New results for the virial coefficients of $D$–dimensional hard spheres

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(Dated: October 31, 2018)

Exact results are given for the fourth virial coefficient of hard spheres in even dimensions up through 12. The fifth and sixth virial coefficients are numerically computed for dimensions 2 through 50 and it is found that the sixth virial coefficient is negative for $D \geq 6$. Numerical studies are made of the contributing Ree Hoover diagrams up to order 17. It is found for $D \geq 3$ that for large order a class of diagrams we call “loose packed” dominates and the rate of growth of these diagrams is used to study bounds on the radius of convergence.

PACS numbers: 05.20.-y

The virial series for the pressure

$$
P(kBT) = \rho + \sum_{k=2}^{\infty} B_k \rho^k, \tag{1}$$

for hard particles of diameter $\sigma$ where the potential $U(r)$ is $+\infty$ for $|r| < \sigma$ and 0 otherwise, has been studied in dimensions two and three for over 100 years. However, despite the long history of this problem, the only rigorous information of the radius of convergence comes from the upper bound of Lebowitz and Penrose [1] that $B_k/B_2^{k-1} \leq 13.8^{k-1}/k$ which in terms of the packing fraction $\eta = B_2 \rho/2^{D-1}$ gives convergence for $|\eta| \leq 0.145/2^D$. For $D = 3$ this gives a lower bound of 0.018 which is much less than the packing fraction at which freezing occurs of $\eta_f = 0.49$ [2, 3].

Our numerical knowledge of the virial expansion for $D = 2, 3$ is compactly summarized in Table I. Virial coefficients have also been calculated for hard spheres in dimensions higher than three in [4–7].

| discs | spheres |
|-------|---------|
| $B_2$ | $\pi \sigma^2/2$ | $2 \pi \sigma^3/3$ |
| $B_3/B_2^2$ | $\frac{4}{3} - \frac{\sqrt{3}}{2}$ [8] | $\frac{5}{8}$ [9] |
| $B_4/B_2^3$ | 0.5322318 $\cdots$ [10, 11] | 0.2869495 $\cdots$ [9, 12, 13] |
| $B_5/B_2^4$ | 0.33355604(4) [14, 15] | 0.110252(1) [14, 16] |
| $B_6/B_2^5$ | 0.19883(1) [14, 17] | 0.038808(55) [14, 18] |
| $B_7/B_2^6$ | 0.114877(11) [18–20] | 0.013046(22) [18–20] |
| $B_8/B_2^7$ | 0.065030(31) [18, 20] | 0.004164(16) [18, 20] |

There have been many attempts to estimate a radius of convergence and to find an approximate low density form for the equation of state based on these first few virial coefficients. In three dimensions these approximates may be grouped into three classes in terms of the location of the leading singularity in the $\eta$ plane. Either there is (1) a high order pole [21–24] at $\eta = 1$, (2) a simple pole [3, 14, 18, 25, 26] at or near the packing fraction $\eta_{cp} = 0.74048 \cdots$ of closest packed spheres, or (3) a fractional power law divergence [27–30] at or near the “random close packed” density $\eta_{rcp} = 0.64$ as defined by [31].

All of these approximates have radii of convergence greater than the endpoints of the numerically determined [2, 3] first order phase transition $\eta_f = 0.49$ and $\eta_r = 0.54$: because of this it is often assumed that the virial expansion for hard spheres is analytic at the freezing density $\eta_f$. This analyticity assumption is incorporated in most of the phenomenological theories used to describe freezing [32–34]. There is clearly a large discrepancy between the lower bound on the radius of convergence and the assumption of analyticity at $\eta_f$.

Furthermore all the known virial coefficients for $D = 2, 3, 4, 5$ are positive and this positivity is often built into the approximate equations of state by having the leading singularity on the positive real axis. But the possibility of negative virial coefficients was suggested by Temperley [35] as far back as 1957, and in 1964 it was shown [4] that $B_4$ is negative for $D \geq 8$. The sixth and seventh virial coefficients are negative for parallel hard cubes [36] and oscillatory signs are found in models of hard squares [37] and hard hexagons [38, 39]. Consequently there is no a priori reason to expect the leading singularity to be on the real axis.

