On a Class of Configuration and Coincidence Problems

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(Manuscript received August 28, 1967)

Let A and B be sets in E^m where B is convex and symmetric about o. Let n points be taken in A and let B_i be the translate of B centered at the i^{th} one. Let Y be the subset of the Cartesian product A^n, corresponding to the configurations $(B_1, \cdots, B_n)$ such that no more than $p - 1$ sets B_i intersect, or corresponding to any similar configuration condition, expressible in purely Boolean terms. The problem of evaluating various integrals over Y generalizes a number of questions in queuing, telephone traffic, statistical mechanics of hard spheres, and so on. This article gives a complete solution for certain special cases, and discusses numerical (Monte Carlo) techniques.

I. INTRODUCTION

We consider here a number of problems of the following general type. Let A and B be two sets in the m-dimensional Euclidean space $E^m (m \geqq 1)$. B is assumed to have a center of symmetry and for any point x $B(x)$ denotes the translate of B centered at x. An integer $n (n \geqq 2)$ is fixed and the n-fold Cartesian product $A \times A \times \cdots \times A$ is denoted by P. If $u \in P$ then $u = (x_1, \cdots, x_n)$ where $x_i \in A$ for $i = 1, \cdots, n$; we shall be interested in the sets $B(x_1), \cdots, B(x_n)$. By a configuration condition we shall understand a statement referring to the relative positions of the sets $B(x_1), \cdots, B(x_n)$ and describing their intersection properties in purely Boolean terms.

Examples of admissible configuration conditions are: (*i*) the n sets are pairwise disjoint, (*ii*) their intersection is empty, (*iii*) their union is connected. A configuration condition which generalizes (*i*) and (*ii*) is: an integer p is given $(2 \leqq p \leqq n)$ and no p of the n sets intersect. Any admissible configuration condition C induces a partition of P into two disjoint and complementary sets $Y = Y(C)$ and $N = N(C)$; if $u = (x_1, \cdots, x_n) \in$

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P then $u \varepsilon Y$ if and only if the condition C holds for $B(x_1), \cdots, B(x_n)$. Finally, a function $F = F(x_1, \cdots, x_n)$ is defined over P and dV denotes the volume element $dx_1 \cdots dx_n$. Our problem is to evaluate the integral

$$J = \int_Y F\, dV.$$

In all cases to be considered the sets A, B, and Y, as well as the function F, will be sufficiently regular so that the questions of measurability and integrability will not arise. In fact, in most cases of interest B turns out to be a ball, a cube, or an m-dimensional regular octahedron. All these are Minkowski balls for a suitable norm $\rho(\xi) = \rho(\xi_1, \ldots, \xi_n)$. We get the Euclidean ball with

$$\rho(\xi) = \left(\sum_1^n \xi_i^2\right)^{\frac{1}{2}},$$

the cube with $\rho(\xi) = \max_i (\xi_1, \ldots, \xi_n)$, and the octahedron with

$$\rho(\xi) = \sum_1^n | \xi_i | .$$

It will be therefore assumed throughout that B is a Minkowski ball. This amounts simply to assuming that B is a convex symmetric body. The precise shape of A is of no particular importance, only its content and sufficient regularity are.

The integrand F will be usually of some highly symmetric type such as

$$F = 1, \qquad F = \prod_{i=1}^n f(x_i), \qquad F = \prod_{1 \leq i < j \leq n} f(| x_i - x_j |),$$

where f is a suitable sufficiently regular function.

In this part of the paper we are concerned with certain special configuration conditions which lead to an explicit expression for J in terms of the so-called cluster-integrals. Later we consider a related expansion of the form

$$J = \sum_{j=0}^{\infty} J_j \lambda^j \tag{1}$$

where the parameter λ measures the ratio of sizes of B to A. We shall take up the questions of the existence of the expansion (1) and the regularity of J as a function of λ.

II. EXAMPLES

Example 1

Let $m = 1$, A is the interval $[0, L]$ and B is the interval $[0, a]$, n is any integer such that $(n - 1)a \leqq L$, the configuration condition is that the sets $B(x_1), \cdots, B(x_n)$ are disjoint, and $F \equiv 1/L$. J is now the probability that with n points at random on the interval $[0, L]$ no two points are closer than a.

Example 2

Let m, A, and B be as above,

$$F(x_1, \cdots, x_n) = \prod_1^n f(x_i)$$

where $f(x)$ is a probability density on A. The configuration condition is: p is an integer $(2 \leqq p \leqq n)$ and some p-tuple of the sets $B(x_1), \cdots, B(x_n)$ is to have a nonempty intersection. Here we have the following interpretation: $[0, L]$ is a basic time interval and n events occur during that time. Each event occurs independently of the others with the probability density $f(x)$. A p-fold coincidence is defined to be the compound event arising when some p events occur closely together—on a time-interval of length a. Now J is the probability that a p-fold coincidence occurs.

The above examples show that problems of our type might be of interest in queuing theory, telephone traffic, the theory of particle counters, and in similar areas. The next example is a scattering problem for a random linear array of n identical isotropic point-scatters, no two of which can be too close together.

Example 3

Let m, A, B, and C be as in example 1. We suppose that the wave-length is 2π and that L is an integral multiple of it. Aside from proportionality factors the signal scattered by the array is the vector (ξ, η) where

$$\xi = \sum_1^n \cos x_i, \qquad \eta = \sum_1^n \sin x_i .$$

We are here interested in the probability $P(u, v)$ that

$$u \leqq \xi \leqq u + du \quad \text{and} \quad v \leqq \eta \leqq v + dv.$$

The Markov method[1] gives

$$P(u, v) = (2\pi)^{-2} J_A^{-1} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-i(ru+sv)} B(r, s)\, dr\, ds$$

where

$$B(r, s) = \int_{Y_A} \exp\left[i\left(r \sum_1^n \cos x_i + s \sum_1^n \sin x_i \right) \right] dV.$$

J_A and Y_A are the integral and the region of example 1, respectively. Therefore the spectrum $B(r, s)$ is obtained in the form of our integral J if we take

$$F = \prod_1^n f(x_i), \qquad f(x) = e^{i(r \cos x + s \sin x)}.$$

When $a = 0$ then $P(u, v)$ reduces to the probability density for the isotropic plane random walk of n unit displacements in arbitrary directions.

Example 4

Let $m = 3$, let A be any large and sufficiently regular portion of space, and let B be the ball of radius a. The configuration condition is that no two sets $B(x_i)$ and $B(x_j)$ overlap. There is a suitable given function $\varphi(x)$ and

$$F(x_1, \cdots, x_n) = \prod_{1 \leq i < j \leq n} e^{-\varphi(|x_i - x_j|)}.$$

Now, aside from some simple normalization factors, J is the so-called partition function for a hard-sphere model of idealized gas with intermolecular potential φ and the hard core radius a.[2]

The knowledge of J is here of considerable importance in statistical mechanics and a great deal of work has been done on the subject of evaluating J in the form (1) which is closely associated with the so-called virial expansion.

