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A Correction to a Remark in a Paper by Procacci and Yuhjtman: New Lower Bounds for the Convergence Radius of the Virial Series

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Abstract In this note we deduce a new lower bound for the convergence radius of the Virial series of a continuous system of classical particles interacting via a stable and tempered pair potential using the estimates on the Mayer coefficients obtained in the recent paper by Procacci and Yuhjtman (Lett Math Phys 107:31–46, 2017). This corrects the wrongly optimistic lower bound for the same radius claimed (but not proved) in the above cited paper (in Remark 2 below Theorem 1). The lower bound for the convergence radius of the Virial series provided here represents a strong improvement on the classical estimate given by Lebowitz and Penrose in 1964.

Keywords Classical continuous gas · Virial series · Cluster expansion · Penrose tree-graph identity

Mathematics Subject Classification 82B05 · 82B21

1 Introduction

The n-order coefficient of the Mayer series of a continuous system of classical particles at inverse temperature $\beta > 0$ confined in a box $\Lambda \subset \mathbb{R}^d$ and interacting via a pair potential V is explicitly given by

$$
C_n(\beta, \Lambda) = \begin{cases} \frac{1}{n!} \frac{1}{|\Lambda|} \int_\Lambda dx_1 \ldots \int_\Lambda dx_n \sum_{g \in G_n} \prod_{\{i,j\} \in E_g} \left[e^{-\beta V(x_i - x_j)} - 1 \right] & \text{if } n \geq 2 \\ 1 & \text{if } n = 1 \end{cases}
$$
(1.1)

where G_n is the set of the connected graphs in $[n]$ and E_g denotes the edge set of $g \in G_n$. In our recent paper [7] it is proved that if the potential V is stable and tempered with stability constant B (see (2.4) ahead) the following upper bound holds.

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$$|C_n(\Lambda, \beta)| \le e^{\beta Bn} \frac{n^{n-2}}{n!} [\tilde{C}(\beta)]^{n-1} \qquad (1.2)$$

where

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

This improves the classical estimates for the same coefficients obtained by Penrose and Ruelle in 1963 [5,8], namely

$$|C_n(\Lambda, \beta)| \le e^{\beta 2B(n-2)} \frac{n^{n-2}}{n!} [C(\beta)]^{n-1} \qquad (1.3)$$

with

$$C(\beta) = \int_{\mathbb{R}^d} dx \left|1 - e^{-\beta V(x)}\right|$$

The pressure $P_\Lambda(\beta, \lambda)$ and the density $\rho_\Lambda(\beta, \lambda)$ of the system can be written in terms of these coefficients as power series in the fugacity λ as

$$\beta P_\Lambda(\beta, \lambda) = \sum_{n=1}^{\infty} C_n(\beta, \Lambda) \lambda^n \qquad (1.4)$$

$$\rho_\Lambda(\beta, \lambda) = \lambda \frac{\partial}{\partial \lambda} (\beta P_\Lambda(\beta, \lambda)) = \sum_{n=1}^{\infty} n C_n(\beta, \Lambda) \lambda^n \qquad (1.5)$$

and by estimates (1.2) one immediately concludes that $P_\Lambda(\beta, \lambda)$ and $\rho_\Lambda(\beta, \lambda)$ are analytic functions of λ for all complex values of λ satisfying

$$|\lambda| < R^* \doteq \frac{1}{e^{\beta B+1} \tilde{C}(\beta)}$$

The lower bound R^* for the convergence radius of the Mayer series obtained in [7] improves the one given by Ruelle and Penrose [5,8] derived from estimates (1.3).

