Virial series for a system of classical particles interacting through a pair potential with negative minimum

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Abstract
In this note we revisit the recent developments concerning rigorous results on the virial series of a continuous system of classical particles interacting via a stable and tempered pair potential and we provide new lower bounds for its convergence radius when the potential has a strictly positive stability constant. As an application we obtain a new estimate for the convergence radius of the virial series of the Lennard-Jones gas which improves sensibly previous estimates present in the literature.

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1. Introduction: Model and results
In this note we consider a system of classical identical particles confined in a box $\Lambda \subset \mathbb{R}^d$ interacting via a translational invariant and even pair potential $v : \mathbb{R}^d \to \mathbb{R} \cup \{+\infty\}$. This system is described in the Grand Canonical Ensemble by a probability measure on $\cup_n \Gamma_n(\Lambda)$ where $\Gamma_n(\Lambda) = \{(x_1, \ldots, x_n) \in \Lambda^{dn}\}$ whose restriction to $\Gamma_n(\Lambda)$ is

$$d\mu(x_1, \ldots, x_z) = \frac{1}{\Xi_v^\Lambda(\beta, z)} \frac{z^n}{n!} e^{-\beta \sum_{1 \leq i < j \leq n} v(x_i - x_j)} dx_1 \ldots dx_n$$

(1.1)

where $\beta = (kT)^{-1}$ is the inverse of the temperature in units of the Boltzmann constant and $z$ is the (configurational) fugacity. The normalization constant $\Xi_v^\Lambda(\beta, z)$, i.e. the grand canonical partition function is explicitly written as

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

(1.2)

The series above is an holomorphic function in the complex plane $z \in \mathbb{C}$ as soon as the potential $v$ is stable (see e.g. [22]). We remind that a pair potential $v$ is stable if there exists a finite non-negative number $B_v$ such that

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

(1.3)

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The number $B_v$ is called the stability constant of the potential $v$. We will also consider two more constants associated to the potential $v$. Namely,

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

and

$$
B_v^* = \sup_{x \in \mathbb{R}^d} v^-(x)
$$

where $v^-$ is the negative part of the potential, i.e.

$$
v^-(x) = \frac{1}{2} (|v(x)| - v(x))
$$

**Remark.** The constant $\hat{B}_v$ is called the *Basuev stability constant* of the potential $v$ (after Basuev who was the first to introduce it in [1]) while $B_v^*$ is simply the (absolute value of the) infimum of the potential. For a general stable potential $v$ it holds that $B_v \leq \hat{B}_v \leq \frac{d+1}{d} B_v$ and for any stable potential $v$ in $d \geq 3$ which reaches a negative minimum at some $|x| = r_0$ and is negative for all $|x| > r_0$ it holds $\hat{B}_v \leq \frac{2d(d-1)+1}{2d(d-1)} B_v$ (see [19]). For the majority of potentials used in simulations by chemists and physicists the stability constant and the Basuev stability constant are likely to be very close if not equal. In particular, for the specific case of the Leonard-Jones potential $V_{LJ}(r) = r^{-12} - 2r^{-6}$ in three dimensions to be considered later, according to the tables given in [11], we have that $B_{V_{LJ}} \leq \hat{B}_{V_{LJ}} \leq \frac{1001}{1000} B_{V_{LJ}}$.

Beyond stability, which is the key property standing behind the well-definiteness of the partition function, a standard hypothesis on the pair potential [22] is the so-called *regularity*. Namely, a pair potential $v$ is regular if

$$
\int_{\mathbb{R}^d} |e^{-\beta v(x)} - 1| dx = C_v(\beta) < +\infty
$$

Hereafter we will refer to the constant $C_v(\beta)$ as the *regularity constant* of the potential. Note that (1.7) is equivalent to require that there exists $r_0 > 0$ such that $\int_{|x| \geq r_0} |v(x)| dx < +\infty$ (see [22]). All potentials considered here below are supposed to be stable and regular.

In the present paper we will also consider a very relevant subclass of the stable and regular pair potentials which was first proposed by Basuev in [1]. This class is sufficiently large to embrace the large majority of examples of non purely repulsive pair potential physicists are usually dealing with.

**Definition 1** A regular pair potential $v$ is called Basuev if there exist $\alpha > 0$ such that

$$
v(x) \geq v_\alpha > 0 \quad \text{for all} \quad |x| \leq \alpha
$$

and

$$
v_\alpha > 2 \mu_v(\alpha)
$$

where $v_\alpha = \min_{x \in \mathbb{R}^d} v(x)$ and

$$
\mu_v(\alpha) = \sup_{n \in \mathbb{N}} \sup_{(x_1, \ldots, x_n) \in \mathbb{R}^d} \sum_{1 \leq i < j \leq n} v^-(x_i - x_j)
$$
with \( v^- \) being the negative part of the potential defined in (1.6).

In \([1]\) (see also \([9]\), Appendix B) it is proved the following useful proposition.

**Proposition 1** A Basuev potential \( v \) according to Definition 1 is stable with stability constant 
\[ B_v \leq \frac{1}{2} \mu(\alpha) . \]

We stress that many classical potentials utilized in simulations by physicists and chemists are Basuev. In particular, as shown in \([9]\), a pair potential \( v \) of Lennard-Jones type (for whose definition and properties we refer the reader to references \([5]\), \([6]\), \([22]\), \([14]\)) is Basuev.