III. A SPECIAL CASE

The method to be used involves certain dissections of Cartesian products together with the inclusion-exclusion principle of combinatorics.[3] As an illustration and an introduction to the more complex examples which follow, we consider here at some length example 1 of the previous section. The material is taken from Ref. 4, where some further details can be found. The well-known solution[5, 6] is here

$$J = J(n, a, L) = [1 - (n - 1)a/L]^n \tag{2}$$

and it may be obtained analytically as follows.

Let the coordinates of the n points be $x_1, \cdots, x_n$; these can be ordered in $n!$ ways. Suppose that $0 \leqq x_1 \leqq x_2 \leqq \cdots \leqq x_n \leqq L$; the conditions of the problem are satisfied if and only if

$$0 \leqq x_1 \leqq x_2 - a \leqq x_3 - 2a$$
$$\leqq \cdots \leqq x_n - (n-1)a \leqq L - (n-1)a. \tag{3}$$

Let $y_i = x_i - (i-1)a$ $(i = 1, \ldots, n)$, then the probability that (3) holds is L^{-n} times the volume of the region in E^n consisting of the points $y = (y_1, \ldots, y_n)$ for which

$$0 \leqq y_1 \leqq y_2 \leqq \cdots \leqq y_n \leqq L - (n-1)a.$$

The volume in question is $[L-(n-1)a^n]/n!$; since there are $n!$ equi-probable orderings we get (2) at once.

Consider next an alternative geometrical proof of (2), which is considerably more complicated, but leads to useful generalizations and gives some additional insight.

First, let $n = 2$. The sample space of pairs $(x_1, x_2)(0 \leqq x_1, x_2 \leqq L)$ is the square Q of side-length L, lying in the first quadrant of E^2 and containing the origin as a vertex. Let D be the diagonal of Q through the origin and draw the two lines parallel to D at the distance $2^{-\frac{1}{2}}a$ from it. The hexagonal subset of Q contained between those two lines is the sample space of the forbidden configurations with $|x_1 - x_2| \leqq a$. The remainder of the square Q consists of two congruent triangles which can be moved together so as to form a square Q_1, of side-length $L - a$. By the randomness assumption $J(2, a, L)$ is the ratio of the areas of Q_1 and Q which yields (2) for $n = 2$.

The case of arbitrary n is handled similarly. In E^n we take a Cartesian coordinate system with the n axes $X_1, \ldots, X_n$. The n-dimensional cube

$$H = \{(x_1, \cdots, x_n): 0 \leqq x_i \leqq L, i = 1, \cdots, n\}$$

is then the sample space of all n-tuples of points on the segment $[0, L]$. Let I_i be the interval $[0, L]$ on the X_i- axis. In the two-dimensional square face $Q_{ij} = I_i \times I_j$ of H let D_{ij} be the diagonal through the origin and let H_{ij} be the hexagonal subset of Q_{ij} consisting of all points no further from D_{ij} than $2^{-\frac{1}{2}}a$. Let S_{ij} be the Cartesian product of H_{ij} with all the I_k's for which $k \neq i$ and $k \neq j$.

S_{ij} is now the sample space of the configurations which are forbidden on account of too close approach of the points x_i and x_j for the chosen indices i and j: $|x_i - x_j| \leqq a$. The sample space Y of the allowed configurations is therefore the set

$$H - \bigcup_{1 \leqq i < j \leqq n} S_{ij} .$$

When the $\binom{n}{2}$ paradiagonal slabs S_{ij}, based on the paradiagonal sets H_{ij}, are removed from H, the remainder of the cube H consists of $n!$ congruent simplexes which can be reassembled by suitable translations so as to form a smaller cube H_1 of sidelength $L - (n - 1)a$. By the randomness assumption $J(n, a, L)$ is the ratio of the volumes of the cubes H_1 and H, and so (2) is proved again.

The above procedure works on account of a lucky geometrical accident of the fitting of $n!$ simplexes. If A and B were some other, m-dimensional, sets, we could still form the paradiagonal sets and slabs and we could attempt to find the volume of the union $\bigcup S_{ij}$ of all the paradiagonal slabs. This is essentially what is done in the next section by means of the inclusion-exclusion principle[3].

IV. SIMPLE COINCIDENCE WITH SEPARABLE INTEGRAND

In this section we are concerned with a configuration condition corresponding to simple coincidence: $u = (x_1, \cdots, x_n) \varepsilon Y$ if and only if for some i and j $B(x_i)$ and $B(x_j)$ intersect. Subject to general restrictions, A, B, m, and n are arbitrary. We let $N = \binom{n}{2}$ and we form the N paradiagonal sets

$$H_{ij} = \{(x_i, x_j): B(x_i) \cap B(x_j) \neq \phi\}$$

and the N paradiagonal slabs

$$S_{ij} = \{(x_1, \cdots, x_n): B(x_i) \cap B(x_j) \neq \phi\}.$$

Let the slabs be enumerated by a single index as $\{S_k\}$, $k = 1, \ldots, N$. Then an application of the inclusion-exclusion principle gives

$$J = \int_Y F\, dV = \sum_{r=1}^{n} (-1)^{r+1} \left[\sum_{1 \leqq k_1 < k_2 < \cdots < k_r \leqq N} \cdots \sum \int_{S_{k_1} \cap \cdots \cap S_{k_r}} F\, dV \right] \quad (4)$$

$$= \sum_{r=1}^{n} (-1)^{r+1} K_r .$$

With the general integrand no further elaboration of (4) is possible. Suppose now that F has the separable form

$$F = \prod_1^n f(x_i). \tag{5}$$

With the double-index enumeration of the S_{ij}'s the first term K_1 can be written as

$$K_1 = \sum_{1 \leqq i_1 < j_1 \leqq n} \int_{S_{i_1 j_1}} \prod_1^n f(x_i)\, dV$$

and since all the N paradiagonal sets are congruent, we have

$$K_1 = N\left(\int_A f(x)\, dx\right)^{n-2} \int_{H_{12}} f(x_1)f(x_2)\, dx_1\, dx_2 \,.$$

For reasons which will be clear shortly we write

$$N_{11} = N, \qquad \int_A f(x)\, dx = J_0\,, \qquad \int_{H_{12}} f(x_1)f(x_2)\, dx_1\, dx_2 = J_{11} \tag{6a}$$

so that

$$K_1 = N_{11}J_0^{n-2}J_{11}\,. \tag{6b}$$

Similarly, the second term K_2 in (4) is

$$K_2 = \sum_{(i_1,j_1)} \sum_{(i_2,j_2)} \int_{S_{i_1j_1} \cap S_{i_2j_2}} \prod_1^n f(x_i)\, dV$$

where the summation extends over all distinct pairs (i_1, j_1), (i_2, j_2) such that $1 \leqq i_1 < j_1 \leqq n$, $1 \leqq i_2 < j_2 \leqq n$; no regard is paid to the order of pairs; [(1, 2), (3, 4) is the same as (3, 4), (1, 2)] so that there are exactly

$$\binom{\binom{n}{2}}{2}$$

such pairs of pairs. There are two types of these: N_{21} pairs like (1, 2), (3, 4) with all four indices different, and N_{22} pairs like (1, 2), (1, 3) with one shared index. By a simple calculation