By eliminating the activity λ from Eqs. (1.4) and (1.5) one can write the pressure of the system in the grand canonical ensemble in power of the density $\rho = \rho_\Lambda(\beta, \lambda)$ obtaining the so-called Virial expansion of the pressure, which is usually written as

$$\beta P_\Lambda(\beta, \rho) = \rho - \sum_{k \ge 1} \frac{k}{k+1} \beta_k(\beta, \Lambda) \rho^{k+1} \qquad (1.6)$$

The coefficients $\beta_k(\beta, \Lambda)$ are of course certain algebraic combinations of the Mayer coefficients $C_n(\beta, \lambda)$ with $n \le k+1$ whose explicit expression is long known (see e.g. formula (29) p. 319 of [4] and references therein). In 1964 Lebowitz and Penrose developed an indirect method, based on Lagrange inversion, to derive a lower bound for the convergence radius $\mathcal{R}$ of the Virial series (1.6) from the Penrose–Ruelle estimates (1.3). Namely, they proved that the r.h.s. of (1.6) converges absolutely for all complex ρ such that

$$|\rho| < \mathcal{R}_{\text{LP}} \doteq \frac{g(e^{2\beta B})}{e^{2\beta B} C(\beta)} \qquad (1.7)$$

with the function

$$g(u) = \max_{0 < w < \ln(1+u)} \frac{[(1+u)e^{-w} - 1]w}{u} \qquad (1.8)$$

slightly increasing in the interval $[1, +\infty)$ and such that $g(1) \approx 0.14477$ and $\lim_{u \to \infty} g(u) = e^{-1}$.

Our paper [7] contains a remark (Remark 2, immediately after Theorem 1) claiming that the new bounds for the Mayer coefficients (1.2) also yields an improvement (formula (2.17) in [7]) on $\mathcal{R}_{LP}$. In [7] it is alleged that to get this new lower bound of the convergence radius of the virial series one has just to redo the calculations performed by Lebowitz and Penrose in [3] using the new upper bound of the nth-order Mayer coefficients (1.2) in place of the old ones (1.3) given by Penrose and Ruelle. This assertion is wrong since the new bounds of the n-order Mayer coefficients (1.2) actually improve on (1.3) only as soon as $n \geq 4$, and it happens that the $n = 2$ and the $n = 3$ order Mayer coefficients have a non-negligible influence in the deduction presented in [3]. The purpose of this note is thus to correct this error and explain in details how to deduce a new lower bound of the convergence radius of the virial series (which still strongly improves on (1.7)) from (a slight variant of) the new upper bounds of the Mayer coefficients (1.2) and via the method used in [3].

2 The New Lower Bound for the Convergence Radius of the Virial Series

Let us first of all introduce some notations and definitions. Given a pair potential V we recall that

$$B = \sup_{n \geq 2} \sup_{(x_1, \ldots, x_n) \in \mathbb{R}^{dn}} \left\{ -\frac{1}{n} \sum_{1 \leq i < j \leq n} V(x_i - x_j) \right\} \tag{2.1}$$

is the usual stability constant of V. We also set

$$\bar{B} = \sup_{n \geq 2} \sup_{(x_1, \ldots, x_n) \in \mathbb{R}^{dn}} \left\{ -\frac{1}{n-1} \sum_{1 \leq i < j \leq n} V(x_i - x_j) \right\} \tag{2.2}$$

and call $\bar{B}$ the *Basuev stability constant* of the potential V (after Basuev who was the first to introduce it in [1]). We have clearly, for all $n \geq 2$ and all $(x_1, \ldots, x_n) \in \mathbb{R}^{dn}$

$$\sum_{1 \leq i < j \leq n} V(x_i - x_j) \geq -nB \tag{2.3}$$

$$\sum_{1 \leq i < j \leq n} V(x_i - x_j) \geq -(n-1)\bar{B} \tag{2.4}$$

and

$$\bar{B} \geq B$$

For the majority of realistic stable potentials the constants $\bar{B}$ and B are likely to be very close (if not equal). E.g. for the Leonard–Jones potential in three dimensions $V_{LJ}(x) = |x|^{-12} - 2|x|^{-6}$, according to the tables given in [2], we have that $B \leq \bar{B} \leq \frac{1001}{1000}B$. In any case, that for general stable potentials it holds that

$$\bar{B} \leq \frac{d+1}{d} B \tag{2.5}$$

while for potentials which reach a negative minimum at some $|x| = r_0$ and are negative for all $|x| > r_0$ (e.g. Lennard-Jones type potentials) it holds that

$$\bar{B} \leq \begin{cases} \frac{3}{2}B & \text{if } d = 1 \\ \frac{7}{6}B & \text{if } d = 2 \\ \frac{2d(d-1)+1}{2d(d-1)}B & \text{if } d \geq 3 \end{cases} \tag{2.6}$$

