

Monte Carlo Simulation of Hard Hyperspheres in Six, Seven and Eight Dimensions for Low to Moderate Densities

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The pair correlation function of hard hyperspheres in six, seven and eight dimensions is obtained from Monte Carlo simulations. The value of the pair correlation function at contact is compared with the results from molecular dynamics calculations and a variety of theoretical approaches. Remarkably good agreement is found with the simple, closed-form equations of Y. Song, E. A. Mason and R. M. Stratton, *J. Phys. Chem.*, **93**:6916–6919 (1989). The Monte Carlo results for the equation of state are compared with the theoretical expressions of M. Baus and J. L. Colot, *Phys. Rev. A*, **36**:3912 (1987), M. Luban and J. P. J. Michels, *Phys. Rev. A*, **41**:6796 (1990), and high order virial expansions. In addition, in seven dimensions, comparisons are made with the exact PY solution provided by M. Robles, M. L. de Haro and A. Santos, *J. Chem. Phys.*, **120**:9113 (2004). Very good agreement was observed between theory and computer simulation in all dimensions.

KEY WORDS: hyperspheres, monte carlo, pair correlation function, equation of state

1. INTRODUCTION

Hard hyperspherical systems in arbitrary spatial dimension, D , have been and remain, an active area of research in statistical mechanics.^(1–3) Song, Mason and Stratton⁽⁴⁾ have proposed a theoretical equation which predicts the pair correlation function at contact for any reduced number density, ρ , and any dimension by assuming that the probability that a second particle will be found within a small

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region about a reference particle is the product of independent probabilities for each dimension. Their equation for the pair correlation function at contact, $G(\sigma)$, is

$$G(\sigma) = \frac{1 - \alpha\eta}{(1 - \eta)^D} \quad (1)$$

where σ is the diameter of the D dimensional hypersphere, η is the packing fraction

$$\eta = \frac{B_2\rho}{2^{D-1}} \quad (2)$$

and

$$\alpha = D - 2^{D-1} \frac{B_3}{B_2^2} \quad (3)$$

B_2 and B_3 are the second and third virial coefficients, respectively. These equations have no adjustable parameters.

In a recent publication⁽⁵⁾ we have compared the predictions of their equations with our Monte Carlo, MC, computer simulations in one through five dimensions. Excellent agreement between their theory and the MC data, within statistical errors, was found in all dimensions studied.

One of the major goals of this investigation is to further test their theory in six, seven and eight dimensions. In addition, we report and compare our MC equation of state data to a variety of other theoretical and molecular dynamic simulation results.

The compressibility factor, Z , is defined as

$$Z = P\beta/\rho \quad (4)$$

where β is $1/k_B T$; k_B is Boltzmann's constant, T is the absolute temperature and P is the pressure. The value of the pair correlation function at contact is related to the equation of state, Z as a function of ρ , in D dimensions⁽⁶⁾ by

$$Z = 1 + \rho B_2 G(\sigma) \quad (5)$$

B_2 has the value⁽⁷⁾ of

$$B_2 = \frac{\pi^{D/2} \sigma^D}{2\Gamma(1 + D/2)} \quad (6)$$

where Γ is the Gamma Function. The contact value of the pair correlation function from our simulations was determined by a least-squares fit⁽⁸⁾ with extrapolation to contact. The resultant $G(\sigma)$ values were used to determine the equation of state via Eq. 5. This procedure was employed in our earlier studies.

The virial expansion of the equation of state⁽⁹⁾

$$Z_V = 1 + B_2\rho + B_3\rho^2 + B_4\rho^3 + B_5\rho^4 + \dots + B_{V+1}\rho^V \quad (7)$$

which is expected to describe low and moderate density fluids in all dimensions can be compared to the simulation results. In the case of hard hyperspheres Z_V is independent of the temperature since the virial coefficients, (B_V , $V = 2, 3, \dots$), are independent of temperature. A number of the B's (B_2 , B_3 and B_4) are known exactly^(7,10,11) for D dimensional hyperspheres because the necessary multidimensional integrals can be evaluated analytically. Other values (B_5 , B_6 , B_7 , B_8 , B_9 and B_{10}) are known^(10,12-18) from extensive numerical calculations.

The Z_V expansion, Eq. 7, includes the $V + 1$ -th virial coefficient. Employing all the known values for B_V , Z_9 has been computed for six, seven and eight dimensions. Using the notation that $[n, m]$ indicates an approximant that has a polynomial of degree n for its numerator and a polynomial of degree m for its denominator, both the $[4,5]$ and $[5,4]$ Padé approximants^(19,20) in six through eight dimensions were determined from the virial expansions. In six dimensions we find that

$$Z_{[4,5]} = \frac{1 + 5.6358\rho + 11.648\rho^2 + 10.539\rho^3 + 3.4170\rho^4}{1 + 3.0520\rho + 1.4857\rho^2 - 0.8228\rho^3 + 0.0694\rho^4 + 0.0154\rho^5} \quad (8)$$

$$Z_{[5,4]} = \frac{1 + 5.4689\rho + 10.758\rho^2 + 8.8023\rho^3 + 1.9483\rho^4 - 0.4313\rho^5}{1 + 2.8851\rho + 1.0270\rho^2 - 0.9939\rho^3 + 0.1830\rho^4} \quad (9)$$