$$N_{21} = n(n-1)(n-2)(n-3)/8, \qquad N_{22} = n(n-1)(n-2)/2,$$
$$N_{21} + N_{22} = \binom{\binom{n}{2}}{2} \tag{7a}$$

and in analogy to (6) we set

$$J_{21} = \int_{H_{12}\cap H_{34}} \prod_1^4 f(x_i)\, dx_1\, dx_2\, dx_3\, dx_4$$

$$= \left[\int_{H_{12}} f(x_1)f(x_2)\, dx_1\, dx_2\right]^2 = J_{11}^2 \qquad (7b)$$

$$J_{22} = \int_{H_{12}\cap H_{13}} \prod_1^3 f(x_i)\, dx_1\, dx_2\, dx_3$$

so that

$$K_2 = N_{21}J_0^{n-4}J_{11}^2 + N_{22}J_0^{n-3}J_{22}\,. \qquad (7c)$$

The main purpose of this section is to develop formulae, analogous to (6) and (7), for the general term K_r of (4). The principal difficulty here is that in passing from the single-index formula for K_r

$$K_r = \sum_{1\leq k_1<\cdots<k_r\leq N} \cdots \sum \int_{S_{k_1}\cap\cdots\cap S_{k_r}} \prod_{i=1}^n f(x_i)\, dV \qquad (8a)$$

to the double-index formula

$$K_r = \sum_{(i_1,j_1)} \cdots \sum_{(i_r,j_r)} \int_{S_{i_1j_1}\cap\cdots\cap S_{i_rj_r}} \prod_{i=1}^n f(x_1)\, dV \qquad (8b)$$

we need an adequate description of the different types of r-tuples of pairs of indices occurring in (4), together with a hold on the range of summation in (8b). For instance, with $r = 2$ there are two such types, illustrated by (1, 2), (3, 4) and (1, 2), (1, 3). With $r = 3$ there are five types of index-sharing in triples of pairs:

(1, 2), (3, 4), (5, 6); (1, 2), (1, 3), (4, 5); (1, 2), (2, 3), (3, 4);

(1, 2), (1, 3), (1, 4); (1, 2), (1,3) (2, 3); (9)

We may therefore expect that the formula for $r = 3$, analogous to (7c) for $r = 2$, will have five terms rather than two. The number of such types grows very rapidly with r, and as an aid we introduce certain graphs associated with the terms of (8). These graphs reflect completely the intersection properties of the sets $B(x_1), \ldots, B(x_n)$. For $r = 3$ there are five such graphs corresponding to the five types enumerated in (9). These are given in Fig. 1 together with the corresponding B-configurations. (It is, of course, assumed that $n > 2$.)

Each graph is of the following kind:

(*i*) No vertex is isolated.
(*ii*) No pair of vertices is connected by more than one edge.

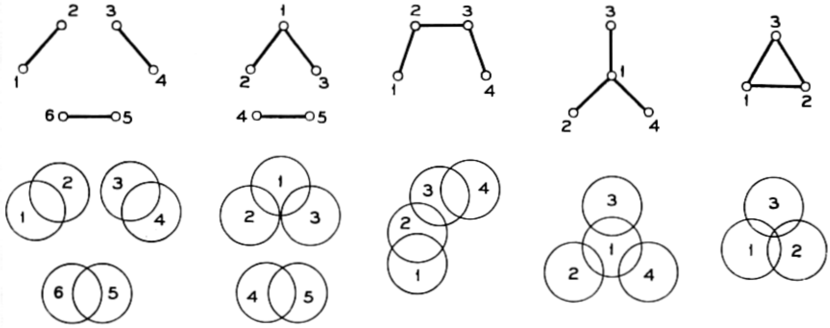


Fig. 1 — Coincidence graphs, $r = 3$.

(*iii*) No edge connects a vertex to itself.
(*iv*) There are exactly r edges.
(*v*) There are exactly v vertices.

One further, and crucial, condition is added:

(*vi*) If the v vertices are enumerated in some order then there exists a configuration of v translates $B_1, \cdots, B_v$ of B, such that B_i and B_j intersect if and only if the i^{th} and the j^{th} vertices are connected by an edge.

For the sake of convenience we make here the following convention: two convex m-dimensional bodies will be said to intersect only if their intersection is itself m-dimensional, otherwise they are to be regarded as disjoint. The reason for this is that we are interested in purely metric properties: the intersections of such sets serve as domains of integration for well-behaved functions in E^m.

A graph satisfying conditions *i* through *vi* will be called a (B, r, v)-graph, one satisfying *i* through *iv* and *vi* a (B, r)-graph, and one satisfying *i* through *iii* and *vi* a B-graph. It must be emphasized that the condition *vi* is not of the usual graph-theoretic kind and it prevents many graphs from being B-graphs. For instance, let $m = 2$ and let B be a circular disk. Since a disk in E^2 cannot intersect six congruent pairwise disjoint disks, the graphs of Fig. 2 are not B-graphs.

The proof of the above assertion for the graph of Fig. 2b is obtained by showing that here the "extreme" configuration is that of Fig. 3.

Similarly, when $m = 2$ and B is a square then B cannot intersect five pairwise disjoint translates of itself (for each translate contains

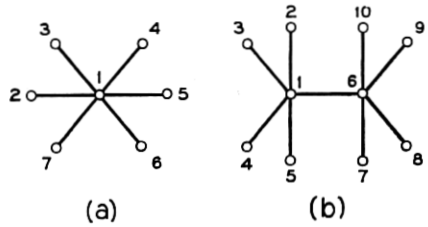


Fig. 2 — Graphs which are not B-graphs. (B is a disk.)

a vertex of B) so that the graph of Fig. 4a is not a B-graph. On the other hand, the graph of Fig. 4b, which corresponds to that of Fig. 2b, is a B-graph as shown by the configuration of Fig. 4c.

Returning to the evaluation of K_r, we start with (8b). Summation there extends over all the

$$\binom{\binom{n}{2}}{2}$$

distinct r-tuples of pairs of indices where for each pair $(i_s, j_s) 1 \leqq i_s < j_s \leqq n$; r-tuples differing only in the order of pairs are not considered distinct. We can now associate the terms of (8b) in a 1 : 1 fashion with the distinct (B, r)-graphs on some n vertices $w_1, \cdots, w_n$. Given a B-graph G let

$$S(G) = \bigcap S_{ij}, \tag{10}$$

where the intersection is taken over all pairs (i, j) for which w_i is connected to w_j by an edge in G. Then (8b) may be written as

$$K_r = \sum_G \int_{S(G)} \prod_{i=1}^{n} f(x_i)\, dV, \tag{11}$$

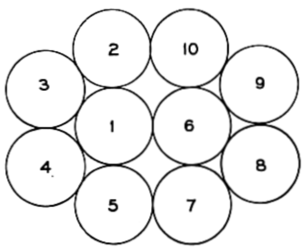


Fig. 3 — An extreme B-configuration.

