Equation of state of a seven-dimensional hard-sphere fluid. Percus–Yevick theory and molecular dynamics simulations

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Following the work of Leutheusser [Physica A 127, 667 (1984)], the solution to the Percus–Yevick equation for a seven-dimensional hard-sphere fluid is explicitly found. This allows the derivation of the equation of state for the fluid taking both the virial and the compressibility routes. An analysis of the virial coefficients and the determination of the radius of convergence of the virial series are carried out. Molecular dynamics simulations of the same system are also performed and a comparison between the simulation results for the compressibility factor and theoretical expressions for the same quantity is presented.

I. INTRODUCTION

In liquid theory there has been a long lasting interest on the equilibrium properties of high-dimensional hard-sphere fluids, especially in the last few years. Such an interest has arisen from many different sources. To begin with, given the relative simplicity of the intermolecular interactions in these hard-core systems, they are amenable to both theoretical and computer simulation studies. In this sense and as it occurs in other problems in theoretical and mathematical physics, it is an asset that one can deal with hard spheres in arbitrary dimensionality and exploit some of the features that these systems have in common, for instance the fact that they all exhibit a first-order freezing transition. Furthermore, and as conjectured by Frisch and Percus, in the case of fluids high spatial dimensionality may have a parallel with limiting high density situations, so that by increasing the dimensionality one may obtain at least a rough idea of any thermodynamic phenomenology that extends to such dimensionality. An example of this expectation is the recent investigation of the demixing problem in mixtures of hard hyperspheres.

Computer simulation studies of hard-sphere fluids in dimensions greater than three are very scarce. To the best of our knowledge, only the four- and five-dimensional simple and multicomponent fluids have been simulated. This is not surprising since the computational effort needed to obtain reliable results increases significantly with the dimensionality.

Exact information on the equation of state (EOS) usually comes from the virial coefficients $B_n$ defined by

$$Z \equiv \frac{p}{\rho k_B T} = 1 + \sum_{n=2}^{\infty} B_n \rho^{n-1} = 1 + \sum_{n=2}^{\infty} b_n \eta^{n-1}. \quad (1)$$

In this equation, $p$ is the pressure, $\rho$ is the number density, $k_B$ is the Boltzmann constant, $T$ is the temperature, and $Z$ is the compressibility factor. The second virial coefficient is $B_2 = 2^{d-1} v_d \sigma^d$, where $d$ is the dimensionality, $\sigma$ is the diameter of a sphere, and $v_d = (\pi/4)^{d/2}/\Gamma(1 + d/2)$ is the volume of a $d$-dimensional sphere of unit diameter. In the second line of Eq. (1) we have introduced the packing fraction $\eta \equiv \rho v_d \sigma^d$ and the reduced virial coefficients $b_n \equiv B_n/(v_d \sigma^d)^{n-1} = 2^{(d-1)(n-1)} B_n/B_2^{n-1}$. The radius of convergence of the virial series $\rho_{\text{conv}} = \lim_{n \to \infty} [B_n/B_{n+1}]$, is the modulus of the singularity of $Z(\rho)$ closest to the origin in the complex $\rho$ plane. If such a singularity were located on the positive real axis, then all the virial coefficients $B_n$ would be positive for large $n$.

The exact expression for the third virial coefficient is

$$\frac{B_3}{B_2^2} = \frac{2 B_3/4 (d/2 + 1, 1/2)}{B(d/2 + 1/2, 1/2)}. \quad (2)$$

where $B(a,b) = \Gamma(a) \Gamma(b)/\Gamma(a + b)$ is the beta function and $B_x(a,b)$ is the incomplete beta function. Both $B_2$ and $B_3$ are positive definite for arbitrary $d$. The analytic evaluation of the fourth virial coefficient is much more involved. Luban and Baram derived exact expressions for two of the three terms contributing to $B_4$ and proposed a semi-empirical formula for the remaining contribution. More recently, Clisby and McCoy showed that $B_4$ can be evaluated exactly for any even dimension $d$ and gave the explicit results for $d = 4, 6, 8, 10, 12$. They also computed numerically the fifth and sixth virial coefficients through $d = 50$. The results show that, while $B_3$ remains positive, $B_4$ and $B_5$ become negative for $d \geq 8$ and $d \geq 6$, respectively. This suggests the possibility that, even in the three-dimensional case, there might be negative virial coefficients $B_n$ for sufficiently large $n$. The fact that the virial coefficients are not positive definite and that they may have alternate signs is of importance in connection with the radius of convergence of the virial expansion, as mentioned before.
A. The scenario for high dimensionality

The high-dimensionality limit of hard hyperspheres has been the subject of several studies. By means of asymptotic methods and heuristic arguments, Frisch and Percus were led to the following scenario in that limit:

- The fourth virial coefficient is negative. Beyond that term, the virial expansion is an alternating series.
- The virial series is convergent for \( \hat{\rho} < 1 \), where \( \hat{\rho} \equiv 2\eta^{1/d} \) is the scaled density per dimension. In terms of the packing fraction, the virial series converges for \( \eta < \eta_{\text{conv}} = 2^{-d} \).
- In the density range \( \hat{\rho} < 1 \) the second virial term dominates over the remaining ones, so that

\[
Z \approx 1 + B_2 \rho = 1 + \frac{\hat{\rho}^d}{2}.
\] (3)

- Even though the virial expansion does not converge for \( \hat{\rho} > 1 \) (oscillatory divergence), the truncated series \( Z(\eta) \) remains valid within the interval \( 1 < \hat{\rho} < (1 - \epsilon)\hat{\rho}_0 \), where \( \epsilon = \mathcal{O}(d^{-1}) \) and

\[
\hat{\rho}_0 = (1.148d^{-1/6}e^{-1.473d^{1/3}})^{-1/d} \sqrt{e/2} \sim \sqrt{e/2} \approx 1.17.
\] (4)

- At the density \( \hat{\rho} = \hat{\rho}_0 \) an infinite compressibility spinodal appears, thus indicating a first-order transition to the high-dimensional solid.