The pressure \( P(v z, \beta) \) and the density \( \rho(v z, \beta) \) of the system under analysis are deduced from the partition function via the relations
\[
\beta P(v z, \beta) = \lim_{\Lambda \to \infty} \frac{1}{|\Lambda|} \log \Xi_{\Lambda}^v(z, \beta) \tag{1.11}
\]
\[
\rho(v z, \beta) = \lim_{\Lambda \to \infty} \frac{z}{|\Lambda|} \frac{\partial}{\partial z} \log \Xi_{\Lambda}^v(z, \beta) \tag{1.12}
\]

where \(|\Lambda|\) denotes the volume of the box \( \Lambda \) and here \( \lim_{\Lambda \to \infty} \) means that the size of the cubic box goes to infinity. It is long known (see \([22]\) and references therein) that the limits above exist whenever \( v \) is stable and regular. It is even longer known (see e.g. \([12]\) and references therein) that, by rewriting \( e^{-\beta \sum_{1 \leq i < j \leq n} v(x_i - x_j)} \) as \( \prod_{1 \leq i < j \leq n} [e^{-\beta v(x_i - x_j)} - 1] + 1 \), it is possible to expand the \( \log \Xi_{\Lambda}^v(z) \) as a power series in the fugacity \( z \). Namely,
\[
\frac{1}{|\Lambda|} \log \Xi_{\Lambda}^v(z) = z + \sum_{n=2}^{\infty} c_n^v(\Lambda, \beta) z^n \tag{1.13}
\]

where, for \( n \geq 2 \), \( c_n(\Lambda, \beta) \), the so-called (finite volume) Mayer (a.k.a. Ursell) coefficients are explicitly given by the formula
\[
c_n^v(\Lambda, \beta) = \frac{1}{|\Lambda| n!} \int_{\Lambda} dx_1 \ldots \int_{\Lambda} dx_n \sum_{g \in G_n} \prod_{\{i,j\} \in E_g} \left[ e^{-\beta v(x_i - x_j)} - 1 \right] \tag{1.14}
\]

with \( G_n \) denoting the set of the connected graphs with vertex set \([n] \equiv \{1, \ldots, n\}\) and \( E_g \) denoting the edge set of \( g \in G_n \). Plugging the expansion (1.13) into (1.11) and (1.12) we get
\[
\beta P^v(z, \beta) = z + \sum_{n=2}^{\infty} c_n^v(\beta) z^n \tag{1.15}
\]
\[
\rho^v(z, \beta) = z + \sum_{n=2}^{\infty} n c_n^v(\beta) z^n \tag{1.16}
\]

where \( c_n^v(\beta) = \lim_{\Lambda \to \infty} c_n^v(\Lambda, \beta) \) which, since the pair potential \( v \) is translational invariant, is given by
\[
c_n^v(\beta) = \frac{1}{n!} \int_{\mathbb{R}^d} dx_2 \ldots \int_{\mathbb{R}^d} dx_n \sum_{g \in G_n} \prod_{\{i,j\} \in E_g} \left[ e^{-\beta v(x_i - x_j)} - 1 \right] \tag{1.17}
\]
Formula (1.15) is known as the Mayer series of the pressure. The coefficients $c_n^\nu(\beta)$ are well defined (i.e. are all finite) as soon as the potential $v$ is regular.

By inverting the series (1.16), i.e. by expressing the fugacity $z$ as power series of the density $\rho = \rho^\nu(z, \beta)$ (which is always possible, at least in a neighbor of $z = 0$, since the first order coefficient of the series (1.16) is non zero), one can write the pressure of the system in the grand canonical ensemble in power of $\rho$ obtaining the so-called virial series, which is usually written as

$$\beta P^\nu(\rho, \beta) = \rho - \sum_{k \geq 1} \frac{k}{k + 1} \beta_k^\nu(\beta) \rho^{k+1}$$

(1.18)

The equation (1.18) is a fundamental one in statistical mechanics: it represents the equation of state of the (non-ideal) gas of classical particles interacting via the pair potential $v$. The coefficients $\beta_k^\nu(\beta)$ of the virial series are of course certain (quite intricate) algebraic combinations of the Mayer coefficients $c_n^\nu(\beta)$. This algebraic combinations are known since a long time (see e.g. formula (49) in [13] or also formula (29), p. 319 of [16]) and thus they can in principle be computed just by knowing the function $v(x)$. The virial coefficients $\beta_k^\nu(\beta)$ also admit a nice representation in terms of connected graphs (see e.g. [12] and references therein), namely

$$\beta_n^\nu(\beta) = \int_{\mathbb{R}^d} dx_2 \ldots \int_{\mathbb{R}^d} dx_n \sum_{g \in G_n^*} \prod_{(i,j) \in E_g} \left[ e^{-\beta v(x_i - x_j)} - 1 \right]$$

(1.19)

where $G_n^*$ is the set of the two-connected graphs with vertex set $[n] \equiv \{1, \ldots, n\}$. We recall that a graph $g$ is two-connected if deleting any vertex $v$ of $g$ plus the edges incident to $v$ the new graph so obtained remains connected.

A fundamental question in statistical mechanics is to establish the convergence radius $R_{Mayer}^v(\beta)$ of the Mayer series (1.15) and the convergence radius $R_{virial}^v(\beta)$ of the virial series (1.18).

As far as the Mayer series is concerned, in 1963 Penrose obtained [17] the following upper bound for its coefficients $|c_n^\nu(\beta)|$ when the pair potential $v$ is stable and regular

$$|c_n^\nu(\beta)| \leq \frac{n^{n-2}}{n!} e^{2\beta B_v(n-2)[C_v(\beta)]^{n-1}}$$

(1.20)

where $B_v$ is the stability constant of the potetial $v$ defined in (1.3) and $C_v(\beta)$ is the regularity constant of the potential $v$ defined in (1.7). From (1.20) it immediately follows that, for a fixed $\beta$, of the series (1.15) and (1.16) are absolutely convergent as soon as $z$ belongs to the open complex disc of radius $R_{PR}(\beta)$ centered at the origin with $R_{PR}(\beta)$ given by

$$R_{PR}(\beta) = (1/e) \frac{e^{-2\beta B_v}}{C_v(\beta)}$$

(1.21)

Therefore we have that $R_{Mayer}^v(\beta) \geq R_{PR}(\beta)$. This lower bound was also obtained in the same year by Ruelle [23].

