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Hard-sphere fluid in infinite dimensions

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We derive the exact Mayer series for the pressure, density, and the equation of state of a hard-sphere fluid in the limit of infinite space dimensions D. The Mayer series can be analytically continued into the full (cut) activity plane and there is no sign of a phase transition. We also treat the quantum-mechanical system. For $D=\infty$ the fluid behaves like an ideal Bose gas and undergoes a Bose-Einstein condensation.

I. INTRODUCTION

There is considerable interest in the system of hard spheres in statistical mechanics, to model the behavior of real fluids at sufficiently high temperatures where attractive forces can be neglected. In particular, this applies to dense fluids.[1]

Classically, the exact (Tonks) equation of state[2] of the one-dimensional hard-sphere fluid is known and the system does not exhibit a phase transition. For two and three dimensions, several of the initial virial coefficients (which are positive) are known, there are also estimates of the radius of convergence of the virial series.[1] Computer simulations[1,3,4] in two and three dimensions indicate a first-order transition which, at least in three dimensions, is from a fluid to a solid phase. There are approximate theories of the equation of state in two and three dimensions which yield results which are in very good numerical agreement with the fluid branch [Percus-Yevick (PY),[5] scaled-particle,[6] Carnahan and Starling (CS),[7] etc.] and the solid branch ("free volume,"[8] etc.) of the computer simulations. There is no analytic theory of a phase transition for dimensions larger then 1.

The physics of this problem is such that one expects considerable simplifications in finding an equation of state in the thermodynamic limit, in the subsequent limit where the dimensionality D becomes infinitely large. This is a general feature of interacting systems on lattices in the thermodynamic limit.

In this paper we consider this infinite dimensional limit of the hard-sphere fluid. In Sec. II we give a diagrammatic analysis of the Mayer and Mayer type[9] of the grand canonical partition function for this system for infinite dimensionality. We obtain infinite series in the fugacity for the pressure p divided by kT, and for the density ρ of the fluid, which are exact for infinite D (with corrections that are exponentially small in D). We also find their analytic continuation and the exact equation of state. In Sec. III we compare our results with the approximate scaled-particle theory equation of state of classical hard spheres in D dimensions. Briefly, we also discuss some previous conjectures concerning the form of the equation of state in D dimensions. Section IV contains a treatment of the quantum-mechanical system. We extend the Yang-Lee-Huang-Bogolyubov theory[10,11] of the degenerate, "almost ideal" Bose gas to D dimensions, and compare with the classical hard-sphere fluid. Section V summarizes and discusses the results. A short account of our work has been published previously.[12]

II. THE EQUATION OF STATE FOR THE $D=\infty$, CLASSICAL HARD-SPHERE FLUID

Our starting point is the expansion of the grand partition function Ξ for a classical fluid in powers of the activity $z=\Lambda^{-D}\exp(\beta\mu)$, where μ is the chemical potential, or Gibbs free energy per particle, $\beta=(kT)^{-1}$, and $\Lambda=[h^2/(2\pi mkT)]^{1/2}$,

$$\Xi=\sum_{n=0}^{\infty}(z^n/n!)\int d^Dx_1\cdots\int d^Dx_n\exp\left[-\beta\sum_{i=1}^{n}\sum_{\substack{j=1\\(j>i)}}^{n}\phi(|\mathbf{x}_i-\mathbf{x}_j|)\right]. \tag{2.1}$$

ϕ is the interaction energy of two particles, which reads for a hard-sphere fluid

$$\phi(\mathbf{x})=\begin{cases}\infty, & |\mathbf{x}|<a\\ 0, & |\mathbf{x}|>a\end{cases} \tag{2.2}$$

where a is the diameter of the hard sphere. From Ξ, one obtains the thermodynamic potential

$$\Omega(T,V,\mu)=-kT\ln\Xi=-pV\ . \tag{2.3}$$

Expansion (1) can be rewritten in terms of linear, local graphs, following Mayer and Mayer,[9] by introducing the function

$$f_{ij}=\exp[-\beta\phi(|\mathbf{r}_i-\mathbf{r}_j|)]-1=-\Theta(a-|\mathbf{r}_i-\mathbf{r}_j|)\ , \quad (2.4)$$

where Θ is the Heaviside (unit step) function. The exponent in (2.1) corresponds to a product of factors $(f_{ij}+1)$, and one can represent it by a graph, that is to every pair of particles or points $\mathbf{r}_i,\mathbf{r}_j$ one associates a line or nothing, depending on whether f_{ij} or 1 enters the product. As usual, graphs with cycles $f_{i_1i_2}f_{i_2i_3}\cdots f_{i_ki_1}$ are called loop graphs (with loops of length k) and graphs without cycle tree graphs. The contribution of the nth order in z to the grand partition function Ξ is then $(z^n/n!)$ times the sum of all linear graphs of n labeled points (the zeroth contribution is 1).

The linked-cluster theorem reduces Ξ to a sum of connected graphs Ξ_c,

$$\Xi=\exp(\Xi_c-1)\ , \quad (2.5)$$

where Ξ_c now contains only graphs with all points connected by at least one line. Thus, $\Xi_c(z)$ is a series in powers of the activity z,

$$\Xi_c(z)=\sum_{n=0}^{\infty} b_n z^n\ , \quad (2.6)$$

whose coefficients b_n are the sum of all possible connected graphs of n labeled points multiplied by their respective weights (integrals over the f'_{ij}'s), and $b_0=1$.

From the thermodynamic potential (2.3) one obtains

$$pV/kT=\Xi_c-1=V\sum_{n=1}^{\infty} b_n z^n\ , \quad (2.7)$$

and, for the average number of particles $\langle N\rangle$ in the grand-canonical ensemble,

$$\langle N\rangle=-\partial\Omega/\partial\mu=z\,\partial\Xi_c/\partial z=V\sum_{n=1}^{\infty} n b_n z^n\ . \quad (2.8)$$

The equation of state $p/(\rho kT)=f(\rho)$, is obtained by eliminating z between (7) and (8).

The evaluation of the weights b_n simplifies considerably as the space dimension D tends to infinity. We shall show that for large D, they are dominated by tree diagrams, in that, at a given order n, any loop reduces exponentially the weight of the diagram by a factor $(\sqrt{3}/2)^D/\sqrt{D}$. An nth-order tree diagram has a weight given by evaluating each integral over $\mathbf{x}_i,\ldots$ in turn. Each integral is restricted by the range a of f_{ij}, except the last, x_1 which extends over the whole volume V. Thus the weight of one given nth-order tree diagram is $V(v)^{n-1}$, where

$$v=\frac{\pi^{D/2}}{\Gamma(1+D/2)}a^D=V_D(a) \quad (2.9)$$

is the volume of a $(D-1)$-sphere (a disk in D-dimensional space) of radius a in D dimensions.