Now, using (2.4) in place of (2.3), with minor changes in the proof given in [7] one can show that the inequality (1.2) can be rewritten in terms of the Basuev constant $\bar{B}$ as follows

$$|C_n(\Lambda, \beta)| \leq e^{\beta \bar{B}(n-1)} n^{n-2} \frac{[\tilde{C}(\beta)]^{n-1}}{n!} \tag{2.7}$$

Using these bounds (2.7) and following the strategy described in [3] we have the following Theorem.

Theorem 1 *Let V be a stable and tempered pair potential with Basuev stability constant $\bar{B}$. Then the convergence radius $\mathcal{R}$ of the Virial series (1.6) admits the following lower bound.*

$$\mathcal{R} \geq \mathcal{R}^* \doteq \frac{g(1)}{\tilde{C}(\beta)e^{\beta \bar{B}}} \tag{2.8}$$

where g is the function defined in (1.8).

Note that the difference with the incorrect announced bound of formula (2.17) of [7] is that in the correct expression (2.8) the Basuev stability constant $\bar{B}$ replaces the usual stability constant $\bar{B}$ and moreover (2.8) contains a $g(1)$, rather than a $g(e^{\beta \bar{B}})$. We will prove Theorem 1 in the next section and, to make this note as self-contained as possible, we will also sketch, in Appendix A, the proof of (2.7) while in Appendix B we will prove bounds (2.5) and (2.6).

We conclude this section by comparing the new bound $\mathcal{R}^*$ (2.8) with the Lebowitz Penrose bound $\mathcal{R}_{LP}$ (1.7). Let us first observe that the ratio $\mathcal{R}^*/\mathcal{R}_{LP}$ is 1 for positive potentials, so there is no improvement when $B = \bar{B} = 0$. On the other hand for potentials with stability constant $B > 0$ (i.e. for potentials with a negative part) the ratio $\mathcal{R}^*/\mathcal{R}_{LP}$ grows exponentially in β, since so do $C(\beta)/\tilde{C}(\beta)$ and $e^{\beta(2B-\bar{B})}$. To give an idea of how significant can be the improvement in a concrete example, let us look at the case of the three-dimensional Lennerd–Jones potential $V_{LJ}(x) = |x|^{-12} - 2|x|^{-6}$ considered in [7]. We have that at inverse temperature $\beta = 1$, using the value $B_{LJ} = 8.61$ for its stability constant and the fact that $\bar{B}_{LJ} \leq \frac{1001}{1000}B_{LJ}$ (see [2]), $\mathcal{R}^*$ is at least 3.3×10^4 larger than $\mathcal{R}_{LP}$, while for $\beta = 10$ $\mathcal{R}^*$ is at least 2.9×10^{43} larger than $\mathcal{R}_{LP}$.

2.1 Proof of Theorem 1

We start by observing that, due to (1.5) and the fact that $C_1(\beta, \Lambda) = 1$, there exists a circle of some radius $R < 1/[\tilde{C}(\beta)e^{\beta \bar{B}+1}]$ and center in the origin $\lambda = 0$ of the complex λ-plane such that $\rho_\Lambda(\beta, \lambda)$ has only one zero in the disc $D_R = \{\lambda \in \mathbb{C} : |\lambda| \leq R\}$ and this zero occurs precisely at $\lambda = 0$. Let now $\rho \in \mathbb{C}$ be such that

