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Intersecting Disks (and Spheres) and Statistical Mechanics. I. Mathematical Basis

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The calculations of a previous paper on intersecting disks are completed. Further quantities of interest in connection with intersecting disks and spheres are defined. The above considerations are extended to spherical boundary conditions. Then two applications are stated: The penetrable-sphere model of Widom and Rowlinson, and the hard-sphere system. Finally, the generalization to D-dimensional spheres is outlined.

KEY WORDS: Intersection of disks; set theory; statistical mechanics; periodic boundary conditions; spherical boundary conditions; penetrable spheres; hard spheres.

1. INTRODUCTION

In a previous paper[1], the area of intersection of n equal circular disks was investigated. The radius of the disks was set equal to unity and will be σ now. Moreover, not only the area of intersection $I(1,2,\ldots,n)$, but also the corresponding length of the boundary $B(1,2,\ldots,n)$ will be considered. The result for two disks 1, 2 is

$$I(1,2)=\left\{\begin{matrix} I_1=I_2 & r_{12}=0 & B_1=B_2 \\ I_{12} & 0<r_{12}<2\sigma & B_{12} \\ 0 & 2\sigma\leqslant r_{12} & 0 \end{matrix}\right\}=B(1,2)$$

$$I_1=\pi\sigma^2, \qquad B_1=2\pi\sigma \tag{1.1}$$

$$I_{12}=2\sigma^2\left\{\cos^{-1}(r_{12}/2\sigma)-(r_{12}/2\sigma)\left[1-(r_{12}/2\sigma)^2\right]^{1/2}\right\}$$

$$B_{12}=4\sigma\left[\cos^{-1}(r_{12}/2\sigma)\right]$$

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For n disks, $I(1,2,\ldots,n)$ is the area on which all n disks intersect. It is denoted by $I_{12\ldots n}$ if it is nonzero and if the removal of any of the disks increases the area. Correspondingly, $B(1,2,\ldots,n)$ is denoted by $B_{12\ldots n}$ in this case.

Direct calculation of B_{123} yields (compared with the known I_{123})

$$I_{123} = \tfrac{1}{2}\left(I_{12} + I_{13} + I_{23} - \pi\sigma^2\right) + \tfrac{1}{4} r_{12} r_{13} r_{23}/R_c \tag{1.2a}$$

$$B_{123} = \tfrac{1}{2}\left(B_{12} + B_{13} + B_{23} - 2\pi\sigma\right) \tag{1.2b}$$

R_c is the circumradius of the triangle (123), see Powell[2] and Kratky.[3] Equations (1.2) show that there is a simple relation between I_{123} and B_{123}. In fact Eqs. (1.2) meet a general relationship: If the locations of the disks are arbitrary, but fixed, $I(1,2,\ldots,n)$ and $B(1,2,\ldots,n)$ can be considered as functions only of the radius σ. Then, the following relation holds:

$$B(1,2,\ldots,n) = dI(1,2,\ldots,n)/d\sigma \tag{1.3}$$

Thus, I_{12} and I_{123} can also be obtained by integrating B_{12} and B_{123}, respectively. The constant of integration C can be evaluated in a simple manner [$r_{12} = \max(r_{ij})$ without loss of generality]:

$$\begin{aligned} &I_{12} \to 0 \quad \text{if} \quad (r_{12}/2\sigma) \to 1, \\ &I_{123} \to A \quad \text{if} \quad (R_c/\sigma) \to 1, \end{aligned} \qquad A\begin{cases} 0: & r_{12}^2 \leqslant r_{13}^2 + r_{23}^2 \\ I_{12}(\sigma = R_c): & r_{12}^2 > r_{13}^2 + r_{23}^2 \end{cases} \tag{1.4}$$

This means a considerable simplification obtaining Eq. (1.2a) compared with other methods[1,4,5] since actual calculation shows that (1.2b) can be obtained easily. $C = 0$ for I_{12}, $C = \frac{1}{4} r_{12} r_{13} r_{23}/R$ for I_{123}; see (1.1) and (1.2), respectively.

It has been shown that the intersection of n disks can always be reduced to intersections of at most three disks[1]. The same relations as for $I(1,2,\ldots,n)$ can now be transcribed for $B(1,2,\ldots,n)$, e.g., Eq. (3.2) of Ref. 1 also holds for B_{1234}:

$$I_{1234} = I_{ikl} + I_{jkl} - I_{kl}, \qquad B_{1234} = B_{ikl} + B_{jkl} - B_{kl} \tag{1.5}$$

In the case $I(1,2,3,4) = I_{1234}$, the disk centers 1, 2, 3, 4 can be interpreted as the corners of a convex quadrangle[1]. Equation (1.5) is true if i and j are connected by a diagonal of the quadrangle. Then k and l are also connected by a diagonal, yielding a second correct expression for I_{1234} and B_{1234} like (1.5). Thus, two of the six permutations (i,j,k,l) of $(1,2,3,4)$ yield the correct result. Incidentally, this means that, e.g., I_{123} can be expressed in terms of the other intersections of three disks and of two intersections of two disks.

Now a fifth disk is added. If $I(1,2,3,4,5) = I_{12345}$, then $(1,2,3,4,5)$ is a convex pentagon with i and j being connected by a diagonal if this was true for (1, 2, 3, 4). Thus,

$$I_{12345} = I_{ikl5} + I_{jkl5} - I_{kl5}, \qquad B_{12345} = B_{ikl5} + B_{jkl5} - B_{kl5} \tag{1.6}$$

and so forth when adding more and more disks. Five of the possible ten relations like (1.6) yield the correct I_{12345} (and B_{12345}) because a pentagon has five diagonals. Generally (n disks), $[\binom{n}{2} - n]$ relations like (1.5) or (1.6) out of the $\binom{n}{2}$ possible relations are correct. Even if all incorrect relations yield the same estimate of $I_{12\ldots n}$ among themselves, the correct solution can be obtained by taking the most degenerate value for $n \geqslant 6$. The advantage of this method is that no geometrical considerations are necessary. In the following, it will be shown that another simple recipe can be used to obtain the correct $I_{12\ldots n}$ for any n ($n \geqslant 4$). If one forms all $\binom{n}{2}$ equations like (1.5) or (1.6) and determines the corresponding estimates of $I_{12\ldots n}$, the maximum value yields the correct intersection.