in seven dimensions that

$$Z_{[4,5]} = \frac{1 + 5.8810\rho + 12.461\rho^2 + 11.291\rho^3 + 3.5776\rho^4}{1 + 3.5187\rho + 2.5736\rho^2 - 0.4615\rho^3 - 0.0638\rho^4 + 0.0261\rho^5} \quad (10)$$

$$Z_{[5,4]} = \frac{1 + 4.6594\rho + 5.8738\rho^2 - 1.3949\rho^3 - 6.6540\rho^4 - 2.7188\rho^5}{1 + 2.2970\rho - 1.1277\rho^2 - 2.4788\rho^3 + 0.4591\rho^4} \quad (11)$$

and in eight dimensions that

$$Z_{[4,5]} = \frac{1 + 5.4951\rho + 10.767\rho^2 + 8.8764\rho^3 + 2.5049\rho^4}{1 + 3.4657\rho + 2.7671\rho^2 - 0.0664\rho^3 - 0.0859\rho^4 + 0.0163\rho^5} \quad (12)$$

$$Z_{[5,4]} = \frac{1 + 7.4067\rho + 20.2895\rho^2 + 25.5900\rho^3 + 14.5259\rho^4 + 2.7554\rho^5}{1 + 5.3774\rho + 8.4107\rho^2 + 3.3474\rho^3 - 0.4047\rho^4} \quad (13)$$

Another possible equation of state is the Baus-Colot⁽²¹⁾ rescaled virial expansion given by

$$Z_{BC} = \frac{1 + (b_2 - D)\eta + (b_3 - b_2D + D(D - 1)/2)\eta^2}{(1 - \eta)^D} \quad (14)$$

where $b_n = 2^{(D-1)(n-1)}B_n/B_2^{n-1}$. This representation of the equation of state has no adjustable parameters and only requires knowledge of b_2 and b_3 .

The Luban-Michels⁽²²⁾ approximation is:

$$Z_{LM} = 1 + \frac{b_2^*X(1 + [(b_3^*/b_2^*) - \zeta(X)(b_4^*/b_3^*)]X)}{1 - \zeta(X)(b_4^*/b_3^*)X + [\zeta(X) - 1](b_4^*/b_2^*)X^2} \quad (15)$$

where $X = \rho/\rho_{cp}$, ζ is a function of X and $b_n^* = B_n\rho_{cp}^{n-1}$. Here ρ_{cp} is the lattice close packed density. $\zeta(X)$ can be determined by using values of $G(\sigma)$ in Eq. 5 to find Z and then inverting Eq. 15 to yield

$$\zeta(X) = \frac{b_3^*[b_2^*X(b_2^* + b_3^*X) - (b_2^* - b_4^*X^2)(Z - 1)]}{b_4^*X[b_2^*X + (b_3^*X - b_2^*)(Z - 1)]} \quad (16)$$

2. METHOD

The hyperspheres are initially arranged in a simple hypercubic lattice. The number of particles, N , the number density of the state and the dimensionality of the system of interest are pre-selected input parameters. These determine the size of the system simulation hyperbox. The hyperspheres are randomly moved using the standard Metropolis Monte Carlo technique⁽²³⁾ to form an equilibrated fluid. We have employed the shuffled, nested Weyl random number generator⁽²⁴⁾ which empirical tests have shown to work well in parallel Monte Carlo calculations.⁽²⁵⁾ In the case of hard hyperspheres the usual Metropolis energy check becomes a simple test for overlaps since the pair potential of the particles separated by the D dimensional distance R is given by

$$U(R) = \begin{cases} \infty & R < \sigma \\ 0 & R \geq \sigma \end{cases} \quad (17)$$

The computer simulation proceeds by attempting to move, in turn, all of the N particles in the simulation hyperbox; this is called a pass. A new trial position is randomly selected from a hyperbox surrounding the current location of the center of mass of the hypersphere. If the new position is not accepted, the hypersphere remains at its current location. The move may or may not be accepted but is always counted in the averaging. The acceptance ratio, the number of accepted moves divided by the number of total moves, is monitored. This ratio, as well as, the maximum magnitude of an allowed displacement for each

Table I. Six Dimensional MC Results

ρ	PreEq	PostEq	Maximum Displacement	Acceptance Ratio	$G(1)$	LM ^a $G(1)$	BC ^b $G(1)$
0.10	1000	10000	5.00	0.58	1.091(3)	1.093	1.092
0.20	1000	10000	4.00	0.31	1.186(1)	1.186	1.190
0.30	1000	10000	0.50	0.29	1.285(6)	1.289	1.297
0.40	1000	10000	0.30	0.32	1.395(8)	1.396	1.412
0.50	1000	10000	0.20	0.34	1.508(0)	1.506	1.536
0.60	1000	10000	0.16	0.33	1.630(7)	1.634	1.669
0.70	1000	10000	0.12	0.35	1.759(9)	1.769	1.814
0.80	1000	10000	0.08	0.42	1.897(6)	1.892	1.970
0.90	2500	10000	0.045	0.55	2.045(3)	2.038	2.139

^aRef. 22.

^bRef. 21.

density and dimension is listed in Tables I, II and IV. Standard periodic boundary conditions⁽²⁶⁾ are employed in testing for overlaps and in maintaining a constant number of particles in the simulation hyperbox. The efficiency of the calculation was increased six-fold by partitioning⁽²⁷⁾ the simulation hyperbox into subcells.