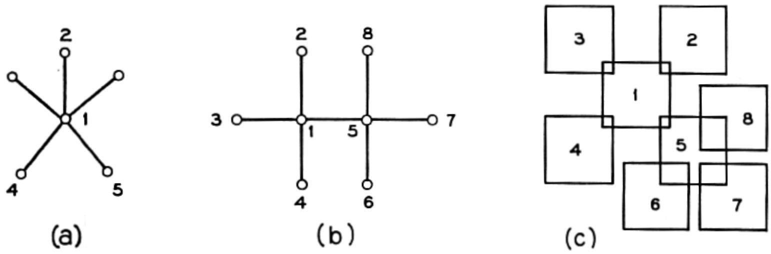


Fig. 4 — Configurations when B is a square.

the summation running over all distinct (B, r)-graphs on n vertices.

Let $v(G)$ denote the number of vertices of G and $C(G)$ a connected component of G. Since the integrand in (11) is completely separable, the integral over $S(G)$ splits into a product of integrals over the connected components and we get

$$K_r = \sum_G J_0^{n-v(G)} \prod_{C(G)} J[C(G)]. \tag{12}$$

Here $J[C(G)]$ is an integral over the connected component and the product is taken over all such components of G. Two examples of integrals $J[C(G)]$ are given in (7b). Owing to the congruence of all the paradiagonal slabs and the form of the integrand, it is not necessary to sum in (12), over all (B, r)-graphs on the vertices $w_1, \ldots,$ w_n, but only over their types.

Suppose that there are exactly $t = t(r)$ types of such graphs and let G_j be any one of the j^{th} type; let also $N_{rj}(n)$ be the number of different (B, r)-graphs on the vertices $w_1, \ldots, w_n$, of the j^{th} type. Then (12) becomes

$$K_r = \sum_{j=1}^{t(r)} N_{rj}(n) J_0^{n-v(G_j)} \prod_{C(G_j)} J[C(G_j)]. \tag{13}$$

Thus the problem of evaluating J has been reduced through (4) and (13) to: the geometrical problem of determining the types of (B, r)-graphs, the combinatorial problem of calculating the coefficients $N_{rj}(n)$, and the analytical problem of evaluating the cluster-integrals over the connected (B, r)-graphs.

V. MULTIPLE COINCIDENCE WITH SEPARABLE INTEGRAND

Formulae analogous to those of the previous section will now be obtained for the case of p-tuple coincidence. Subject to general conditions,

A, B, n, and m are arbitrary and F is of the separable form (5). An integer p is fixed ($2 \leqq p \leqq n$) and the configuration condition is: $u = (x_1, \cdots, x_n) \varepsilon Y$ if and only if there are p indices $i_1, \cdots, i_p (1 \leqq i_1 < \cdots < i_p \leqq n)$ such that

$$\bigcap_{s=1}^{p} B(x_{i_s}) \neq \phi.$$

We observe here our convention that the intersection must be itself m-dimensional. We introduce the analogs of paradiagonal sets and slabs:

$$H_{i_1 \cdots i_p} = \left\{ (x_{i_1}, \cdots, x_{i_p}) : \bigcap_{s=1}^{p} B(x_{i_s}) \neq \phi \right\},$$

$$S_{i_1 \cdots i_p} = \left\{ (x_1, \cdots, x_n) \quad : \bigcap_{s=1}^{p} B(x_{i_s}) \neq \phi \right\},$$

we let $M = \binom{n}{p}$, and we re-enumerate the M sets $S_{i_1, \cdots, i_p}$ with a single index k as $\{S_k\}$, $1 \leqq k \leqq M$. Then we get a formula analogous to (4):

$$J = \int_Y F\, dV = \sum_{r=1}^{n} (-1)^{r+1} \left[\sum_{1 \leqq k_1 < \cdots < k_r \leqq M} \cdots \sum \int_{S_{k_1} \cap \cdots \cap S_{k_r}} F\, dV \right]$$

$$= \sum_{r=1}^{n} (-1)^{r+1} U_r \,. \qquad (14)$$

As in (6a) we let

$$M_{11} = M, \quad \int_A f(x)\, dx = J_0 \,, \quad \int_{H_{12 \cdots p}} \prod_{1}^{p} f(x_i)\, dx_1 \cdots dx_p = J_{11} \,,$$

to get

$$U_1 = M_{11} J_0^{n-p} J_{11} \,.$$

In terms of p-tuple indices the second term U_2 of (14) is

$$U_2 = \sum_{(i_1, \cdots, i_p)} \sum_{(j_1, \cdots, j_p)} \int_{S_{i_1 \cdots i_p} \cap S_{j_1 \cdots j_p}} \prod_{1}^{n} f(x_i)\, dV.$$

The summation extends over the $\binom{n}{2}$ distinct pairs of p-tuples. We have now p types of such pairs, depending on the number of shared indices, which may be 0, 1, $\cdots$, or $p - 1$. Let M_{2j} be the number of p-tuple pairs of type j (that is, with $j - 1$ indices shared) and put

$$J_{2j} = \int_{H_{12 \cdots p} \cap H_{p+2-j \cdots 2p-j+1}} \prod_{i=1}^{2p-j+1} f(x_i)\, dx_1 \cdots dx_{2p-j+1} \,,$$

then

$$U_2 = \sum_{j=1}^{p} N_{2j} J_0^{n-2p+j-1} J_{2j} .$$

Observe that the integral J_{21} splits into a product: $J_{21} = J_{11}^2$. To get an expression for arbitrary U_r we introduce a higher-dimensional equivalent of B-graphs. Let X be a regular simplex in E^{n-1} on the vertices $w_1, \cdots, w_n$. On account of properties *i* through *iii* listed in Section IV, a (B, r)-graph is simply a set of certain r edges (or one-dimensional faces) of X. A d-dimensional hypergraph G will be just a set of some of the $\binom{n}{d+1}$ d-dimensional faces of X. This takes care of properties *i* through *iii*. When there are r such faces in G we shall speak of an (r)-hypergraph and when these faces comprise between them v vertices of X, G will be called an (r, v)-hypergraph.

An equivalent of the important condition (*vi*) is very naturally obtained: there is a B-configuration of v translates $B_1, \cdots, B_v$ of B, such that any $d + 1$ of them, say, $B_{i_1,\ldots,i_{d+1}}$ intersect if and only if $w_{i_1}, \cdots, w_{i_{d+1}}$ are the vertices of a d-dimensional face of X included in G. Components, types, and so on, for (B, r)-hypergraphs are defined in the same way as before. For instance, a hypergraph G is connected if no plane disjoint from it can strictly separate some of its d-faces from others. All quantities such as $C(G)$ and $v(G)$ have the same meaning as before. Let $t = t(r, d)$ be the number of different types of (B, r)-hypergraphs, let G_j be any one hypergraph of the j^{th} type, and let $M_{rj}^d(n)$ be the number of different (B, r)-hypergraphs of the j^{th} type on the n vertices. Then, proceeding as before, we get the equivalent of (13):

$$U_r = \sum^{t(r,p-1)} M_{rj}^{p-1}(n) J_0^{[n-v(G_j)]} \prod_{C(G_j)} J[C(G_j)]. \tag{15}$$

VI. SOME COMBINATORIAL PROPERTIES OF B-GRAPHS AND B-HYPERGRAPHS

Let $\varphi(r)$ and $\psi(r)$ be the smallest and the largest number of vertices, respectively, in a (B, r, v)-graph G. From conditions *i* through *iii* we have at once $\psi(r) = 2r$. G is then minimally connected with r components (Fig. 5a). Suppose that r is a triangular number: $r = s(s-1)/2$; there is then a complete graph on s vertices which is clearly a B-graph for any B, so that $s = v$. If r is not a triangular number let $t(t-1) < 2r < t(t+1)$ and put $e = r - t(t-1)/2$.