Let us now evaluate a diagram containing one closed loop. The simplest one is of order 3, where all points are connected to each other (a triangle). We must calculate

$$C=\int d^Dr_2\int d^Dr_3 f_{12}f_{23}f_{13}\ , \quad (2.10)$$

where $\mathbf{r}_i=\mathbf{x}_i-\mathbf{x}_1$, and the last coordinate $\mathbf{x}_1$ is not integrated over (it is unrestricted and yields a factor V). C will be compared with the tree diagram of same order 3, consisting of three points connected by only two lines,

$$C_0=\int d^Dr_2\int d^Dr_3 f_{12}f_{13}=v^2\ . \quad (2.11)$$

C is evaluated in two steps, setting $\mathbf{s}=\mathbf{r}_2$

$$C=\int d^Ds\, f_s\mathcal{O}(s)\ , \quad (2.12)$$

$$\mathcal{O}(s)=\int d^Dr_3 f_{23}f_{13}\ . \quad (2.13)$$

$\mathcal{O}(s)$ is the overlap or intersection of volumes of two spheres, each of radius a, whose centers ($\mathbf{x}_1$ and $\mathbf{x}_2$) are a distance s apart. Obviously, $\mathcal{O}$ vanishes if $s\geq 2a$. Also, with z as the axis through the centers $\mathbf{x}_1$ and $\mathbf{x}_2$ of the two spheres, and θ, the colatitude angle from that axis, $\frac{1}{2}\mathcal{O}$ equals the volume of a spherical cap whose base is a $(D-2)$-sphere of radius $a\sin\theta$, and whose height is given by $z=a\cos\theta$, i.e.,

$$\tfrac{1}{2}\mathcal{O}=V_{D-1}(a)a\int_0^{\theta_m}d\theta\sin^D\theta\ , \quad (2.14)$$

with $\cos\theta_m=\frac{1}{2}s/a$. Similarly, since the solid angle of a $(D-1)$-sphere is $S_D(1)=DV_D(1)$,

$$C=-2aV_{D-1}(a)DV_D(1)\int_0^a ds\, s^{D-1}\int_0^{\theta_m}d\theta\sin^D\theta\ , \quad (2.15)$$

which can be evaluated after a change of variable, $\frac{1}{2}s/a=\cos\alpha$, and permutation of the orders of integration,

$$C=-(2a)^{D+1}V_D(1)V_{D-1}(a)\times\left[\int_{\pi/3}^{\pi/2}d\alpha\sin^D\alpha\cos^D\alpha+2^{-D}\int_0^{\pi/3}d\alpha\sin^D\alpha\right]\ . \quad (2.16)$$

Finally, using the trigonometric identity $\sin 2\alpha=2\sin\alpha\cos\alpha$, and the obvious symmetry of the integrand, we obtain

$$C=-3V_D(a)V_{D-1}(a)a\int_0^{\pi/3}d\theta\sin^D\theta\ . \quad (2.17)$$

The integral is obviously bounded by $\frac{1}{3}\pi(\sqrt{3}/2)^D$. It can be evaluated exactly when $D\to\infty$. The result is (Appendix A)

$$C=-3V_D(a)V_{D-1}(a)a\left[\frac{1}{2(D+1)}\left[\frac{\sqrt{3}}{2}\right]^{D+1}+\mathcal{O}\left[\frac{1}{D}\left[\frac{\sqrt{3}}{2}\right]^{D+2}\right]\right]\ . \quad (2.18)$$

C_0 can also be evaluated from $\mathcal{O}(s)$,

$$C_0=\int d^Ds\,\mathcal{O}(s)=2V_D(a)V_{D-1}(a)a\int_0^{\pi/2}d\theta\sin^D\theta=v^2\ . \quad (2.19a)$$

Thus

$$|C/C_0| = \frac{3}{2\sqrt{\pi}}[\Gamma(1+\tfrac{1}{2}D)/\Gamma(1+\tfrac{1}{2}(D-1))] \times \frac{1}{D+1}\left[\frac{\sqrt{3}}{2}\right]^{D+1} + O\left[\frac{1}{D}\left[\frac{\sqrt{3}}{2}\right]^{D+2}\right]$$
$$\simeq \frac{3}{2}\left[\frac{e}{2\pi}\right]^{1/2}\frac{1}{\sqrt{D}}\left[\frac{\sqrt{3}}{2}\right]^{D+1}, \tag{2.19b}$$

using Stirling's formula. Thus, the one-loop triangle graph is bounded by α^D, $\alpha<1$. If the closed loop contains more than three vertices, say m, it will be bounded at least by $D^k\alpha^D$, $\alpha<1$, $k\sim 1$ (this holds, because the integration over alternating variables in the analog of Eq. (2.10) involves $\lceil\frac{1}{2}m\rceil$ overlaps, $\lceil\frac{1}{2}m\rceil$ being the nearest integer $\leq m/2$, each of which is bounded by $\theta_m \sin^D\theta_m$ [see Eq. (2.14)]). The contribution of the square loop ($m=4$) is calculated explicitly in Appendix B.

Thus, as long as the Mayer series [(2.6)–(2.8)] has bounded coefficients and a finite radius of convergence—which it has, according to Groeneveld's theorem (Ref. 13, p. 95)— and the proportion of loops to tree diagrams of order n does not increase too fast as $n\to\infty$—as will be shown below—it is dominated, as D tends to infinity by tree graphs, order by order, and

$$\Xi_c - 1 = V\sum_{n=1}^{\infty}[c_n z^n(-v)^{n-1}/n!][1+O((\alpha<1)^D)], \tag{2.20}$$

where c_n is the number of labeled tree graphs of order n, given by Cayley[14,15] as

$$c_n = n^{n-2}. \tag{2.21}$$

Now, the activity expansion of the thermodynamic quantities (7) and (8) is

$$\frac{pv}{kT} = -\sum_{n=1}^{\infty}\frac{n^{n-2}}{n!}(-zv)^n, \tag{2.22}$$

$$\rho v = -\sum_{n=1}^{\infty}\frac{n^{n-1}}{n!}(-zv)^n. \tag{2.23}$$

Both series have the same radius of convergence R,

$$\frac{1}{R} = \lim_{n\to\infty}\left[1+\frac{1}{n}\right]^{n-2} = e. \tag{2.24}$$

For $zv<R$, the series (2.22) and (2.23) are absolutely convergent since the majorant series

$$\sum\frac{n^{n-2}}{n!}e^{-n} \simeq \frac{1}{\sqrt{2\pi}}\zeta\left[\frac{5}{2}\right] \simeq 0.535, \tag{2.25}$$

$$\sum\frac{n^{n-1}}{n!}e^{-n} \simeq \frac{1}{\sqrt{2\pi}}\zeta\left[\frac{3}{2}\right] \simeq 1.042 \tag{2.26}$$

are convergent. Here $\zeta(s)=\sum_{n=1}^{\infty}n^{-s}$ is the Riemann ζ function and Stirling's approximation, $n! = \sqrt{2\pi}n^{n+1/2}e^{-n}$ has been used. Groeneveld's theorem (Ref. 13, p. 95) for hard-sphere systems gives bounds for the Mayer coefficient

$$\frac{1}{n} \leq |b_n| \leq \frac{n^{n-2}}{n!}, \tag{2.27}$$

and the radius of convergence of the Mayer series. Our classical system of hard spheres at $D=\infty$ realizes the upper bound on b_n (the Ford model[16] realizes the lower bound) and the lower bound on the radius of convergence (2.24).