As is well-known the Metropolis MC algorithm requires many passes in order to converge to an equilibrium state. Hence, some number of passes must be discarded; we refer to these discarded passes as the pre-equilibrium stage (PreEq in the tables). Typically, on the order of one to five thousand passes are needed in order to reach the equilibrated state. Then an additional one to ten thousand passes are generated (labelled PostEq) for analysis.

Even in the equilibrated regime there is still serial correlation between the passes. One way in which we addressed this issue was to sample $G(R)$ only at a “save” interval of 10 passes. This procedure allows some of the serial correlation

Table II. Seven Dimensional MC Results

ρ	PreEq	PostEq	Maximum Displacement	Acceptance Ratio	$G(1)$
0.10	1000	10000	1.50	0.61	1.066(2)
0.20	1000	10000	2.00	0.35	1.138(2)
0.30	1000	10000	0.50	0.30	1.208(0)
0.40	1000	10000	0.30	0.33	1.280(8)
0.50	1000	10000	0.18	0.40	1.353(4)
0.60	1000	10000	0.15	0.38	1.431(5)
0.70	1000	10000	0.11	0.41	1.510(7)
0.80	1000	10000	0.07	0.50	1.594(0)
0.90	4000	10000	0.04	0.63	1.680(7)

Table III. Seven Dimensional Theoretical Results for $G(1)$

ρ	PYV ^a	PYC ^a	CS ^a	LM ^a	BC ^a
0.10	1.066	1.068	1.068	1.067	1.068
0.20	1.133	1.139	1.138	1.137	1.139
0.30	1.199	1.212	1.210	1.210	1.214
0.40	1.267	1.289	1.286	1.286	1.291
0.50	1.335	1.370	1.364	1.367	1.372
0.60	1.404	1.454	1.446	1.453	1.457
0.70	1.475	1.543	1.531	1.544	1.545
0.80	1.547	1.635	1.620	1.641	1.637
0.90	1.620	1.732	1.713	1.743	1.733

^aRef. 33.

to dissipate from the previously sampled value of $G(R)$. In addition, at least 15 statistically independent sets of simulations were performed in parallel and averaged together. This results in very small error bars in $G(R)$, on the order of 10^{-3} to 10^{-4} .

The MC method was implemented using the SWC^(28–30) (small Web computing) Java framework. This framework is a Master-Worker MIMD (Multiple-Instruction, Multiple-Data) parallel programming model and can be used as Web-based collaborative software or as a multi-threaded process on a SMP (symmetric multi-processing) machine or even as a set of distributed, independent processes on separate machines.

Table IV. Eight Dimensional MC Results

ρ	PreEq	PostEq	Maximum Displacement	Acceptance Ratio	$G(1)$	LM ^a $G(1)$	BC ^b $G(1)$
0.10	400	1000	2.00	0.66	1.050(0)	1.049	1.048
0.20	400	1000	2.00	0.42	1.100(3)	1.099	1.097
0.30	400	1000	1.70	0.26	1.144(5)	1.151	1.148
0.40	400	1000	0.40	0.28	1.192(0)	1.206	1.199
0.50	500	1000	0.30	0.27	1.239(3)	1.264	1.252
0.60	500	1000	0.15	0.42	1.288(4)	1.325	1.306
0.70	1000	1000	0.105	0.48	1.338(7)	1.391	1.361
0.80	1000	1000	0.055	0.63	1.390(5)	1.461	1.417
0.90	4500	1000	0.027	0.77	1.440(9)	1.537	1.475

^aRef. 22.^bRef. 21.

An order parameter⁽³¹⁾, O ,

$$O = \frac{\sum_{j=1}^D \sum_{i=1}^N \cos[4\pi X_i(j)Q^{1/D}]}{DN} \tag{18}$$

was used to monitor when the system had reached equilibrium. Here, $X_i(j)$ is the j -th position component of the i -th hypersphere. The order parameter has a value of 1 for a completely ordered lattice and randomly oscillates about 0 when the system has equilibrated in the fluid state.

To calculate $G(R)$ a histogram of the number of pair separations as a function of separation distance, R , was accumulated on a grid with spacing ΔR . Normalization of $G(R)$ required the number density of pairs, $0.5\rho(N-1)$ and their occupied differential volume, $V_D((R + \Delta R)^D - R^D)$, where V_D is related to the surface area of a D dimensional hypersphere⁽³²⁾

$$V_D = \frac{\pi^{D/2}}{\Gamma(1 + D/2)}. \tag{19}$$

3. RESULTS

In all of this work, the hard hypersphere diameter, σ , is set equal to one and therefore, all quantities are reported in reduced units. Tables I, II and IV present the simulation results for six, seven and eight dimensions, respectively; in six dimensions $N = 4096$, in seven dimensions $N = 2187$ and in eight dimensions $N = 6561$. The pair correlation functions at contact, $G(1)$, are listed in the tables. To estimate an empirical error on the extrapolated $G(1)$ value, the first five $G(R)$ points for which R is greater than 1.0 are refit by a linear least-squares line varying each point by 1.96 standard deviations; i.e. the 95% confidence interval. These error estimates range between 1×10^{-4} and 5×10^{-4} . The data reported in Tables I, II and IV indicate the magnitude of the uncertainty of the last decimal place by the number in parentheses. In addition, Tables I, III and IV show theoretical results for $G(1)$.