To show this, only set-theoretical arguments are necessary. Two general results of set theory are:

$$\mu(A \cap B) = \mu(A) + \mu(B) - \mu(A \cup B) \tag{1.7a}$$

$$(C \cup D) \cap E = (C \cap E) \cup (D \cap E) \tag{1.7b}$$

where A, B, C, D, E are sets, μ is a measure, $\cup$ is the union, and $\cap$ is the intersection. We number now the considered sets as I_1^s, I_2^s, I_3^s, I_4^s (s stands for "set") and define

$$\begin{aligned} &A \doteqdot I_1^s \cap (I_3^s \cap I_4^s), \quad B \doteqdot I_2^s \cap (I_3^s \cap I_4^s) \\ &C \doteqdot I_1^s, \qquad D \doteqdot I_2^s, \quad E \doteqdot (I_3^s \cap I_4^s) \end{aligned} \tag{1.8}$$

Using equations (1.7) gives

$$\begin{aligned} \mu\left[(I_1^s \cap I_2^s) \cap (I_3^s \cap I_4^s)\right] &= \mu\left[I_1^s \cap (I_3^s \cap I_4^s)\right] + \mu\left[I_2^s \cap (I_3^s \cap I_4^s)\right] \\ &\quad - \mu\left[(I_3^s \cap I_4^s) \cap (I_1^s \cup I_2^s)\right] \end{aligned} \tag{1.9}$$

In a more convenient way (I being the measure of I^s), this can be written as

$$\begin{aligned} I(1,2,3,4) &= I(1,3,4) + I(2,3,4) - \mu\left[(I_3^s \cap I_4^s) \cap (I_1^s \cup I_2^s)\right] \\ &\geqslant I(1,3,4) + I(2,3,4) - I(3,4) \end{aligned} \tag{1.10}$$

Relation (1.10) is generally valid for any sets with, e.g., $I(1, 2, 3)$ being the measure of the intersection of the first, second, and third set. The equality is valid if and only if $(I_3^s \cap I_4^s) \subseteq (I_1^s \cup I_2^s)$. Now we assume that we have four equal disks with $I(1, 2, 3, 4) = I_{1234}$. In this case, (1.10) becomes

$$I_{1234} \geqslant I_{ikl} + I_{jkl} - I_{kl} \tag{1.11}$$

for any permutation (i, j, k, l). Since we know that for at least one (really two) relations like (1.11) the equality sign is valid, one has only to take the maximum value of the six lower bounds of I_{1234} to obtain the correct I_{1234}. By the way, the geometrical condition that i and j are connected by diagonals now turns out to be equivalent to $I_{kl}^s \subseteq (I_i^s \cup I_j^s)$.

For B_{1234}, the equivalent of (1.11) and thus the "maximum method" is not valid generally. But from I_{1234} one knows which indices one has to take. To obtain for I_{12345} a formula analogous to (1.10) for I_{1234}, one has to define

$$\begin{aligned} A &\doteq I_1^s \cap (I_3^s \cap I_4^s \cap I_5^s), \quad B \doteq I_2^s \cap (I_3^s \cap I_4^s \cap I_5^s) \\ C &\doteq I_1^s, \qquad D \doteq I_2^s, \qquad E \doteq (I_3^s \cap I_4^s \cap I_5^s) \end{aligned} \tag{1.12}$$

Doing the same calculation as above, this ends up in

$$\begin{aligned} I(1,2,3,4,5) &= I(1,3,4,5) + I(2,3,4,5) - \mu\left[(I_3^s \cap I_4^s \cap I_5^s) \cap (I_1 \cup I_2)\right] \\ &\geqslant I(1,3,4,5) + I(2,3,4,5) - I(3,4,5) \end{aligned} \tag{1.13}$$

and so on for $n \geqslant 5$ disks. If for (1.10) the equality sign is valid, this is also the case for (1.13). This is now clear without any geometrical consideration, since

$$\left[(I_3^s \cap I_4^s) \subseteq (I_1^s \cup I_2^s)\right] \Rightarrow \left[(I_3^s \cap I_4^s \cap I_5^s) \subseteq (I_1^s \cup I_2^s)\right] \tag{1.14}$$

The above considerations split up into two groups: First, purely set-theoretical arguments have been used which are valid generally, cf., (1.9) or (1.10). Second, geometrical considerations[1] yield the result that for at least one combination of indices the equality sign is true in (1.11) with I_{1234} being the intersection of four equal disks.

It is interesting to compare the results for disks with the general case of D-dimensional equal spheres ($D = 1,2,3$). For $D = 1$ (i.e., for overlapping intervals),

$$\left.\begin{aligned} I(1,2,\ldots,n) &= I(p,q) \\ B(1,2,\ldots,n) &= B(p,q) \end{aligned}\right\} \qquad r_{pq} = \max(r_{ij}), \qquad 1 \leqslant i < j \leqslant n \tag{1.15}$$

That means that a reduction to the intersection of two intervals is always possible. For $D = 2$ (disks), a reduction to the intersection of at most three disks is always possible; see above. For $D = 3$ (spheres), the knowledge of $I(1,2,3,4)$ would be necessary to solve the general case.