We have studied these questions of sign change and rate of growth of the virial coefficients by numerically, and for $B_4$ analytically, evaluating selected Ree Hoover diagrams for orders up through 17. We use the definitions and notations adapted from [40]. In particular, for diagrams of $k$ points which contribute to $B_k$, each point is connected to each other point either by an $f$ bond that corresponds to the function $f(r)$ which is $-1$ for $|r| < \sigma$ and 0 otherwise, or by a bond $\tilde{f} = 1 + f$. In drawing the diagrams we need only specify either $f$ bonds (represented by solid lines) or $\tilde{f}$ bonds, not both. For example the fourth virial coefficient is given by

$$
B_4 = \frac{1}{4} \cdot 0 - \frac{3}{8} \cdot \overline{1} = \frac{1}{4} \overline{\infty} - \frac{3}{8} \overline{\infty}. \tag{2}
$$

The first expression in Eq. 2 is the expansion in Ree-
Hoover graphs with \( \tilde{f} \) bonds, while the second is the same expansion but with only \( f \) bonds shown.

The integrals in Eq. 2 have been previously evaluated analytically only for \( D = 2 \) [10, 11] and 3 [9, 12, 13]. We have extended these analytic computations for even dimensions up through \( D = 12 \). The results are shown in Table II. Details of the computation will be published elsewhere.

| TABLE II: Analytical results for \( B_k/B_2^k \) in even dimensions. |
|-----------------------|-----------------------|
| \( D \) | Analytic Value | Numerical Value |
| 2 | \( 2 - \frac{9\sqrt{3}}{4\pi} + \frac{10}{\pi} \) | 0.53223180 \( \cdots \) |
| 4 | \( 2 - \frac{9\sqrt{3}}{4\pi} + \frac{32}{\pi} \) | 0.15184606 \( \cdots \) |
| 6 | \( 2 - \frac{3\sqrt{3}}{2\pi} + \frac{8\pi}{3} \) | 0.0336314 \( \cdots \) |
| 8 | \( 2 - \frac{27\sqrt{3}}{8\pi} + \frac{170}{3\pi} \) | -0.00255768 \( \cdots \) |
| 10 | \( 2 - \frac{7\sqrt{3}}{8\pi} + \frac{80}{\pi} \) | -0.010962 \( \cdots \) |
| 12 | \( 2 - \frac{3\sqrt{3}}{4\pi} + \frac{152}{\pi} \) | -0.01067028 \( \cdots \) |

To investigate the phenomena of negative virial coefficients further we have made a Monte-Carlo evaluation of \( B_4, B_5, \) and \( B_6 \) for dimensions up to 50. The method used allows the calculation of \( B_k \) for dimensions \( D \geq k - 1 \), including non-integer dimensions, and will be reported elsewhere. The results for integer dimensions up to 12 are shown in Table III where the entries for \( B_6 \) in \( D = 4 \) and 5 are from [7]. For dimensions higher than 12 these \( B_6/B_2^{k-1} \) approach zero in a monotonic fashion. From an interpolation of these results we see that \( B_k \) becomes negative at \( D = 7.73 \), \( B_6 \) becomes negative at \( D \sim 5.3 \), and that while \( B_6/B_2^4 \) is always positive it is not monotonic. The fact that the zero crossing of \( B_k \) has decreased from 7.73 to 5.3 as \( D \) increases from 4 to 6 suggests that it is plausible that the zero crossing for \( B_8 \) occurs close to \( D = 4 \).