R serves also as a lower bound for the radius of convergence $R(V)$ of the finite-volume Mayer expansion, $R(V)\geq R = \lim_{V\to\infty}R(V)$.[17]

The Mayer series (2.22) and (2.23) have a singularity at the unphysical value $zv=-1/e$. An analytic continuation of the series can be performed as follows, although this may not contain the full physical information. The approximate series (use again Stirling's approximation)

$$\rho v = -\frac{1}{\sqrt{2\pi}}\sum\frac{(-zve)^n}{n^{3/2}},$$
$$\frac{pv}{kT} = -\frac{1}{\sqrt{2\pi}}\sum\frac{(-zve)^n}{n^{5/2}}, \tag{2.28}$$

which have the same radius of convergence as the original series, can be analytically continued in the complex z plane, cut along $-\infty\leq z\leq -1/(ev)$, by using Appell's integral[18]

$$-\sum_{n=1}^{\infty}\frac{(-zev)^n}{n^s} = \frac{zev}{\Gamma(s)}\int_0^{\infty}dt\frac{t^{s-1}}{e^t+zev}, \tag{2.29}$$

which is an analytic function of z everywhere in the cut complex z plane if $\mathrm{Re}z>0$.

There is therefore no sign of a phase transition in the Mayer series. We shall see in Sec. IV that at high densities corresponding to zv outside the radius of convergence of the Mayer series, the physical $D=\infty$ hard-sphere fluid is quantum mechanical except at infinite temperatures.

To obtain the equation of state, p/kT as a function of ρ, one needs to invert series (2.22) and (2.23). This can be done in either of two ways. First (Ref. 19, pp. 149–51) one writes

$$\frac{p}{\rho kT} = 1 + \sum_{m=1}^{\infty}B_m\rho^{m-1}, \tag{2.30}$$

where the virial coefficients B_m have a diagrammatic representation (Ref. 9, Chap. 13)

$$B_m = -\frac{m-1}{m}\beta_{m-1},$$
$$\beta_m = \lim_{V\to\infty}V^{-1}\frac{1}{(m-1)!}\times\int d^Dr_1\int d^Dr_2\cdots\int d^Dr_m\sum\left[\prod f_{ij}\right], \tag{2.31}$$

and the sum runs over connected graph's of order m, $m>2$ such that there are at least two paths of lines connecting two points (graphs which cannot be disconnected by cutting one single line, sometimes called "blocks"). Among all tree graphs, only those of second order remain if $D\to\infty$. We have

$$\beta_1 = -v,$$

and consequently,

$$B_2=\tfrac{1}{2}v[1+O((\alpha^D))] ,$$

$$B_{m>2}=O((\alpha^D)) .$$

Recently, Frisch and Percus[20] have generalized this result to arbitrary finite-range repulsive interactions and nonuniform densities.

The equation of state is simply

$$\frac{p}{\rho kT}=1+\tfrac{1}{2}v\rho . \tag{2.32}$$

This equation is exact for $D=\infty$, and the corrections are exponentially small in D. p/kT is an analytic function of ρ.

Alternatively, one can use Langrange's method of series reversion:[21] The Mayer series (2.23) is the unique root of the implicit equation (in ρv)

$$\rho v e^{\rho v}=zv \tag{2.33}$$

inside a contour in the ρv plane around the origin such that $|zv||e^{-\rho v}|<|\rho v|$ for ρv on the contour. Equation (2.33) yields $d(\rho v)/d(zv)=e^{-\rho v}(1+\rho v)^{-1}$, whereas (2.22) and (2.23) imply that $zv[d(pv/kT)/d(zv)]=\rho v$; thus $d(pv/kT)/d(\rho v)=\rho v/\{zv[d(\rho v)/d(zv)]\}$. Combining these two expressions with (2.33), we obtain $d(pv/kT)/d(\rho v)=1+\rho v$ and thus (2.32).

At this point we must discuss the influence of other diagrams, besides trees, on the Mayer coefficients b_n. Enumeration of all diagrams ("labeled star trees") contributing to b_n is discussed in Ref. 22.

Consider first one-loop diagrams of order n, containing one closed loop of length k. Their number is given by[14]

$$\frac{1}{2}\frac{n!}{(n-k)!}n^{n-k-1} . \tag{2.34}$$

Comparing now with the number of tree diagrams of the same order, n^{n-2}, we obtain, summing over k from 3 to n,

$$\sum_k \frac{1}{2}\frac{n!}{(n-k)!}n^{1-k}=\frac{n!n}{2n^n}\sum_k \frac{1}{(n-k)!}n^{n-k} \tag{2.35}$$

more one-loop diagrams than tree diagrams. The sum is bounded by e^n and $n!$ is approximated by Stirling's formula. As a result there are less than $n^{3/2}$ times more one-loop graphs than tree graphs of order n. The corresponding Mayer series clearly converges within R (2.24) and we can, as $D\to\infty$, omit this contribution. The point is that the number of such graphs grows only as a power of n.

For c loops ($c=e-n+1$, e = number of lines, n = order of diagrams), the weight of a diagram is suppressed by a factor $(\alpha^D)^n$ rather than by $(\alpha^D)^c$ because loops with a common line do not have independent restrictions on overlaps (see Appendix B).

At every order, the total number of labeled star trees is finite [the overwhelming majority of all $2^{\binom{n}{2}}$ graphs, connected or not, are stars for large n and c (Ref. 22). If one restricts the diagrams to consist of stars containing no more than a given number of loops $c=e-n+1$, their number is[22]

$$\frac{b}{2\sqrt{\pi}}x_0^{-n+1/2}n^{-5/2}n! , \tag{2.36}$$

where b and $x_0<1$ are finite. Since

$$\frac{b}{2\sqrt{\pi}}x_0^{-n+1/2}n^{-5/2}n!/n^{n-2}\simeq\frac{b}{\sqrt{2}}(x_0e)^{-n} \tag{2.37}$$

(Stirling's formula), we see that their contribution, compared to those of tree graphs is $\simeq(\alpha^D/x_0e)^n$; for D large enough this can be again neglected. In the case of polygonal stars (mixed Husimi trees), $b=0.87$, $x_0=0.24$. Therefore, as long as $\alpha^D<0.66$, the corresponding graphs can be neglected. Note that the above restriction to (an infinite collection of) stars with a finite number of loops is, according to Ref. 22, not necessary for Eq. (2.36) to be valid. The weaker, necessary condition is not known.