Up to now, the D-dimensional spheres were assumed to be thoroughly penetrable. If, however, the restriction $r_{ij} \geqslant \sigma$ is placed, then $I(1,2,\ldots,n) > 0$ cannot be fulfilled for $n > \bar{n}$, $\bar{n}$ being a function of D. The problem is equivalent to filling n points ($r_{ij} \geqslant \sigma$) within an open D-dimensional sphere of radius σ. The solution is[6-8]

$$\bar{n}(D = 1) = 2, \qquad \bar{n}(D = 2) = 5, \qquad \bar{n}(D = 3) = 12 \tag{1.16}$$

Equation (1.16) will be used in Section 4.

Some applications of the knowledge of $I(1,2,\ldots,n)$ have already been discussed by the author.[1] Melnyk and Rowlinson[9] also considered several aspects of "overlapping figures." Before further applications can be treated, more quantities in connection with intersecting disks have to be defined.

2. DEFINITION OF THE QUANTITIES $I_{(j)}, B_{(j)}, V_{(k)}, S_{(k)}, \bar{S}_{(k)}$

The quantities defined in this section refer to D-dimensional equal spheres (in the following called "spheres") so that the three-dimensional diction ("volume," "surface") will be used.

n spheres of radius σ are assumed. The location of the spheres is arbitrary, but fixed. For j out of the n spheres, the set-theoretical intersection $I^s(i_1,\ldots,i_j)$ and the corresponding measure (volume) $I(i_1,\ldots,i_j)$ is given by

$$I^s(i_1,i_2,\ldots,i_j) \doteqdot \{p/r(p,i_l)<\sigma, l=1,2,\ldots,j\} \tag{2.1a}$$

$$I(i_1,i_2,\ldots,i_j) \doteqdot \mu\left[I^s(i_1,i_2,\ldots,i_j)\right], \qquad 1\leqslant i_1<i_2\cdots<i_j\leqslant n \tag{2.1b}$$

$r(p,i_l)$ is the distance between an arbitrary point p of the intersection and sphere center i_l. It is convenient to define

$$I_{(j)} \doteqdot \sum_{1\leqslant i_1<i_2\cdots<i_j\leqslant n} I(i_1,\ldots,i_j) \tag{2.2}$$

i.e., the sum of all volumes of intersection of j spheres. The quantities defined in (2.1) are independent of the location of the $(n-j)$ remaining spheres. This is not the case for the following quantities:

$$\begin{aligned} V^s(i_1,i_2,\ldots,i_k) \doteqdot \{p/r(p,i_l)<\sigma,\quad & l=1,2,\ldots,k \\ r(p,i_m)\geqslant\sigma,\quad & m=k+1,\ldots,n\} \end{aligned} \tag{2.3a}$$

$$V(i_1,i_2,\ldots,i_k) \doteqdot \mu\left[V^s(i_1,i_2,\ldots,i_k)\right] \tag{2.3b}$$

Unlike $I^s(i_1,\ldots,i_j)$, it follows that all $V^s(i_1,\ldots,i_k)$ are disjoint. Therefore, forming the union of V^s corresponds to summing up the V:

$$\begin{aligned} &\left[V^s_{(k)} \doteqdot \bigcup_{1\leqslant i_1<\cdots<i_k\leqslant n} V^s(i_1,\ldots,i_k)\right] \\ &\quad\Rightarrow\left[V_{(k)} = \sum_{1\leqslant i_1<\cdots<i_k\leqslant n} V(i_1,\ldots,i_k)\right] \end{aligned} \tag{2.4}$$

if $V_{(k)} \doteqdot \mu[V^s_{(k)}]$ as usual. Correspondingly, the whole volume $V_\cup \doteqdot \mu(V^s_\cup)$ covered by the union of spheres is the sum of all $V_{(k)}$; see (1.7a):

$$\left[V^s_\cup \doteqdot \bigcup_{1\leqslant k\leqslant n} V^s_{(k)}\right]\Rightarrow\left[V_\cup = \sum_{1\leqslant k\leqslant n} V_{(k)}\right] \tag{2.5}$$

(2.4) is valid since different $V^s(i_1, \ldots, i_k)$ with the same k are disjoint. Since moreover different $V^s(i_1, \ldots, i_k)$ with different k are disjoint, (2.5) is valid. $V_{(k)}$ is the total volume covered by k and only k spheres. According to (2.5), the union volume $V_\cup$ can be split up into volumes $V_{(k)}$.

Because of the property of being disjoint, the V^s are more convenient than the I^s. On the other hand, the intersections $I(i_1, \ldots, i_j)$ are known explicitly (see Section 1). Making use of (1.7), however, it is easy to relate $I_{(j)}$ to $V_{(k)}$:

$$\left.\begin{aligned} V_{(k)} &= \sum_j \binom{j}{k}(-1)^{j+k} I_{(j)} \\ I_{(j)} &= \sum_k \binom{k}{j} V_{(k)} \end{aligned}\right\} \qquad \begin{aligned} &\tbinom{r}{t} \doteq 0 \quad \text{if } t > r \\ &1 \leqslant (j,k) \leqslant n \end{aligned} \tag{2.6}$$

$$V_\cup = \sum_{j=1}^{n} (-1)^{j+1} I_{(j)} \tag{2.7}$$

The restriction $1 \leqslant (j,k)$ in (2.6) can be removed easily by introducing $I_{(0)}$ and $V_{(0)}$ in a consistent way. To do this, it is necessary to assume that the interacting spheres are enclosed in a volume V. The boundary of V is arbitrary but must not intersect with any of the spheres. Then,

$$I_{(0)} \doteq V, \qquad V_{(0)} \doteq V - V_\cup \tag{2.8}$$

Both definitions are only extensions of the above $I_{(j)}$ and $V_{(k)}$. $I_{(0)}$ means that there is no restriction $r(p, i_l) < \sigma$, thus it is the whole volume V. $V_{(0)}$ means the total volume which is covered by no sphere, which is just $V - V_\cup$. Using (2.8), equations (2.6) are valid for $0 \leqslant (j,k) \leqslant n$. Even the upper limit n may be dropped since $V_{(m)}$ and $I_{(m)}$ are zero for $m > n$.