The upper bound (1.20) on the absolute value of Mayer coefficients $|c_n^\nu(\beta)|$ for a general stable and regular pair potential $v$ has been recently improved by Procacci and Yuhjtman [20] who proved that

$$|c_n^\nu(\beta)| \leq \frac{n^{n-2}}{n!} e^{\beta B_v n}[\tilde{C}_v(\beta)]^{n-1}$$

(1.22)
where
\[
\tilde{C}_v(\beta) = \int_{\mathbb{R}^d} (1 - e^{-\beta|v(x)|}) dx
\]  
(1.23)

Bound (1.22) forthwith implies that the Mayer series (1.15) of a system of classical particles interacting via a stable and regular potential \( v \) is absolutely convergent at fixed \( \beta \) as soon as \( |z| < R_{\text{PY}}^v(\beta) \) where
\[
R_{\text{PY}}^v(\beta) = \left( \frac{1}{e} \right) \frac{e^{-\beta B_v}}{\tilde{C}_v(\beta)}
\]  
(1.24)

and hence \( R_{\text{Mayer}}^v(\beta) \geq R_{\text{PY}}^v(\beta) \). Note that, for any \( \beta > 0 \), it holds that \( R_{\text{PY}}^v(\beta) \geq R_{\text{PR}}^v(\beta) \) and the equality holds only if \( B_v = 0 \). We remind the reader that a stable and a regular pair potential \( v \) such that \( B_v = 0 \) is necessarily non-negative, that is to say, \( v(x) \geq 0 \) for all \( x \in \mathbb{R}^d \).

When the pair potential \( v \) is Basuev (i.e. \( v \) satisfies Definition \( \boxed{1} \)), it is possible to obtain an alternative lower bound for the Mayer coefficients using the procedure illustrated by Basuev in [2] and revisited in [9]. In these two references the alternative estimate of the Mayer coefficients when Basuev potentials are involved was given in the following form.

\[
|c_n^v(\beta)| \leq \frac{n^{n-2}}{n!} \left[ \frac{e^{\beta B_v} - 1}{\beta B_v} \right]^{n-1} \left[ \tilde{C}_v(\beta) \right] n^{-1}
\]  
(1.25)

where \( \tilde{B}_v \) is the Basuev stability constant defined in (1.4) and
\[
\tilde{C}_v(\beta) = \int_{|x| \leq \alpha} dx |v(x)| \beta \beta B_v (1 - e^{-\beta|v(x) - v_\alpha - B_v|}) \beta (v(x) - v_\alpha - B_v) (e^{\beta B_v} - 1) + \int_{x \geq \alpha} dx \beta |v(x)|
\]  
(1.26)

with \( \alpha \) and \( v_\alpha \) being the parameters (to be optimized) appearing in the Definition \( \boxed{1} \) The estimate (1.25) can be rewritten, after simple algebraic manipulations, in an alternative and more convenient way for later use. Namely, inequality (1.25) can be rewritten as

\[
|c_n^v(\beta)| \leq \frac{n^{n-2}}{n!} e^{\beta B_v (n-1)} |\tilde{C}_v(\beta)| n^{-1}
\]  
(1.27)

where
\[
\tilde{C}_v(\beta) = e^{-\beta B_v} \int_{|x| \leq \alpha} dx \beta |v(x)| \left( 1 - e^{-\beta|v(x) - v_\alpha - B_v|} \right) \beta (v(x) - v_\alpha - B_v) + \int_{x \geq \alpha} dx \beta |v(x)|
\]  
(1.28)

Bound (1.27) immediately implies that series (1.15) and (1.16) are absolutely convergent if \( |z| < R_{\text{Ba}}^v(\beta) \) where
\[
R_{\text{Ba}}^v(\beta) = \left( \frac{1}{e} \right) \frac{e^{-\beta B_v}}{\tilde{C}_v(\beta)}
\]  
(1.29)

Therefore, when \( v \) is a Basuev potential according to Definition \( \boxed{1} \) we have that \( R_{\text{Mayer}}^v(\beta) \geq R_{\text{Ba}}^v(\beta) \). As discussed in [20], in several relevant cases (e.g. if \( v \) is the Lennard-Jones potential) the lower bound \( R_{\text{Ba}}^v(\beta) \) for the convergence radius of the Mayer series is larger that the value \( R_{\text{PY}}^v \) found in [20].
To conclude the discussion about the Mayer series, it is important to stress that the bounds (1.22) and (1.25) for the Mayer coefficients are less than or equal to the old Penrose bounds given in the r.h.s. of (1.20) only if \( n \geq 4 \). When \( n = 2, 3 \) the bound (1.20) beats both bounds (1.22) (1.25). Of course this has no impact on the estimate of the lower bound of the convergence radius of the Mayer series but, as we will see in Section 2 below, tighter bounds for \( c^v_2(\beta) \) and \( c^v_3(\beta) \) are crucial to get efficient estimates of the convergence radius of the virial series.

Turning to the virial series (1.18), unfortunately a direct upper bound on its coefficients, as given in (1.19), is so far unavailable. Neverthless, lower bounds for the convergence radius \( R^v_{\text{virial}}(\beta) \) of the virial series (1.18) of a system of particles interacting via a pair potential \( v \) have been obtained during the last six decades. The best lower bound for was, until very recently, the one given by Lebowitz and Penrose in 1964 \([7]\) who, assuming that the pair potential \( v \) is stable and regular, proved that

\[
R^v_{\text{virial}}(\beta) \geq R^v_{\text{LP}}(\beta) = F(0) e^{-\beta B_v} \frac{C_v(\beta)}{\bar{C}_v(\beta)}
\]

(1.30)

where, for \( s \geq 0 \)

\[
F(s) = \max_{w \in (0,1)} \frac{[(1 + e^{2s})e^{-w} - 1]w}{e^{2s}}
\]

(1.31)

The function \( F(s) \) is increasing in the interval \( s \in [0, +\infty) \) with

\[
F(s = 0) = 0.144767 \quad \text{and} \quad \lim_{s \to \infty} F(s) = \frac{1}{e}
\]

The bound (1.30) was obtained via a complex analysis argument using explicitly the upper bounds on the absolute value of the Mayer coefficients \( |c^v_n(\beta)| \) given in (1.20). Therefore one can reasonably expect that the estimates (1.22) on \( |c^v_n(\beta)| \), which represent a clear advance with respect to the old estimates (1.20), should naturally result in an equally strong increase of the lower bound for \( R^v_{\text{virial}}(\beta) \). Indeed, recently \([19]\) the Lebowitz-Penrose bound (1.30) has been improved for system interacting via a stable and regular pair potential \( v \) using a slight variant of the bound for \( |c^v_n(\beta)| \) given in (1.22). The upper bound for \( |c^v_n(\beta)| \) proved in \([19]\) is as follows.

\[
|c^v_n(\beta)| \leq \frac{n^{n-2}}{n!} e^{\beta B_v(n-1)}[\tilde{C}_v(\beta)]^{n-1}
\]

(1.32)

where \( \bar{B}_v \) is the Basuev stability constant defined in (1.4) and \( \tilde{C}_v(\beta) \) is the constant defined in (1.23). As shown in \([19]\), the bound (1.32) implies that

\[
R^v_{\text{virial}}(\beta) \geq R^v_{\text{Pr}}(\beta) \equiv F(0) e^{-\beta \bar{B}_v} \frac{\tilde{C}_v(\beta)}{\bar{C}_v(\beta)}
\]

(1.33)

where \( F(0) \) is the function defined in (1.31) evaluated at \( s = 0 \).