To predict a value of Z_{LM} following the analysis of Luban and Michels⁽²²⁾ and Robles, de Haro and Santos⁽³³⁾, a linear fit to $\zeta(X)$ vs X was made for $0.5 \leq \rho$. Figure 1 shows that this linear approximation is reasonable at higher densities. This fit line was then substituted into Eq. 15. Thus, Z_{LM} requires two adjustable parameters (since one performs a straight line fit) in addition to knowledge of b_2^* , b_3^* and b_4^* .

Figure 2 displays the pair correlation function in six dimensions for a representative range of densities: $\rho = 0.3, 0.5$ and 0.7 . One notes that there is little structure present; there is no second peak even at the highest density. Note that the error bars at all values of R , and at all densities, are less than 10^{-3} .

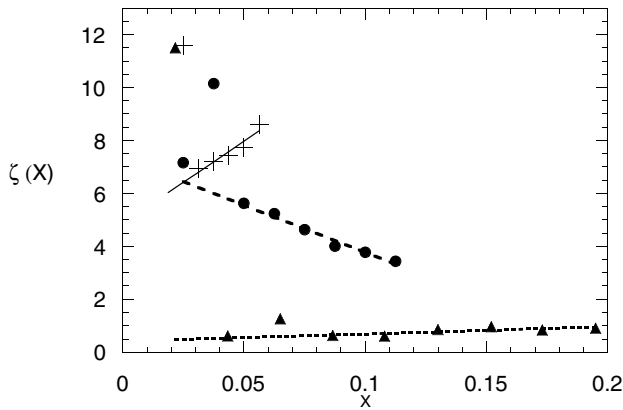


Fig. 1. The variation of $\zeta(X)$ with X at different densities and dimensions. The Luban-Michels linear fit for each dimension is presented: Filled triangles 6D MC data, (...) fit; filled circles 7D MC data, (---) fit; and + 8D MC data, (—) fit.

Figure 3 presents a variety of Z vs ρ data for six dimensional hyperspheres. The MC simulation data is in excellent agreement with the MD data of Lue and Bishop⁽³⁴⁾ and the theoretical [4,5] and [5,4] Padé approximants. The error bars on the MC results are smaller than the plotted symbols. In Table I the Z_{LM} approximation employed the six dimensional lattice close-packed density⁽¹⁸⁾ $8/\sqrt{3}$. The Z_{BC} approximation followed directly from Eq. 14. These Z values have been used in Eq. 5 to predict $G(1)$ and the results are listed in Table I. As was found

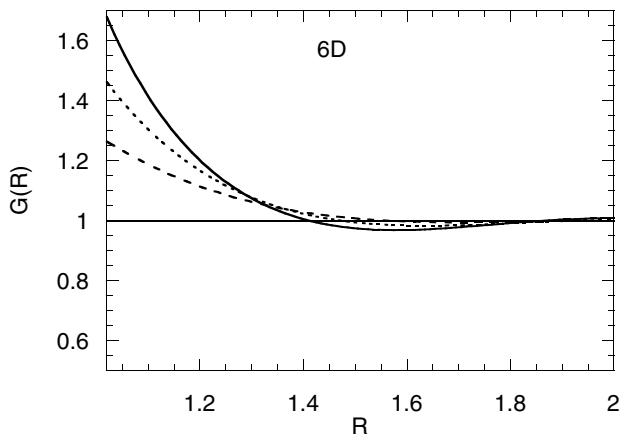


Fig. 2. The pair correlation function in six dimensions for $\rho = 0.30$ (---) $\rho = 0.50$ (...) and $\rho = 0.70$ (—).

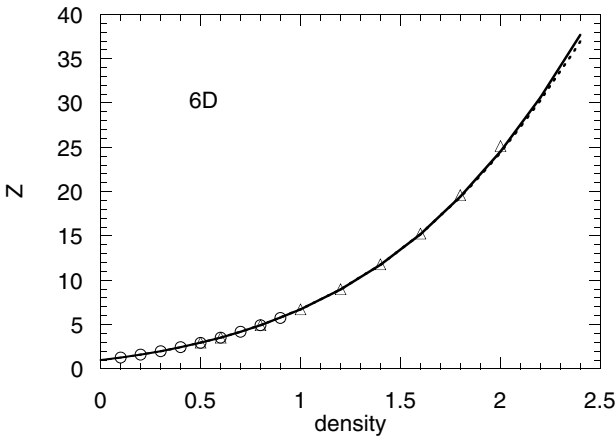


Fig. 3. Equation of State in Six Dimensions MC (○), MD⁽³⁴⁾ (△), Z_[4,5] Padé (—), Z_[5,4] Padé (⋯).

in the earlier work of Bishop, Masters and Vlasov⁽¹⁶⁾ in four and five dimensions, the Luban-Michels approximation agrees more closely with the MC data than the Baus-Colot approximation. This reflects the fact that the linear approximation is well justified over a wide range of densities in six dimensions.

Figure 4 presents the pair correlation function in seven dimensions for the same representative range of densities as in Fig. 2. In seven dimensions one observes even less structure than was the case in six dimensions. Robles, de Haro

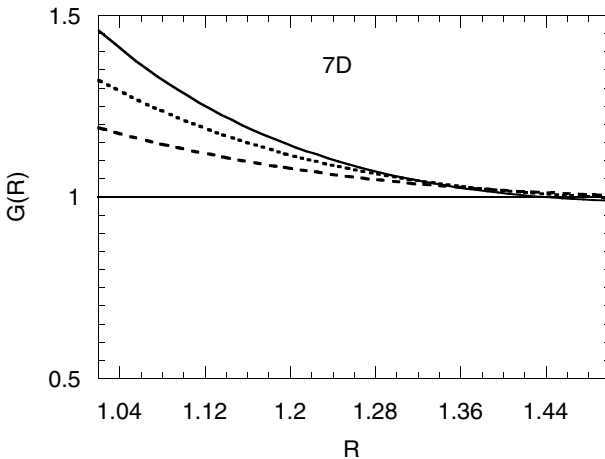


Fig. 4. The pair correlation function in seven dimensions for $\rho = 0.30$ (---) $\rho = 0.50$ (⋯) and $\rho = 0.70$ (—).