Let G be the complete graph on t vertices. For the corresponding B-configuration we may assume that the translates $B_1, \cdots, B_t$ of B

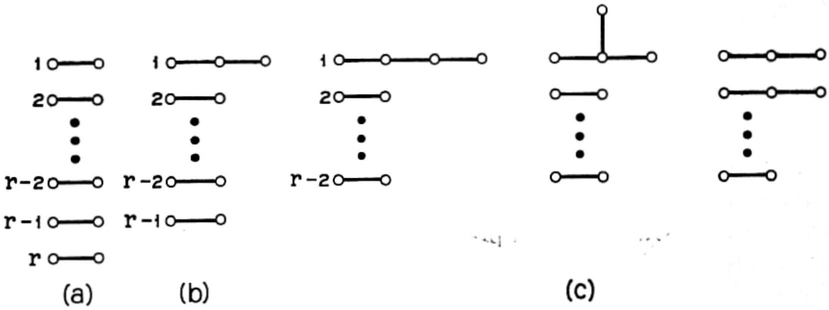


Fig. 5 — (B, r, v)—graphs with high v.

have an interior point in common. We check that $e < t$ and that $B_1, \cdots, B_t$ may be arranged so that a point $z \in \bigcap_1^e B_i$ can be strictly separated from $\bigcup_{e+1}^t B_i$ by a plane P. Let B_{t+1} be a translate of B which contains z and lies strictly on the same side of P as z. Then the resulting B-configuration $B_1, \cdots, B_{t+1}$ corresponds to a (B, r, v)-graph G with $v = t + 1$. This G may be said to be a maximally connected (B, r, v)-graph. We have now

$$\psi(r) = 2r, \qquad \varphi(r) = \min_j \{j : j \geqq [1 + (1 + 8r)^{\frac{1}{2}}]/2\}.$$

Similarly, let $\varphi(r, d)$ and $\psi(r, d)$ be the corresponding minimum and maximum of v for a (B, r, v)-hypergraph. Then clearly $\psi(r, d) = (d + 1)r$. To determine $\varphi(r, d)$ we suppose first that $r = \binom{s}{d+1}$. There is then a complete hypergraph on s vertices, consisting of all the d-dimensional faces of an $(s - 1)$-dimensional simplex. This hypergraph is a B-hypergraph for any B and so $v = s$. If

$$\binom{t}{d+1} < r < \binom{t+1}{d+1}$$

we proceed as before and find that $v = t + 1$. Hence

$$\psi(r, d) = (d + 1)r, \ \varphi(r, d) = \min_j \{j :$$
$$j \geqq \text{largest pos. root of } x(x - 1) \cdots (x - d) = (d + 1)!r\}.$$

The bounds $\varphi(r)$ and $\psi(r)$ lead us to the possibility of a combinatorial identity

$$\binom{\binom{n}{2}}{r} = \sum_{k=\varphi(r)}^{\psi(r)} A_{rk} \binom{n}{k} \tag{16}$$

and its relation to B-graphs and the numbers $N_{rj}(n)$. For instance, we find for $r = 2$

$$\binom{\binom{n}{2}}{2} = 3\binom{n}{4} + 3\binom{n}{3},$$

$\binom{\binom{n}{2}}{2}$ is the total number $N_{21} + N_{22}$ of graphs of (7a) and

$$3\binom{n}{4} = N_{21}, \qquad 3\binom{n}{3} = N_{22}.$$

To prove the validity of an expansion like (16) for all n observe that the left-hand side is a polynomial in n of degree $2r = \psi(r)$ so that

$$\binom{\binom{n}{2}}{r} = \sum_{k=0}^{2r} A_{rk}\binom{n}{k}.$$

Further, $A_{rk} = 0$ for $k < \varphi(r)$, for we substitute successively $n = 0, 1, \cdots, \varphi(r) - 1$ in (16) and recall that $\binom{p}{r} = 0$ for $p < r$. By expanding both sides of (16) in powers of n and comparing the coefficients we find

$$A_{r\,2r} = (2r)!/2^r r!, \quad A_{r\,2r-1} = (2r-1)!/2^{r-1}(r-2)!,$$
$$A_{r\,2r-2} = (2r-2)!(3r-1)/3.2^{r-1}(r-3)!$$

and so on. Therefore (16) may be written as

$$\binom{\binom{n}{2}}{r} = (n)_{2r}/(2^r r!) + (n)_{2r-1}/[2^{r-1}(r-2)!]$$
$$+ (n)_{2r-2}/[3.2^{r-1}(r-3)!\,(3r-1)] + \cdots \qquad (17)$$
$$= \sum_{i=0}^{2r-\varphi(r)} (n)_{2r-i}/D_i .$$

$(n)_p$ stands for $n(n-) \ldots (n-p+1)$.

The denominators D_i have the following interpretation. Consider first the $(B, r, 2r)$-graph of Fig. 5a. The $2r$ vertices can be chosen out of $w_1, \ldots, w_n$ *in* $(n)_{2r}$ ways. We define the symmetry number for a (B, r, v)-graph to be the number of ways in which its vertices can be labelled with integers $1, 2, \ldots, v$, all of which ways are to correspond to the same B-configuration. Here the symmetry number is $2^r r!$, as there are 2^r ways of permuting the labels on the two vertices of a component and $r!$ ways of permuting their components. This leads us to the first term $(n)_{2r}/2^r r!$ in (17) which is precisely the number $N_{r1}(n)$ of (13) provided that we consider G_1 in (13) to be of the type of Fig. 5a.

Similarly, for the $(B,r,2r-1)$-graph of Fig. 5b we find the symmetry number to be $2^{r-1}(r-2)!$. The number of ways to choose the $2r-1$ vertices is $(n)_{2r-1}$ and so we get the second term $(n)_{2r-1}/2^{r-1}(r-2)!$ of (17). The situation gets somewhat more complicated for the $(B,r,2r-2)$-graphs. Here we have three types instead of one, illustrated in Fig. 5c. The $2r-2$ vertices can be selected in $(n)_{2r-2}$ ways, the symmetry numbers for the three types are

$$2^{r-2}(r-3)!, \quad 3.2^{r-2}(r-3)!, \text{ and } 2^{r-1}(r-4)!. \tag{18}$$

Therefore, the corresponding numbers of graphs, say $N_{r3}(n)$, $N_{r4}(n)$, $N_{r5}(n)$ are

$$(n)_{2r-2}/[2^{r-2}(r-3)!], \ (n)_{2r-2}/[3.2^{r-2}(r-3)!], \ (n)_{2r-2}/[2^{r-1}(r-4)!]$$

and their sum is precisely the third term of (17). The corresponding denominator D_2 is therefore three times the harmonic mean of the three symmetry numbers in (18).