The bound (1.33) represents a very strong improvement on the old Lebowitz-Penrose bound (1.30) when the pair potential \( v \) has stability constant \( B_v \) strictly positive (i.e \( v \) assumes negative values somewhere), especially for large \( \beta \). On the other hand, for systems of particles interacting via non-negative potential \( v \), for which \( \bar{B}_v = B_v = 0 \) and \( C_v(\beta) = \tilde{C}_v(\beta) \), the bound above coincides with the old Lebowitz-Penrose bound, namely

\[
R^v_{\text{virial}}(\beta) \geq \frac{0.144767}{C_v(\beta)} \quad \text{when} \quad v \geq 0
\]

(1.34)
In this regard it is worth to mention that for the specific case of positive pair potentials, the bound \((1.34)\) has very recently been improved, first by Jansen, Kuna and Tsagkarogiannis \([10]\) who replaced the constant \(0.144767\) by \(\frac{1}{2} \approx 0.183939\), and then by Fernández and Nyoung \([15]\) who, inspired on an unpublished work by S. Ramawadth and S. Tate \([21]\), further improved the same constant up to the value \(0.237961\) which coincides with that claimed (but never proved) long time ago by Groeneveld \([8]\).

However, these recent results on the convergence radius of the virial series obtained in \([10]\) and \([15]\), as far as non purely repulsive pair potentials are concerned, leave the situation practically unchanged at the point where it was after the paper \([19]\). The purpose of this note is to show that, by carefully revisiting results obtained in papers \([9]\), \([20]\), \([19]\) and \([25]\), it is possible to get new lower bounds of the convergence radius of systems of classical particles interacting via stable and tempered pair potentials with non-zero stability constant. These new bounds may become even better when Basuev pair potentials according to Definition \(1\) are involved.

To convince the reader of goodness of our new estimates, we pick as an example the important case where \(C_\beta = 2\) (and even for the \(d = 2\) case it holds strictly \(\bar{B}_{\nu} > \frac{3}{2}B_{\nu}^*\)) if the potential \(v\) reaches the negative minimum \(B_{\nu}^*\) at some \(x_0\) with \(|x_0| = r_0\) and is non-positive for all \(|x| > r_0\). Moreover, by straightforward calculations (e.g. using Wolframalpha to find the minimum) we have that

\[
F_v^*(\beta = 0) \approx 0.144767 \quad \lim_{\beta \to +\infty} F_v^*(\beta) \approx 0.241857
\]

Note that in general the function \(F_v^*(\beta)\) tends to increase rapidly from its minimum value to its maximum value as \(\beta\) increases because for most of the physical potentials the ratio \(\bar{B}_{\nu}/B_{\nu}^*\) is large (e.g. is of the order on 10 for the Lennard-Jones potentials). Bound \((1.35)\) given in Theorem \(1\) is clearly an improvement on the best lower bound \((1.33)\) obtained in \([19]\) for convergence radius of the virial series as far as stable and regular potentials with strictly positive stability constant are concerned. On the other hand, when positive potentials are considered, for which \(\bar{B}_{\nu} = B_{\nu} = 0\) and \(C_{\nu}(\beta) = \tilde{C}_{\nu}(\beta)\), the bound \((1.35)\) above, similarly to bound \((1.33)\), coincides with Lebowitz-Penrose bound \((1.34)\).
Theorem 2  Let $v$ be a Basuev potential according to Definition 1. Then the convergence radius of the virial series (1.18) of a system of classical particles interacting via the potential $v$ admits the following lower bound.

$$R_{\text{virial}}^v(\beta) \geq \max \left\{ R_{\text{stab}}^v(\beta), R_{\text{Bas}}^v(\beta) \right\}$$  \hspace{1cm} (1.37)

where $R_{\text{stab}}^v(\beta)$ is defined in (1.35) and

$$R_{\text{Bas}}^v(\beta) = \tilde{F}_v(\beta) \frac{e^{-\beta B_v}}{\hat{C}_v(\beta)}$$  \hspace{1cm} (1.38)

with $\hat{C}_v(\beta)$ being defined in (1.28) and

$$\tilde{F}_v(\beta) = \max_{w \in (0,1)} w \left[ 2e^{-w} + \left( 1 - e^{-\beta(\tilde{B}_v - B_v^*)} \frac{\hat{C}_v(\beta)}{\hat{C}_v(\beta)} \right) we^{-2w} + + \frac{3}{2} \left( 1 - e^{-\beta(2B_v - 3B_v^*)} \left[ \frac{\hat{C}(\beta)}{\hat{C}_v(\beta)} \right]^2 \right) w^2 e^{-3w} - 1 \right]$$  \hspace{1cm} (1.39)

Note that the quantity $\tilde{F}_v(\beta)$ is always strictly greater than zero since for any real $c_1$ and $c_2$ the function $f(w) = w(2e^{-w} + c_1 we^{-2w} + c_2 w^2 e^{-3w} - 1)$ has always a positive maximum in the interval $w \in (0,1)$. We will see ahead through a popular example (the Lennard-Jones fluid) that for systems of particles interacting via a Basuev potential we may have that $R_{\text{Bas}}^v(\beta) > R_{\text{stab}}^v(\beta)$.

2. Proof of Theorem 1

First of all we want to point out that in doing the estimate of the convergence radius of the virial series a la Lebowitz-Penrose as described below, it is crucial to have upper bounds for $|c_n(\beta)|$ defined in (1.17) as tight as possible when $n = 2$ and $= 3$. We thus prove the following preliminary lemma.

