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On a probability distribution function arising in stochastic neutron transport theory

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Abstract

In a recently developed method for understanding the transport of neutrons in spatially stochastic media, it is necessary to prescribe a random distribution for the fissile lumps. In most practical cases the lumps are assumed to be uniformly distributed within the container. However, the associated centre-to-centre separation distances are not uniformly distributed and this paper describes a method for calculating that distribution function. Two methods are used: an analytical approach which is exact for lumps of zero size and a numerical simulation which accounts for finite size and excludes the possibility of more than one particle occupying the same space.

The numerical simulations are compared with the analytical expression and we find excellent agreement for small spheres, which in the limit will be exact. Deviations from the theoretical curve become larger as the sphere becomes larger and size effects become significant.

Results are presented for a rectangular box, spherical container, square and one-dimensional rod.

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1. Introduction

In the transport of neutrons in spatially stochastic media, we encounter the problem of calculating the probability distribution function of the separation distances between two points, when the positions of the points themselves are uniformly distributed in a rectangular box of sides L_1, L_2 and L_3 (Williams 2000a, b). An important example of this problem arises in the prediction of the behaviour of fissile and absorbing lumps distributed randomly within a background matrix in a container. Such an arrangement simulates closely a radioactive waste container, the contents of which may only be known within prescribed upper and lower bounds, and for which it is desirable to calculate regulatory safety limits for criticality and for surface dose rate. This is the physical background to the present problem which we now formulate mathematically.

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For an arbitrarily shaped body of volume V, the probability that two points $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ are separated by a distance R is given by

$$P(R) = \int_V \mathrm{d}\boldsymbol{r}_1 \int_V \mathrm{d}\boldsymbol{r}_2\, p\,(\boldsymbol{r}_1, \boldsymbol{r}_2)\, \delta\,(R - |\boldsymbol{r}_1 - \boldsymbol{r}_2|) \tag{1a}$$

where $p\,(\boldsymbol{r}_1,\boldsymbol{r}_2)$ is the probability distribution that the two points lie within the volume V.

In the special case of the rectangular box discussed above, equation (1a) may be written explicitly in Cartesian coordinates as

$$P(R) = \int_0^{L_1} \mathrm{d}x_1 \int_0^{L_1} \mathrm{d}x_2 \int_0^{L_2} \mathrm{d}y_1 \int_0^{L_2} \mathrm{d}y_2 \int_0^{L_3} \mathrm{d}z_1 \int_0^{L_3} \mathrm{d}z_2\, p(x_1, x_2, y_1, y_2, z_1, z_2) \\ \times \delta \left(R - \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2} \right). \tag{1b}$$

In this equation, $P(R)$ is the desired probability distribution function of the separation distance R between the two points with Cartesian coordinates (x_1, y_1, z_1) and (x_2, y_2, z_2). $p(\cdots)$ is the probability distribution that the two Cartesian points lie within the box.

If we assume that

$$p(x_1, x_2, y_1, y_2, z_1, z_2) = p\,(|x_1 - x_2|, |y_1 - y_2|, |z_1 - z_2|) \tag{2}$$

then equation (1) can be reduced to the following simpler result:

$$P(R) = 8 \int_0^{L_1} \mathrm{d}\bar{u}\,(L_1 - \bar{u}) \int_0^{L_2} \mathrm{d}\bar{v}\,(L_2 - \bar{v}) \int_0^{L_3} \mathrm{d}\bar{w}\,(L_3 - \bar{w})\, p\,(\bar{u}, \bar{v}, \bar{w}) \\ \times \delta \left(R - \sqrt{\bar{u}^2 + \bar{v}^2 + \bar{w}^2} \right) \tag{3}$$

which is a general expression for the probability of a separation R. In the present problem, we are concerned with the case when the lumps are distributed uniformly in the box, such that

$$p(x_1, x_2, y_1, y_2, z_1, z_2) = \frac{1}{L_1^2 L_2^2 L_3^2} \qquad (x_i, y_i, z_i) \in (0, L_1) \times (0, L_2) \times (0, L_3). \tag{4}$$

In that case, and scaling variables such that $\bar{u} = uL_1$, $\bar{v} = vL_2$, $\bar{w} = wL_3$, we find

$$P(R) = 8 \int_0^1 \mathrm{d}u\,(1 - u) \int_0^1 \mathrm{d}v\,(1 - v) \int_0^1 \mathrm{d}w\,(1 - w)\, \delta \left(R - \sqrt{u^2 L_1^2 + v^2 L_2^2 + w^2 L_3^2} \right). \tag{5}$$

It is our purpose to obtain an analytical expression for $P(R)$ and to compare it with a numerical result by simulation with random numbers.