In the absence of any restriction on the types of constituting stars, the number of connected graphs of order n is, asymptotically, $2^{\binom{n}{2}}\simeq\sqrt{2^{n^2}}$. From the above discussion, we have a suppression factor of at least α^{Dn}, $\alpha<1$. Thus, at the very least, at every order n there is a D_n above which the Mayer coefficient is dominated by tree graphs. Since the Mayer series is uniformly convergent within its (finite) radius of convergence, the operations $D\to\infty$ and $\sum_n$ can be interchanged.

Note that Eq. (2.32) has a nontrivial virial coefficient and that the hard-sphere system is still interacting as $D\to\infty$. Nevertheless, there are no premonitory signs of a phase transition in the classical fluid phase described by the equation of state (2.32) (which is analytic and does not exhibit any pressure divergence or maximum) or by the Mayer series (2.22) and (2.23) and its analytic continuation, Eq. (2.29).

Consider, however, the characteristic densities of a hard-sphere fluid in $D=\infty$ dimensions. v is the natural scale of volume for the Mayer cluster expansions (2.1),[13] so that ρv is the relevant dimensionless density. $\rho v\approx 1$ corresponds, as we have seen, to the radius of convergence of the Mayer series.

A hypercubic lattice of touching hard spheres has an utterly negligible density

$$\rho v_{\text{HC}}=\frac{1}{\sqrt{\pi}}\left[\frac{\pi e}{2D}\right]^{D/2} .$$

On the other hand, close (dense) packings of spheres in $D=\infty$ dimensions have a density given by Roger's bound[23]

$$cD<\rho v_{\text{CP}}<2^{D/2-1}D ,$$

where c is a number less than 2. Consequently, the dimensionless close-packing density ρv_{CP} is infinite as $D\to\infty$. We shall see in Sec. IV that the physical hard-sphere fluid, at $\rho v>1$, is quantum mechanical for all finite temperatures. The quantum hard-sphere fluid does undergo a phase transition (Bose-Einstein condensation).

III. COMPARISON WITH APPROXIMATE THEORIES OF CLASSICAL HARD-SPHERE FLUIDS

The exact equation of state (2.32) can be compared with the results of approximate theories. The scaled-particle theory (SPT) (Ref. 6) is a simple, yet accurate method to determine the equation of state of hard-sphere fluids. It is based on evaluating the reversible work, hence the entropy produced in creating a spherical cavity in the fluid. In a hard-sphere fluid, a cavity of radius a has precisely the same effect on the rest of the system as a particle itself, so that there is a relation between macroscopic thermodynamic quantities and the microscopic structure of the system. The scaled-particle theory is easily generalized to arbitrary dimensions.[24] As $D\rightarrow\infty$, the equation of state is

$$\frac{p^{\rm SPT}}{\rho kT}=(1+\tfrac{3}{8}\rho v)/(1-\tfrac{1}{8}\rho v)+O(2^{-D}\rho v)\ . \tag{3.1}$$

The second virial coefficient, $\frac{1}{2}v$, is identical in both SPT and exact theory (2.30). The exact pressure, at given density, is lower than that given by (3.1), as may be expected from an approximate calculation.

Carnahan and Starling[7] (CS) have suggested a semiempirical modification to the SPT equation of state in $D=3$, to make it yield the exact next virial coefficient. It has also been conjectured that such a correction, and the approximate equation of state itself, must be of a specific form (Y form) of monomials in $Y=y/(1-y)$ [where $y=\rho V_D(a/2)=\rho v/2^D$] so that the CS approximate equation of state in D dimensions should be a polynomial of degree D in Y,[25]

$$\frac{p}{kT}=\sum_{n=1}^{D}a_n Y^n\ . \tag{3.2}$$

The conjecture is based on calculations in $D=1,2,3$.

For $D=\infty$, the canonical Y form can be rewritten as

$$\frac{p}{\rho kT}=\frac{1}{1-2^{D-3}y}(\alpha+\beta Y+\gamma Y^2+\cdots)\ , \tag{3.3}$$

since

$$y(1-2^{D-3}y)^{-1}=Y[1-(2^{D-3}-1)Y]^{-1}\ .$$

The SPT equation (3.1) is obtained for $\alpha=1$, $\beta=\frac{3}{8}2^D$; all other coefficients vanish. The exact equation of state (all higher-order virial coefficients) is recovered by adding to $p^{\rm SPT}/\rho kT$, the Y-form term $-4(\frac{1}{8}\rho v)^2/(1-\frac{1}{8}\rho v)$. Then $\gamma=-4(\frac{1}{8}2^D)^2$, and the other coefficients remain zero. Thus, the conjecture of Barboy and Gelbart[25] is satisfied by the exact expressions for $D=1$ and $D=\infty$.

IV. THE HARD-SPHERE BOSE FLUID

In Sec. II we have seen that the Mayer series and the equation of state are analytic within the classical fluid phase. Analytic continuation of the Mayer series could also be performed outside the circle of convergence, $|zev|=1$, i.e., for densities higher than $(\rho v)^*=0.305$. However, classical mechanics may no longer be applicable at such high densities.

The physical situation indeed requires a quantum-mechanical treatment. The radius of convergence of the Mayer series $|zve|=1$ corresponds, at low temperature (for maximal value $\mu=0$ of the chemical potential) to a thermal wavelength Λ of the order of the hard-sphere diameter $v^{1/D}$. Given a classical Hamiltonian for N hard spheres, both first *and* second quantization are required. The hard spheres are spinless so that they should be regarded as bosons. Their mutual repulsion is a dynamical effect of the hard-sphere potential, not a statistical one (which would be reminiscent of Fermi-Dirac statistics).

In this section we shall show that the hard-sphere Bose gas becomes ideal in the limit $D=\infty$, in that the particles are effectively noninteracting. The difficulty with an infinite interaction potential at small interparticle distances, is circumvented in the standard fashion, by calculating the scattering amplitude or t matrix, and using it as a pseudopotential whose effect can be treated in the Born approximation.[11].