Lemma 1  Given a regular pair potential $v$, let $c_n^v(\beta)$ be defined as in (1.17). Then the following bounds hold.

$$|c_2^v(\beta)| \leq \frac{1}{2} e^{\beta B_v^*} \hat{C}_v(\beta)$$  \hspace{1cm} (2.1)

$$|c_3^v(\beta)| \leq \frac{1}{2} \left[ e^{\frac{3}{2} \beta B_v^*} \hat{C}_v(\beta) \right]^2$$  \hspace{1cm} (2.2)

Proof. Let first analyze the case $n = 2$. By (1.17) we have that

$$|c_2^v(\beta)| = \frac{1}{2!} \left| \int_{\mathbb{R}^d} (e^{-\beta v(x)} - 1) dx \right| \leq \frac{1}{2!} \int_{\mathbb{R}^d} |e^{-\beta v(x)} - 1| \ dx$$  \hspace{1cm} (2.3)

Now observe that

$$|e^{-\beta v(x)} - 1| = \begin{cases} (1 - e^{-\beta |v(x)|}) & \text{if } v(x) \geq 0 \\ e^{-\beta v(x)} (1 - e^{-\beta |v(x)|}) & \text{if } v(x) < 0 \end{cases}$$
and since $e^{-\beta v(x)} \leq e^{+\beta B^*_v}$ for all $x \in \mathbb{R}^d$ by definition of $B^*_v$, we have in any case

$$|e^{-\beta v(x)} - 1| \leq e^{+\beta B^*_v} (1 - e^{-\beta |v(x)|})$$  \hfill (2.4)

Plugging (2.4) into (2.3) we get (2.1).

Let us now consider the case $n = 3$. By (1.17) we have

$$|c^v_3(\beta)| = \frac{1}{3!} \left| 3 \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} dy (e^{-\beta v(x)} - 1)(e^{-\beta v(y)} - 1) + \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} dy (e^{-\beta v(x)} - 1)(e^{-\beta v(y)} - 1)(e^{-\beta v(x-y)} - 1) \right| =$$

$$= \frac{1}{3!} \left| 2 \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} dy (e^{-\beta v(x)} - 1)(e^{-\beta v(y)} - 1) + \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} dy (e^{-\beta v(x)} - 1)(e^{-\beta v(y)} - 1)e^{-\beta v(x-y)} \right| \leq$$

$$\leq \frac{1}{3!} \left( 2 \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} dy |e^{-\beta v(x)} - 1||e^{-\beta v(y)} - 1| + \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} dy |e^{-\beta v(x)} - 1||e^{-\beta v(y)} - 1|e^{-\beta v(x-y)} \right)$$

Therefore, using again (2.4) we get

$$|c^v_3(\beta)| \leq \frac{1}{3!} \left[ 2e^{2\beta B^*_v} |\tilde{C}_v(\beta)|^2 + e^{3\beta B^*_v} |\tilde{C}_v(\beta)|^2 \right] \leq \frac{1}{2} e^{3\beta B^*_v} |\tilde{C}_v(\beta)|^2 = \frac{1}{2} \left[ e^{2\beta B^*_v} \tilde{C}_v(\beta) \right]^2$$

and the proof of Lemma 1 is concluded. $\square$

For $n \geq 3$, we will bound $|c^v_n(\beta)|$ either as in (1.32) if $v$ is stable and regular or as in (1.27) if $v$ is Basuev.

We now follow the steps done by Lebowitz and Penrose in [7] to obtain a lower bound for $R^v_{\text{virial}}(\beta)$. We start by observing that, due to (1.16) and the fact that $c_1(\beta) = 1$, there exists a circle $C$ of some radius $R < 1/|\tilde{C}(\beta)e^{\beta B^*_v}|$ and center in the origin $z = 0$ of the complex $z$-plane such that $\rho^v(\beta, z)$ has only one zero in the disc $D_R = \{ z \in \mathbb{C} : |\lambda| \leq R \}$ and this zero occurs precisely at $z = 0$. Let now $\rho \in \mathbb{C}$ be such that

$$|\rho| < \min_{z \in C} |\rho^v(\beta, z)|$$  \hfill (2.5)

Then by Rouche’s Theorem $\rho^v(\beta, z)$ and $\rho^v(\beta, z) - \rho$ have the same number of zeros (i.e. one) in the region $D_R = \{ z \in \mathbb{C} : |z| \leq R \}$. In other words, for any complex $\rho$ satisfying (2.5) there is only one $z \in D_R$ such that $\rho = \rho^v(\beta, z)$ and therefore we can invert the equation $\rho = \rho^v(\beta, z)$ and write $z = z(\beta, \rho)$. Thus, according to Cauchy’s argument principle, we can write the pressure $\beta P^v(\beta, z)$ as a function of the density $\rho = \rho(\beta, z)$ as

$$P^v(\rho, \beta) = \frac{1}{2\pi i} \oint_{\gamma} P^v(\beta, z) \frac{d\rho^v(\beta, z)}{dz} \frac{dz}{\rho^v(\beta, z) - \rho}$$  \hfill (2.6)

where $\gamma$ can be any circle centered at the origin in the complex plane fully contained in the region $D_R$ and such that