Thus the first few terms of (17) give the total numbers

$$\sum_j N_{rj}(n)$$

of (B,r,v)-graphs for $v = 2r, 2r-1$, and so on. However, this pleasing circumstance breaks down as soon as we reach the smallest term i for which one of the types of graphs in question is not a B-graph.

For the case $m = 2$, B a circular disk, this occurs for $i = 7$ and the graph in question is then that of Fig. 2a together with other components containing one edge each. When B is a square the graph of Fig. 4a shows that the breakdown occurs for $i = 6$. On the other hand, the quantity $(n)_{2r-i}/D_i$ from (17) always provides an upper bound for the sum $\sum N_{rj}(n)$, the summation extending over all types j of $(B, r, 2r - i)$-graphs.

The explicit form of (16) is

$$\binom{\binom{n}{2}}{r} = \sum_{k=q}^{2r} A_{rk}\binom{n}{k} \tag{19}$$

where $q = \varphi(r)$ and

$$A_{rk} = \sum_{j=0}^{k-q} (-1)^j \binom{k}{j}\binom{\binom{k-j}{2}}{r}. \tag{20}$$

We prove (2) by induction on k. For $k = q$, (20) holds, suppose it to be proved for $k \leqq q + s - 1$. Let $n = q + s$ in (19), then

$$A_{rq+s} = \binom{\binom{q+s}{2}}{r} - \sum_{i=0}^{s-1} \binom{q+s}{q+i} A_{rq+i}$$

which by the induction hypothesis may be written as

$$A_{rq+s} = \binom{\binom{q+s}{2}}{r} - \sum_{i=0}^{s-i} \sum_{j=0}^{i} (-1)^j \binom{q+s}{q+i} \binom{\binom{q+i-j}{2}}{r}.$$

In the double sum we may sum first over those terms for which the difference $u = i - j$ is constant, then over u. In this way one gets

$$A_{rq+s} = \binom{\binom{q+s}{2}}{r} + \sum_{u=0}^{s-1} (-1)^{s-u} \binom{q+s}{q+u} \binom{\binom{q+s}{2}}{r}$$

which after some simple algebra becomes (20) with $k = q+s$. This completes the induction and the proof of (20).

Some combinatorial identities may be obtained from the above. For example, we know that $A_{r2r} = (2r)!/2^r r!$. Hence, on putting $k = 2r$ in (20), we get

$$\sum_{j=0}^{2r-q} (-1)^j \binom{2r}{j} \binom{\binom{2r-j}{2}}{r} = (2r)!/2^r r!. \tag{21}$$

Similarly, with $k = 2r - 1$ and $k = 2r - 2$ we get

$$\sum_{j=0}^{2r-q-1} (-1)^j \binom{2r-1}{j} \binom{\binom{2r-j-1}{2}}{r} = (2r-1)!/2^{r-1}(r-2)! \tag{22}$$

and

$$\sum_{j=0}^{2r-q-2} (-1)^j \binom{2r-2}{j} \binom{\binom{2r-j-2}{2}}{r} = [(2r-2)!\,(r-1/3)]/2^{r-1}(r-3)!. \tag{23}$$

For hypergraphs we have the identity

$$\binom{\binom{n}{d}}{r} = \sum_{k=q}^{dr} A_{rk}(d) \binom{n}{k} \tag{24}$$

where $q = \varphi(r,d)$. The explicit expression for the coefficients $A_{rk}(d)$ can be found in the same way as (20):

$$A_{rk}(d) = \sum_{j=0}^{k-q} (-1)^j \binom{k}{j} \binom{\binom{k-j}{d}}{r}. \tag{25}$$

Some of the higher coefficients $A_{r\,dr}$, $A_{r\,dr-1}$, . . . can be evaluated by comparing the powers of n in (24):

$$A_{r\,dr}(d) = (dr)!/r!(d!)^r, \quad A_{r\,dr-1}(d) = (dr)!d(r-1)/2.r!(d!)^r$$

and so on, so that by putting $k = rd$ and $k = rd - 1$ in (25) we get

$$\sum_{j=0}^{dr-q} (-1)^j \binom{\binom{dr-j}{d}}{r} = (dr)!/r!\,(d!)^r \tag{26}$$

and

$$\sum_{j=0}^{dr-q-1} (-1)^j \binom{dr-1}{j} \binom{\binom{dr-j-1}{d}}{r} = (dr)!\,d(r-1)/2.r!\,(d!)^r. \tag{27}$$

The coefficients $A_{kr}(d)$ have the same interpretation with hypergraphs as the A_{kr} have with ordinary graphs, and they refer to symmetry numbers.

VII. SIMPLE COINCIDENCE IN A CUBE

We consider here the problem of evaluating the probability $P(n,a,L)$ that when n points are taken at random (uniform distribution) in a three-dimensional cube of edge-length L, then no two points are closer than a. The problem occurs in deriving the van der Waals equation from a primitive hard-sphere gas model. See, for instance, Ref. 2, where the problem is termed "very difficult" and the crude (though sufficient) approximation

$$P(n, a, L) \cong \prod_{j=1}^{n-1} (1 - 4\pi j a^3/3L^3) \cong 1 - 2\pi n^2 (a/L)^3/3 \tag{28}$$

is used.

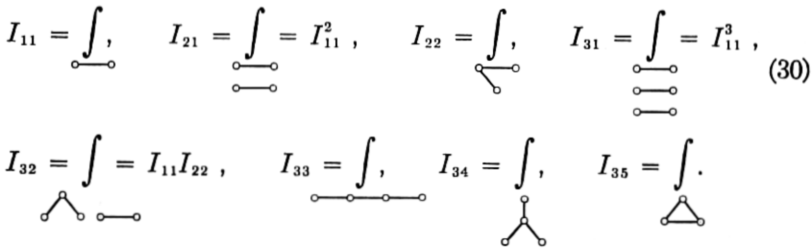
From our formulation we find that

$$L^{3n}[1 - P(n, a, L)]$$

is the J integral for the case $m = 3$, A is a cube of volume L^3, B a ball of radius $a/2$, and the configuration condition is that not all sets $B(x_i)$ be disjoint; in other words, a simple coincidence. Therefore by (4), (13), and an inspection of Fig. 1 we have

$$\begin{aligned} L^{3n}[1 - P(n, a, L)] = {} & N_{11}L^{3n-6}I_{11} - (N_{21}L^{3n-12}I_{21} + N_{22}L^{3n-9}I_{22}) \\ & + (N_{31}L^{3n-18}I_{31} + N_{32}L^{3n-15}I_{32} + N_{33}L^{3n-12}I_{33} \\ & + N_{34}L^{3n-12}I_{34} + N_{35}L^{3n-9}I_{35}) - \cdots \end{aligned} \tag{29}$$

where the integrals I_{11}, I_{21}, . . . can be symbolically represented as follows



$$I_{11} = \int, \quad I_{21} = \int = I_{11}^2, \quad I_{22} = \int, \quad I_{31} = \int = I_{11}^3, \tag{30}$$

$$I_{32} = \int = I_{11}I_{22}, \quad I_{33} = \int, \quad I_{34} = \int, \quad I_{35} = \int.$$

To obtain an explicit Cartesian expression for an integral, I, we consider its signature graph G which is a (B,r,v)-graph. If the v vertices are enumerated as 1,2, . . . , v in an arbitrary order then I becomes a $3v$-tuple integral

$$I = \int \underset{R_I}{\cdots} \int dr_1 \cdots dr_v \tag{31a}$$

where r_i is the vector (x_i, y_i, z_i), dr_i stands for $dx_i\, dy_i\, dz_i$, and the region of integration R_I is given by $3v + r$ inequalities:

$$0 \leqq x_i \leqq L,\ 0 \leqq y_i \leqq L,\ 0 \leqq z_i \leqq L,\ (i = 1, \cdots, v), \tag{31b}$$

$$|r_i - r_j|^2 \leqq a^2 \text{ if the } i^{\text{th}} \text{ and the } j^{\text{th}} \text{ vertices are connected} \tag{31c}$$

in G by an edge.