In an independent paper, Parisi and Slanina reached similar conclusions from a toy model based on simplified HNC equations. They obtained that, while in the limit \( d \to \infty \) the EOS for \( \hat{\rho} < 1 \) is given by Eq. (3), in the interval \( 1 < \hat{\rho} < \hat{\rho}_0 = \sqrt{e/2} \), one has

\[
Z(\hat{\rho}) = 1 + \hat{\rho}^d \left[ \frac{1}{2} + \Delta(\hat{\rho}) \right],
\] (5)

where

\[
\Delta(\hat{\rho}) = \left[ \frac{e\kappa(\hat{\rho})}{2\hat{\rho}^2} \right]^d.
\] (6)

\( \kappa(\hat{\rho}) \) being the solution to

\[
\ln \frac{2\hat{\rho}^2}{e} = \ln \left( 1 + \sqrt{1 - \kappa^2} \right) - \sqrt{1 - \kappa^2}.
\] (7)

Note that, since \( \ln \kappa < \ln (1 + \sqrt{1 - \kappa^2}) - \sqrt{1 - \kappa^2} \) for \( 0 < \kappa < 1 \), one has \( \lim_{d \to \infty} \Delta(\hat{\rho}) = 0 \) for \( \hat{\rho} < \hat{\rho}_0 \). Although, strictly speaking, Eq. (7) cannot be extended to \( \hat{\rho} > \hat{\rho}_0 \), Eq. (6) suggests that \( \lim_{d \to \infty} \Delta(\hat{\rho}) = \infty \) in that density domain, in agreement with the phase transition noted by Frisch and Percus.

B. Approximate equations of state

As in two and three dimensions, one can make use of approximate schemes to represent the EOS of hard hyperspheres. Several proposals have been made in the literature for the EOS based on the knowledge of the first few virial coefficients. For illustration, we review here a few of them making use of the first three virial coefficients. The extension to higher virial coefficients is straightforward.

1. Truncated virial series

The first obvious choice is the truncated virial expansion

\[
Z_{[2,0]}(\eta) = 1 + b_2 \eta + b_3 \eta^2.
\] (8)

As discussed above, this simple approximation becomes more and more accurate in the stable fluid domain as the dimensionality increases. In a way analogous to Eq. (8) it is possible to define a truncated expansion \( Z_{[n,0]} \) from the knowledge of the first \( n + 1 \) virial coefficients.

2. Padé approximants

One can also construct Padé approximants of the form \( Z_{[n,m]}(\eta) \) from the first \( n + m + 1 \) virial coefficients. For instance,

\[
Z_{[1,1]}(\eta) = \frac{b_2 + (b_3^2 - b_3)\eta}{b_2 - b_3 \eta},
\] (9)

\[
Z_{[0,2]}(\eta) = \left[ 1 - b_2 \eta + (b_2^2 - b_3)\eta^2 \right]^{-1}.
\] (10)

3. Colot–Baus approximation

Colot and Baus proposed (truncated) rescaled virial expansions, where the series expansion of \( (1 - \eta)^d Z(\eta) \), rather than that of \( Z(\eta) \), is truncated. Let us denote by \( Z_{[n,0]}^{BC}(\eta) \) the truncated rescaled virial expansion that makes use of the first \( n + 1 \) virial coefficients. For example,

\[
Z_{[2,0]}^{BC}(\eta) = \frac{1 + (b_2 - d)\eta + [b_3 - b_2(d + d(d - 1)/2)]\eta^2}{(1 - \eta)^d}.
\] (11)

The pole of order \( d \) at the (unphysical) packing fraction \( \eta = 1 \) is suggested by the scaled particle theory.

4. Maeso–Solana–Amorós–Villar approximation

Maeso et al. combined the advantages of Padé approximants and rescaled expansions by proposing Padé
of exact first four virial coefficients, regardless of the choice of the EOS, since Eq. (14) is consistent with the knowledge of the function \(Z(n,0)(\eta)\).

\[ Z(n,0)(\eta) = Z_{BC}(\eta). \]

By construction, \(Z_{BC}(\eta) = Z_{BC}(\eta).\)

5. Song–Mason–Stratt approximation

Using simple arguments, Song et al.\(^{10,12}\) proposed the following generalization to \(d\) dimensions of the celebrated Carnahan–Starling (CS) EOS for three-dimensional hard spheres:\(^{35}\)

\[ Z_{SMS}(\eta) = 1 + b_2\eta \frac{1 + (b_3/b_2 - \zeta(\eta)/b_4/b_3)(\eta)}{(1 - \eta)^2}. \]

6. Luban–Michels approximation

On a different vein, Luban and Michels\(^{13}\) wrote the compressibility factor as

\[ Z_{LM}(\eta) = 1 + b_2\eta \frac{1 + [b_3/b_2 - \zeta(\eta)/b_4/b_3](\eta)}{(1 - \eta)^2}. \]

The knowledge of the function \(\zeta(\eta)\) is equivalent to that of \(Z(\eta)\). However, \(\zeta(\eta)\) focuses on the high density behavior of the EOS, since Eq. (13) is consistent with the first exact four virial coefficients, regardless of the choice of \(\zeta(\eta)\). The approximation \(\zeta(\eta) = 1\) is equivalent to assuming a Padé approximant \(Z_{[2,1]}(\eta)\). Instead, Luban and Michels observed that the computer simulation data for \(d = 2–5\) favor a linear approximation \(\zeta(\eta) = a + b\eta\), with coefficients obtained by a least-square fit to the simulation results for each dimensionality.

7. Percus–Yevick theory

It is noteworthy that the Percus–Yevick (PY) integral equation can be solved analytically in odd dimensions, as first pointed out by Freasier and Isbister\(^{1}\) and, independently, Leutheusser.\(^{2}\) The latter concluded that, in general, the problem reduces to an algebraic equation of degree \(d-3\). Following his procedure, however, we find that for \(d = 9\) this is not so (see the Appendix) and our calculations suggest that such degree should rather be \(2(d-3)/2\) for \(d \geq 3\). In any case, in five dimensions one has to deal with a quadratic equation\(^{14}\) and explicit expressions for the virial and compressibility routes to the EOS can be obtained\(^{22}\). A simple analysis of the solution for \(d = 5\), that as far as we know has not been carried out before, shows that the virial route incorrectly gives a negative value for \(B_6\): \(B_6 = -0.00286\). The compressibility route yields \(B_6 = 0.00094\). Both routes consistently predict that \(B_6\) is negative, with subsequent coefficients alternating in sign. On the other hand, the virial route gives values for the magnitude of \(B_6\) (\(n \geq 8\)) increasingly larger than the compressibility route: \(B_6 \approx 0.00094\). The alternating character of the virial series predicted by the PY equation for \(d = 5\) is due to a branch singularity located on the negative real axis at \(\eta_{\text{branch}} = -(9 - 5\sqrt{3})/6 \approx -0.0566243\). The radius of convergence \(\eta_{\text{conv}} \approx 0.0566243\) of the PY solution for \(d = 5\) is larger than the value \(2^{-5} = 0.03125\) extrapolated from the radius limit \(\eta_{\text{conv}} = 2^{-d}\), but is close to the estimate \(\eta_{\text{conv}} \approx 0.0529\) made by Clisby and McCoy on the basis of Monte Carlo evaluation of sets of Ree–Hoover diagrams\(^{29,30}\). All these estimates are sensibly smaller than the packing fraction \(\eta_f = 0.19\) at which freezing occurs for \(d = 5, 3, 2\).