$$|\rho| < \min_{\lambda \in C} |\rho_\Lambda(\beta, \lambda)| \tag{2.9}$$

Then by Rouché's theorem $\rho_\Lambda(\beta, \lambda)$ and $\rho_\Lambda(\beta, \lambda) - \rho$ have the same number of zeros (i.e. one) in the region $D_R = \{\lambda \in \mathbb{C} : |\lambda| \leq R\}$. In other words, for any complex ρ satisfying (2.9) there is only one $\lambda \in D_R$ such that $\rho = \rho_\Lambda(\beta, \lambda)$ and therefore we can invert the equation $\rho = \rho_\Lambda(\beta, \lambda)$ and write $\lambda = \lambda_\Lambda(\beta, \rho)$. Thus, according to Cauchy's argument principle, we can write the pressure $\beta P_\Lambda(\beta, \lambda)$ as a function of the density $\rho = \rho_\Lambda(\beta, \lambda)$ as

$$P_\Lambda(\rho, \beta) = \frac{1}{2\pi i} \oint_\gamma P_\Lambda(\beta, \lambda) \frac{d\rho_\Lambda(\beta, \lambda)}{d\lambda} \frac{d\lambda}{\rho_\Lambda(\beta, \lambda) - \rho} \tag{2.10}$$

where γ can be any circle centered at the origin in the complex λ-plane fully contained in the region D_R and such that

$$|\rho| < \min_{\lambda \in \gamma} |\rho_\Lambda(\beta, \lambda)| \tag{2.11}$$

By standard complex analysis $P_\Lambda(\rho, \beta)$ is analytic in ρ in the region (2.11). Indeed, once (2.11) is satisfied we can write

$$\frac{1}{\rho_\Lambda(\beta, \lambda) - \rho} = \sum_{n=0}^\infty \frac{\rho^n}{[\rho_\Lambda(\beta, \lambda)]^{n+1}} \tag{2.12}$$

and inserting (2.12) in (2.10) we get

$$P_\Lambda(\rho, \beta) = \sum_{n=1}^\infty c_n(\beta, \Lambda) \rho^n \tag{2.13}$$

with

$$
\begin{aligned}
c_n(\beta, \Lambda) &= \frac{1}{2\pi i} \oint_\gamma P_\Lambda(\beta, \lambda) \frac{d\rho_\Lambda(\beta, \lambda)}{d\lambda} \frac{d\lambda}{[\rho_\Lambda(\beta, \lambda)]^{n+1}} \\
&= -\frac{1}{2\pi i n} \oint_\gamma P_\Lambda(\beta, \lambda) \frac{d}{d\lambda} \left[\frac{1}{[\rho_\Lambda(\beta, \lambda)]^n} \right] d\lambda \\
&= \frac{1}{2\pi i n} \oint_\gamma \frac{d P_\Lambda(\beta, \lambda)}{d\lambda} \frac{1}{[\rho_\Lambda(\beta, \lambda)]^n} d\lambda \\
&= \frac{1}{2\pi i n \beta} \oint_\gamma \frac{1}{[\rho_\Lambda(\beta, \lambda)]^{n-1}} \frac{d\lambda}{\lambda}
\end{aligned}
$$

Therefore

$$|c_n(\beta, \Lambda)| \leq \frac{1}{n\beta} \frac{1}{\left[\min_{\lambda \in \gamma} |\rho_\Lambda(\beta, \lambda)| \right]^{n-1}} \tag{2.14}$$

Inequality (2.14) shows that the convergence radius $\mathcal{R}$ of the series (2.13) (i.e. of the virial series (1.6)) is such that

$$\mathcal{R} \geq \min_{\lambda \in \gamma} |\rho_\Lambda(\beta, \lambda)| \tag{2.15}$$

Therefore the game is to find an optimal circle γ in the region D_R which maximizes the r.h.s. of (2.15). We proceed as follows. Recalling (1.5) we have, by the triangular inequality, that

$$|\rho_\Lambda(\beta, \lambda)| \geq |\lambda| - \sum_{n=2}^\infty n |C_n(\beta, \Lambda)| |\lambda|^n \tag{2.16}$$