$$|\rho| < \min_{z \in \gamma} |\rho^v(\beta, z)|$$  \hfill (2.7)
The function \( P(\rho, \beta) \) is clearly analytic in \( \rho \) in the region (2.7). Indeed, once (2.7) is satisfied we can write
\[
\frac{1}{\rho^n(\beta, z) - \rho} = \sum_{n=0}^{\infty} \frac{\rho^n}{[\rho^n(\beta, z)]^{n+1}}
\]  
(2.8)
and inserting (2.8) in (2.6) we get
\[
P^\nu(\rho, \beta) = \sum_{n=1}^{\infty} k_n(\beta)\rho^n
\]  
(2.9)
with
\[
k_n(\beta) = \frac{1}{2\pi i} \oint_\gamma P^\nu(\beta, z) \frac{d\rho^\nu(\beta, z)}{\rho^\nu(\beta, z) + \rho} \frac{dz}{d\rho^\nu(\beta, z)\rho^n[\rho^n(\beta, z)]^{n+1}} = \frac{1}{2\pi imB} \oint_\gamma \frac{1}{\rho^\nu(\beta, z)\rho^n[\rho^n(\beta, z)]^{n+1}} dz = \frac{1}{2\pi imB} \oint_\gamma \frac{1}{\rho^\nu(\beta, z)\rho^n[\rho^n(\beta, z)]^{n+1}} dz
\]  
Therefore
\[
|k_n(\beta, \Lambda)| \leq \frac{1}{n\beta} \frac{1}{\min_{z \in \gamma} |\rho^n(\beta, z)|^{n-1}}
\]  
(2.10)
Inequality (2.10) shows that the convergence radius \( \mathcal{R}_\text{virial}^\nu(\beta) \) of the series (2.9) (i.e. of the virial series (1.18)) is such that
\[
\mathcal{R}_\text{virial}^\nu(\beta) \geq \frac{1}{\min_{z \in \gamma} |\rho^n(\beta, z)|}
\]  
(2.11)
The game is thus to find a circle \( \gamma \) of optimal radius \( r_\gamma \) in the region \( D_R \) in such a way to maximize the r.h.s. of (2.11). We proceed as follows. Recalling (1.16) we have, by the triangular inequality, that
\[
|\rho^\nu(\beta, z)| \geq |z| - \sum_{n=2}^{\infty} n|c_n^\nu(\beta)||z|^n
\]  
(2.12)
We now use estimates (2.1) and (2.2) and to bound the first two coefficients of the sum in the r.h.s. of (2.12) and estimates (1.32) for the remaining coefficients. Therefore we get
\[
\max_{r \in D_R} \min_{|z| = r} |\rho^\nu(\beta, z)| \geq \max_{r \in D_R} \left\{ r - e^{\beta B_v} \tilde{C}_v(\beta) r^2 - \frac{3}{2} \left[ e^{2\beta B_v} \tilde{C}_v(\beta) \right]^2 r^3 - \sum_{n=4}^{\infty} \frac{n^{n-1}}{n!} [\tilde{C}_v(\beta) e^{\beta B_v}]^{n-1} r^n \right\} = \max_{r \in D_R} \left\{ 2r + \tilde{C}_v(\beta) (e^{\beta B_v} - e^{\beta B_v^*}) r^2 + \frac{3}{2} [\tilde{C}_v(\beta)]^2 (e^{2\beta B_v} - e^{2\beta B_v^*}) r^3 - \frac{1}{\tilde{C}_v(\beta) e^{\beta B_v}} \sum_{n=1}^{\infty} \frac{n^{n-1}}{n!} [\tilde{C}_v(\beta) e^{\beta B_v}]^{n-1} r^n \right\} \geq \max_{x \in (0,1/e)} \frac{1}{\tilde{C}_v(\beta) e^{\beta B_v}} \left[ 2x + (1 - e^{-\beta B_v - B_v^*}) x^2 + \frac{3}{2} (1 - e^{-2\beta(B_v - \frac{1}{2} B_v^*)}) x^3 - \sum_{n=1}^{\infty} \frac{n^{n-1}}{n!} x^n \right]
\]  
(2.13)
where we have set \( x = e^{\beta B_v} \tilde{C}_v(\beta) r \) and we have taken \( x \in (0,1/e) \) which surely inside the convergence region since \( \tilde{B}_v \geq B_v \) and \( \tilde{C}_v(\beta) e^{\beta B_v} |\lambda| < 1/e \). The r.h.s. of (2.13) can be written in a closed form by the change of variables
\[
x = we^{-w}
\]
10
which is one-to one as \( x \) varies in the interval \([0, \frac{1}{e}]\) and \( w \) varies in the interval \([0, 1]\). Indeed using Euler formula

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

valid for all \( w \in [0, 1] \). We thus can rewrite the r.h.s. of (2.13) as

\[
\frac{1}{C_v(\beta)e^{\beta B_v}} \max_{w \in (0,1)} \left\{ w \left[ 2e^{-w} + (1 - e^{-\beta(B_v - B_v^*)})we^{-2w} + \frac{3}{2}(1 - e^{-2\beta(B_v - \frac{3}{2}B_v^*)}w^2e^{-3w} - 1) \right] \right\}
\]

In conclusion we get that

\[
\mathcal{R}_{\text{virial}}(\beta) \geq \frac{F_{v^*}(\beta)}{C_v(\beta)e^{\beta B_v}}
\]

(2.15)

where \( F_{v^*}(\beta) \) is precisely the constant defined in (1.36).

3. Proof of Theorem 2

The proof of Theorem 2 can be done along the same lines of the previous section. First of all, since a Basuev potential \( v \) is stable and regular, by Theorem 1 we have that \( \mathcal{R}_{\text{virial}}(\beta) \geq \mathcal{R}_{\text{stab}}(\beta) \). Thus to prove (1.37) we need to show that it also holds that \( \mathcal{R}_{\text{virial}}(\beta) \geq \mathcal{R}_{\text{Ba}}(\beta) \). We use once again estimates (2.1) and (2.2) to bound the first two coefficients of the sum in the r.h.s. of (2.12) but now we use estimates (1.27) for the remaining coefficients. We get

\[
|\rho^v(\beta, z)| \geq |z| - e^{\beta B_v^*} \tilde{C}_v(\beta)|z|^2 - \frac{3}{2} \left[ e^{2\beta B_v^*} \tilde{C}_v(\beta)^2 \right]^2 |z|^3 - \sum_{n=4}^{\infty} \frac{n^{n-1}}{n!} \left[ \tilde{C}_v(\beta)e^{\beta B_v} \right]^{n-1} |z|^n =
\]

\[
= 2|z| + \left[ \tilde{C}_v(\beta)e^{\beta B_v} - e^{\beta B_v^*} \tilde{C}_v(\beta) \right] |z|^2 + \frac{3}{2} \left[ \left[ \tilde{C}_v(\beta)e^{\beta B_v} \right]^2 - \frac{3\beta B_v^*}{2} \tilde{C}_v(\beta) \right] |z|^3 - \\
- \frac{1}{C_v(\beta)e^{\beta B_v}} \sum_{n=1}^{\infty} \frac{n^{n-1}}{n!} \left[ \tilde{C}_v(\beta)e^{\beta B_v} \right]^n
\]

i.e. we can bound

\[
\max_{r \in D_R} \min_{|z|=r} |\rho^v(\beta, z)| \geq \frac{1}{C_v(\beta)e^{\beta B_v}} \max_{x \in (0, \frac{1}{e})} \left\{ 2x + \left( 1 - e^{-\beta(B_v - B_v^*)} \tilde{C}_v(\beta) \right) x^2 + \frac{3}{2} \left( 1 - e^{-\beta(2B_v - 3B_v^*)} \left[ \tilde{C}_v(\beta) \right]^2 \right) x^3 - \sum_{n=1}^{\infty} \frac{n^{n-1}}{n!} x^n \right\}
\]

