rouen,
Avenue de l'Universite, BP.12, 76801 Saint-Etienne-du-Rouvray, France

A. Procacci (✉)
Departamento de Matemática, UFMG, 30161-970 Belo Horizonte, MG, Brazil
e-mail: aldo@mat.ufmg.br

B. Scoppola
Dipartimento di Matematica, Universitá "Tor Vergata" di Roma, V.le della Ricerca Scientifica,
00100 Roma, Italy

where $|x-y|$ denotes the euclidean distance between the sphere centers x and y. The corresponding pressure is $\lim_{\Lambda\to\mathbb{R}^d} P(z,\Lambda)$ (limit in van Hove sense), where

$$P(z,\Lambda)=\frac{1}{|\Lambda|}\log \Xi(z,\Lambda)$$

($|\Lambda|$ denotes the volume of the region Λ). The cluster expansion, in this setting, amounts to writing the preceding logarithm as the power series (see e.g. [1])

$$\log \Xi(z,\Lambda)=\sum_{n=1}^{\infty}\frac{z^n}{n!}\int_{\Lambda^n} dx_1\cdots dx_n \sum_{\substack{g\subset g(x_1,\dots,x_n)\\ g\in G_n}}(-1)^{|g|} \tag{1}$$

where the graph $g(x_1,\dots,x_n)$ has vertex set $\{1,\dots,n\}$ and edge set $E(x_1,\dots,x_n)=\{\{i,j\}: |x_i-x_j|\le R\}$ (that is, if the spheres centered at x_i and x_j intersect), G_n is the set of all the connected graphs with vertex set $\{1,\dots,n\}$, and $|g|$ denotes the cardinality of the edge set of the graph g. Only families $(x_1,\dots,x_n)$ for which $g(x_1,\dots,x_n)$ is connected contribute to (1); such families represent "clusters" of spheres.

The standard way to estimate the radius of analyticity of the pressure is to obtain a Λ-independent lower bound of the radius of convergence of the series

$$|P|(z,\Lambda)=\frac{1}{|\Lambda|}\sum_{n=1}^{\infty}\frac{|z|^n}{n!}\int_{\Lambda^n} dx_1\cdots dx_n \Bigg|\sum_{\substack{g\subset g(x_1,\dots,x_n)\\ g\in G_n}}(-1)^{|g|}\Bigg|. \tag{2}$$

This strategy leads to the classical estimation (see e.g. [6], Sect. 4) that the pressure is analytic if

$$|z|<\frac{1}{eV_d(R)}, \tag{3}$$

where $V_d(R)$ is the volume of the d-dimensional sphere of radius R (excluded volume).

Our approach is based on a well known tree identity. Let us denote by T_n the subset of G_n formed by all tree graphs with vertex set $\{1,\dots,n\}$. Given a tree $\tau\in T_n$ and a vertex i of τ, we denote by d_i the *degree* of the vertex i in τ, i.e. the number of edges of τ containing i. We regard the trees $\tau\in T_n$ as rooted in the vertex 1. This determines the usual partial order of vertices in τ by generations: If u,v are vertices of τ, we write $u\prec v$—and say that u precedes v—if the (unique) path from the root to v contains u. If $\{u,v\}$ is an edge of τ, then either $v\prec u$ or $u\prec v$. Let $\{u,v\}$ be an edge of τ and assume without loss of generality that $u\prec v$, then u is the called the *predecessor* and v the *descendant*. Every vertex $v\in\tau$ has a unique predecessor and $s_v=d_v-1$ descendants, except the root that has no predecessor and $s_v=d_v$ descendants. For each vertex v of τ we denote by v' the unique predecessor of v and by $v^1,\dots,v^{s_v}$ the s_v descendants of v. The number s_v is called the branching factor; vertices with $s_v=0$ are called end-points or "leaves".

Penrose [4] showed that the sum in (1) is equal, up to a sign, to a sum over trees satisfying certain constraints. We shall keep only the "single-vertex" constraints: descendants of a given sphere must be mutually non-intersecting. This implies that

$$\Bigg|\sum_{\substack{g\subset g(x_1,\dots,x_n)\\ g\in G_n}}(-1)^{|g|}\Bigg|\le\sum_{\tau\in T_n} w_\tau(x_1,\dots,x_n) \tag{4}$$

where

$$w_\tau(x_1,\dots,x_n)=\begin{cases}1 & \text{if } |x_v-x_{v'}|\le R \text{ and } |x_{v^i}-x_{v^j}|>R,\\ & \quad \forall v \text{ vertex of } \tau, \{i,j\}\subset\{1,\dots,s_v\},\\ 0 & \text{otherwise.}\end{cases} \tag{5}$$

Hence from (2) and (4) we get

$$|P|(z,\Lambda)\le\sum_{n=1}^{\infty}\frac{|z|^n}{n!}\sum_{\tau\in T_n}S_\Lambda(\tau) \tag{6}$$

with

$$S_\Lambda(\tau)=\frac{1}{|\Lambda|}\int_{\Lambda^n}w_\tau(x_1,\dots,x_n)dx_1\cdots dx_n. \tag{7}$$