We now use estimate (2.7) to bound the sum in the r.h.s. of (2.16). Therefore we get

$$
\begin{aligned}
|\rho_\Lambda(\beta, \lambda)| &\geq |\lambda| - \sum_{n=2}^\infty \frac{n^{n-1}}{n!} [\tilde{C}(\beta) e^{\beta \bar{B}}]^{n-1} |\lambda|^n \\
&= 2|\lambda| - \frac{1}{\tilde{C}(\beta) e^{\beta \bar{B}}} \sum_{n=1}^\infty \frac{n^{n-1}}{n!} [\tilde{C}(\beta) e^{\beta \bar{B}} |\lambda|]^n
\end{aligned}
$$

Now following [3] let us set w to be the first positive solution of

$$we^{-w} = \tilde{C}(\beta)e^{\beta\bar{B}}|\lambda| \tag{2.17}$$

If we take $|\lambda| < 1/e^{\beta\bar{B}+1}\tilde{C}(\beta)$ (which is surely inside the convergence region since $\bar{B} \geq B$) then $\tilde{C}(\beta)e^{\beta\bar{B}}|\lambda| < 1/e$ and since the function we^{-w} is increasing in the interval $[0, 1]$ and takes the value $1/e$ at $w = 1$, there is a unique w in the interval $[0, 1]$ which solves (2.17). Now we use the Euler's formula

$$w = \sum_{n=1}^{\infty} \frac{n^{n-1}}{n!}(we^{-w})^n$$

to get

$$|\rho_\Lambda(\beta, \lambda)| \geq \frac{w}{\tilde{C}(\beta)e^{\beta\bar{B}}}\left[2e^{-w} - 1\right] \tag{2.18}$$

Observe that the r.h.s. (2.18) is greater than zero when w varies in the interval $(0, \ln 2)$. Therefore, any circle γ around the origin with radius R_γ between zero and $\ln 2/(2e^{\beta\bar{B}+1}\tilde{C}(\beta))$, which corresponds, in force of (2.17), to any w in the interval $(0, \ln 2)$, is surely in the region D_R. So we have

$$\max_{\gamma \subset D_R} \min_{\lambda \in \gamma} |\rho_\Lambda(\beta, \lambda)| \geq \max_{w \in (0, \ln 2)} \frac{w}{\tilde{C}(\beta)e^{\beta\bar{B}}}\left[2e^{-w} - 1\right] \tag{2.19}$$

which, recalling (2.15) and (1.8), concludes the proof.

Appendix A: Proof of (2.7)

Estimate (2.7) is basically the bound (1.2) proved in [7] with the unique difference that the factor $e^{\beta\bar{B}(n-1)}$ replaces the factor $e^{\beta Bn}$. Of course, since $\bar{B} \geq B$, this is a bad deal for someone interested in an upper bound the Mayer series. On the other hand, as shown in Sec. 3, the use (2.7) instead of (1.2) happens to be a good deal towards an upper bound the Virial series. Inequality (2.7) relies on two lemmas originally proved in [7] (see there Lemma 1 and Lemma 2). For completeness we report these lemmas and their proofs here below.

The first of these two lemmas involves the concept of partition scheme, which, we remind, is a map M from the set T_n of the labeled trees in $[n]$ to the set G_n of the connected graphs in $[n]$ such that $G_n = \biguplus_{\tau \in T_n}[\tau, M(\tau)]$ with $\biguplus$ disjoint union and $[\tau, M(\tau)] = \{g \in G_n : \tau \subseteq g \subseteq M(\tau)\}$.