8. Generalized Carnahan–Starling approximation

As is well known, the CS EOS for three-dimensional hard spheres can be interpreted as a weighted average between the PY virial and compressibility routes:

\[ Z_{CS}(\eta) = \alpha Z_{PY-c}(\eta) + (1 - \alpha) Z_{PY-v}(\eta), \]

where \(\alpha = 1/2\). Given that the PY equation can be solved for odd dimensions, it is then natural to speculate about whether or not the prescription \(\alpha = 1/2\), with an adequate choice of the mixing parameter \(\alpha\), keeps being reliable for \(d > 3\), even though the internal inconsistency between both routes seems to increase dramatically with the dimensionality.\(^\star\) In the five-dimensional case, one of us\(^\star\) showed that the choice \(\alpha = 1/2\) leads to values of \(Z_{CS}\) in excellent agreement with computer simulations.\(^\star\) This suggested that the choice \(\alpha = (d + 1)/2d\) might provide a good description for \(d > 3\). Note that, while Eqs. (13) and (15) coincide at \(d = 3\), they differ for \(d > 3\), so they generalize the original CS EOS along different directions. An alternative generalization of the CS EOS was made by Gonzalez et al.\(^{16}\) They proposed a simple ansatz for the direct correlation function \(c(r)\), which reduced exactly to the PY theory for \(d = 1\) and \(d = 3\) and gave results very close to the PY theory for other dimensions. Their generalized CS EOS consisted of a weighted average between the virial and compressibility routes obtained from their theory with a mixing parameter \(\alpha = 2/(2d-1)/5d\).

C. Aim of the paper

The aim of this paper is threefold. First, we present the explicit solution to the PY equation in the case of a
seven-dimensional hard-sphere fluid following the procedure introduced by Leutheusser. This allows us to derive the EOS of the fluid both through the virial and the compressibility routes, as well as to analyze the behavior of the virial coefficients stemming out of them. As we will see, the singularity closest to the origin is again a branch point on the negative real axis, so the radius of convergence of the PY virial series is \( \eta_{\text{conv}} \approx 0.0100625 \). We conjecture that this value might be close to the (unknown) exact radius. Moreover, a Carnahan–Starling-like equation of state of the form (13) with \( \alpha = \frac{5}{6} \) is proposed. Secondly, we provide molecular dynamics results for the compressibility factor. To the best of our knowledge, this is the first time that simulation results are presented for hard hyperspheres in seven dimensions. The twenty densities considered range from the dilute regime \((\rho \sigma ^ 7 = 0.1 \text{ or } \eta = 0.0037)\) to our estimated freezing point \((\rho \sigma ^ 7 \approx 1.95 \text{ or } \eta \approx 0.072)\). Finally, we perform a comparison between different proposals for the EOS of a seven-dimensional hard-sphere fluid with the simulation data. We observe that the proposals [11] and [13] (which do not have any empirical parameter), [14] (which contains two fitting parameters), and [15] (with one fitting parameter) reproduce fairly well the simulation data.

The paper is organized as follows. In Section [II] we provide the solution of the PY equation for a seven-dimensional hard-sphere fluid as well as the analysis of the virial coefficients arising from the derivation of the EOS using the virial and the compressibility routes. This is followed in Section [III] by a description of the molecular dynamics simulation that was carried out to obtain the compressibility factor of the fluid. The results of the simulation are then used to assess the merits of various proposals that have been made in the literature for the EOS. The paper is closed in Section [IV] with further discussion of the results and some concluding remarks.

II. SOLUTION OF THE PERCUS–YEVICK EQUATION FOR A SEVEN-DIMENSIONAL HARD-SPHERE FLUID

As mentioned in Sec. [I] the solution to the PY equation for hard hyperspheres with \( d = \text{odd} \) reduces to an algebraic equation of degree \( 2^{(d-3)/2} \). The case \( d = 5 \), which yields a quadratic equation, has been analyzed by several authors [1,4,14,20,21]. The highest dimensionality for which the algebraic problem certainly lends itself to an analytic solution is \( d = 7 \). A sketch of the general solution and some details of the particular cases \( d = 7 \) and \( d = 9 \) are provided in the Appendix. It is shown there that the solution of the PY equation for seven-dimensional hard hyperspheres is given by the physical solution to the quartic equation (A19). In the Appendix it is also shown that for \( d = 9 \) the resulting algebraic equation is of eighth degree.

A study of the solutions of Eq. (A19) shows that in the interval \( 0.446469 \leq \eta < 1 \) the four roots are real. On the other hand, for \( 0 \leq \eta \leq 0.446469 \) two of the roots become complex conjugates and only the other two roots remain real, the physical one being finite in the limit \( \eta \to 0 \). The explicit solution to Eq. (A19) involves the term \( [P_5(\eta) P_5(\eta)]^{1/2} \), where \( P_5(\eta) = 1 + 94\eta + 202\eta^2 + \frac{1369}{30} \eta^3 + 50\eta^4 \) and \( P_5(\eta) = 1 + 99\eta^2 - \frac{366}{5}\eta^3 - \frac{378}{5}\eta^4 + \frac{305}{3}\eta^5 + \frac{25}{3}\eta^6 \). As a consequence, the solution possesses branch points at the zeroes of \( P_5(\eta) \) and \( P_5(\eta) \). The zero of \( P_5(\eta) \) closest to the origin is \( \eta_{\text{branch}} \approx -0.0100625 \), while that of \( P_5(\eta) \) is \( \eta_{\text{branch}} \approx -0.0100625 \). Therefore, the radius of convergence of the virial series for a seven-dimensional hard-sphere fluid described by the PY approximation is \( \eta_{\text{conv}}^\text{PY} = |\eta_{\text{branch}}| \approx 0.0100625 \).