$I_{(0)} = V$ and $I_{(1)} = \sum_{i=1}^n I(i) = nI^*$ (I^* being the volume of a sphere) are independent of the configuration. Thus, there exist two combinations of the $V_{(k)}$ which are independent of the given configuration, too [cf. (2.6)]:

$$V = I_{(0)} = \sum_{k=0}^{n} V_{(k)}, \qquad nI^* = I_{(1)} = \sum_{k=0}^{n} kV_{(k)} \tag{2.9}$$

Relations (2.9) are of some help in the hard-disk case[10].

The above-mentioned condition that the spheres must not intersect the boundary of V is too restrictive in many cases. Therefore periodic boundary conditions will be assumed in the following. The length of the (cubic) cell must be at least 4σ to avoid the case that a sphere intersects another from two sides. Then, the results of the paper are valid for any n, r_{ij} being the minimum distance of centers i, j.

Analogous considerations as for the volumes can be made for the corresponding surfaces of the volumes. The analog of (2.2) is evident:

$$B_{(j)} \doteq \sum B(i_1, \ldots, i_j) \tag{2.10}$$

$B(i_1, \ldots, i_j)$ being the surface of $I(i_1, \ldots, i_j)$, see (2.1b). In the case of $V_{(k)}$, the natural way of defining a surface seems to be

$$\bar{S}^s(i_1, \ldots, i_k) = \text{surface of } V^s(i_1, \ldots, i_k) \tag{2.11a}$$

$$\bar{S}^s_{(k)} = \cup \bar{S}^s(i_1, \ldots, i_k) \tag{2.11b}$$

compare (2.4). Since all $\bar{S}^s(i_1, \ldots, i_k)$ with the same k are disjoint the analog of (2.4) for $\bar{S}$ is also valid, $\bar{S}(\cdots)$ being $\mu[\bar{S}^s(\cdots)]$:

$$\bar{S}_{(k)} \doteq \sum_{1 \leq i_1 < \cdots < i_k \leq n} \bar{S}(i_1, \ldots, i_k) \tag{2.12}$$

However, not all $\bar{S}^s$ are disjoint since volumes of the type $V^s(i_1, \ldots, i_j)$ and $V^s(i_1, \ldots, i_k)$ may have a common border[10] if $k = j \pm 1$. To obtain only disjoint surfaces, it is convenient to define a set $S^s(i_1, \ldots, i_k)$ as the subset of the surface of $V^s(i_1, \ldots, i_k)$ which borders on a $V^s(i_1, \ldots, i_k, i_{k+1})$, i_{k+1} being any of the remaining $(n-k)$ spheres:

$$S^s(i_1, \ldots, i_k) \doteq \bar{S}^s(i_1, \ldots, i_k) \cap \left[\bigcup_{i_{k+1}} \bar{S}^s(i_1, \ldots, i_k, i_{k+1}) \right] \tag{2.13}$$

$S_{(n)} = 0$ because of (2.13). All sets S^s are disjoint now. Only for $S_\cup$ it is convenient to define $S^s_\cup = \bar{S}^s_\cup = \mu(\text{surface of } V^s_\cup)$. The quantities $S_{(k)} = \mu(S^s_{(k)}) = \mu[\cup S^s(i_1, \ldots, i_k)]$ and $B_{(j)}$ are related in a way very close to the relation between $V_{(k)}$ and $I_{(j)}$, Eqs. (2.6), (2.7):

$$\left.\begin{aligned} S_{(k)} &= \sum_j \binom{j}{k} (-1)^{j+k} B_{(j+1)} \\ B_{(j+1)} &= \sum_k \binom{k}{j} S_{(k)} \end{aligned}\right\} \qquad 0 \leq (j,k) \leq n-1 \tag{2.14}$$

$$S_\cup = \sum_{j=1}^{n} (-1)^{j+1} B_{(j)} \tag{2.15}$$

$B_{(0)}$ need not be defined, but a consistent definition would be $B_{(0)} = 0$ since the periodic cell has no surface. $S_{(0)}$ is—as a consequence of definition (2.13)—just the boundary between $V^s_\cup$ and $V^s_{(0)}$. Comparison between (2.14) and (2.15) shows indeed that

$$S_{(0)} = S_\cup \tag{2.16}$$

compared with $V_{(0)} = V - V_\cup$, see (2.8). There exists one relation between the $S_{(k)}$. $B_{(1)} = \sum_{i=1}^{n} B(i) = nB^*$ (B^* being the surface of a sphere) is independent of the configuration. Thus, from (2.14) follows

$$nB^* = B_{(1)} = \sum_{k=0}^{n-1} S_{(k)} \tag{2.17}$$

Now, the relation between $S_{(k)}$ and $\bar{S}_{(k)}$ will be stated:

$$\left.\begin{aligned} \bar{S}_{(k)} &= S_{(k)} + S_{(k-1)} \\ S_{(k)} &= \sum_j (-1)^{j+k} \bar{S}_{(j)} \end{aligned}\right\} \quad \begin{aligned} 0 \leqslant j \leqslant k \leqslant n \\ S_{(-1)} \doteq 0 \end{aligned} \tag{2.18 }$$

From the definition $S_{(-1)} \doteq 0$, $\bar{S}_{(0)} = S_{(0)} = S_{\cup}$ results; cf. (2.16).