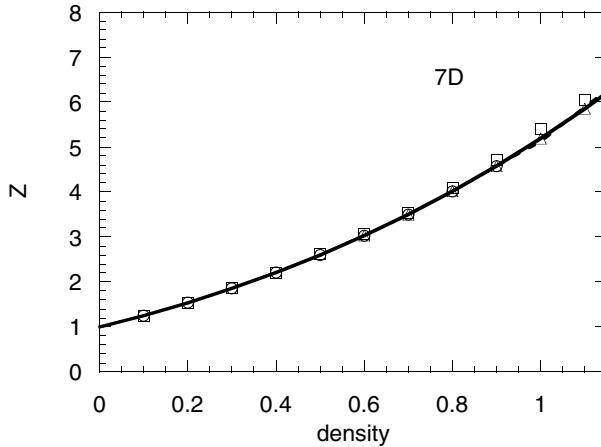


Fig. 5. Equation of State in Seven Dimensions MC (\circ), MD⁽³⁴⁾ (\triangle), MD⁽³³⁾ (\square), $Z_{[4,5]}$ Padé (—), $Z_{[5,4]}$ Padé (---).

and Santos⁽³³⁾ have made an extensive study of seven dimensional hard spheres and have obtained equation of state values from many different approximations, including their own exact solution to the Percus Yevick virial equation, PYV , and the Percus Yevick compressibility equation, PYC . They presented a new Carnahan-Starling⁽³⁵⁾ approximation, Z_{CS} , by weighting the Z_{PYV} and Z_{PYC} values

$$Z_{CS} = \alpha Z_{PYV} + (1 - \alpha) Z_{PYC} \quad (20)$$

with $\alpha = 5/6$. This empirical form was suggested by the observation that the two different PY calculations bracket the simulation data in three dimensions,⁽⁴⁾ five dimensions⁽³⁶⁾ and seven dimensions.⁽³³⁾ Also they performed MD simulations for $N = 64$ over a wide range of reduced densities (0.1 up to 1.95). We have used their reported Z values (their Table II) to determine the corresponding $G(1)$ predictions which are listed in Table III. The $G(1)$ resulting from the published Z_{PYC} and Z_{PYV} values bracket the MC numerical data and the new Z_{CS} approximation displays good agreement with the MC results. Comparing the other theoretical results, the Baus-Colot $G(1)$ agrees better with the MC results at higher densities. The linearization of $\zeta(X)$ is less justified in seven dimensions than was the case in six dimensions.

Figure 5 illustrates the excellent agreement of Z in seven dimensions among the present MC investigations, the MD studies by Robles, de Haro and Santos⁽³³⁾ and Lue and Bishop⁽³⁴⁾ and the Padé approximants for seven dimensional hyperspheres. Again, the error bars in the MC results are smaller than the plotted symbols. The fine agreement of the Padé approximants is the result of the availability

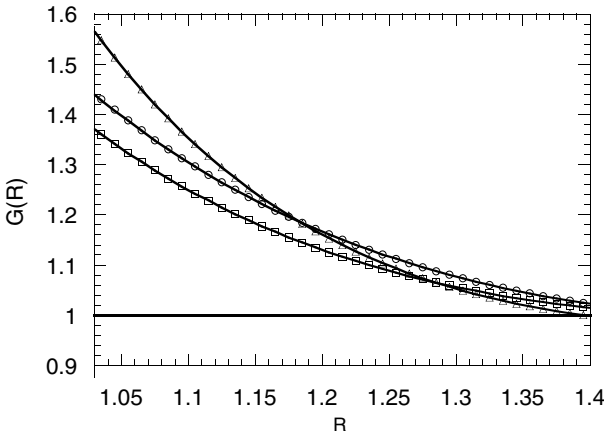


Fig. 6. The pair correlation function. The symbols are the MD data of Lue and Bishop⁽³⁷⁾ triangles $D = 7, \rho = 0.9$ and $N = 2187$; circles $D = 6, \rho = 0.5$ and $N = 4000$; squares $D = 7, \rho = 0.6$ and $N = 4000$. The lines are the current MC data.

of the higher order virial coefficients. Also note the good agreement, especially at low and moderate densities, of the Robles, de Haro and Santos⁽³³⁾ MD data which used only 64 particles. At the high dimensions studied here particles will not influence each other very much until the system approaches the freezing density and even a small number of particles will display behavior typical of a larger sample.

The pair correlation function $G(R)$ in six and seven dimensions has also been computed by Lue and Bishop⁽³⁷⁾ using MD and their results are compared to the Monte Carlo data in Fig. 6. The agreement with the MC results is excellent and this is consistent with the agreement of the equation of state computed by both simulation methods.

Figure 7 presents the pair correlation function in eight dimensions for the same representative range of densities as in Figs. 2 and 4. Again one observes very little structure.