Table [I] gives the first few values of the PY virial coefficients obtained from the virial and the compressibility routes. As far as we know, the exact values \( B_n^{\text{ex}} \) of the virial coefficients of seven-dimensional hard spheres are known up to \( n = 6 \) only [29,30]. They are listed in Table [I] as well, which also gives the CS-like values \( B_n^{\text{CS}} / B_n^{-1} \), where \( B_n^{\text{CS}} = \alpha B_n^{\text{PY-c}} + (1 - \alpha) B_n^{\text{PY-v}} \), with the simple choice \( \alpha = \frac{5}{6} \). Note that the choice \( \alpha \approx 0.6 \) would make \( B_n^{\text{CS}} / B_n^{\text{ex}} \), whereas the choice \( \alpha \approx 0.7 \) would make \( B_n^{\text{CS}} / B_n^{\text{ex}} \). However, comparison with molecular dynamics simulations (see Section [III]) favors \( \alpha \approx 0.8 \).

From Table [I] we observe that the virial route of the PY approximation incorrectly yields a negative value for the fourth virial coefficient (which actually becomes negative for \( d \geq 8,29,30 \)) while the compressibility route predicts the correct sign [30]. We have computed \( B_n^{\text{PY-v}} / B_n^{\text{PY-c}} \) for values of \( n \) much larger than those displayed in Table [I]. The results indicate that \( \text{sgn}(B_n^{\text{PY-v}}) = (-1)^n \) for \( 5 \leq n \leq 97 \) but \( \text{sgn}(B_n^{\text{PY-v}}) = (-1)^n \) for \( n \geq 98 \); analogously, \( \text{sgn}(B_n^{\text{PY-c}}) = (-1)^n \) for \( 5 \leq n \leq 80 \) but \( \text{sgn}(B_n^{\text{PY-c}}) = (-1)^n \) for \( n \geq 81 \). Therefore, both routes synchronize their signs for \( 5 \leq n \leq 80 \) and again for \( n \geq 98 \). This peculiar behavior of the alternating character of the virial series seems to be a consequence of the proximity between the two branch point singularities closest to the origin, \( \eta_{\text{branch}} \approx -0.0100625 \) and \( \eta_{\text{branch}} \approx -0.0100625 \), both located on the negative real axis. To confirm this interpretation, we plot in Fig. [I] the ratios \( [b_n^{\text{PY-v}} / b_n^{\text{PY-c}}] \), \( [b_n^{\text{PY-c}} / b_n^{\text{PY-v}}] \), and \( [b_n^{\text{CS}} / b_n^{\text{CS}}] \). Recall that the radius of convergence of the virial series is \( \eta_{\text{conv}} = \lim_{n \to \infty} b_n / b_{n+1} \). Figure [I] shows that for \( n \leq 50 \) the ratio \( b_n / b_{n+1} \) seems to converge from above to the apparent radius of convergence \( \eta_{\text{conv}} \approx \eta_{\text{branch}} \approx 0.0100625 \). However, the true radius \( \eta_{\text{conv}} \approx \eta_{\text{branch}} \approx 0.0100625 \) is reached from below for \( n \geq 100 \).

As mentioned in Sec. [I] the radius of convergence predicted by the PY approximation in the five-dimensional case is \( \eta_{\text{conv}} \approx 0.0566243 \). When going to the next odd dimensionality, the radius of convergence has shrunk to \( \eta_{\text{conv}} \approx 0.0100625 \). In terms of the scaled density per di-
TABLE I: Values of $B_n/B_2^{n-1}$ for $n = 3$–8, according to the virial route of the PY approximation, the compressibility route of the PY approximation, the CS-like approximation \(\text{(15)}\) with $\alpha = \frac{2}{3}$, and the known exact results \(\text{[29]30}\).

| $n$ | $B_n^{\text{PY-v}}/B_2^{n-1}$ | $B_n^{\text{PY-c}}/B_2^{n-1}$ | $B_n^{\text{CS}}/B_2^{n-1}$ | $B_n^{\text{ex}}/B_2^{n-1}$ |
|-----|-------------------------------|--------------------------------|-----------------------------|-----------------------------|
| 3   | 0.2822265625                  | 0.2822265625                  | 0.2822265625                | 0.2822265625                |
| 4   | $-7.499694824 \times 10^{-3}$ | 2.155081431 $\times 10^{-2}$  | 1.670906279 $\times 10^{-2}$ | 9.873(4) $\times 10^{-3}$   |
| 5   | 1.235022893 $\times 10^{-2}$  | 5.116807918 $\times 10^{-3}$  | 6.322378086 $\times 10^{-3}$ | 7.071(7) $\times 10^{-3}$   |
| 6   | $-8.17705666 \times 10^{-3}$  | $-1.865328120 \times 10^{-3}$ | $-2.917274378 \times 10^{-3}$ | $-3.52(2) \times 10^{-3}$   |
| 7   | $6.55313160 \times 10^{-3}$   | $1.384246670 \times 10^{-3}$  | $2.245724148 \times 10^{-3}$ | $2.45724148 \times 10^{-3}$ |
| 8   | $-5.762797816 \times 10^{-3}$ | $-1.078783146 \times 10^{-3}$ | $-1.859452258 \times 10^{-3}$ | $-1.859452258 \times 10^{-3}$ |

FIG. 1: Plot of the ratios $|B_n^{\text{PY-v}}/B_{n+1}^{\text{PY-v}}|$ (diamonds), $|B_n^{\text{PY-c}}/B_{n+1}^{\text{PY-c}}|$ (triangles), and $|B_n^{\text{CS}}/B_{n+1}^{\text{CS}}|$ (circles). The horizontal lines correspond to the apparent radius of convergence $\eta_{\text{conv}} \approx 0.0108868$ and to the true radius of convergence $\eta_{\text{conv}} \approx 0.0100625$.

FIG. 2: Plot of the virial coefficients $B_n^{\text{PY-v}}/B_2^{n-1}$ (diamonds), $B_n^{\text{PY-c}}/B_2^{n-1}$ (triangles), and $B_n^{\text{CS}}/B_2^{n-1}$ (circles).

n = 10, and then grow with $n$. The fact that the PY solution in the three-dimensional case does not possess a branch point singularity, so that all the virial coefficients remain positive, casts some doubts as to whether the true virial series fails to converge for densities close to the freezing density $\eta_f \approx 0.494$. In any case, the true radius of convergence for $d = 3$ cannot be larger than the crystalline close-packing value $\eta_{\text{CP}} = \pi/\sqrt{2}/6 \approx 0.7405$, while the PY solution has $\eta_{\text{conv}} = 1$.