Further, such an integral occurs in (29) with the multiplier $N_{rj}L^{3n-3v}$ where N_{rj} is the number of distinct graphs on n vertices, which are of the same type as G. Together with each such integral $I = I_{pq}$ we may also consider the corresponding integral K_{pq} given by

$$K_{pq} = \int \underset{Q_I}{\cdots} \int dr_1 \cdots dr_v,$$

where the region Q_I is given by the $(v^2 + 5v)/2$ inequalities (31b), (31c) and

$$|r_i - r_j|^2 \geqq a^2 \text{ if the } i^{\text{th}} \text{ and the } j^{\text{th}} \text{ vertices are not connected in } G \tag{31d}$$

by an edge.

It turns out that the I integrals are expressible in terms of the K integrals, and conversely. For instance, consider the K integral with the signature graph which has four vertices 1, 2, 3, and 4, and edges

12, 13, 23, and 24. We write it in a self-explanatory terminology as

$$(12)(13)(23)(24)[1 - (14)][1 - (34)]$$

and multiply this out to get

$$(12)(13)(23)(24) - (12)(13)(23)(24)(14) - (12)(13)(23)(24)(34) + (12)(13)(23)(24)(14)(24)(34)$$

which yields at once a representation of K as a sum of four I-integrals.

The first integral I_{11} is sixtuple and can be reduced to an iterated integral as follows:

$$I_{11} = \int_{m_6}^{M_6} \cdots \int_{m_1}^{M_1} dx_1\, dx_2\, dy_1\, dy_2\, dz_1\, dz_2 \tag{32}$$

where

$$m_2 = m_4 = m_6 = 0, \quad M_2 = M_4 = M_6 = L$$

and

$$\begin{aligned}
m_1 &= \max \{0, x_2 - [a^2 - (y_1 - y_2)^2 - (z_1 - z_2)^2]^{\frac{1}{2}}\}, \\
m_1 &= \min \{L, x_2 + [a^2 - (y_1 - y_2)^2 - (z_1 - z_2)^2]^{\frac{1}{2}}\}, \\
m_3 &= \max \{0, y_2 - [a^2\}(z_1 - z_2)^2]^{\frac{1}{2}}\}, \\
M_3 &= \min \{L, y_2 + [a^2 - (z_1 - z_2)^2]^{\frac{1}{2}}\}, \\
m_5 &= \max \{0, z_2 - a\}, \\
M_5 &= \min \{L, z_2 + a\}.
\end{aligned}$$

This arrangement of the limits of integration corresponds to taking two balls of radii $a/2$ and centers (x_1, y_1, z_1) and (x_2, y_2, z_2), and letting the center of the first ball move freely over the cube while the coordinates of the second center vary so that the balls intersect. Accordingly, I_{11} has a simple probabilistic interpretation: $I_{11} = L^6[1 - P(2,a,L)]$, where $P(2,a,L)$ is the probability that two points taken at random in the cube of edge-length L are no nearer than a. Similar probabilistic interpretation holds for any other K integral. If G is its (B,r,v)-graph then K *is* L^{3v} times the probability that when v balls of radius $a/2$ are taken with their centers at random in the cube, then the balls are in the configuration of G (so that two of them intersect if and only if the corresponding vertices of G are connected by an edge).

We evaluate now the integral (32) subject to the condition $a \leqq L$.

Integration with respect to x_1 and x_2 gives

$$L^2 - [\max(0, L - D)]^2 \tag{33}$$

where

$$D^2 = a^2 - (y_1 - y_2)^2 - (z_1 - z_2)^2.$$

Since $a \leqq L$ we have $D \leqq L$ and therefore (33) is $2LD - D^2$. Integrating this with respect to y_1 and y_2 we get first, on putting $y_1 - y_2 = u$,

$$\int_0^L \int_{-m}^M [2L(b^2 - u^2)^{\frac{1}{2}} - (b^2 - u^2)]\, du\, dy_2$$

where

$$b^2 = a^2 - (z_1 - z_2)^2,\ m = \min(y_2, b),\ M = \min(L - y_2, b).$$

Again, $a \leqq L$ implies $b \leqq L$ and the double integral is therefore

$$\pi L^2 b^2 - 8Lb^3/3 + b^4/2.$$

Finally, integrating with respect to z_1 and z_2 we get

$$I_{11} = 4\pi a^3 L^3/3 - 3\pi a^4 L^2/2 + 8a^5 L/5 - a^6/6, \quad 0 \leqq a \leqq L. \tag{34}$$

There are two more forms of I_{11}, corresponding to the ranges $L \leqq a \leqq 2^{\frac{1}{2}}L$ and $2^{\frac{1}{2}}L \leqq a \leqq 3^{\frac{1}{2}}L$, but they do not appear to be expressible in terms of elementary or standard transcendental functions. It may be observed that the leading term in (34) is the product of the volumes of the cube and the ball of radius a.

To get a better approximation to $P(n,a,L)$ than (28), we examine (29) and find that for small a every integral I_{ij}, beyond I_{11}, is $O(a^6)$. Therefore

$$P(n, a, L) = 1 - \binom{n}{2}[4\pi/3(a/L)^3 - 3\pi/2(a/L)^4 + 8/5(a/L)^5] + O[(a/L)^6]. \tag{35}$$

It is possible to find the exact limit of $P(n,a,L)$ as

$$n \to \infty,\ a \to 0,\ (4\pi/3)(n^2/2)(a^3/L^3) \to b.$$

For we have then $P(n,a,L) = P(b)$ and

$$1 - P(b) = N_{11}I_{11}/L^6 - N_{21}I_{21}/L^{12} + N_{31}I_{31}/L^{18} - \cdots$$

and

$$N_{k1} \cong \binom{\binom{n}{2}}{k} \cong n^{2k}/2^k k^2$$

$$I_{k1} = (I_{11})^k.$$

This amounts to neglecting all graphs other than the "principal" one, for each k, that is, the one corresponding to the configuration of Fig. 5a. Hence

$$1 - P(b) = \sum_{j=1}^{\infty} (-1)^{j+1}[(4\pi/3)(n^2/2)(a/L)^3]^j/j! = 1 - e^{-b}$$

so that

$$P(b) = e^{-b}. \tag{36}$$

VIII. NUMERICAL EVALUATION OF THE I-INTEGRALS

Since no I integral beyond I_{11} appears to be explicitly evaluable in terms of standard functions, the possibility was investigated of computing those integrals numerically by the Monte Carlo method. The first set of trial calculations was performed on I_{11} itself, in order to be able to compare the results with the known true value. We assume as before that $a \leq L$ and we put $L = 1$ (homogeneity!) to get

$$I_{11}(a) = 4.1888a^3 - 4.7129a^4 + 1.6000a^5 - 0.1667a^6, \quad 0 \leqq a \leqq 1.$$