Figure 8 illustrates the expected agreement of Z between the MC investigations and the Padé approximants for eight dimensional hyperspheres. In Table IV the Z_{LM} approximation employed the eight dimensional lattice close-packed density,⁽¹⁸⁾ 16. The Baus-Colot form is a more accurate approximation to the MC data than the Luban-Michels equations. More high density states and/or a non-linear functional form of $\zeta(X)$ may be needed to enhance the behavior of the Luban-Michels theory.

Figure 9 presents the predictions of the Song, Mason and Stratt⁽⁴⁾ (SMS) theory for $1/G(1)$ versus the packing fraction compared with our MC data. The

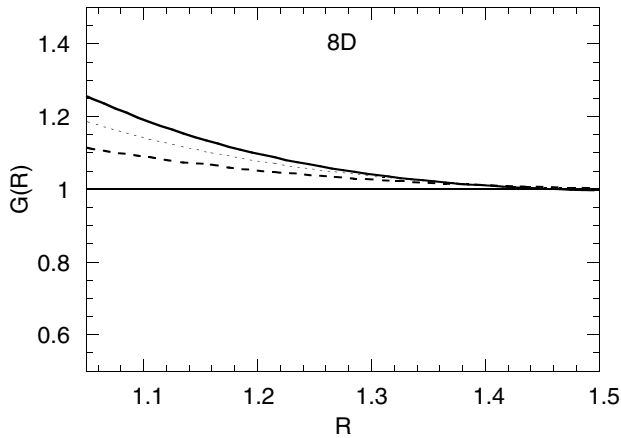


Fig. 7. The pair correlation function in eight dimensions for $\rho = 0.30$ (---) $\rho = 0.50$ (...) and $\rho = 0.70$ (—).

results clearly show, as was found previously in four and five dimensions, that the SMS prediction is excellent at low densities and quite close to the simulation data at higher densities for six through eight dimensions. Their method based upon mean field theory, the Carnahan-Starling equation of state, and independence in each dimension has remarkable predictive power for the fluid states. Moreover, their closed-form equations are very simple.

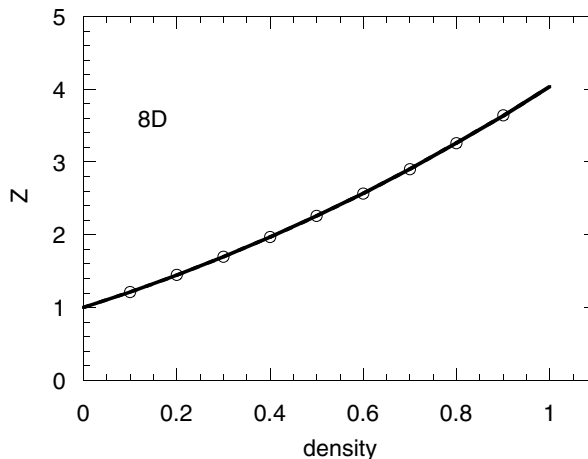


Fig. 8. Equation of State in Eight Dimensions MC (\circ), $Z_{[4,5]}$ Padé (—), $Z_{[5,4]}$ Padé (...).

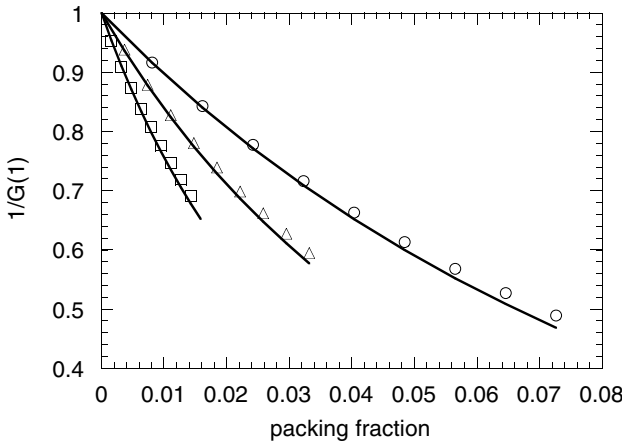


Fig. 9. Comparison of the MC data to the theory of SMS (Song, Mason and Strat⁽⁴⁾) MC $D = 6$: (\circ), MC $D = 7$: (Δ), MC $D = 8$: (\square) and theory (—).

4. CONCLUSION

Despite the simplicity of the hard hypersphere fluid system, an exact solution for its equation of state has not been derived for finite dimensions except for the case⁽³⁸⁾ of $D = 1$. However, $D = \infty$ has been extensively analyzed⁽¹⁻³⁾ and it has been shown that the higher order virial coefficients vanish identically. Thus, the equation of state becomes:

$$Z = 1 + B_2\rho \tag{21}$$

But by Eq. 5 this means that $G(1) = 1$.

Equation 21 implies that fluctuations become less important as the dimension increases and this is readily apparent from a perusal of Figs. 2, 4 and 7. Also, the value of $G(1)$ is expected to decrease as $D \rightarrow \infty$. Our Monte Carlo results are consistent with this expectation. For example, at a constant number density of $\rho = 0.70$, in 6D, $G(1) = 1.759(9)$; in 7D, $G(1) = 1.510(7)$; and in 8D, $G(1) = 1.338(7)$. Similar results are observed at all number densities computed, in agreement with this theoretical prediction.