Lemma 1 *For fixed V and $(x_1, \ldots, x_n) \in \mathbb{R}^{dn}$, choose a total order $\succ$ in the set of edges E_n of the complete graph K_n in such a way that $\{i, j\} \succ \{k, l\} \Longrightarrow V(x_i - x_j) \geq V(x_k - x_l)$ and let $T : G_n \to T_n$ be the map that associates to $g \in G_n$ the tree $T(g) \in T_n$ constructed by starting from $\emptyset$ and keeping adding the lowest edge in g that does not create a cycle (Kruskal algorithm).*

Let $M : T_n \to G_n$ be the map that associates to $\tau \in T_n$ the graph $M(\tau) \in G_n$ whose edges are the $\{i, j\} \in E_n$ such that $\{i, j\} \succeq \{k, l\}$ for every edge $\{k, l\} \in E_\tau$ belonging to the path from i to j through τ.

Then $T^{-1}(\tau) = \{g \in \mathcal{G}_n : \tau \subseteq g \subseteq M(\tau)\}$ and therefore M is a partition scheme in $\mathcal{G}_n$.

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

Remark The proof of Lemma 1 above, as well as the definition of the partition scheme M, are identical to those given in the homonymous lemma of [7], but the map $T : \mathcal{G}_n \to T_n$ appearing in the enunciate, based on Kruskal's algorithm, replaces a similar (but more involved) map constructed in [7] via so-called admissible functions with values in a tomonoid. The idea to use the Kruskal's algorithm, which eases the definition of the "minimal tree" map T, has been suggested during an Oberwolfach meeting by David Brydges, Tyler Helmuth and Daniel Ueltschi (see [10]).

Using the partition scheme M defined in Lemma 1 we now state and prove the second key lemma of [7].

Lemma 2 *Let V be stable with Basuev stability constant $\bar{B}$, and let $\tau \in T_n$. Let $(x_1, ..., x_n) \in \mathbb{R}^{dn}$ and let M be the partition scheme given above, then*

$$\sum_{\{i,j\} \in E_{M(\tau)} \setminus E_\tau^+} v(x_i - x_j) \geq -\bar{B}(n-1) \tag{2.20}$$

Proof . The set of edges $E_\tau \setminus E_\tau^+$ forms the forest $\{\tau_1, ..., \tau_k\}$. Let us denote V_{τ_s} the vertex set of the tree τ_s from the forest. Assume $i \in V_{\tau_a}$, $j \in V_{\tau_b}$. If $a \neq b$, the path from i to j through τ involves an edge $\{k, l\}$ in E_τ^+. Thus, if in addition $\{i.j\} \in E_{M(\tau)}$, we have $\{i, j\} \succeq \{k, l\}$ and therefore $v(x_i - x_j) \geq v(x_k - x_l) \geq 0$. If $a = b$, the path from i to j through τ is contained in τ_a. Thus, if in addition $\{i, j\} \notin E_{M(\tau)}$, there must be at least one edge $\{r, s\}$ in that path such that $\{i, j\} \prec \{r, s\}$ and therefore $v(x_i - x_j) \leq v(x_r - x_s) < 0$. This allows to bound:

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

where to get the last inequality we have used (2.4). $\quad\square$

We are now ready to conclude the proof of (2.7). By the so-called Penrose tree-graph identity [6], given a pair potential V and $(x_1, ..., x_n) \in \mathbb{R}^{dn}$, one has that

$$\sum_{g \in \mathcal{G}_n} \prod_{\{i,j\} \in E_g} \left[e^{-\beta V(x_i - x_j)} - 1 \right] = \sum_{\tau \in T_n} e^{-\beta \sum_{\{i,j\} \in E_{M(\tau)} \setminus E_\tau} V(x_i - x_j)} \prod_{\{i,j\} \in E_\tau} \left(e^{-\beta V(x_i - x_j)} - 1 \right)$$
$$\tag{2.21}$$

where $M : T_n \to \mathcal{G}_n$ is any map such that $\mathcal{G}_n = \biguplus_{\tau \in T_n} [\tau, M(\tau)]$ with $\biguplus$ disjoint union and $[\tau, M(\tau)] = \{g \in \mathcal{G}_n : \tau \subseteq g \subseteq M(\tau)\}$ (partition scheme) and T_n is the set of all trees with vertex set $[n]$.