| TABLE III: Numerical values for \( B_k/B_2^k \), \( B_5/B_2^5 \) and \( B_6/B_2^6 \). Local minima and maxima are underlined. |
|-----------------------|-----------------------|
| \( D \) | \( B_k/B_2^k \) | \( B_5/B_2^5 \) | \( B_6/B_2^6 \) |
| 3 | 0.2869495 \( \cdots \) | 0.110252(1) | 0.03881(6) |
| 4 | 0.1518460 \( \cdots \) | 0.03565(5) | 0.00769(3) |
| 5 | 0.075978(4) | 0.01297(1) | 0.00094(3) |
| 6 | 0.0336314 \( \cdots \) | 0.007528(8) | -0.00176(2) |
| 7 | 0.009873(4) | 0.007077(7) | -0.00352(2) |
| 8 | -0.0025576 \( \cdots \) | 0.00429(6) | -0.00451(2) |
| 9 | -0.008575(3) | 0.00743(6) | -0.00478(1) |
| 10 | -0.0109624 \( \cdots \) | 0.00696(5) | -0.00452(1) |
| 11 | -0.011334(3) | 0.006176(4) | -0.00395(1) |
| 12 | -0.0109624 \( \cdots \) | 0.005244(4) | -0.003261(7) |

To proceed further we separate the Ree-Hoover diagrams with \( k \) points into classes with \( m \leq k \) points which are the end points of \( f \) bonds. We designate the value of a diagram in this class, including its combinatorial coefficient, as \( B_k[m, i] \) where \( i \) is an arbitrary label specifying the graph with given \( k \) and \( m \). If the graph \( B_k[m, i] \) exists for \( k = m \) then it will continue to exist for \( k > m \). There is one graph in the class \( B_k[0, i] \), one in the class \( B_k[4, i] \) three in the class \( B_k[5, i] \), and 18 in the class \( B_k[6, i] \).

For the diagram with \( m = 0 \) the absence of \( f \) bonds forces the points to all lie within a distance \( \sigma \) of each other. We define any sequence of diagrams with increasing number of points as being “close packed” if the maximal volume of the convex hull of \( k \) points approaches a constant as \( k \to \infty \). As such, any sequence with \( m \) and \( i \) fixed is a close packed sequence of diagrams. We have numerically studied \( B_k[0,1], B_k[4,1], \) and all graphs in \( B_k[5, i] \) for many values of \( k \) and \( D \). Two examples are shown in Tables IV and V.

| TABLE IV: \( B_k[0,1]/B_2^k = 0/B_2^{k-1} \). |
|-----------------------|-----------------------|
| \( k \) | \( D = 2 \) | \( D = 3 \) | \( D = 4 \) | \( D = 5 \) |
| 4 | 0.5488(4) | 0.3166(3) | 0.1888(2) | 0.1153(2) |
| 5 | 0.3620(3) | 0.1420(2) | 0.0591(2) | 0.0252(8) |
| 6 | 0.2292(3) | 0.0593(2) | 0.0164(6) | 0.0047(6) |
| 7 | 0.1412(3) | 0.0233(2) | 0.0042(6) | 0.0007(1) |
| 8 | 0.0844(4) | 0.0087(2) | 0.00101(2) | 0.00129(3) |
| 9 | 0.0505(4) | 0.00315(6) | 0.000226(5) | 1.78(7) \( \times 10^{-5} \) |
| 10 | 0.0293(4) | 0.00111(2) | 5.2(2) \( \times 10^{-5} \) | 2.5(4) \( \times 10^{-6} \) |
| 11 | 0.0170(3) | 0.000380(8) | 1.0(1) \( \times 10^{-5} \) |
| 12 | 0.0097(2) | 0.000128(3) | 2.7(7) \( \times 10^{-6} \) |
| 13 | 0.0053(1) | 5.2(4) \( \times 10^{-5} \) |
| 14 | 0.00304(6) | 1.7(3) \( \times 10^{-5} \) |
| 15 | 0.00179(4) |