III. MOLECULAR DYNAMICS SIMULATIONS

A. Method

The numerical simulation was implemented by using the same algorithm as described in Ref. [25], which is also based on the work of Michel and Trappenberg\(\text{[22]}\) and Luban and Michel\(\text{[23]}\) for four- and five-dimensional hyperspheres. We are not aware of any previous computer simulation of hard hyperspheres of a dimension higher than $d = 5$. We have chosen the molecular dynamics method instead of the Monte Carlo method because that gives us the possibility of testing our code by applying it to $d = 4$ and $d = 5$ and comparing with the results of Refs. [22-25].

For our simulations, in order to keep the computing time within reasonable limits and at the same time being able to examine a wide density range, the initial con-
B. Results

We have computed the compressibility factor for densities $0.1 \leq \rho^* \leq 1.90$ with a step $\Delta \rho^* = 0.1$, as well as for $\rho^* = 1.95$. The simulation data obtained by our molecular dynamics simulations are listed in Table II at the largest density $\rho^* = 1.95$ ($\eta = 0.0720$) the compressibility factor presents a dramatic drop. We interpret this as an indication of the freezing transition. Consequently, the density at which the seven-dimensional fluid of hard spheres freezes can be estimated as $\rho^*_f \lesssim 1.95$ or, equivalently, $\eta_f \lesssim 0.072$. From Fig. 5 of Ref. 26 one can observe that $\ln \eta_f(d)$ is almost a linear function of the dimensionality $d$, with a slight negative curvature. According to this, knowing the freezing densities $\eta_f(d)$ and $\eta_f(d+2)$, one can estimate the freezing density $\eta_f(d+4) = \eta_f(d+4) \lesssim \eta_f^2(d+2)/\eta_f(d)$. Given that $\eta_f(3) \approx 0.494$ and $\eta_f(5) \approx 0.19$, one has $\eta_f(7) \lesssim 0.19^2/0.494 \approx 0.073$, in close agreement with our estimate. An independent estimate based on a conjecture by Colot and Baus confirms again this value. These authors suggested that the ratio of length scales $[\eta_f(d)/\eta_f(d)]^{1/d}$ is practically independent of $d$, so that $\eta_f(d+2) \approx \eta_f(d+2)[\eta_f(d)/\eta_f(d)]^{(d+2)/d}$. The general expression for the close-packing fraction $\eta_f(d)$ is not known, but for $d < 25$ the values are not far from Blichfeldt’s upper estimate. An independent estimate based on a conjecture by Colot and Baus confirms again this value. These authors suggested that the ratio of length scales $[\eta_f(d)/\eta_f(d)]^{1/d}$ is practically independent of $d$, so that $\eta_f(d+2) \approx \eta_f(d+2)[\eta_f(d)/\eta_f(d)]^{(d+2)/d}$. The general expression for the close-packing fraction $\eta_f(d)$ is not known, but for $d < 25$ the values are not far from Blichfeldt’s upper estimate. An independent estimate based on a conjecture by Colot and Baus confirms again this value. These authors suggested that the ratio of length scales $[\eta_f(d)/\eta_f(d)]^{1/d}$ is practically independent of $d$, so that $\eta_f(d+2) \approx \eta_f(d+2)[\eta_f(d)/\eta_f(d)]^{(d+2)/d}$. The general expression for the close-packing fraction $\eta_f(d)$ is not known, but for $d < 25$ the values are not far from Blichfeldt’s upper estimate.
Luban–Michels EOS \cite{14} one fits \( \zeta(\eta) \) to a linear function. Figure 3 shows the simulation values of \( \zeta(\eta) \). As in the five-dimensional case \cite{13} \( \zeta(\eta) \) is an increasing function of \( \eta \), while it is a decreasing function for \( d = 2-4 \). A linear fit in the interval \( 0.5 \leq \rho^* \leq 1.9 \) \( (0.0185 \leq \eta \leq 0.0701) \) yields

\[
\zeta(\eta) = -5.81 + 88.2\eta. \quad (18)
\]

The column labeled \( Z_{LM} \) in Table II has been evaluated using the fit \cite{18}. On the other hand, our simulation data in Fig. 3 seem to indicate a negative curvature of \( \zeta(\eta) \).

Table II shows that up to \( \rho^* = 0.8 \) \( (\eta = 0.0295) \) all the different theoretical results tabulated, including the simple truncated virial expansion \( Z_{4,0} \), behave relatively well. For larger densities, \( Z_{4,0} \) tends to overestimate the simulation data, while the Pade approximants \( Z_{2,2} \) and \( Z_{3,2} \) tend to underestimate them. The best global agreement is presented by \( Z_{CS} \), \( Z_{LM} \), \( Z_{BC, 0} \), and \( Z_{SMS} \). This is especially noteworthy in the case of the two latter approximations, since they do not contain fitting parameters and, moreover, only the knowledge of the first three virial coefficients is exploited. This contrasts with \( Z_{LM} \), which includes the fourth virial coefficient and contains two fitting parameters. On the other hand, \( Z_{CS} \) belongs in a different class of approximations. Given the involved algebraic structure of the PY solution, \( Z_{CS} \) does not intend to represent a practical recipe to the EOS of a seven-dimensional hard-sphere fluid. Instead, its role is to highlight the fact that the two PY routes keep bracketing the simulation data, so that an interpolation between them with a density-independent parameter \( \alpha \) is rather accurate, as graphically illustrated in Fig. 4. This gives some confidence on the expectation that some of the analytical properties of the PY solution (e.g., alternating character of the virial series, branch points located on the negative real axis, ...) may shed light on the true behavior of the exact series.