Set now $E_\tau^+ = \{\{i, j\} \in E_\tau : V(x_i - x_j) \geq 0\}$, then from (2.21) one immediately gets

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

$$\leq \sum_{\tau \in T_n} e^{-\beta \sum\limits_{\{i,j\} \in E_{M(\tau)} \setminus E_\tau^+} V(x_i - x_j)} \prod_{\{i,j\} \in E_\tau} \left(1 - e^{-\beta |V(x_i - x_j)|} \right) \quad (2.22)$$

Let us now choose the partition scheme defined in Lemma 1. Then from Lemma 2, inserting (2.20) into (2.22), one obtains, for any $n \geq 2$ and any $(x_1, \ldots, x_n) \in \mathbb{R}^{dn}$, the following inequality

$$\left| \sum_{g \in G_n} \prod_{\{i,j\} \in E_g} (e^{-\beta V(x_i - x_j)} - 1) \right| \leq e^{\beta \bar{B}(n-1)} \sum_{\tau \in T_n} \prod_{\{i,j\} \in E_\tau} (1 - e^{-\beta |V(x_i - x_j)|}) \quad (2.23)$$

Now (2.7) follows easily from (2.23) recalling that $|T_n| = n^{n-2}$ and observing that, for any $\tau \in T_n$, it holds

$$\int_\Lambda dx_1 \ldots \int_\Lambda dx_n \prod_{\{i,j\} \in E_\tau} \left(1 - e^{-\beta |v(x_i - x_j)|} \right) \leq |\Lambda| \left[\tilde{C}(\beta) \right]^{n-1} \quad (2.24)$$

Appendix B: Proof of (2.5) and (2.6)

Proof of (2.5)

Let assume that $V(|x|)$ is a stable and tempered pair potential in d dimensions with stability constant B and Basuev stability constant $\bar{B}$. Let

$$B_n = \sup_{(x_1, \ldots, x_n) \in \mathbb{R}^{dn}} \left\{ -\frac{1}{n} \sum_{1 \leq i < j \leq n} V(x_i - x_j) \right\}$$

and

$$\bar{B}_n = \sup_{(x_1, \ldots, x_n) \in \mathbb{R}^{dn}} \left\{ -\frac{1}{n-1} \sum_{1 \leq i < j \leq n} V(x_i - x_j) \right\}$$

so that $B = \sup_{n \in \mathbb{N}} B_n$ and $\bar{B} = \sup_{n \in \mathbb{N}} \bar{B}_n$.
Let us first prove that if

$$\bar{B} = \limsup_{n \to \infty} \bar{B}_n \quad (2.25)$$

then

$$\bar{B} = B$$

Suppose by contradiction that $\bar{B} - B = \delta > 0$. If this holds then necessarily there exists a finite $m \geq 2$ such that $B = B_m$ otherwise if $B = \limsup_{n \to \infty} B_n$ then $B = \bar{B}$. Now, due to the hypothesis (2.25), for all $\varepsilon > 0$ there exists n_0 such that for infinitely many $n > n_0$

$$\bar{B}_n > \bar{B} - \varepsilon \quad \Longrightarrow \quad B_n > \frac{n-1}{n}(\bar{B} - \varepsilon) = \frac{n-1}{n}(B + \delta - \varepsilon)$$

Choose $\varepsilon = \frac{\delta}{2}$, then for infinitely many n we have that

$$B_n > \frac{n-1}{n}(B + \frac{\delta}{2}) > B \qquad \text{as soon as } n > \frac{2B}{\delta} + 1$$

in contradiction with the assumption that $B = B_m$. Hence we must have $B = \limsup B_n = \limsup \bar{B}_n = \bar{B}$.

So let us suppose that the sup $\bar{B}_n$ is reached at some finite integer m, i.e. $\bar{B} = \bar{B}_m$.