Combining (2.14) with (2.18) yields the relation between $\bar{S}_{(k)}$ and $B_{(j)}$:

$$\left.\begin{aligned} \bar{S}_{(k)} &= \sum_j (-1)^{j+k} \left[\binom{j}{k} - \binom{j}{k-1} \right] B_{(j+1)} \\ B_{(j+1)} &= \sum_k (-1)^k \left[\sum_{i=k}^{n} \binom{i}{j} (-1)^i \right] \bar{S}_{(k)} \end{aligned}\right\} \quad \begin{aligned} & 0 \leqslant j \leqslant n-1 \\ & 0 \leqslant k \leqslant n \\ & \binom{m}{-1} \doteq 0 \\ & \text{for any } m \end{aligned} \tag{2.19}$$

The upper bounds $(n-1)$ or n of the variables i, j, and k occurring in Eqs. (2.14)–(2.19) are only set for convenience to avoid identities as $0 = 0$. If one sets arbitrary higher bounds, these equations remain valid. This is relevant when searching for relations between the $\bar{S}_{(k)}$. Since $B_{(1)} = nB^*$ is independent of the special configuration, see (2.17), from (2.19) it follows that

$$\begin{aligned} nB^* = B_{(1)} &= \sum_{k=0}^{n} (-1)^k \left[\sum_{i=k}^{n} (-1)^i \right] \bar{S}_{(k)} \\ &= \begin{cases} \bar{S}_{(0)} + \bar{S}_{(2)} + \bar{S}_{(4)} + \cdots & \text{if } n \text{ even} \\ \bar{S}_{(1)} + \bar{S}_{(3)} + \bar{S}_{(5)} + \cdots & \text{if } n \text{ odd} \end{cases} \end{aligned} \tag{2.20}$$

But since the upper limit for i does not matter, both relations must be true for any n, yielding the additional relation

$$\sum_{k=0}^{n} (-1)^k \bar{S}_{(k)} = 0 \tag{2.21}$$

This yield together with (2.20)

$$2nB^* = 2B_{(1)} = \sum_{k=0}^{n} \bar{S}_{(k)} \tag{2.22}$$

(2.22) meets the fact that every part of the surface $\bar{S}$ is the common border of two volumes and is thus counted twice. The disjoint surfaces S, however, yield (2.17). By the way, (2.18) directly yields

$$\sum_{k \geqslant 0} \bar{S}_{(k)} = 2 \sum_{k \geqslant 0} S_{(k)} \tag{2.23}$$

At last, the relation between the volumes and the surfaces will be studied.

Equation (1.3) can easily be generalized to

$$\frac{\partial}{\partial \sigma} I(i_1, \ldots, i_j) = B(i_1, \ldots, i_j) \tag{2.24a}$$

$$\frac{\partial}{\partial \sigma} I_{(j)} = B_{(j)} \tag{2.24b}$$

(2.24b) is an immediate consequence of (2.24a); see (2.2). $(\partial/\partial\sigma)$ means that the location of the centers of the spheres is held fixed. If one wants to relate S and V in an analogous way, the equations

$$S_{\cup} = \frac{\partial}{\partial \sigma} V_{\cup} \qquad S_{(0)} = -\frac{\partial}{\partial \sigma} V_{(0)} \tag{2.25}$$

are obvious and furthermore connected by $(V_{(0)} + V_{\cup} = V)$, Eq. (2.8), V being independent of σ. The generalization of (2.25) is

$$\frac{\partial}{\partial \sigma} V_{(k)} = S_{(k-1)} - S_{(k)} \tag{2.26}$$

Whenever a volume of the type $V(i_1, \ldots, i_k)$ borders a volume of the type $V(i_1, \ldots, i_k, i_{k+1})$, increase of σ increases the latter volume at this border to the debit of the former.

Using (2.24) and (2.26), the two combinations of $V_{(k)}$ which are independent of the configuration, see (2.9), yield

$$0 = \sum S_{(k)} - \sum S_{(k-1)}; \qquad B_{(1)} = \sum S_{(k)} \tag{2.27}$$

i.e., one trivial relation $0 = 0$ and the known relation (2.17).

3. SPHERICAL BOUNDARY CONDITIONS

Up to now, periodic boundary conditions have been assumed. The above considerations can be extended to spherical boundary conditions (spherical BC) which have been introduced by the author.[11] In the following, explicit formulas are given for disks.

The spherical BC are defined in the following way: The D-dimensional volume of the system lies on the surface of a $(D + 1)$-dimensional sphere of radius R. Now, equal disks on the surface of a sphere are considered $(V = 4\pi R^2)$. The distances on the sphere are geodesic distances corresponding to the shorter segment of a great circle through two points. If the (geodesic) radius of the disks is σ, then

$$\left.\begin{aligned} I_1 &= 4\pi R^2 \sin^2(\tfrac{1}{2}\beta) \\ B_1 &= 2\pi R \sin\beta \end{aligned}\right\} \beta \doteqdot \sigma/R, \qquad 0 \leqslant \beta \leqslant \pi \tag{3.1}$$

A great circle corresponds to $\beta = \frac{1}{2}\pi$. To avoid anomalous intersections which only occur when $\beta > \frac{1}{2}\pi$, i.e., $\sigma^2/V > \pi/16$, $\beta \leqslant \frac{1}{2}\pi$ shall be assumed in the following. This may be compared with the condition $\sigma^2/V \leqslant 1/16$ for disks with periodic BC, Section 2.