2. Reduction to analytical form

We may write the delta function in equation (5) in the following way:

$$\delta \left(R - \sqrt{u^2 L_1^2 + v^2 L_2^2 + w^2 L_3^2} \right) = 2R\delta \left(R^2 - u^2 L_1^2 - v^2 L_2^2 - w^2 L_3^2 \right). \tag{6}$$

Denoting the delta function by a Fourier integral, we have

$$P(R) = \frac{8R}{\pi} \int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}tR^2} H\big(tL_1^2\big) H\big(tL_2^2\big) H\left(tL_3^2\right) \tag{7}$$

where

$$H(t) = \int_0^1 \mathrm{d}u\,(1 - u)\, \mathrm{e}^{-\mathrm{i}tu^2}. \tag{8}$$

We also note from the argument of the delta function that $P(R)$ is non-zero in the range $0 < R < \sqrt{L_1^2 + L_2^2 + L_3^2}$. The maximum value is simply the corner-to-corner distance in the box.

A special case of equation (7) arises when $L_1 = L_2 = L_3 = L$, i.e. we have a cube, then

$$P(R) = \frac{8R}{\pi} \int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}tR^2} H(tL^2)^3 \tag{9}$$

and $0 < R < \sqrt{3}L$.

By the simple transformation $tL^2 = x$, equation (9) may be reduced to

$$P(R) = \frac{1}{L}\frac{8R}{\pi L} \int_{-\infty}^{\infty} \mathrm{d}x\, \mathrm{e}^{\mathrm{i}x(R/L)^2} H(x)^3 = \frac{1}{L} G\left(\frac{R}{L}\right) \tag{10}$$

where $G(R/L)$ is a universal function of R/L. $H(t)$ can be evaluated as

$$H(t) = \int_0^1 \mathrm{d}w \cos(tw^2) - \frac{\sin(t)}{t} + \mathrm{i}\left(\frac{1-\cos(t)}{2t} - \int_0^1 \mathrm{d}w \sin(tw^2)\right). \tag{11}$$

But according to the IMSL mathematical library (IMSL 1998), the Fresnel sine and cosine integrals are defined as

$$S(x) = \int_0^x \mathrm{d}t \sin\left(\frac{\pi}{2}t^2\right) \tag{12}$$

and

$$C(x) = \int_0^x \mathrm{d}t \cos\left(\frac{\pi}{2}t^2\right). \tag{13}$$

We shall adopt these definitions but the reader should be aware of the fact that the definitions in Gradsteyn and Ryzhik (1994) are slightly different such that

$$C_I(x) = C_{GR}\left(\sqrt{\frac{\pi}{2}}x\right) \tag{14}$$

where I refers to IMSL and GR to Gradsteyn and Ryzhik. Similarly for $S(x)$.

Thus we have

$$\begin{aligned} H(t) &= \sqrt{\frac{\pi}{2t}} C\left(\sqrt{\frac{2t}{\pi}}\right) - \frac{\sin(t)}{t} + \mathrm{i}\left(\frac{1-\cos(t)}{2t} - \sqrt{\frac{\pi}{2t}} S\left(\sqrt{\frac{2t}{\pi}}\right)\right) \\ &\equiv H_0(t) + \mathrm{i}H_1(t). \end{aligned} \tag{15}$$

It is then readily shown that

$$P(R) = \frac{16R}{\pi} \int_0^{\infty} \mathrm{d}t \left\{F_0(t)\cos(tR^2) - F_1(t)\sin(tR^2)\right\} \tag{16}$$

where

$$\begin{aligned} F_0(t) = {} & H_0(tL_1^2)\, H_0(tL_2^2)\, H_0(tL_3^2) - H_0(tL_3^2)\, H_1(tL_1^2)\, H_1(tL_2^2) \\ & - H_0(tL_2^2)\, H_1(tL_1^2)\, H_1(tL_3^2) - H_0(tL_1^2)\, H_1(tL_2^2)\, H_1(tL_3^2) \end{aligned} \tag{17}$$

and

$$\begin{aligned} F_1(t) = {} & H_0(tL_2^2)\, H_0(tL_3^2)\, H_1(tL_1^2) + H_0(tL_1^2)\, H_0(tL_3^2)\, H_1(tL_2^2) \\ & + H_0(tL_1^2)\, H_0(tL_2^2)\, H_1(tL_3^2) - H_1(tL_1^2)\, H_1(tL_2^2)\, H_1(tL_3^2). \end{aligned} \tag{18}$$