Since V is stable, it is bounded from below and since V is tempered inf V cannot be positive. Let $\inf_{x \in \mathbb{R}^d} V(x) = -C$ with $C \geq 0$. Then for any $\varepsilon > 0$ there exists r_ε such that $V(r_\varepsilon) < -(C - \varepsilon)$. Take the configuration $(x_1, x_2, \ldots, x_{d+1}) \in (\mathbb{R}^d)^{d+1}$ such that $x_1, x_2, \ldots, x_{d+1}$ are vertices of a d-dimensional hypertetrahedron with sides of length r_ε. Recall that a d-dimensional hypertetrahedron has $d+1$ vertices and $d(d+1)/2$ sides. Then $U(x_1, x_2, \ldots, x_{d+1}) < -\frac{d(d+1)}{2}(C - \varepsilon)$, which implies that $B > \frac{d}{2}(C - \varepsilon)$ and by the arbitrariness of ε we get $B \geq \frac{d}{2}C$. On the other hand we also have, for any $(x_1, \ldots, x_m) \in \mathbb{R}^{dm}$ that $U(x_1, \ldots, x_m) \geq -m(m-1)C/2$ which implies that $\bar{B}_m = \bar{B} \leq \frac{m}{2}C$. Hence we can write $\frac{d}{2}C \leq B \leq \bar{B} = \bar{B}_m \leq \frac{m}{2}C$ which implies $m \geq d+1$ and so $\bar{B} = \bar{B}_m = \frac{m}{m-1}B_m \leq \frac{m}{m-1}B \leq \frac{d+1}{d}B$. $\qquad \square$

Proof of (2.6)

Let us assume that $V(|x|)$ is a stable pair potential in d dimensions with stability constant B and Basuev stability constant $\bar{B}$ and that $V(|x|)$ reaches its negative minimum $-C$ at some $|x| = r_0$ and it is negative for all $|x| > r_0$. We want to prove that the inequalities (2.6) hold.

First note that $d(d-1)C$ is always a lower bound for B when $d \geq 3$. Just consider a configuration in which n particle (with n as large as we want) are arranged in close-packed configuration at the sites of a d-dimensional face-centered cubic lattice with step r_0. The energy of such configuration is (asymptotically as $n \to \infty$) less than or equal to $-d(d-1)Cn$ since in a d-dimensional face-centered cubic lattice each site has $2d(d-1)$ neighbors (see e.g. [9]) and so there are (asymptotically) $d(d-1)n$ pairs of neighbors in the configuration. On the other hand, for any n-particle configuration $(x_1, \ldots, x_n) \in \mathbb{R}^{dn}$, it holds that $U(x_1, \ldots, x_n) \geq -n(n-1)C/2$, i.e. $\bar{B}_n \leq nC/2$. Now, if $\bar{B} = \sup_n \bar{B}_n$ is attained at $n \to \infty$ then, as previously seen, we have $\bar{B} = B$. So let us suppose that $\bar{B} = \sup_n \bar{B}_n$ is attained at a certain finite m. Then we must have that $d(d-1)C \leq B \leq \bar{B} \leq mC/2$ and so $m \geq 2d(d-1)$. Now if $m = 2d(d-1)$ then $\bar{B} = B$. So when $\bar{B} > B$ then $m > 2d(d-1)$ and so we have $\bar{B} = \frac{m}{m-1}B_m \leq \frac{2d(d-1)+1}{2d(d-1)}B$. The case $d = 1$ and $d = 2$ are treated analogously by just observing that the close-packed arrangement in $d = 1$ is simply the cubic lattice with 2 neighbors for each site while for $d = 2$ is the triangular lattice with 6 neighbors for each site. So $d(d-1)$ must be replaced by 1 for $d = 1$ and by 3 for $d = 2$ yielding $m > 2$ and $m > 6$ for $d = 1$ and $d = 2$ respectively. $\qquad \square$

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