By (5) we have

$$S_\Lambda(\tau)\le g_d(d_1)\prod_{i=2}^{n}g_d(d_i-1) \tag{8}$$

where d_i is the degree of the vertex i in τ,

$$g_d(k)=\int_{\substack{|x_i|\le R\\ |x_i-x_j|>R}}dx_1\cdots dx_k=R^{dk}\int_{\substack{|y_i|\le 1\\ |y_i-y_j|>1}}dy_1\cdots dy_k$$

for k positive integer, and $g_d(0)=1$ by definition. It is convenient to write

$$g_d(k)=[V_d(R)]^k\tilde{g}_d(k) \tag{9}$$

with

$$\tilde{g}_d(k)=\frac{1}{[V_d(1)]^k}\int_{\substack{|y_i|\le 1\\ |y_i-y_j|>1}}dy_1\cdots dy_k \tag{10}$$

for k positive integer and $\tilde{g}_d(0)=1$. We observe that $\tilde{g}_d(k)\le 1$ for all values of k. From (8)–(10) we conclude that

$$\begin{aligned}S_\Lambda(\tau)&\le[V_d(R)]^{d_1}\tilde{g}_d(d_1)\prod_{i=2}^{n}[V_d(R)]^{d_i-1}\tilde{g}_d(d_i-1)\\ &=[V_d(R)]^{n-1}\tilde{g}_d(d_1)\prod_{i=2}^{n}\tilde{g}_d(d_i-1).\end{aligned}$$

The last identity follows from the fact that for every tree of n vertices, $d_1+\cdots+d_n=2n-2$. The τ-dependence of this last bound is only through the degree of the vertices, hence it leads, upon insertion in (6), to the inequality

$$|P|(z,\Lambda)\le\frac{1}{V_d(R)}\sum_{n=1}^{\infty}\frac{(|z|V_d(R))^n}{n!}\sum_{\substack{d_1,\dots,d_n\\ d_1+\cdots+d_n=2n-2}}\tilde{g}_d(d_1)\prod_{i=2}^{n}\tilde{g}_d(d_i-1)\frac{(n-2)!}{\prod_{i=1}^{n}(d_i-1)!}.$$

The last quotient of factorials is, precisely, the number of trees with n vertices and fixed degrees $d_1, \ldots, d_n$, according to Cayley formula.

At this point we can bound the last sum by a power in an obvious manner. The convergence condition so obtained would already be an improvement over the classical estimate (3). We can, however, get an even better result through a trick used by two of us in [3]. We multiply and divide by a^{n-1} where $a > 0$ is a parameter to be chosen in an optimal way. This leads us to the inequality

$$|P|(z, \Lambda) \leq \frac{a}{V_d(R)} \sum_{n=1}^{\infty} \frac{(|z|V_d(R))^n}{a^n n(n-1)} \sum_{\substack{d_1,\ldots,d_n \\ d_1+\cdots+d_n=2n-2}} \frac{\tilde{g}_d(d_1)a^{d_1}}{d_1!} \prod_{i=2}^{n} \frac{\tilde{g}_d(d_i-1)a^{d_i-1}}{(d_i-1)!}$$

$$\leq \frac{a}{V_d(R)} \sum_{n=1}^{\infty} \frac{1}{n(n-1)} \left(\frac{|z|}{a} [V_d(R)] \left[\sum_{s\geq 0} \frac{\tilde{g}_d(s)a^s}{s!} \right] \right)^n.$$

The last series converges if

$$|z|V_d(R) \leq \frac{a}{C_d(a)}$$

where

$$C_d(a) = \sum_{s\geq 0} \frac{\tilde{g}_d(s)}{s!} a^s$$

(this is a finite sum!). The pressure is, therefore, analytic if

$$|z|V_d(R) \leq \max_{a>0} \frac{a}{C_d(a)}. \tag{11}$$

This is our new condition.

Let us show that for $d = 2$ the quantitative improvement given by this condition can be substantial. In this case

$$C_2(a) = \sum_{s=0}^{5} \frac{\tilde{g}_2(s)}{s!} a^s$$

where, by definition, $\tilde{g}_2(0) = \tilde{g}_2(1) = 1$. The factor $\tilde{g}_2(2)$ can be explicitly evaluated in terms of straightforward integrals and we get

$$\tilde{g}_2(2) = \frac{3\sqrt{3}}{4\pi}.$$

The other terms of the sum can be numerically evaluated using a simple Monte Carlo simulation, obtaining

$$\tilde{g}_2(3) = 0.0589, \qquad \tilde{g}_2(4) = 0.0013, \qquad \tilde{g}_2(5) \leq 0.0001.$$

Choosing $a = [\frac{8\pi}{3\sqrt{3}}]^{1/2}$ (a value for which $\frac{a}{C_d(a)}$ is close to its maximum) we get

$$|z|V_2(R) \leq 0.5107.$$

This should be compared with the bound $|z|V_2(R) \leq 0.36787\ldots$ obtained through the classical condition (3).

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