IV. DISCUSSION

The results of the previous sections deserve further discussion. To begin with, to our knowledge this is the first time that a molecular dynamics simulation has been carried out on a seven-dimensional hard-sphere fluid. The simulation strategy that we adopted implied a compromise between computer process time and density range to be explored and the outcome is rather encouraging. The availability of simulation data for the EOS of the fluid allowed us to locate the freezing transition and also to assess the merits and limitations of various proposals that have been made in the literature for the compressibility factor of hard hyperspheres. From this analysis it is clear that even simple approximations such as \( Z_{BC, 0} \) and \( Z_{SMS} \) do a reasonably good job and that, as it occurs in other dimensionalities, the virial and compressibility routes to the EOS in the PY approximation keep bracketing the simulation data, so that a Carnahan–Starling-like recipe of the form of Eq. \cite{15} turns out to be rather accurate. However the parameter \( \alpha \) seems not to follow a simple relation as the ones suggested by González et al. \cite{16,17} or Santos. \cite{21}

We also presented the explicit solution of the PY equation for a hard-sphere fluid in 7D. Such a solution allowed us to carry out an analysis of the virial coefficients arising both in the virial and in the compressibility routes and to determine the radius of convergence of both virial series. The results indicate some peculiar behavior of the virial coefficients with the virial route incorrectly predicting a negative fourth virial coefficient. The radius of convergence of the virial series is due to a singularity (branch point) located on the negative real axis and therefore what one has is an alternating series. Because of the good agreement between our value of the radius of convergence of the virial series and other independent estimates and the similar results obtained for \( d = 5 \), it is tempting to conjecture that the PY solution for even
higher dimensionalities should provide a rather accurate estimate of the radius of convergence of the true virial series and that it is the existence of singularities on the negative real axis (either poles or branch points) which determines such radius. 

As a final point it is worth commenting that in this case our analysis was facilitated by the fact that we could combine both the analytical and the simulation results. And due to the common features such as the freezing transition that hard-core systems in different dimensionalities share, the expectation and the hope is that the present results shed some more light on the thermodynamic properties of such systems. As far as the high dimensionality limit is concerned, our results provide some support to the scenario of Frisch and Percus mentioned in the Introduction in the following sense. The solution to the PY equation predicts an alternating virial series. Further, the values of the scaled density \( \hat{\rho} \) that one obtains for the radius of convergence (\( \hat{\rho} = 1.13 \) for \( d = 5 \), \( \hat{\rho} = 1.04 \) for \( d = 7 \), and the number \( \hat{\rho} \approx 1.02 \) coming out of our preliminary calculations for \( d = 9 \)) are consistent with a limiting value of \( \hat{\rho} = 1 \) for \( d \to \infty \). Also, the fluid range in \( d = 7 \) is reasonably well accounted for by the first three or four virial coefficients so that it is conceivable that for infinite dimensionality only the second virial coefficient will be the dominant term.

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Appendix A: Solution of the Percus–Yevick equation for hard hyperspheres

For simplicity, in the remainder of this Appendix we set \( \sigma = 1 \).

In the Percus–Yevick approximation, the structure factor \( S(q) \) of a hard-sphere fluid in \( d = 2k + 1 \) dimensions is

\[
S(q) = \frac{1}{\tilde{Q}(q)\tilde{Q}(-q)},
\]

where

\[
\tilde{Q}(q) = 1 - \lambda \int_0^1 dr e^{iqr} Q(r), \quad \lambda \equiv (2\pi)^d \rho = 2^{2k}(2k + 1)!! \eta,
\]

\[Q(r) \text{ having the form}
\]

\[
Q(r) = \begin{cases} 
\sum_{m=0}^{k} Q_m (r-1)^{m+k}, & 0 \leq r \leq 1, \\
0, & r \geq 1.
\end{cases}
\]

The \( k + 1 \) coefficients \( \{Q_m\} \) are functions of the density determined by the two linear equations

\[
(-1)^k = -k!2^k Q_k + \lambda \sum_{m=0}^{k} (-1)^m \frac{Q_m}{k + m + 1}, \quad k \geq 0,
\]

\[(-1)^k = -(k-1)2^{k-1} Q_{k-1} - \lambda \sum_{m=0}^{k} (-1)^m \frac{Q_m}{k + m + 2}, \quad k \geq 1,
\]

plus the \( k - 1 \) nonlinear equations

\[
Q^{(2m+1)}(0) = \frac{1}{2} \lambda (-1)^{m+1} \left[ Q^{(m)}(0) \right]^2
\]

\[+ \lambda \sum_{\nu=0}^{m-1} (1-\nu)Q^{(\nu)}(0)Q^{(2m-\nu)}(0),
\]

\[
0 \leq m \leq k - 2.
\]

Here \( Q^{(\nu)}(r) \) represents the \( \nu \)-th derivative of the function \( Q(r) \). For \( k = 0 \) (\( d = 1 \), Eq. (A1) gives the exact solution for hard rods. For \( k = 1 \) (\( d = 3 \), Eqs. (A4) and (A5) are sufficient to find the solution of the PY equation. However, for \( k \geq 2 \) (\( d \geq 5 \)) one needs in addition Eq. (A6), so that the problem reduces to solving an algebraic equation which, as we will argue below, is likely to be of degree \( 2^{k-1} = 2^{(d-3)/2} \).

In the limit \( \eta \to 0 \), it is easy to verify that

\[
\lim_{\eta \to 0} Q_m = (-1)^{k+1} \frac{2^{m-1}}{m} \frac{k}{m(k-m)},
\]

\[
\lim_{\eta \to 0} Q(r) = (-1)^k \frac{2^{m-1} (2m-1)!}{m!(k-m)!} r^k,
\]

\[
\lim_{\eta \to 0} Q^{(2m)}(0) = (-1)^{m+1} 2^{m-1} \frac{(2m)!}{m!(k-m)!},
\]

\[\lim_{\eta \to 0} Q^{(2m+1)}(0) = 0.
\]

In general, one can expand the coefficients \( Q_m \) in powers of \( \eta \):

\[
Q_m(\eta) = \sum_{n=0}^{\infty} Q_{m,n} \eta^n,
\]

where \( Q_{m,0} \) is given by the first equation of (A7). Of course, the full nonlinear dependence of the coefficients \( Q_m(\eta) \) can be obtained from the solution to the set of equations (A4)–(A6), either analytically (\( k \leq 3 \)) or numerically (\( k \geq 4 \)).