In D dimensions, the Born approximation for the scattering amplitude is established as follows (we shall only be interested in s waves). The scattered wave $u(r)$ satisfying the radial Schrödinger equation for zero angular momentum,

$$\left[\frac{1}{r^{D-1}}\frac{d}{dr}r^{D-1}\frac{d}{dr}+k^2-\frac{2\mu}{\hbar^2}\tilde{V}\right]u=0 \tag{4.1}$$

[where $\mu=\frac{1}{2}m$ is the reduced mass in a collision of two particles of mass m, $E=\hbar^2k^2/(2\mu)$ the eigenenergy, and $\tilde{V}$ the scattering pseudopotential], can be written as $u(r)=(f_0/r^{D-2})g(r)$ in the region $\tilde{V}=0$, where $g(r)$ satisfies the Bessel equation

$$g''+\frac{D-3}{r}g'+k^2g=0\ , \tag{4.2}$$

and f_0 is the s-wave scattering amplitude. The total wave function is the sum of the incident plane wave $\psi_0=e^{i\mathbf{k}\cdot\mathbf{r}}$ and the scattered wave $u(r)$, $\psi=\psi_0+u$. It is also the solution of the Schrödinger equation, which can be written in the Born approximation, using the Green's function, as $\psi_B=\psi_0+\int(m/\hbar^2)G_0\tilde{V}\psi_0 d^Dr$, where G_0 is the solution of

$$(\nabla^2+k^2)G_0(\mathbf{r},\mathbf{r}')=\delta^{(D)}(\mathbf{r}-\mathbf{r}')\ , \tag{4.3}$$

which is

$$G_0(\mathbf{r},\mathbf{r}')=-[(D-2)S_D]^{-1}\exp(ik|\mathbf{r}-\mathbf{r}'|)\times(|\mathbf{r}-\mathbf{r}'|)^{2-D}\ . \tag{4.4}$$

The numerical factors $[S_D=D\pi^{D/2}/\Gamma(1+D/2)]$ are obtained by integrating (4.3) over a spherical volume $V_D(r)$ enclosing the source point $\mathbf{r}'=0$, neglecting k^2 beside ∇^2 for the singular behavior at $|\mathbf{r}|=0$, and using Gauss's formula. By putting G_0 into the integral equation for ψ_B in the asymptotic region $|\mathbf{r}|\gg a$, one obtains f_0 in the Born approximation. For slow collisions $|\mathbf{q}|a\ll 1$, where $\mathbf{q}$ is the momentum transfer and a the range of the pseudopotential, it reads

$$f_0 = -\frac{m}{(D-2)S_D\hbar^2}\int d^D r\,\tilde{V}(r)$$
$$= -\frac{m}{(D-2)\hbar^2}\int_0^\infty dr\,r^{D-1}\tilde{V}(r)\ . \qquad (4.5)$$

For $D=3$, $-f_0$ is called the scattering "length." Here f_0 has dimensions (length)$^{D-2}$.

The hard-sphere Bose gas has been analyzed in three dimensions by Lee, Huang, and Yang.[11] Despite the hard-sphere potential being infinite for small interparticle distances, the scattering amplitude, or t matrix, remains finite and plays the part of the pseudopotential $\tilde{V}$.

In the Born approximation (4.5), $Aa^2 \sim DS_D\rho a^2 |f_0| \ll 1$ is the small parameter of the perturbation scheme. [$\rho=N/V$ is the density of Bose particles, and the approximation symbol stands for numerical factors given below in Eq. (4.10).] In this sense, the hard-sphere Bose gas is regarded as almost ideal in three dimensions. We shall see that it becomes ideal as D tends to infinity.

The main physical quantity measuring the effect of interactions between particles is the depletion of the zero-momentum condensed state, given by $1-\langle N_0\rangle/N$, where $\langle N_0\rangle/N$ is the fraction of particles in the condensed state at absolute zero.

Let us recall the main results of Bogolyubov's theory,[10,26] straightforwardly generalized to D dimensions. The energy of elementary excitations of momentum $\mathbf{p}$ is

$$\varepsilon_p = [(p^2/2m)^2 + u^2p^2]^{1/2}\ , \qquad (4.6)$$

$$mu^2 = (D-2)S_D\hbar^2 |f_0|\rho/m\ , \qquad (4.7)$$

where u is the sound velocity in the Bose gas. The coherent mixing between Bose particles and antiparticles is given by

$$L_p = (\varepsilon_p - p^2/2m - mu^2)/mu^2\ , \qquad (4.8)$$

and the $\mathbf{p}\neq 0$ momentum distribution of the Bose particles at $T=0$ by

$$\langle N_p\rangle = L_p^2/(1-L_p^2)\ ,$$

so that the depletion of the condensate is

$$1-\langle N_0\rangle/N = \frac{S_D}{(2\pi\hbar)^D}\frac{1}{\rho} \times \int_0^\infty dp\,p^{D-1}\left[\frac{(mu^2)^2}{2\varepsilon_p(p^2/2m+mu^2-\varepsilon_p)}-1\right] \qquad (4.9)$$

(Eq. 78.20 of Ref. 26 is misprinted). Here we have made the standard transformation to a continuum $\mathbf{p}$ spectrum,

$$N^{-1}\sum_p \to \frac{1}{\rho(2\pi\hbar)^D}\int d^Dp\ .$$

The change of variable, $p=2mu\sinh t$, eliminates m and $\hbar$ from Eq. (4.9), which now reads

$$1-\langle N_0\rangle/N = A^{D/2}(S_D/\rho)2^{(1/2)D-2}H_D\ ,$$

where

$$A = [mu/(\sqrt{2}\pi\hbar)]^2 = (D-2)S_D|f_0|\rho/(2\pi^2)\ , \qquad (4.10)$$

and H_D is the dimensionless integral

$$H_D = \int_0^\infty dt\,\exp(-2t)(\sinh t)^{D-2}\ . \qquad (4.11)$$

H_D diverges at large t for $D\geq 4$, and a cutoff t_{max} is required at large momentum. It is given by the obvious sum rule $N^{-1}\sum_p = 1$, equating the number of modes to the number of particles, that is

$$1 = A^{D/2}S_D/(D\rho)(\sqrt{2}\sinh t_{max})^D\ . \qquad (4.12)$$

Note that the cutoff, $\sinh t_{max} \propto D^{1/2}$, becomes very large as $D\to\infty$. It is unnecessary at $D=3$, where H_3 is easily evaluated and Eq. (4.9) yields the classic result[26]

$$1-\langle N_0\rangle/N = \frac{8}{3\sqrt{\pi}}(\rho|f_0|^3)^{1/2}\ .$$

For $D\to\infty$, the integral in H_D is dominated by the large t contribution, where $\sinh t \sim (1/2)e^t$, and

$$H_D \simeq \frac{1}{2^{D/2}(D-4)}\left[\frac{D\rho}{A^{D/2}S_D}\right]^{1-4/D}\ , \qquad (4.13)$$

by using the cutoff (4.12); so that, finally,

$$1-\langle N_0\rangle/N = \frac{1}{4}\left[\frac{D}{D-4}\right]\left[\frac{S_D}{\rho D}\right]^{4/D}A^2$$
$$\simeq \frac{1}{D^{D-1}}(e^2/4\pi^3)(2\pi e)^D(|f_0|\rho^{1-2/D})^2\ , \qquad (4.14)$$

which is negligibly small at $D=\infty$. The hard-sphere Bose fluid behaves therefore like an ideal Bose gas, with classical Bose-Einstein condensation, in infinite space dimensions.