| TABLE V: \( B_k[4,1]/B_2^k = i/B_2^{k-1} \). |
|-----------------------|-----------------------|
| \( k \) | \( D = 2 \) | \( D = 3 \) | \( D = 4 \) | \( D = 5 \) |
| 4 | -0.01644(5) | -0.02984(9) | -0.0370(1) | -0.0391(1) |
| 5 | -0.0264(3) | -0.0316(2) | -0.0270(2) | -0.0189(2) |
| 6 | -0.0285(5) | -0.0219(4) | -0.0117(2) | -0.0059(1) |
| 7 | -0.0239(5) | -0.0114(2) | -0.00403(8) | -0.00130(3) |
| 8 | -0.0183(4) | -0.0056(1) | -0.00120(5) |
| 9 | -0.0123(3) | -0.0025(1) |
| 10 | -0.0086(4) |
| 11 | -0.0056(2) |
| 12 | -0.0038(2) |
| 13 | -0.0023(3) |

In contrast to the close packed diagrams, we call diagrams \( B_k[k, i] \) for which many points are forced to be more than a distance \( \sigma \) apart “loose packed”. One sequence of loose packed diagrams is the \( k \) point ring of \( f \) bonds which we denote by \( R_k \), for which numerical values are shown in Table VI. We have found numerically for fixed \( k \) that as \( D \to \infty \) this ring diagram is larger than all other studied. We therefore make the following
Conjecture: For fixed $k$, $\lim_{D \to \infty} B_k/R = 1$. In particular the sign of $B_k$ for large $D$ is $(-1)^{k-1}$.

For fixed $D$, we find that for $k$ up to 7 the largest diagrams are of the form of a ring with “insertions” where one point of the ring is replaced by a cluster of points connected by $f$ and $\bar{f}$ bonds. We thus may define a sequence of loose packed diagrams which consist of ring diagrams with an inserted diagram. Note that the contribution of these sequences to the virial coefficient alternate in sign, whereas close packed diagrams always contribute with the same sign. The smallest possible insertions have 4 points, of which there are two examples. The larger of these is given in Table VII where the type of insertion is indicated in the figure caption. Multiple insertions are possible but never dominate for the values of $k$ we have studied.

| Table VI: $B_k[k,1]/B_k^{d-1} = R/B_k^{d-1}$. The underline marks the approximate location of the minimum value. |
|---|---|---|---|---|
| $k$ | $D = 2$ | $D = 3$ | $D = 4$ | $D = 5$ |
| 4 | $-0.01639(9)$ | $-0.0298(1)$ | $-0.0371(1)$ | $-0.0392(5)$ |
| 5 | 0.00869(6) | 0.01623(9) | 0.0214(2) | 0.0230(1) |
| 6 | $-0.00526(8)$ | $-0.0109(1)$ | $-0.0150(2)$ | $-0.0168(9)$ |
| 7 | 0.00335(6) | 0.0078(2) | 0.0124(2) | 0.0142(3) |
| 8 | $-0.00234(5)$ | $-0.0064(1)$ | $-0.0106(2)$ | $-0.0129(3)$ |
| 9 | 0.000177(4) | 0.0053(1) | 0.0098(2) | 0.0126(2) |
| 10 | $-0.00125(3)$ | $-0.00452(9)$ | $-0.0091(2)$ | $-0.0126(3)$ |
| 11 | 0.00095(2) | 0.00392(8) | 0.0089(2) | 0.0128(3) |
| 12 | $-0.00074(1)$ | $-0.00333(7)$ | $-0.0083(2)$ | $-0.0134(3)$ |
| 13 | 0.00005(1) | 0.00313(8) | 0.0086(2) | 0.0142(3) |
| 14 | $-0.00041(1)$ | $-0.0027(1)$ | $-0.0086(2)$ | $-0.0166(3)$ |
| 15 | 0.00033(2) | 0.00226(1) | 0.0087(3) | 0.0183(4) |