Once one has determined the function \( Q(r) \), the structural properties of the fluid are given by Eqs. (A1) and (A2). In particular, the long wavelength limit of the
structure factor and the contact value of the radial distribution function are, respectively,

\[ S(q = 0) = \frac{1}{[k!2kQ_k]^2}, \quad (A10) \]

\[ g(1^+) = (-1)^{k+1} k! Q_0. \quad (A11) \]

The virial route to the EOS is given by

\[ Z = 1 + 2^{d-1} \eta g(1^+), \quad (A12) \]

while the compressibility route is

\[ \chi \equiv k_B T \left( \frac{\partial \rho}{\partial \rho} \right)_T = S(q = 0). \quad (A13) \]

Inserting the expansion into Eqs. (A12) and (A13) we get the virial coefficients along both routes:

\[ \rho_{PY-v}^{(n+2)} = 2^{2k} (-1)^{k+1} k! Q_{0,n}, \]

\[ \rho_{PY-c}^{(n+1)} = 2^{2k} (k!)^2 \frac{1}{n+1} \sum_{m=0}^{n} Q_{k,m} Q_{k,n-m}. \quad (A14) \]

Table III shows the first few coefficients \(Q_{m,n}\). The exact values are rational numbers, but they become more and more involved as the order \(n\) increases and so they are expressed in real form in Table III. From Eq. (A14) we can obtain the virial coefficients corresponding to the virial and the compressibility routes. The first few values are listed in Table I.

1. The case \(d = 7\)

Now we particularize to the seven-dimensional case \((k = 3)\), the unknowns being \(Q_m, m = 0, 1, 2, 3\). Since the two nonlinear equations \((A6)\) involve the derivatives \(Q^{(m)} \equiv Q^{(m)}(0)\), it is more advantageous to work with the set \(\{Q^{(m)}\}\) rather than with the set \(\{Q_m\}\). The latter can be expressed in terms of the former as

\[ \left( \begin{array}{c} Q_0 \\
Q_1 \\
Q_2 \\
Q_3 \\
Q_4 \\
Q_5 \\
Q_6 \\
Q_7 \\
Q_8 \\
Q_9 \\
\end{array} \right) = \left( \begin{array}{c}
20 \\
20 \\
20 \\
20 \\
20 \\
20 \\
20 \\
20 \\
20 \\
20 \\
\end{array} \right) \left( \begin{array}{c}
Q^{(0)} \\
Q^{(1)} \\
Q^{(2)} \\
Q^{(3)} \\
Q^{(4)} \\
Q^{(5)} \\
Q^{(6)} \\
Q^{(7)} \\
Q^{(8)} \\
Q^{(9)} \\
\end{array} \right). \quad (A15) \]

Equations (A4) and (A5), plus Eq. (A6) with \(m = 0\) yield

\[ Q^{(1)} = -3360 \eta Q^{(0)^2}, \quad (A16) \]

\[ Q^{(2)} = -\frac{1 + 96Q^{(0)} \left(1 - 5\eta \left[3 + 112Q^{(0)}(3 - 10\eta)\right]\right)}{8(1 - \eta)}, \quad (A17) \]

\[ Q^{(3)} = \frac{8 - 15\eta + 192Q^{(0)} \left(2 - \eta \left[53 + 280Q^{(0)}(3 - 10\eta)^2 - 100\eta\right]\right)}{8(1 - \eta)^2}. \quad (A18) \]

Thus, the parameters \(Q^{(1)}, Q^{(2)}, \text{ and } Q^{(3)}\) are given as explicit quadratic functions of \(Q^{(0)} = Q(0)\). Finally, insertion of Eqs. (A16)–(A18) into Eq. (A6) with \(m = 1\) leads to the quartic equation

\[ 8 - 15\eta + 192Q^{(0)} \left(2 - \eta \left[88 - 135\eta + 1960Q^{(0)} \left[3 - 4\eta \left[9 - 10\eta + 240Q^{(0)}(1 - \eta)\right] \right] \right] \right) \times \left[3 - 10\eta \left(1 + 84Q^{(0)}(1 - \eta)\right)\right] = 0. \quad (A19) \]

Although an explicit expression exists for the physical root of Eq. (A19), it is of course too cumbersome and will be omitted here.

2. The case \(d = 9\)

We will now sketch the result for the case \(d = 9\) following the same procedure. For \(k = 4\), the set \(\{Q_m\}\) can be expressed in terms of the set \(\{Q^{(m)}\}\) as

\[ \left( \begin{array}{c} Q_0 \\
Q_1 \\
Q_2 \\
Q_3 \\
Q_4 \\
Q_5 \\
Q_6 \\
Q_7 \\
Q_8 \\
Q_9 \\
\end{array} \right) = \left( \begin{array}{c}
70 \\
224 \\
280 \\
160 \\
35 \\
20 \\
5 \\
\frac{1}{4} \\
\frac{1}{8} \\
\frac{1}{16} \\
\end{array} \right) \left( \begin{array}{c}
Q^{(0)} \\
Q^{(1)} \\
Q^{(2)} \\
Q^{(3)} \\
Q^{(4)} \\
\end{array} \right). \quad (A20) \]
In addition, the fifth derivative $Q^{(5)}$ is a linear combination of $\{Q_m\}$ and hence of the first four derivatives:

$$Q^{(5)} = -20 \left( 336Q^{(0)} + 210Q^{(1)} + 60Q^{(2)} + 10Q^{(3)} + Q^{(4)} \right).$$  

(A21)

The nonlinear equations (A6) with $m = 0, 1, 2$ allow one to express the odd derivatives in terms of the even ones as

$$Q^{(1)} = -\frac{\lambda}{2}Q^{(0)^2}, \quad Q^{(3)} = \frac{\lambda^3}{8}Q^{(0)^4} - \lambda Q^{(0)}Q^{(2)}, \quad Q^{(5)} = \frac{\lambda^5}{16}Q^{(0)^6} + \frac{\lambda^3}{2}Q^{(0)^3}Q^{(2)} - \frac{\lambda}{2}Q^{(2)^2} - \lambda Q^{(0)}Q^{(4)},$$  

(A22)

where $\lambda = 241.9207$. Next, insertion of Eqs. (A22) and (A23) into the linear equations (A4) and (A5) yields $Q^{(2)}$ and $Q^{(4)}$ as nonlinear functions of $Q^{(0)}$. Finally, by equating the right-hand sides of Eqs. (A21) and (A24) one gets a closed algebraic equation of eighth degree for $Q^{(0)}$. A preliminary analysis of this equation indicates that its physical solution possesses a branch point at $\eta_{\text{branch}} \approx -0.0023945$, so that the radius of convergence of the PY virial series would be $\eta_{\text{conv}} = |\eta_{\text{branch}}| \approx 0.0023945$.

We have checked that for $d = 11$ the resulting equation is of degree 16. Therefore, it seems plausible that in the general case $d = 2k + 1$ the degree of the equation for $Q^{(0)}$ is $2k - 1 = 2(d - 3)/2$.