The cases for $I(1,2)$ are $I_1 = I_2$, I_{12}, and 0, as usual. The different regions of r_{12} are the same as in Eq. (1.1). The result for I_{12} and B_{12} is

$$I_{12} = 4R^2\left[\cos^{-1}\left(\frac{\sin\alpha_{12}}{\sin\beta}\right) - \cos\beta\cos^{-1}\left(\frac{\tan\alpha_{12}}{\tan\beta}\right)\right]$$

$$B_{12} = 4R\sin\beta\cos^{-1}\left(\frac{\tan\alpha_{12}}{\tan\beta}\right) \tag{3.2}$$

$$\alpha_{12} \doteqdot r_{12}/2R, \qquad 0 \leqslant \alpha_{12} < \beta \leqslant \tfrac{1}{2}\pi$$

I_{12} has been obtained by integrating B_{12} and using (1.4) to determine the integration constant C. In Ref. 11, I_{12} has been calculated directly; the complicated result given there may be compared with the simpler representation of I_{12} now.

The cases for $I(1,2,3)$ are $I_1 = I_2 = I_3$, I_{12}, I_{13}, I_{23}, I_{123}, and 0, respectively. In the following, r_{12} is arbitrary, but fixed within the limits $0 < r_{12} < 2\sigma$. Thus, $I(1,2) = I_{12}$, and the trivial case $I(1,2,3) = I_1$, i.e., $r_{12} = r_{13} = r_{23} = 0$, cannot occur. The possible locations of center 3 can be divided into several regions according to the corresponding type of $I(1,2,3)$. A discussion of the regions for disks (or spheres) in Euclidean space has been given in the Appendix of Ref. 12, where "$-g_{ij}$" means I_{ij}. Analogous considerations can be done for spherical BC. To simplify the problem, it is now assumed without loss of generality that $r_{12} = \max(r_{12}, r_{13}, r_{23})$, $0 < r_{12} < 2\sigma$. Then, only the cases I_{12}, I_{123}, and 0 occur. They can be characterized in the following way: Points P and Q are the two solutions of the equation

$$\left.\begin{matrix} r_{P1} = r_{P2} = \sigma \\ r_{Q1} = r_{Q2} = \sigma \end{matrix}\right\} \qquad r_{12} = \max(r_{12}, r_{13}, r_{23}) \tag{3.3}$$

P is assumed to lie at the same side of the straight line (great circle) through 1 and 2 as center 3. Then it follows

$$\begin{array}{llll} I_{12}: & r_{P3} \leqslant \sigma & \text{and} & r_{Q3} \leqslant \sigma \\ I_{123}: & r_{P3} < \sigma & \text{and} & r_{Q3} > \sigma \\ 0: & r_{P3} \geqslant \sigma & \text{and} & r_{Q3} > \sigma \end{array} \tag{3.4}$$

Equations (3.3) and (3.4) are valid to characterize the regions of center 3 for spherical BC as well as in Euclidean space. Employing spherical geometry, these relations can be used to define the borders of the regions analytically also for spherical BC. If $\theta \geqslant 0$ is the angle at center 1 of the (spherical) triangle (123), $\theta \leqslant \frac{1}{2}\pi$ follows from $r_{12} = \max(r_{ij})$. θ can be expressed as a function of the distances r_{ij} in the following way ($\alpha_{ij} \doteqdot r_{ij}/2R$):

$$\text{Euclidean:} \quad \theta = \cos^{-1}\left[\left(r_{12}^2 + r_{13}^2 - r_{23}^2\right)/(2r_{12}r_{13})\right]$$

$$\text{Spherical:} \quad \theta = \cos^{-1}\left[(\cos 2\alpha_{23} - \cos 2\alpha_{12}\cos 2\alpha_{13})/(\sin 2\alpha_{12}\sin 2\alpha_{13})\right] \tag{3.5}$$

If θ_P and θ_Q correspond to segments of circles with radius σ around points P and Q, respectively, the regions of disk 3 are as follows:

$$\begin{aligned} I_{12}&: \quad 0 \leqslant \theta \leqslant \theta_Q \\ I_{123}&: \quad \theta_Q < \theta < \theta_P \\ 0&: \quad \theta_P \leqslant \theta \end{aligned} \tag{3.6}$$

$$\text{Euclidean:} \quad \theta_{P,Q} = \pm\cos^{-1}(r_{12}/2\sigma) + \cos^{-1}(r_{13}/2\sigma)$$

$$\text{Spherical:} \quad \theta_{P,Q} = \pm\cos^{-1}\left(\frac{\tan\alpha_{12}}{\tan\beta}\right) + \cos^{-1}\left(\frac{\tan\alpha_{13}}{\tan\beta}\right)$$

$\theta_P \leqslant \theta$ is not compatible with $r_{12} = \max(r_{ij})$ if $\cos 2\alpha_{12} > (1 - \frac{3}{2}\sin^2\beta)$, i.e., $r_{12} < \sqrt{3}\sigma$ in Euclidean space. For this range of r_{12}, $I(1,2,3) \neq 0$.

Considering the spherical triangle (123) results in explicit formulas for B_{123} and via integration for I_{123}:

$$\begin{aligned} I_{123} &= \tfrac{1}{2}(I_{12} + I_{13} + I_{23}) + (\pi + \epsilon)R^2(\cos\beta - 1) + C \\ B_{123} &= \tfrac{1}{2}(B_{12} + B_{13} + B_{23}) - (\pi + \epsilon)R\sin\beta \end{aligned} \tag{3.7}$$