We now choose a suitable integer M and set the value of a at $1/M$. Next, two points $p_1(x_1, y_1, z_1)$ and $p_2(x_2, y_2, z_2)$ are taken at random in the unit cube by choosing each coordinate to be a random number from the rectangular distribution on [0, 1]. Such pairs of random points are selected N times; suppose that in N_1 of them the distance between the random points does not exceed $1/M$, then the quotient N_1/N is taken as the Monte-Carlo approximation to $I_{11}(1/M)$. Then the whole procedure is repeated with $1/M$ replaced by $2/M$, $3/M$, and so on, until the value $3^{1/2}$ is passed. The whole calculation will be referred to as an N by M Monte Carlo run.

In the first set of trial computations N by M Monte Carlo runs were executed for various values of N and M, and in each case a least-squares fit was done on these data by a polynomial of the form

$$\sum_{j=3}^{6} A_j a^j.$$

The results are shown in Table 1.

TABLE I—FIRST TRIAL COMPUTATIONS

	True value of A_j	4.1888	−4.7129	1.6000	−0.1667
1st	1000 by 20 run	3.1873	−1.0742	−2.5488	1.3448
2nd	1000 by 20 run	3.3296	−1.6727	−1.9088	1.1584
	10000 by 20 run	4.4765	−5.9918	3.4012	−0.9760
	1000 by 200 run	4.3008	−5.2689	2.4437	−0.5641
	10000 by 200 run	4.1974	−4.7337	1.6358	−0.1911
	100000 by 20 run	4.1546	−4.5615	1.4043	−0.0879

It appears from this polynomial that very long and large runs are necessary to determine the coefficients with fair accuracy. However, the values of the integral itself can be computed quite well. To check this we have computed the standard deviations, both for the Monte Carlo data, from

$$\sigma_1^2 = 1/M \sum_{j=1}^{M} [(N_j/N) - I_{11}(j/M)]^2$$

and for the least squares fit from

$$\sigma_2^2 = 1/M \sum_{j=1}^{M} [\bar{I}_{11}(j/M) - I_{11}(j/M)]^2$$

where

$$\bar{I}_{11}(a) = \sum_{j=3}^{6} A_j a^j$$

is the least-squares fit to I_{11}. The results are shown in Table 2.

As a compromise between accuracy and length of the Monte Carlo run, the values $N = 10000$ and $M = 20$ were selected. In this way there were computed the two integrals I_{31} and I_{32} corresponding to the two $(B,r,3)$-graphs, the six integrals $I_{41}, \ldots, I_{46}$ corresponding to the six $(B,r,4)$-graphs, and the 21 integrals $I_{51}, \ldots, I_{521}$ corresponding to the 21 $(B,r,5)$-graphs. The first two series are shown in Figs. 6 and 7. The programming was quite simple and no details need be given. The total time taken up on the CDC 6600 computer was about one hour; this, however, includes a lot of trial runs and tests.

TABLE II—STANDARD DEVIATIONS

N	Monte Carlo σ_1	Least Squares σ_2
1000	0.01154	0.00753
10000	0.00257	0.00183
100000	0.000922	0.000554

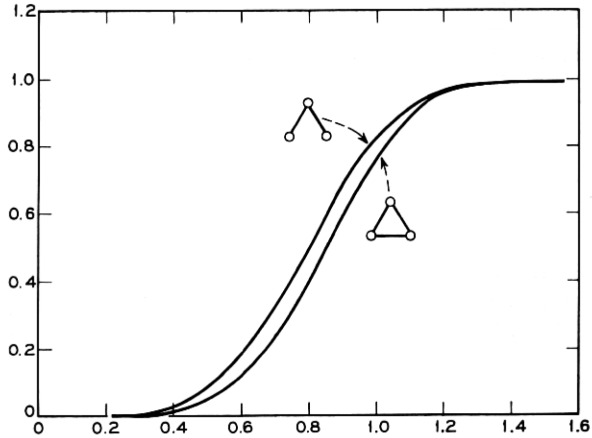


Fig. 6 — Cluster integrals for $v = 3$.

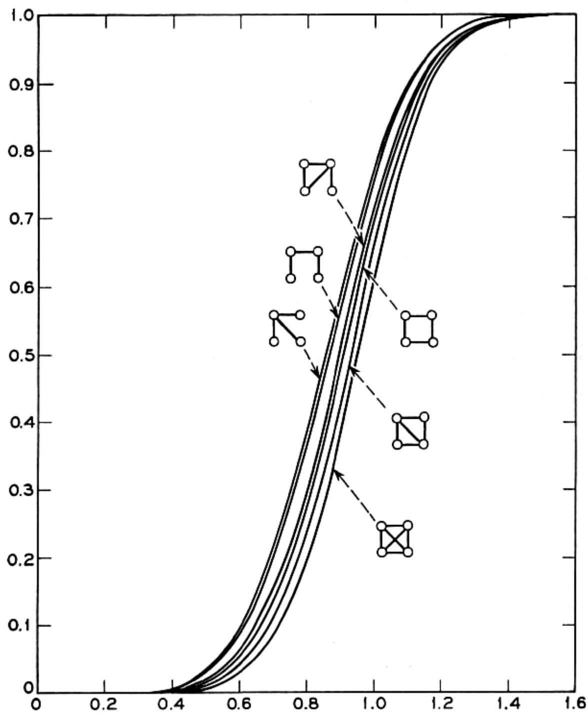


Fig. 7 — Cluster integrals for $v = 4$.

To sum up, it appears that numerical computation of J-type integrals is quite feasible, with the help of an automatic computer, to fairly good approximation. One well known advantage of the Monte Carlo method of evaluating multiple integrals was clearly brought out; namely, its relative independence of the dimension.

IX. ACKNOWLEDGEMENTS

Professors M. Bloom, L. Sobrino, and W. Opechowski, of the Physics Department, University of British Columbia, discussed with the author certain physical problems which led to the general formulation of Section 1. Dr. Max Goldstein, director of the A. E. C. Computation Laboratory at New York University, and his staff, helped with programming and with their CDC 6600 computing machine. Dr. Frank Stillinger of Bell Telephone Laboratories, Murray Hill, pointed out a serious error in the original use of the inclusion-exclusion principle, and suggested the correct version.

The work reported was started while the author was on leave from the University of British Columbia for the year 1966–67 at the Courant Institute of Mathematical Sciences, New York University. During that time he held a Senior Fellowship of the National Research Council. The work was continued while the author was visiting Bell Laboratories in the summer of 1967. I sincerely thank all these persons and institutions.

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