| Table VII: $B_k[k,2]/B_k^{d-1} = R(\boldsymbol{\Delta})/B_k^{d-1}$. The underline marks the approximate location of the minimum value. |
|---|---|---|---|---|
| $k$ | $D = 2$ | $D = 3$ | $D = 4$ | $D = 5$ |
| 5 | $-0.00107(4)$ | $-0.01654(7)$ | $-0.01748(6)$ | $-0.01551(4)$ |
| 6 | 0.00756(6) | 0.01191(8) | 0.01257(6) | 0.01067(6) |
| 7 | $-0.00607(8)$ | $-0.01003(7)$ | $-0.0106(1)$ | $-0.00936(9)$ |
| 8 | 0.0051(1) | 0.0088(2) | 0.0100(1) | 0.00902(8) |
| 9 | $-0.00427(8)$ | $-0.0083(1)$ | $-0.0100(1)$ | $-0.0095(2)$ |
| 10 | 0.00381(8) | 0.0082(2) | 0.0106(2) | 0.0106(2) |
| 11 | $-0.00309(3)$ | $-0.0075(1)$ | $-0.0109(2)$ | $-0.0116(2)$ |
| 12 | 0.00259(3) | 0.00728(7) | 0.0112(5) | 0.0136(3) |
| 13 | $-0.00220(3)$ | $-0.0071(3)$ | $-0.0125(3)$ | $-0.0156(3)$ |
| 14 | 0.00188(4) | 0.0068(4) | 0.0140(5) | 0.0172(4) |
| 15 | $-0.00151(5)$ | $-0.0060(5)$ | $-0.0145(7)$ | $-0.0227(7)$ |

The data of Tables IV–VII differ in the two cases $D = 2$ and $D \geq 3$ in the following respect. For $D = 2$ the close packed diagrams $B_k[0,1]$ and $B_k[4,1]$ are larger than the loose packed diagrams $B_k[k,i]$ we have considered, whereas for $D \geq 3$ the loose packed diagrams rapidly dominate the close packed diagrams for large $k$. Consequently we will consider the two cases separately.

For $D = 2$ an examination of Tables IV–VII indicates that all diagrams are roughly of the same order of magnitude. A measure of the relative size of the close packed to the loose packed diagrams is given by the ratio $|B_k[k,1]/B_k[0,1]|$ which increases from 0.0299 to 0.184 as $k$ increases from 4 to 15 (0.382 when $k = 17$). It can be argued that if this increase continues then eventually the loose packed diagrams will dominate, but such a conclusion requires further computations. The data can be interpreted to say there is a qualitative difference between $D = 2$ and $D \geq 3$. This interpretation may be correct but is not compelling.

For $D \geq 3$ the loose packed diagrams $B_k[k,i]$ rapidly dominate for large $k$ the close packed diagrams $B_k[m,i]$ for fixed $m$ and in particular $|B_k[k,1]|$ first becomes larger than $B_k[0,1]$ for $k = 9$ in $D = 3$, $k = 7$ in $D = 4$, and $k = 6$ in $D = 5$. Further studies indicate that $B_k[k,i]$ even dominates $B_k[k-1,i]$ for large $k$. Thus in order to determine the radius of convergence we will restrict our attention to the diagrams belonging to $B_k[k,i]$.

We see in Table VI that the Ree-Hoover ring diagram $B_k[k,1]/B_k^{d-1}$ increase in magnitude for $D \geq 4$ when $k$ is sufficiently large. In $D = 3$ the data of Table VI can be interpreted as either having a minimum near $k = 1$ or possibly approaching a constant as $k \to \infty$.

The largest diagram shown is the four point insertion $B_k[2,0]$ of Table VII. It seems clear that for $D \geq 4$ this diagram will always be bigger than the Ree-Hoover ring but the ratio seems to grow only as a power of $k$. We believe the same behavior happens for $D = 3$ but it is more difficult to see with the precision given in the tables.

From these and other numerical studies we conjecture that the exponential rate of growth of the ring and ring diagrams with insertions is the same.