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As mentioned in Section I, a similar situation takes place with the PY solution for \( d = 5 \), where \( B_6^{PY-v} < 0 \) but \( B_6^{PY-c} > 0 \).

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A code written in Mathematica which provides the explicit expression for this physical root is available from any of the authors upon request.
TABLE II: Compressibility factor as a function of \( \eta \) from the simulation data and for different approximations. The numbers in parentheses indicate the statistical error in the last significant digit.

| \( \eta \) | \( Z_{\text{simul}} \) | \( Z_{\text{CS}} \) | \( Z_{\text{PY-V}} \) | \( Z_{\text{PY-C}} \) | \( Z_{[4,2]} \) | \( Z_{[3,2]} \) | \( Z_{\text{BC}}^{[2,2]} \) | \( Z_{\text{MSAV}}^{[2,2]} \) | \( Z_{\text{SMS}} \) | \( Z_{\text{LM}} \) |
|---|---|---|---|---|---|---|---|---|---|---|
| 0.0037 | 1.25366(2) | 1.25223 | 1.25192 | 1.25229 | 1.25214 | 1.25214 | 1.25214 | 1.25233 | 1.25214 | 1.25233 |
| 0.0074 | 1.5337(1) | 1.53751 | 1.53516 | 1.53797 | 1.53687 | 1.53687 | 1.53681 | 1.53829 | 1.53685 | 1.53827 |
| 0.0111 | 1.8646(3) | 1.85767 | 1.84997 | 1.85921 | 1.85577 | 1.85576 | 1.85534 | 1.86008 | 1.85562 | 1.86003 |
| 0.0148 | 2.2103(3) | 2.21482 | 2.19691 | 2.21840 | 2.21093 | 2.21094 | 2.20930 | 2.20936 | 2.21033 | 2.21003 |
| 0.0185 | 2.6174(2) | 2.61124 | 2.57674 | 2.61814 | 2.60499 | 2.60513 | 2.60047 | 2.60271 | 2.60328 | 2.60247 |
| 0.0221 | 3.0650(4) | 3.04946 | 2.99039 | 3.06128 | 3.04111 | 3.04170 | 3.03080 | 3.03647 | 3.03716 | 3.06423 |
| 0.0258 | 3.5449(5) | 3.53219 | 3.43890 | 3.55085 | 3.52928 | 3.52481 | 3.50243 | 3.55469 | 3.51502 | 3.55399 |
| 0.0295 | 4.0989(7) | 4.06234 | 3.92342 | 4.09012 | 4.05480 | 4.05948 | 4.01769 | 4.09372 | 4.04037 | 4.09264 |
| 0.0332 | 4.7013(5) | 4.64302 | 4.44519 | 4.68258 | 4.64133 | 4.65183 | 4.57911 | 4.68483 | 4.61713 | 4.68326 |
| 0.0369 | 5.3891(1) | 5.27757 | 5.00555 | 5.33198 | 5.28785 | 5.30924 | 5.18944 | 5.33130 | 5.24971 | 5.32910 |
| 0.0406 | 6.051(1) | 5.96955 | 5.60592 | 6.04228 | 6.00015 | 6.04073 | 5.85164 | 6.03659 | 5.94307 | 6.03358 |
| 0.0443 | 6.8179(6) | 6.72276 | 6.24777 | 6.81775 | 6.78456 | 6.85731 | 6.56896 | 6.80433 | 6.70273 | 6.80033 |
| 0.0480 | 7.6325(1) | 7.54121 | 6.93269 | 7.66292 | 7.64794 | 7.77255 | 7.34490 | 7.63837 | 7.53489 | 7.63317 |
| 0.0517 | 8.5133(2) | 8.42922 | 7.66233 | 8.58259 | 8.59769 | 8.80333 | 8.18328 | 8.54278 | 8.44645 | 8.53613 |
| 0.0554 | 9.4294(3) | 9.39134 | 8.43841 | 9.58192 | 9.64172 | 9.97083 | 9.08829 | 9.52186 | 9.44519 | 9.51348 |
| 0.0591 | 10.492(1) | 10.4324 | 9.62265 | 10.6664 | 10.7885 | 11.3020 | 10.0645 | 10.5801 | 10.5398 | 10.5697 |
| 0.0628 | 11.570(3) | 11.5577 | 10.1372 | 11.8417 | 12.0496 | 12.8317 | 11.1168 | 11.7224 | 11.7400 | 11.7096 |
| 0.0664 | 12.694(1) | 12.7275 | 11.0638 | 13.1142 | 13.4266 | 14.6056 | 12.2507 | 12.9537 | 13.0569 | 12.9381 |
| 0.0701 | 13.907(3) | 14.0828 | 12.0446 | 14.4904 | 14.9374 | 16.6847 | 13.4722 | 14.2794 | 14.5029 | 14.2607 |
| 0.0720 | 9.03944(6) | 9.47756 | 12.5559 | 15.2196 | 15.7454 | 17.8637 | 14.1178 | 14.9794 | 15.2786 | 14.9589 |

TABLE III: Values of the coefficients \( Q_{m,n} \), defined by Eq. (A9), for \( n = 0 \)–6.

| \( n \) | \( Q_{0,n} \) | \( Q_{1,n} \) | \( Q_{2,n} \) | \( Q_{3,n} \) |
|---|---|---|---|---|
| 0 | 0.166666667 | 0.250000000 | 0.125000000 | 0.020833333 |
| 1 | 3.010416667 | 7.888020833 | 5.812500000 | 1.333333333 |
| 2 | −5.119791667 | −59.313802833 | −41.072916667 | −6.541666667 |
| 3 | 5.395897352 \( \times 10^2 \) | 4.247567790 \( \times 10^3 \) | 3.201932292 \( \times 10^3 \) | 6.540590278 \( \times 10^2 \) |
| 4 | −2.286456505 \( \times 10^4 \) | −2.488562475 \( \times 10^5 \) | −1.884527380 \( \times 10^5 \) | −3.841568446 \( \times 10^4 \) |
| 5 | 1.17272501 \( \times 10^6 \) | 1.635350292 \( \times 10^7 \) | 1.241794603 \( \times 10^7 \) | 2.538798289 \( \times 10^6 \) |
| 6 | −6.600274174 \( \times 10^7 \) | −1.143524052 \( \times 10^9 \) | −8.688923174 \( \times 10^8 \) | −1.778764760 \( \times 10^8 \) |