The physical reason for this ideal Bose-Einstein behavior can be seen by comparing the kinetic energy of free bosons $p^2/2m$, with their collision energy

$$mu^2 \simeq \frac{(2\pi\hbar)^2}{2m}A \sim DS_D|f_0|\rho(\hbar^2/m)\ ,$$

as defined in Eqs. (4.6) and (4.7) at large momenta. The collision energy becomes negligible as $D\to\infty$ because the ratio between the volumes of a D sphere and its circumscribed D cube becomes itself negligible.

The Bose-Einstein condensation temperature T_c can be obtained by calculating the depletion of the condensate at finite temperatures, $T<T_c$, so that $\mu=0$. The $\mathbf{p}\neq 0$ momentum distribution is given by[26]

$$\langle N_p\rangle(T) = [n_p + L_p^2(n_p+1)]/(1-L_p^2)\ , \qquad (4.15)$$

where the coherent mixing L_p is defined in Eq. (4.8), and n_p is the Bose-Einstein occupation number at $\mu=0$,

$$n_p(T) = 1/[\exp(\beta\varepsilon_p)-1]\ .$$

ε_p is given by Eq. (4.6). Depletion of the condensate

$$\sum_{\mathbf{p}\,(\neq 0)}\langle N_p\rangle(T)/N = A^{D/2}(S_D/\rho)2^{D/2-2}(H_D+H_T)$$

is due to two contributions, (i) nonideality of the Bose fluid H_D, corresponding to $n_p=0$ in (4.15), and shown above to be negligibly small at $D=\infty$ [Eqs. (4.9)–(4.14)], and (ii) the thermal contribution

$$H_T=\frac{kT}{mu^2}\int_0^\infty dx\frac{1}{\exp(x)-1}[S(x)]^{D/2-1}\ , \quad (4.16)$$

with

$$S(x)=\{[1+(xkT/mu^2)^2]^{1/2}-1\}/2\ .$$

Here the change of variable $x=\beta\varepsilon_p$ has been made. Bounds for $S(x)$,

$$\tfrac{1}{2}[(xkT/mu^2)-1]\Theta(x-mu^2/kT)\le S(x)\le xkT/mu^2\ ,$$

where Θ is the Heaviside (unit step) function, yield excellent bounds for H_T,

$$2\left[\frac{kT}{2mu^2}\right]^{(1/2)D}\Gamma(D/2)F_{D/2}(mu^2/kT) < H_T < 2\left[\frac{kT}{2mu^2}\right]^{(1/2)D}\Gamma(D/2)\zeta(D/2)\ , \quad (4.17)$$

where $F_{D/2}(x)=\sum_{n=1_\infty}e^{-nx}/n^{D/2}$. For $D\to\infty$,

$$F_{D/2}(0)=\zeta(D/2)\to 1\ ,$$

and

$$F_{D/2}(x)=e^{-x}[1+O(2^{-D/2})]\ ,$$

so that

$$\exp\left[-\frac{mu^2}{kT}\right]<H_T\Big/\left[2\left[\frac{kT}{2mu^2}\right]^{(1/2)D}\Gamma(D/2)\right]<1\ . \quad (4.18)$$

We shall show later [Eq. (4.21)] that $kT_c=(2\pi\hbar^2/m)\rho^{2/D}$, so that, from Eqs. (4.7) and (4.14),

$$\begin{aligned}kT_c/mu^2&=\{(2\pi)^{3/2}/[D^{1/2}(D-2)]\}\\&\quad\times(D/2\pi e)^{D/2}(|f_0|\rho^{1-2/D})^{-1}\\&=[e/(D-2)](1-\langle N_0\rangle/N)^{-1/2}\end{aligned} \quad (4.19)$$

is very large, and

$$H_T=2\left[\frac{kT}{2mu^2}\right]^{D/2}\Gamma(D/2)\ , \quad (4.20)$$

except at the very lowest temperatures $kT\ll mu^2$.

At $T=T_c$, the occupation of the condensate is no longer macroscopic, and

$$\begin{aligned}1&=\sum_{\mathbf{p}\,(\neq 0)}\langle N_p\rangle(T)/N\\&=\tfrac{1}{2}A^{D/2}(S_D/\rho)\Gamma(D/2)(kT_c/mu^2)^{D/2}\end{aligned}$$

yields the Bose-Einstein condensation temperature

$$kT_c=(2\pi\hbar^2/m)\rho^{2/D},\quad \Lambda_c=\rho^{-1/D}\ . \quad (4.21)$$

This is exactly the condensation temperature of an ideal Bose gas in D dimensions (Ref. 27, p. 248)

$$\rho=[\Lambda_c^{-D}/\Gamma(D/2)]\int_0^\infty dx\,x^{D/2-1}(e^x-1)\ , \quad (4.22)$$

$x=p^2/(2mkT)$, thereby confirming the ideality of the $D=\infty$ Bose fluid.

T_c, given by Eq. (4.21) or (4.22), is best expressed in terms of the linear density $\rho=(n_1/l_1)^D$. Let N be the atomic weight, m_p, the proton mass, $m=Nm_p$. Then, if l_1 is expressed in angstroms,

$$T_c=302.6(n_1/l_1)^2N^{-1}[\zeta(D/2)]^{-2/D}\ \text{(K)}\ .$$

(This yields $T_c=3.11$ K for He in $D=3$.) Recall that for $D\to\infty$, $\Gamma(D/2)\to 1$.

At, and above the (high) density $\rho=1/v$, corresponding to $zv=e$, that is near the radius of convergence of the classical Mayer series (2.23), T_c is, typically, in Kelvin,

$$T_c\ge 302.6N^{-1}(2\pi e)^{-1}a^{-2}D,\quad \rho\ge 1/v \quad (4.23)$$

for $D\to\infty$, with a in angstroms. At high densities, therefore, the hard-sphere fluid is an ideal Bose condensate in an overwhelming range of temperatures.

To discuss the phase diagram, consider the classical hard-sphere fluid described in Sec. II [Eq. (2.32)], and decrease its temperature at constant density ρ, or activity z. The fluid becomes (smoothly) quantum mechanical at T_D, whenever the thermal de Broglie wavelength Λ reaches a typical atomic ($v^{1/D}$) or interatomic distance ($\rho^{-1/D}$), or, for statistical reasons (validity of the Boltzmann distribution), when the chemical potential $|\mu|\simeq kT$, i.e., $\Lambda\simeq(ez)^{-1/D}$, whichever is the condition encountered first when decreasing the temperature. Thus, the degeneracy temperature T_D is given by

$$\Lambda(T_D)=\min[v^{1/D},\rho^{-1/D},(ez)^{-1/D}]\ . \quad (4.24)$$

Because $\rho<z$ [Eq. (2.33)], $\rho^{-1/D}>(ez)^{-1/D}$, and the interatomic distance is irrelevant in determining the degeneracy temperature, which is always larger than the Bose-Einstein temperature $\Lambda_c=\rho^{-1/D}$ (4.21).