Our Monte Carlo results in six, seven and eight dimensions have been extensively compared with results from molecular dynamics and many different theoretical predictions for $G(1)$. Excellent agreement is observed with the MD results of Lue and Bishop.^(34,37) In dimensions six and seven the Luban-Michels approximation agrees more closely with the MC results than the Baus-Colot prediction except for the two highest densities in seven dimensions. The Baus-Colot approximation is better throughout the density range explored except at the two lowest densities in eight dimensions. In seven dimensions, the new

Robles et al.⁽³³⁾ Carnahan-Starling approximation agrees best with the Monte Carlo values.

Our Monte Carlo results were also compared to the theory of Song, Mason and Street⁽⁴⁾ which is based on the Carnahan-Starling mean field theory. Since the mean field theory of critical phenomena becomes exact above the critical dimension, $D = 4$, for fluids, it is not surprising that the Monte Carlo results agree with the SMS predictions at lower densities for six, seven and eight dimensions.

A variety of intriguing questions arise as the number density is increased towards the transition density. It is well-known that systems even with only pure repulsive interactions undergo a phase transition from the fluid to solid state in dimensions two through five^(39–43) and this is hypothesized at higher dimensions as well.^(44–46) The transition density increases⁽²²⁾ from a value of $\rho \approx 0.88$ in two dimensions, to ≈ 0.95 in three dimensions, to ≈ 1.0 in four dimensions and then to ≈ 1.19 in five dimensions. These transitions were observed by following the variation of the compressibility with density. Alternatively, the onset of the transition is mirrored in the behavior of pair correlation function, e.g. a split second neighbor peak is a signature of the phase transition. The trend of increasing number densities for the freezing transition continues in six, seven and eight dimensions. This is reflected in the lack of structure observed in the higher density pair correlation functions reported here. One of our goals is to extend the MC simulations to higher densities in order to probe the nature of this phase transition.

NOTE ADDED IN PROOF

A paper by Skoge et al.⁽⁴⁷⁾ on packing hyperspheres in high-dimensional Euclidean spaces has recently appeared. In that work they study jammed hard-sphere packings in four, five and six dimensional systems via a molecular dynamics method. They find, in agreement with our MC simulations, that the pair correlation function indicates that short-ranged ordering appreciably decreases with increasing dimension.

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REFERENCES

1. H. L. Frisch, N. Rivier, and D. Wyler, Classical Hard-Sphere Fluid in Infinitely Many Dimensions. *Phys. Rev. Lett.* **54**:2061–2063 (1985).

2. H. L. Frisch and J. K. Percus, Nonuniform classical fluid at high dimensionality. *Phys. Rev. A* **35**:4696–4702 (1987).
3. H. L. Frisch and J. K. Percus, High dimensionality as an organizing device for classical fluids. *Phys. Rev. E* **60**:2942–2948 (1999).
4. Y. Song, E. A. Mason, and R. M. Stratt, Why does the Carnahan-Starling equation work so well? *J. Phys. Chem.* **93**:6916–6919 (1989).
5. M. Bishop, P. A. Whitlock, and D. Klein, The structure of hyperspherical fluids in various dimensions. *J. Chem. Phys.* **122**:074508-1-7 (2005).
6. M. Bishop and P. A. Whitlock, The equation of state of hard hyperspheres in four and five dimensions. *J. Chem. Phys.* **123**:014507-1-3 (2005).
7. M. Luban and A. Baram, Third and fourth virial coefficients of hard hyperspheres of arbitrary dimensionality. *J. Chem. Phys.* **76**:3233–3241 (1982).
8. P. R. Bevington, *Data Reduction and Error Analysis for the Physical Sciences* (McGraw-Hill, New York, 1969).
9. D. A. McQuarrie, *Statistical Mechanics* (Harper and Row, New York, 1976).
10. N. Clisby and B. M. McCoy, Analytical Calculation of B_4 for Hard Spheres in Even Dimensions. *J. Stat. Phys.* **114**:1343–1361 (2004).
11. I. Lyberg, The fourth virial coefficient of a fluid of hard spheres in odd dimensions. *J. Stat. Phys.* **119**:747–764 (2005).
12. N. Clisby and B. M. McCoy, Negative virial coefficients and the dominance of loose packed diagrams for D-dimensional hard spheres. *J. Stat. Phys.* **114**:1361–1392 (2004).
13. M. Bishop, A. Masters, and J. H. R. Clarke, Equation of state of hard and Weeks-Chandler-Anderson hyperspheres in four and five dimensions. *J. Chem. Phys.* **110**:11449–11453 (1999).
14. N. Clisby and B. M. McCoy, New results for virial coefficients of hard spheres in D-dimensions. *Pramana-J. Phys.* **64**:775–783 (2005).
15. N. Clisby, Negative virial coefficients for hard spheres. Ph.D. Thesis, Department of Physics, SUNY at Stony Brook (2004).
16. M. Bishop, A. Masters, and A. Yu. Vlasov, Higher virial coefficients of four and five dimensional hard hyperspheres. *J. Chem. Phys.* **121**:6884–6886 (2004).
17. M. Bishop, A. Masters, and A. Yu. Vlasov, The eighth virial coefficient of four- and five-dimensional hard hyperspheres. *J. Chem. Phys.* **122**:154502-1-2 (2005).
18. N. Clisby and B. M. McCoy, Ninth and tenth order virial coefficients for hard spheres in D-dimensions. *J. Stat. Phys.* **122**:15–57 (2006).
19. G. A. Baker and P. Graves-Morris, *Padé Approximants* (Cambridge University Press, Cambridge, 1996).
20. W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical Recipes* (Cambridge University Press, Cambridge, 1992).
21. M. Baus and J. L. Colot, Thermodynamics and structure of a fluid of hard rods, disks, spheres or hyperspheres from rescaled virial expansions. *Phys. Rev. A* **36**:3912–3925 (1987).
22. M. Luban and J. P. J. Michels, Equation of state of hard D-dimensional hyperspheres. *Phys. Rev. A* **41**:6796–6804 (1990).
23. N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, Equation of state calculations by fast computing machines. *J. Chem. Phys.* **21**:1087–1092 (1953).
24. B. L. Holian, O. E. Percus, T. T. Warnock, and P. A. Whitlock, Pseudorandom number generator for massively parallel molecular dynamics simulations. *Phys. Rev. E* **50**:1607–1615 (1994).
25. T. Gurov and P. A. Whitlock, Investigation of the sensitivity of the Monte Carlo solution for the Barker-Ferry equation using different sequential and parallel pseudorandom number generators. In *Lecture Notes in Computer Science*, Number 3039, M. Bubak, G.D. van Albada, and P.M.A. Sloot (eds.) (Springer Verlag, Heidelberg, 2004).