(3.1)

where we have set \( x = \tilde{C}(\beta)e^{\beta B_v}r \) and \( x \in (0, 1/e) \) is inside the convergence region due to (1.29). Setting as before \( x = we^{-w} \) and using again Euler formula (2.14) we get

\[
\max_{r \in D_R} \min_{|z|=r} |\rho^v(\beta, z)| \geq \frac{1}{C_v(\beta)e^{\beta B_v}} \max_{w \in (0,1)} \left\{ w \left[ 2e^{-w} + \left( 1 - e^{-\beta(B_v - B_v^*)} \tilde{C}_v(\beta) \right) we^{-2w} + \cdots \right] \right\}
\]
\[
\begin{aligned}
+ \frac{3}{2} \left(1 - e^{-\beta (2B_v - 3B_v^*)} \left[ \frac{\tilde{C}_v(\beta)}{\bar{C}_v(\beta)} \right]^2 \right) w^2 e^{-3w} - 1
\end{aligned}
\]

In conclusion we get that
\[
R_v^{\text{virial}}(\beta) \geq \frac{1}{\bar{C}_v(\beta) e^{\beta B_v} \tilde{F}_v(\beta)}
\]

with \(\tilde{F}_v(\beta)\) coinciding with the function defined in (1.39) and therefore (1.37) is proved.

4. An application: the three-dimensional Lennard-Jones potential

Let us compare in this final section our new bounds \(R_v^{\text{stab}}(\beta)\) defined in (1.35) and \(R_v^{\text{Bas}}(\beta)\) defined in (1.38) with the bound \(R_v^{\text{PY}}(\beta)\) given in (1.33) for the convergence radius of the virial series of systems of particles interacting through a pair potential \(v\) with strictly positive stability constant. We will specifically examine the case of the Lennard-Jones potential, usually written as
\[
v(r) = 4\varepsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right]
\]
with \(\varepsilon\) being the depth of the potential well and \(\sigma\) being the distance at which the potential is zero. This potential is by far the most used to model interaction between molecules in simulations by chemists and physicists. As showed in [9], the Lennard-Jones potential is Basuev (see Proposition 2 in [9]), so we are free to use also the estimate (1.37) for \(R_v^{\text{virial}}(\beta)\).

By suitably rescaling inverse temperature and distances, we may assume without loss of generality that the Lennard-Jones potential has the following expression
\[
V_{\text{LJ}}(x) = \frac{1}{|x|^{12}} - \frac{2}{|x|^6}
\]

We remind the reader that we considering here only the three-dimensional case, so in (4.1) it is understood that \(x \in \mathbb{R}^3\). Moreover, for simplicity, we will do the calculations setting the (rescaled) inverse temperature at the value \(\beta = 1\).

First of all it is known that the stability constant \(B_{V_{\text{LJ}}} \) of the three-dimensional rescaled Lennard-Jones potential \(V_{\text{LJ}}\) given in (4.1) is bounded as follows.
\[
8.61 \leq B_{V_{\text{LJ}}} \leq 14.316
\]

The current lower bound has been obtained in [24] while the current upper bound has been obtained in [25]. Concerning the estimate of the Basuev stability constant \(\bar{B}_{V_{\text{LJ}}} \) of the potential \(V_{\text{LJ}}\), we use the data made available in [3] which show that \(B_{V_{\text{LJ}}} \leq (1.001) B_{V_{\text{LJ}}} \) and thus,
\[
8.61 \leq \bar{B}_{V_{\text{LJ}}} \leq 14.331 \quad (4.2)
\]

In regard to value of \(\tilde{C}_{V_{\text{LJ}}}(\beta = 1)\) defined in (1.23) to be plugged in (1.33), a straightforward (computer assisted) calculation gives
\[
\tilde{C}_{V_{\text{LJ}}}(\beta = 1) = 4\pi \int_0^\infty r^2 (1 - e^{-1.5r} - \frac{2}{r}) dr \approx 9.1864 \quad (4.3)
\]

To compute \(R_{V_{\text{LJ}}}^{\text{Bas}}(\beta = 1)\) we will need to estimate \(\tilde{C}_{V_{\text{LJ}}}(\beta)\) defined in (1.28) at \(\beta = 1\). Observe that for any Basuev potential \(v\) and any \(\alpha\) satisfying conditions (1.8) and (1.9), the quantity
\[
e^{-\beta B_v} \frac{(1 - e^{-\beta [v(x) - v_{\alpha} - B_v]})}{\beta (v(x) - v_{\alpha} - B_v)}
\]

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appearing in the integrand of the first term of the r.h.s. of (1.28) is monotone decreasing as a function of $\hat{B}_v$ for any $v(x) - v_a \geq 0$. So, recalling that 8.61 is a lower bound for $\hat{B}_{\text{LJ}}$, we have that

$$e^{-\hat{B}_{\text{LJ}}} \frac{(1 - e^{-[V_{\text{LJ}}(x) - V_{\text{LJ}}(x) - \hat{B}_{\text{LJ}}]})(V_{\text{LJ}}(x) - v_a - \hat{B}_{\text{LJ}})}{(V_{\text{LJ}}(x) - V_{\text{LJ}}(x) - 8.61)} \leq e^{-8.61} \frac{(1 - e^{-[V_{\text{LJ}}(x) - V_{\text{LJ}}(x) - 8.61]})(V_{\text{LJ}}(x) - V_{\text{LJ}}(x) - 8.61)}{(V_{\text{LJ}}(x) - V_{\text{LJ}}(x) - 8.61)}$$