ϵ is the spherical excess, $(\pi + \epsilon)$ is the sum of the angles of the spherical triangle (123) which can be calculated via relations like (3.5). Equation (1.4) can be used to determine C. Inserting the circumradius R_c of the spherical triangle (123) instead of σ yields

$$C = R^2\left\{2\sum_{1\leqslant i<j\leqslant 3} A^{ij}\left[\cos\beta_c\cos^{-1}\left(\frac{\tan\alpha_{ij}}{\tan\beta_c}\right) - \cos^{-1}\left(\frac{\sin\alpha_{ij}}{\sin\beta_c}\right)\right]\right.$$
$$\left. + (\pi + \epsilon)(1 - \cos\beta_c)\right\}, \qquad \beta_c \doteqdot R_c/R \tag{3.8}$$

$$A^{13} = A^{23} = 1, \qquad A^{12} = \text{sign of}\left(\sin^2\alpha_{13} + \sin^2\alpha_{23} - \sin^2\alpha_{12}\right)$$

However, R_c has not yet been determined. To do this, we compare the spherical triangle (123) with the plane triangle $(123)_p$. The circumradius of

$(123)_p$, $\bar{R}_c$, is related to the edges of $(123)_p$, $\bar{r}_{ij}$, as usual [2,3]:

$$\bar{R}_c = \bar{r}_{12}\bar{r}_{13}\bar{r}_{23}\big[(\bar{r}_{12}+\bar{r}_{13}+\bar{r}_{23})(-\bar{r}_{12}+\bar{r}_{13}+\bar{r}_{23}) \times (\bar{r}_{12}-\bar{r}_{13}+\bar{r}_{23})(\bar{r}_{12}+\bar{r}_{13}-\bar{r}_{23})\big]^{-\frac{1}{2}} \tag{3.9}$$

$$\bar{r}_{ij} = 2R\sin(r_{ij}/2R) = 2R\sin\alpha_{ij}, \qquad \beta_c = (R_c/R) = \sin^{-1}(\bar{R}_c/R)$$

Thus, the intersections up to three disks have been solved for spherical BC. Extension to more disks is possible in the same way as exhibited in Section 1 and Ref. 1 for Euclidean geometry. Especially the "maximum method," see (1.11) and (1.13), is again useful for actual calculations. Relations (1.16) change for $D > 1$ into

$$\bar{n}_{\text{spherical}} \leqslant \bar{n}_{\text{Euclidean}} \tag{3.10}$$

$\bar{n}_{\text{spherical}}$ being a function of β ($\beta = 0$: Euclidean). By the way, all relations of Section 2 are also valid for spherical BC. Again, $B_{(0)} = 0$ since the volume of the system has no surface as for periodic BC.

4. DISCUSSION

In this paper, several results concerning intersecting equal D-dimensional spheres—especially disks—have been given. Before some mathematical aspects of these results will be discussed, the connection to statistical mechanics shall be briefly outlined. In a further paper, this connection will be treated more strictly.

One connection to statistical mechanics concerns the penetrable-sphere model of Widom and Rowlinson.[13,14] N thoroughly penetrable D-dimensional spheres of radius σ are assumed. The interaction energy U of a configuration can be written as

$$U = \left[V_{\cup} - I_{(1)}\right]\epsilon \tag{4.1}$$

$\epsilon > 0$ is an energy parameter. For $V_{\cup}$ and $I_{(1)}$, compare (2.7). The pressure P is given by

$$\frac{PV}{NkT} = 1 + \frac{\epsilon}{I_{(1)}kT}\left[\frac{\sigma}{D}\langle S_{\cup}\rangle - \langle V_{\cup}\rangle\right] \tag{4.2}$$

T being the temperature. For $D > 1$, there is a gas–liquid transition characterized by

$$\langle S_{\cup}/V\rangle_{\text{gas}} = \langle S_{\cup}/V\rangle_{\text{liquid}} \tag{4.3}$$

In the case $D = 2$, the quantities $S_{\cup}$ and $V_{\cup}$ can now be calculated explicitly, so that a Monte Carlo computer experiment can be carried on for penetrable disks.

Now, the statistical mechanics of N D-dimensional hard spheres with radius $\frac{1}{2}\sigma$ is considered. This system can be interpreted [10,15] as a system of N "exclusion spheres" with radius σ. These spheres are partly penetrable, $r_{ij} \geqslant \sigma$. Thus, the conditions for the validity of (1.16) are fulfilled. $V_{(0)} = (V - V_{\cup})$ is the total volume of the "holes" of a given configuration. The chemical potential μ can be expressed in terms of $V_{(0)}$ (λ: thermal wavelength):

$$\mu/kT = \ln(\lambda^D N) - \ln\langle V_{(0)}\rangle \tag{4.4}$$

This yields for the phase transition ($D > 1$):

$$\langle V_{(0)}\rangle_{\text{fluid}} = \langle V_{(0)}\rangle_{\text{solid}} \tag{4.5}$$

The pressure is given by [10,16]

$$\frac{PV}{NkT} = 1 + \frac{\sigma}{2D}\,\frac{\langle S_{(0)}\rangle}{\langle V_{(0)}\rangle} = 1 + \frac{\sigma}{2D}\left\langle \frac{s_f}{v_f}\right\rangle \tag{4.6}$$

where v_f is the free volume and s_f is its surface. For high fluid densities, s_f and v_f can be related to $S_{(i)}$ and $V_{(i)}$. A computer experiment for hard disks using (4.4)–(4.6) is being done now. The actual calculation of $V_{(i)}$ and $S_{(i)}$ is efficient for disks since $\bar{n}(D = 2)$ is at most 5 for both boundary conditions, see (1.16) and (3.10). Thus, at most intersections of five disks have to be considered. $V_{(i)}$ and $S_{(i)}$ are correlated with the structure of the system. For instance, $V_{(5)}$ is zero in the ideal hard-disk lattice and is expected to be much less in the solid than in the fluid.