26. M. P. Allen and D. J. Tildesley, *Computer Simulation of Liquids* (Clarendon Press, Oxford, 1993).
27. B. Quentrec and C. Brot, New method for searching for neighbors in molecular dynamics computations. *J. Comp. Phys.* **13**:430–432 (1973).
28. K. Ying, D. Arnow, and D. Clark, Evaluating Communication Protocols for WebComputing. In Proceedings of the 1999 International Conference on Parallel and Distributed Processing Techniques and Applications, CSREA Press, Las Vegas, June, 1999.
29. D. Arnow, G. Weiss, K. Ying, and D. Clark, SWC: A Small Framework for WebComputing. In Proceedings of the International Conference on Parallel Computing, Delft, Netherlands, August, 1999.
30. P. A. Whitlock, M. Bishop, and D. Klein, Small Web Computing Applied to Distributed Monte Carlo Calculations. In *Lecture Notes in Computer Science*, Number 3993, V.N. Alexandrov, G.D. van Albada, P.M.A. Sloot, and J. Dongarra (eds.) (Springer Verlag, Heidelberg, 2006).
31. J. M. Haile, *Molecular Dynamics Simulation* (John-Wiley and Sons, New York, 1992).
32. R. Kubo, *Statistical Mechanics* (North-Holland, Amsterdam, 1965).
33. M. Robles, M. L. de Haro, and A. Santos, Equation of state of a seven-dimensional hard-sphere fluid. Percus-Yevick theory and molecular-dynamics simulations. *J. Chem. Phys.* **120**:9113–9122 (2004).
34. L. Lue and M. Bishop, Molecular Dynamics Study of the Thermodynamics and Transport Coefficients of Hard Hyperspheres in Six and Seven Dimensions. *Phys. Rev. E* **74**:021201-1-6 (2006).
35. N. F. Carnahan and K. E. Starling, Equation of state of nonattracting rigid spheres. *J. Chem. Phys.* **51**:635–636 (1969).
36. A. Santos, An equation of state à la Carnahan-Starling for a five-dimensional fluid of hard hyperspheres. *J. Chem. Phys.* **112**:10680–10681 (2000).
37. L. Lue and M. Bishop, Private Communication.
38. L. Tonks, The Complete Equation of State of One, Two and Three-Dimensional Gases of Hard Elastic Spheres. *Phys. Rev.* **50**:955–963 (1936).
39. B. J. Alder and T. E. Wainwright, Phase Transition in Elastic Disks. *Phys. Rev.* **127**:359–361 (1962).
40. W. W. Wood, *Physics of Simple Liquids*. H.N.V. Temperley, J.S. Rowlinson, and G.S. Rushbrooke (eds.) (North-Holland, Amsterdam, 1968).
41. B. J. Alder and T. E. Wainwright, Phase transition for a hard sphere system. *J. Chem. Phys.* **27**:1208–1211 (1957).
42. W. W. Wood and J. D. Jacobson, Preliminary Results from a Recalculation of the Monte Carlo Equation of State of Hard Spheres. *J. Chem. Phys.* **27**:1207 (1957).
43. J. P. J. Michels and N. J. Trappeniers, Dynamical Computer Simulations on Hard Hyperspheres in Four- and Five-Dimensional Space. *Phys. Lett.* **104**:425–429 (1984).
44. J. L. Colot and M. Baus, The Freezing of Hard Disks and Hyperspheres. *Phys. Lett. A* **119**:135–139 (1986).
45. B. Bagchi and S. A. Rice, On the stability of the infinite dimensional fluid of hard hyperspheres: a statistical mechanical estimate of the density of closest packing of simple hypercubic lattices in spaces of large dimensionality. *J. Chem. Phys.* **88**:1177–1184 (1988).
46. R. Finken, M. Schmidt, and H. Lowen, Freezing transition of hard hyperspheres. *Phys. Rev. E* **65**:016108-1-9 (2001).
47. M. Skoge, A. Donev, F. H. Stillinger, and S. Torquato, Packing Hyperspheres in high-dimensional Euclidean spaces. *Phys. Rev. E* **74**: 041127-1-11 (2006).