Within the radius of convergence of the Mayer series, $ze<1/v$, the degeneracy temperature T_D corresponds to a metric condition

$$\Lambda(T_D)=v^{1/D},\quad ze<1/v\ .$$

Outside ($ze>1/v$), it is statistical,

$$\Lambda(T_D)=(ez)^{-1/D},\quad ze>1/v\ ,$$

that is, if a is expressed in angstroms,

$$T_D>302.6N^{-1}(2\pi e)^{-1}a^{-2}D\ \text{(K)}\ ,$$

an infinite degeneracy temperature, as $D\to\infty$. The *classical* hard-sphere fluid fails to describe the $D=\infty$ real fluid when $zev>1$, outside the radius of convergence of the Mayer series. In that region of high density and activity, we are dealing with a quantum Bose fluid, which undergoes a Bose-Einstein condensation and becomes ideal at T_c, given by Eq. (4.21). It is therefore idle to speculate[28] on the validity of the classical hard-sphere fluid, and on its exact equation of state (2.32) at very high densities, notably near Rogers's bounds for close packing.[22] The fluid is quantum mechanical except at infinite temperatures.

On the other hand, the high-density configurations of the classical hard-sphere fluid for $D=\infty$ can be analyzed as a mathematical problem; indeed very recent work has focused on spatial fluctuations of the density in this picture. Above a critical density the system reaches a Kirkwood (or softmode) instability.[20,29] However, the form of the resulting nonuniform structure and its thermodynamic manifestations are unknown.

Thus the $D=\infty$ hard-sphere fluid, is a "physical" manifestation of the ideal Bose-Einstein condensation, which had not hitherto found a concrete representation. We have not yet calculated the equation of state and the virial expansion of the Bose gas at all temperatures above the Bose-Einstein condensation temperature, and checked whether they are identical with those of the classical fluid [Eq. (2.31)].

V. SUMMARY AND CONCLUSIONS

We have presented an analytic theory of the fluid branch of the infinite dimensional hard-sphere system, including its low-temperature behavior. For the classical hard-sphere fluid in the limit $D\to\infty$, the fluid branch remains analytic for *all* finite values of ρv (ρ is the density, v the volume of a sphere with the double radius). The equation of state is

$$\frac{p}{\rho kT}=1+\tfrac{1}{2}\rho v \ , \tag{5.1}$$

which shows that the system is still interacting. The $D=\infty$ hard-sphere system realizes Groeneveld's upper bound for the Mayer coefficients.

Failure to detect a phase transition in the Mayer expansion does not necessarily imply that there is no phase transition. Indeed, such failure also befalls the Ford model (Ref. 16), a grand partition function written down *ad hoc* as an example of a Yang-Lee phase transition, but which has not yet been attributed to any physical potential.

There, as for Eq. (2.29), the Mayer series can be analytically continued throughout the cut, complex z plane, but continuation beyond the radius of convergence does not yield the condensed phase branch. In the Ford model, no pressure maxima have been obtained by Padé approximation of the virial series, indicating again the failure of the fluid equation of state to supply any information about the condensed phase,[30] exactly as in the present $D=\infty$ hard-sphere model. Incidentally, the Ford model realizes Groeneveld's lower bound (2.7).

Nevertheless, if the hard-sphere fluid is kept classical as a mathematical artifice, one would expect a phase transition into a condensed phase to occur. This is because fluctuations are averaged out, and mean-field theory becomes exact, as the dimensionality of the system increases. The simple form of the $D=\infty$ fluid equation of state, with only one nonvanishing virial coefficient to represent the interaction between hard spheres, indicates that a mean-field limit has been reached, with a finite effective interaction. It is retained for nonuniform density profiles,[20] which, at higher densities, leads the system to a Kirkwood instability.[20,29]

But any classical condensation is physically hidden at $D=\infty$, because by then the hard-sphere system has become quantum mechanical. Indeed, we have shown that, at high densities $\rho\geq 1/v$ beyond the radius of convergence of the classical Mayer series, the $D=\infty$ hard-sphere fluid is an *ideal* Bose condensate at all finite temperature: The Bose-Einstein condensation temperature T_c is proportional to D when $\rho\geq 1/v$ [Eq. (4.23)]. At all densities, the hard-sphere system behaves as a nonideal classical fluid, which undergoes a Bose-Einstein condensation, where 100 percent of the particles occupy the condensate at $T=0$, despite a finite second virial coefficient and a finite interaction.

An obvious, but hard extension of this work would be to carry out the $1/D$ expansion, thereby including the first effects of finite D. This might settle the question of the existence of classical solid phases, and also of metastable, "glassy" states[24] which have been observed in computer simulations of the three dimensional hard-sphere system.[31] One can also ask for the phase behavior of mixtures of hard spheres of different diameters in the $D\to\infty$ limit. It should be possible to generalize our theory to this case.

In this paper we have been solely interested in the (mechanical) equation of state of infinite dimensional hard-sphere fluid. It seems relatively straightforward to carry out the kinetic theory in the Boltzmann-Grad limit of this system and to compute the transport coefficients (self-diffusion, viscosity, and thermal conductivity) from a suitably modified Boltzmann equation using either the Chapman-Enskog or Grad thirteen-moment expansion methods.

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APPENDIX A: EVALUATION OF SOME INTEGRALS $I_D(\varphi)=\int_0^\varphi d\theta \sin^D\theta$

A recursion relation can be obtained

$$I_D(\varphi)=\frac{D-1}{D}I_{D-2}(\varphi)-\frac{1}{D}\sin^{D-1}x\,\cos x \,\Big|_{x=0}^{x=\varphi} \ . \tag{A1}$$

This yields simply

$$\begin{aligned}2I_D(\pi/2)=I_D(\pi)&=\begin{cases}\dfrac{2(D-1)!!}{D!!}, & D \text{ odd}\\[2ex] \dfrac{2(D-1)!!}{D!!}\,\dfrac{\pi}{2}, & D \text{ even}\end{cases}\\ &=\sqrt{\pi}\,\frac{\Gamma(1+(D-1)/2)}{\Gamma(1+D/2)}\\ &=V_D(1)/V_{D-1}(1)\simeq(2\pi/D)^{1/2}\end{aligned} \tag{A2}$$

in the limit $D\to\infty$. For $\varphi\neq\pi/2$, the integral $I_D(\varphi)$ is more easily evaluated for an odd $D=2l+1$. From (A1) we obtain

$$I_{2l+1}(\varphi)=\frac{2^l l!}{(2l+1)!!}-\frac{\cos\varphi}{(2l+1)}\left[\sin^{2l}\varphi+\sum_{k=0}^{l-1}\frac{2^{k+1}l(l-1)\cdots(l-k)}{(2l-1)(2l-3)\cdots(2l-2k-1)}(\sin\varphi)^{(2l-2k-2)}\right]. \tag{A3}$$