Finally, the results of the paper shall be discussed from a mathematical point of view. Two types of boundary conditions have been considered, the periodic BC and the spherical BC. In one dimension ($D = 1$), both BC are equivalent (length of the cell $L = 2\pi R$). For $D \geqslant 2$, it is no longer possible to represent the spherical BC in Cartesian coordinates. In Sections 2 and 3, upper limits for σ (the radius of the considered spheres) with respect to a typical length of the cell have been stated for $D = 2$. Generally, $4\sigma \leqslant 2\pi R$ for spherical BC and $4\sigma \leqslant L_{\min}$ for periodic BC, $L_{\min}$ being the minimal length of the edges of the rectangular cell. For a cubic cell, this corresponds to $4\sigma \leqslant V^{1/D}$. This restriction guarantees that the finiteness of the system does not come in explicitly. For hard disks with spherical BC, the above restriction is certainly fulfilled if the system contains at least six disks, but this is automatically the case in practice. Obeying the restriction for periodic BC means that all formulas concerning intersections of the spheres become the same as in Euclidean space; compare, e.g., the expression "Euclidean" in (3.6), r_{12} being the minimum distance of 1,2 for periodic BC.

The results of Section 2 are mainly based on set theory. Thus, they can be generalized to equal or not equal arbitrarily shaped bodies with ($4\sigma_{\max} \leqslant L_{\min}$) or ($4\sigma_{\max} \leqslant 2\pi R$) for periodic and spherical BC, respectively. $\sigma_{\max}$ is the largest diameter of the bodies. Only Eqs. (2.1a) and (2.3a) have to be generalized in an obvious way:

$$\begin{aligned} I^s(i_1, i_2, \ldots, i_j) &= \bigcap_{l=1}^{j} I^s(i_l) \\ V^s(i_1, i_2, \ldots, i_k) &= I^s(i_1, i_2, \ldots, i_k) \cap \bigcap_{m=k+1}^{n} I_c^s(i_m) \end{aligned} \tag{4.7}$$

$I^s(i_j)$ is the set-theoretical volume of the i_jth body; $I_c^s(i_j)$ is its complement relative to the total volume.

Strictly speaking, there is a problem concerning the surfaces $S_{\ldots}$ and $\bar{S}_{\ldots}$ defined in Section 2. For instance, in (2.13) it was used that two volumes of the type $V^s(i_1, \ldots, i_j)$ and $V^s(i_1, \ldots, i_k)$ may only have a common border if $k = j \pm 1$. However, where the surfaces of two bodies intersect, also $k = j \pm 2$. Since the set of points where this is the case has the measure zero, this does not change the results. In special cases, parts of the surfaces of two bodies may coincide with nonvanishing measure. Then several relations of Section 2 become inconsistent. However, the theoretical probability is zero that a random configuration includes such special cases. In computer experiments, the probability is not zero (because of the finite accuracy) but very small.

Example: Only two equal spheres are considered. The two surfaces coincide if and only if $r_{12} = 0$. Then $V_{(1)} = 0$ and $\bar{S}_{(1)} = 0$, see Eqs. (2.3), (2.4), (2.11), and (2.12), but $\bar{S}_{(1)} = B_{(2)} = 4\pi R^2 \neq 0$ because of (2.19). For equal D-dimensional spheres, the relevant formulas could be changed easily in order to include these special cases. This has not been done since the main application is the hard-sphere case where $r_{ij} > 0$.

Apart from general considerations concerning intersections of D-dimensional equal spheres, the case $D = 2$ has been solved explicitly for periodic and spherical BC (Sections 1 and 3). The case $D = 1$ shall be stated now for completeness:

$$I_1 = 2\sigma, \qquad B_1 = 2; \qquad I_{12} = 2\sigma(1 - r_{12}), \qquad B_{12} = 2 \tag{4.8}$$

The types of $I(1,2)$ and the corresponding range of r_{12} are the same as for disks, Eq. (1.1). Equation (1.15) solves the general case $I(1, \ldots, n)$ and $B(1, \ldots, n)$. Since $B(1,2)$ is not continuous now at $r_{12} = 2\sigma$ [$B(1,2) = 2$

and 0, respectively], Eq. (1.3) has to be changed into

$$B(1,2,\ldots,n) = \lim_{\epsilon\to 0}\left\{(1/\epsilon)\left[I(1,2,\ldots,n)/_{\sigma} - I(1,2,\ldots,n)/_{\sigma-\epsilon}\right]\right\},\qquad \epsilon > 0 \tag{4.9}$$

The same modification is necessary for Eqs. (2.24)–(2.26). The choice of this limit is consistent with the definition that the D-dimensional spheres are open.[1]

The special values for the intersections of spheres depend on dimension D and on the BC. However, $I(1,2,\ldots,n)$ can be reduced to intersections of less than $(D+2)$ spheres independent of the BC if $D<3$, compare Eqs. (1.5)–(1.15), Section 3, and Ref. 1. This leads to the conjecture that the above fact is also valid for $D=3$. The corresponding work is in progress; the main result is that the conjecture is true. As an example, we turn to the intersection of five spheres ($D=3$). We consider only the nontrivial case that $I(i,j,k,l) = I_{ijkl}$ for all intersections of four of the spheres. If, e.g., center 1 lies within the tetrahedron of the others, then $I(1,2,3,4,5) = I_{2345}$. If, however, the five centers form a convex polyhedron, then one of the ten permutations (i,j,k,l,m) yields the correct I_{12345} (i.e., the equality is valid):

$$I_{12345} \geqslant I_{iklm} + I_{jklm} - I_{klm} \tag{4.10}$$

compare (1.13). Thus, the results for five spheres are very close to the results for four disks, see Section 1 and Ref. 1. Powell[17] proved that the reduction of $I(1,2,\ldots,n)$ to intersections of less than $(D+2)$ spheres works in any dimension, even for spheres with different radii. An extension to convex bodies seems to be possible.

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