where

$$V_{\text{LJ}}(x) = \frac{1}{\alpha^2} - \frac{2}{\alpha^6}$$

On the other hand the quantity $(1 - e^{-\hat{B}_v})/\hat{B}_v$ multiplying the second integral in the r.h.s. of (1.28) is also decreasing as a function of $\hat{B}_v$. Therefore, once the constant $\alpha > 0$ satisfying conditions (1.8) and (1.9) in Definition 1 has been established, we can bound $\hat{C}_{\text{LJ}}(\beta = 1, \hat{B}_{\text{LJ}})$ as follows

$$\hat{C}_{\text{LJ}}(\beta = 1) \leq e^{-8.61} \int_{\mathbb{R}^3} dx \frac{V_{\text{LJ}}(|x|)(1 - e^{-[V_{\text{LJ}}(x) - V_{\text{LJ}}(x) - 8.61]})(1 - e^{-8.61})}{(V_{\text{LJ}}(x) - V_{\text{LJ}}(x) - 8.61)} + \frac{1}{8.61} \int_{\mathbb{R}^3} dx \left| V_{\text{LJ}}(x) \right|^2$$

(4.4)

The game now is to find a clever choice of the parameter $\alpha$ for the Lennard-Jones potential $V_{\text{LJ}}$. That is to say, $\alpha$ should be a number which satisfies (1.8) and (1.9) and at the same time makes the r.h.s. of (4.4) as small as possible. This can be achieved by using a recent result obtained by Yuhjtman specifically of the Lennard-Jones potential [25]. Namely, Yuhjtman proved (see Proposition 3.1 in [25]) that for Lennard-Jones potential $V_{\text{LJ}}$ given by (4.1), taking $\alpha \in [0, 0.7]$, the number $\mu_{\text{LJ}}(\alpha)$ defined in (1.10) is such that

$$\mu_{\text{LJ}}(\alpha) \leq \frac{24.05}{\alpha^3}$$

This immediately implies that $V_{\text{LJ}}(\alpha) \geq 2\mu(\alpha)$ as soon as $\alpha \leq 0.6397$. Thus, by choosing $\alpha \in [0.6, 0.6397]$, the Lennard-Jones potential (4.1) satisfies conditions (1.8) and (1.9) in Definition 1. Taking $\alpha = 0.6397$, which is the value in the interval $[0.6, 0.6397]$ that minimizes the r.h.v. of (4.4), we get

$$\hat{C}_{\text{LJ}}(\beta = 1) \leq 4\pi e^{-8.61} \int_0^{0.6397} dr \left[ \frac{1}{r^{10}} - \frac{2}{r^4} \right] \frac{(1 - e^{-\frac{14331}{14.331}})}{(1 - e^{-\frac{14331}{14.331}})} +$$

$$+ \frac{4}{8.61} \int_{0.6397}^{\infty} dx \left| \frac{1}{r^{10}} - \frac{2}{r^4} \right| \leq 0.0345876 + 7.15664 \leq 7.2$$

(4.5)

on the other hand, recalling (4.2), we have also that

$$\hat{C}_{\text{LJ}}(\beta = 1) \geq \frac{4(1 - e^{-14331})}{14.331} \pi \int_{0.6397}^{\infty} dx \left| \frac{1}{r^{10}} - \frac{2}{r^4} \right| \geq 4.3$$

We also need to evaluate the quantities $F_{\text{LJ}}(\beta)$ and $\tilde{F}_{\text{LJ}}(\beta)$ defined in (1.36) and (1.39) when $\beta = 1$. Considering that $B_{\text{LJ}}^* = 1$ and that $\hat{B}_{\text{LJ}} \geq 8.61$ for the Lennard-Jones potential (4.1), we can estimate

$$F_{\text{LJ}}(\beta = 1) \geq \max_{w \in (0, 1)} \left[ 2e^{-w} + (1 - e^{-7.61})we^{-2w} + \frac{3}{2}(1 - e^{-14.22})w^2e^{-3w} - 1 \right] \geq 0.2418$$

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On the other hand, the quantity $\tilde{F}_{VLJ}(\beta = 1)$ can be bounded below, as far as the rescaled Lennard-Jones potential is concerned, by the following value.

$$\tilde{F}_{VLJ}(\beta = 1) \geq \max_{w \in (0,1)} \left\{ w \left[ 2e^{-w} + \left( 1 - e^{-(7.61) \frac{9.2}{4.3}} \right) we^{-2w} + \frac{3}{2} \left( 1 - e^{-(14.22) \frac{9.2}{4.3}} \right)^2 w^2 e^{-3w} - 1 \right] \right\}$$

(4.6)

A straightforward (computer assisted) computation gives

$$\tilde{F}_{VLJ}(\beta = 1) \geq 0.2417$$

We can now compare the best previous lower bound $R_{Pr}^{VLJ}(\beta)$ given in (1.33) for the convergence radius $R_{virial}^{VLJ}(\beta)$ of the virial series of a system of particles at $\beta = 1$ interacting via the rescaled Lennard-Jones potential given in (4.1) with the new bounds $R_{stab}^{VLJ}(\beta)$ and $R_{Ba}^{VLJ}(\beta)$ produced by (1.35) and (1.38). First, according to bound (1.33) given in [19] we have

$$R_{Pr}^{VLJ}(\beta = 1) \approx \frac{0.144767}{9.1864} e^{-B_{LJ}} \approx 0.015759 e^{-B_{LJ}} \approx \frac{e^{-B_{LJ}}}{63.45}$$

(4.7)

On the other hand, the new bound (1.35) given in Theorem 1 yields

$$R_{stab}^{VLJ}(\beta = 1) \approx \frac{0.2418}{9.1864} e^{-B_{LJ}} = 0.02632 e^{-B_{LJ}} \approx \frac{e^{-B_{LJ}}}{38}$$

(4.8)

which represent an improvement by a factor 1.67 with respect to bound (1.35).

An ever better bound is obtained using the bound (1.38) given in Theorem 2. Doing so we get

$$R_{Ba}^{VLJ}(\beta = 1) \geq \frac{0.2417}{7.2} e^{-B_{LJ}} \geq 0.03369 e^{-B_{LJ}} \geq \frac{e^{-B_{LJ}}}{29.8}$$

(4.9)

which represents an improvement more than twice better than bound (4.7).

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