To estimate the rate of growth we concentrate on the Ree-Hoover ring of Table VI. We note that the absolute value of this diagram must be strictly less than the absolute value of the Mayer ring diagram which is obtained by replacing all the $\bar{f}$ bonds by unity. The Mayer ring may be expressed as a single integral [41], and from this we obtain

$$\frac{B_k[k,1]}{B_k^{d-1}} \leq \frac{(k-1)(2\pi)^{D/2}}{2k\Omega_{D-2}^{\frac{D-2}{2}}} \int_0^\infty dx x^{D-1} \left[ \frac{J_{D/2}(x)}{x^{D/2}} \right]^k,$$

where $\Omega_{D-1} \equiv 2\pi^{D/2}/\Gamma(D/2)$ and $J_{D/2}(k)$ is the Bessel function of the first kind. The large $k$ behavior of this integral is obtained by steepest descents and thus we have as $k \to \infty$

$$\frac{B_k[k,1]}{B_k^{d-1}} \leq \frac{(k-1)(1+D/2)^{D/2}}{k^{1+D/2}\Gamma(1+D/2)} 2^{k-2}.$$

From Table VI we see that for all $D$ the ratios $B_{k+1}[k+1,1]/(B_2B_k[k,1])$ are all substantially below this bound.
of 2. If the data in Table VI are extrapolated to say for 
$D = 3$ that $B_8[k, 1]$ goes to a constant (or a power of $k$) 
as $k \to \infty$ then we see that the radius of convergence of 
the sum of Ree-Hoover ring diagrams is $\eta_f = 0.25$. At 
worst the ratios in Table VI for $D = 3$ are bounded below 
by 0.91 as $k \to \infty$ which leads to a radius of convergence 
of $\eta_f = 0.27$. This radius of convergence is substantially 
less than the freezing density of $\eta_f = 0.49$. Similarly we 
estimate from Table VI that in $D = 4$ the radius of conver-
gence of Ree-Hoover rings is $\eta_f \sim 0.12$ and in $D = 5$ 
is $\eta_f \sim 0.052$ which are to be compared with the freezing 
densities $\eta_f = 0.31$ in $D = 4$ and $\eta_f = 0.19$ in $D = 5$ ob-
tained from [42–44]. The alternation of sign of the ring 
means that the leading singularity of the sum of these 
diagrams is on the negative $\eta$ axis.

If all loose packed diagrams $B_k[k, i]$ had the sign 
$(−1)^k−1$ of the Ree-Hoover ring diagram then the esti-
mates of $\eta_f$ found above would be an upper bound on 
the radius of convergence of the virial expansion. How-
ever for every order $k$ both signs occur in the class $B_k[k, i]$ 
and in particular the diagram $B_k[k, 2]$ is larger than and 
has the opposite sign from $B_k[k, 1]$. Therefore cancella-
tions of diagrams within the class $B_k[k, i]$ can occur and 
as evidence of such cancellation we note that the virial 
coefficient $B_8/B_2^2$ of Table I for $D = 3$ is smaller than both 
$B_8[8, 1]$ and $B_8[8, 2]$, and has the opposite sign to the 
ring diagram $B_8[8, 1]$.

However, the diagrams $B_k[k, 2]$ also alternate in sign, 
and by themselves lead to a singularity on the negative 
real axis. If this singularity is to be avoided extensive 
cancellation must take place beyond what can be seen 
in the virial coefficients up through order 8 as given in 
Table I. From this point of view we see that a detailed 
study of diagrams for orders substantially greater than 
8 is needed to substantiate any claim concerning the ra-
dius of convergence of the virial series for hard spheres. 
None of the approximate equations of state for hard 
spheres [3, 14, 18, 21–30] includes diagrams of such high 
or-der. We therefore conclude that there is no existing 
evidence to support the claim that the virial expansion 
converges beyond the freezing density $\eta_f$ of hard spheres.

This work was supported in part by the National 
Science Foundation under DMR-0073058. We thank 
Prof. R. J. Baxter and Prof. G. Stell for useful discus-
sions.

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