The series in (A3) can be rewritten as

$$\Sigma=\frac{2^l l!}{(2l-1)!!}\sum_{k=0}^{l-1}\frac{(2l-2k-3)!!}{(l-k-1)!2^{l-k-1}}(\sin\varphi)^{2l-2k-2}$$
$$=\frac{2^l l!}{(2l-1)!!}\sum_{m=0}^{l-1}\frac{(2m-1)!!}{2^m m!}\sin^{2m}\varphi\ , \tag{A4}$$

with the convention $(-1)!!=1$, and the change of variable $m=l-k-1$. But

$$\sum_{m=0}^{\infty}\frac{(2m-1)!!}{2^m m!}x^{2m}=\frac{1}{(1-x^2)^{1/2}} \tag{A5}$$

for $x<1$; hence,

$$\Sigma=\frac{2^l l!}{(2l-1)!!}\left[\frac{1}{\cos\varphi}-\frac{(2l-1)!!}{2^l l!}\sin^{2l}\varphi-\sum_{m=l+1}^{\infty}\frac{(2m-1)!!}{2^m m!}\sin^{2m}\varphi\right]. \tag{A6}$$

The first two terms in (A6) cancel out the first two terms of $I_{2l+1}(\varphi)$, and only the last term in (A6) contributes to $I_{2l+1}(\varphi)$. Term by term, it yields

$$I_{2l+1}(\varphi)=\frac{1}{2l+2}\cos\varphi\sin^{2l+2}\varphi+O\left[\frac{1}{2l+2}\sin^{2l+4}\varphi\right]$$
$$=\frac{1}{D+1}\cos\varphi\sin^{D+1}\varphi+O\left[\frac{1}{D+1}\sin^{D+3}\varphi\right]. \tag{A7}$$

For arbitrary D, we have the trivial bound

$$I_D(\varphi)<\varphi\sin^D\varphi\ . \tag{A8}$$

For even D, $I_{2l}(\varphi)$ interpolates between I_{2l-1} and I_{2l+1}. Consequently, $I_D(\varphi)$ decreases exponentially with D, except for $\varphi=\pi/2$, where $I_D(\pi/2)\sim D^{-1/2}$.

APPENDIX B: SQUARE-LOOP MAYER DIAGRAM

We wish to show that all one-loop diagrams are vanishing exponentially as $D\to\infty$. The square loop diagram is of order 4,

$$Q=\square=\int d^Ds\,\mathcal{O}^2(s)=DV_D(1)\int_0^\infty ds\,s^{D-1}\mathcal{O}^2(s)\ , \tag{B1}$$

where s denotes the distance between diagonal points 1 and 2, and $\mathcal{O}(s)$ is the overlap between the two spheres at 1 and 2, given by Eq. (2.14). Let $\cos\zeta=(1/2)s/a$. The overlap is bounded by

$$\mathcal{O}(s)=2V_{D-1}(a)a\int_0^\zeta d\theta\sin^D\theta<\pi aV_{D-1}(a)\sin^D\zeta\ , \tag{B2}$$

and Q by

$$Q<DV_D(a)[V_{D-1}(a)a]^2\pi^2 J\ , \tag{B3}$$

where

$$J=2^D\int_0^{(1/2)\pi}d\zeta\sin^{2D+1}\zeta\cos^{D-1}\zeta$$
$$=2^{D-1}\frac{\Gamma(1+D)\Gamma(1+\frac{1}{2}(D-2))}{\Gamma(1+\frac{3}{2}D)}$$
$$\simeq\left[\frac{2\pi}{3D}\right]^{1/2}\left[\frac{4}{3^{3/2}}\right]^D[1+O(1/D)] \tag{B4}$$

by Stirling's approximation.

By comparison with the tree diagram of order 4, $Q_0=v^3$,

$$\frac{Q}{Q_0}<\pi^2 D[V_{D-1}(1)/V_D(1)]^2 J$$
$$\simeq(\pi^2/\sqrt{6}\pi)D^{3/2}\left[\frac{4}{3^{3/2}}\right]^D[1+O(1/D)] \tag{B5}$$

decreases exponentially with D.

APPENDIX C: TWO-LOOP MAYER DIAGRAM

In this appendix we calculate the simplest two-loop Mayer diagram and compare it with the one square loop diagram evaluated in Appendix B. These diagrams are given, respectively, by

$$Q'=\boxslash=\int_0^a d^Ds\,\mathcal{O}^2(s)\ ,$$
$$Q=\square=\int_0^\infty d^Ds\,\mathcal{O}^2(s)\ , \tag{C1}$$

where s, as in Appendix B, denotes the diagonal distance. Using the bound (B2) for $\mathcal{O}(s)$, we obtain

$$Q'<DV_D(a)[aV_{D-1}(a)]^2\pi^2[J(\pi/2)-J(\pi/3)]\ ,$$
$$Q<DV_D(a)[aV_{D-1}(a)]^2\pi^2 J(\pi/2)\ , \tag{C2}$$

where

$$J(\varphi)=2^D\int_0^\varphi d\zeta\sin^{2D+1}\zeta\cos^{D-1}\zeta\ . \tag{C3}$$

Clearly, $Q'<Q$.

For $J(\varphi)$, the obvious bounds

$$[2^D/(2D+2)]\sin^{2D+2}\varphi\cos^{D-2}\varphi<J(\varphi)<[2^D/(2D+2)]\sin^{2D+2}\varphi \tag{C4}$$

suffice, except for $\varphi=\pi/2$, where

$$J(\pi/2)=(2\pi/3D)^{1/2}(4/3^{3/2})^D[1+O(1/D)] \tag{C5}$$

was derived in Appendix B. Consequently,

$$J(\pi/3)>[3/(2D+2)](3/4)^D\ . \tag{C6}$$

Hence

$$Q'<DV_D(a)[aV_{D-1}(a)]^2\pi^2(2\pi/3D)^{1/2}(4/3^{3/2})^D\times\{1-(27/8\pi)^{1/2}D^{-1/2}[(3^{5/2}/16)]^D\}\ . \tag{C7}$$

Thus Q' and Q have the same asymptotic behavior as the triangular diagram evaluated in the main text (2.18): They decrease roughly as α^{nD}, where $n=4$ (for Q,Q') or 3, respectively (for the triangular diagram) and $\alpha<1$, as stated in the text. For large n, the weight of a diagram of order n with e edges, containing $c=e-n+1$ independent loops is smaller than that of a tree diagram of the same order by a factor $(\alpha^D)^n$ rather than $(\alpha^D)^c$ (recall that $c\sim n^2/2$ for large n).

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