The special case of a cube reduces to

$$F_0(t) = H_0(tL^2)\left(H_0^2(tL^2) - 3H_1^2(tL^2)\right)$$

$$F_1(t) = H_1(tL^2)\left(3H_0^2(tL^2) - H_1^2(tL^2)\right)$$

whence

$$P(R) = \frac{16R}{\pi L^2}\int_0^\infty \mathrm{d}s\left\{F_0\left(\frac{s}{L^2}\right)\cos\left(s\left(\frac{R}{L}\right)^2\right) - F_1\left(\frac{s}{L^2}\right)\sin\left(s\left(\frac{R}{L}\right)^2\right)\right\}. \tag{19}$$

3. Moments of the distribution

The moments of the distribution can be written directly from equation (3) as

$$\langle R^n\rangle = 8\int_0^{L_1}\mathrm{d}\bar{u}\,(L_1-\bar{u})\int_0^{L_2}\mathrm{d}\bar{v}\,(L_2-\bar{v})\int_0^{L_3}\mathrm{d}\bar{w}\,(L_3-\bar{w})p\,(\bar{u},\bar{v},\bar{w})\left(\bar{u}^2+\bar{v}^2+\bar{w}^2\right)^{n/2}. \tag{20}$$

Alternatively, an expression for the even moments with the uniform distribution for $p(\cdots)$ can be obtained from equation (7) in terms of the generating function,

$$\bar{P}(k) = \int_0^\infty \mathrm{d}R\,\mathrm{e}^{-\mathrm{i}kR^2}P(R) = 8H\left(kL_1^2\right)H\left(kL_2^2\right)H\left(kL_3^2\right). \tag{21}$$

Clearly, $\bar{P}(0) = 1$ as we expect, and

$$\langle R^2\rangle = \mathrm{i}\left.\frac{\partial\bar{P}}{\partial k}\right|_{k=0} = \frac{1}{6}\left(L_1^2+L_2^2+L_3^2\right). \tag{22}$$

For the special case of a cube in which $L_1 = L_2 = L_3 = L$, the calculation of the mean value is more difficult but can be evaluated analytically. Using *Mathematica* (Wolfram 1991), we find

$$\begin{aligned}\frac{\langle R\rangle}{L} = {} & \frac{8+34\sqrt{2}-12\sqrt{3}}{210} - \frac{\pi}{45} + \frac{28}{105}\left(\tan^{-1}\left(\frac{16-17\sqrt{3}}{47}\right) - \cot^{-1}(4)\right)\\ & + \frac{1}{30}\left(8\log\left(\frac{1+\sqrt{3}}{\sqrt{2}}\right) + 4\log\left(1+\sqrt{2}\right)\right.\\ & \left. - 9\log(2) + \log\left(\frac{3+2\sqrt{2}}{2+\sqrt{3}}\right) + 18\log\left(1+\sqrt{3}\right)\right).\end{aligned} \tag{23}$$

The value of this expression is 0.661 707 . . . , the variance is

$$\sigma_R^2 = \langle R^2\rangle - \langle R\rangle^2 = 0.062\,144\ldots L^2 \tag{24}$$

and the standard deviation

$$\sigma_R = 0.249\,29\ldots L. \tag{25}$$

Higher even moments are obtained easily, but the odd ones require some effort.

The case of the distribution function in a rectangle ($L_1 \times L_2$) is an interesting limiting case of equations (16) and (21) and can be obtained by allowing $L_3 \to 0$. The results are

$$\langle R^2\rangle = \tfrac{1}{6}\left(L_1^2+L_2^2\right) \tag{26}$$

which for a square becomes

$$\langle R^2\rangle = \frac{L^2}{3}. \tag{27}$$

For the mean we find

$$\langle R\rangle = \frac{L_1^5+L_2^5}{15L_1^2L_2^2} - \frac{L_1^4+L_2^4-3L_1^2L_2^2}{15L_1^2L_2^2}\sqrt{L_1^2+L_2^2} + \frac{L_1^2}{6L_2}\log\left(\frac{L_2}{L_1}+\sqrt{1+\frac{L_2^2}{L_1^2}}\right) + \frac{L_2^2}{6L_1}\log\left(\frac{L_1}{L_2}+\sqrt{1+\frac{L_1^2}{L_2^2}}\right) \tag{28}$$

which for a square reduces to

$$\langle R\rangle = \frac{L}{15}\left(2+\sqrt{2}+5\log\left(1+\sqrt{2}\right)\right) = 0.521\,405\ldots \tag{29}$$

leading to $\sigma_R^2 = 0.061\,4697\ldots L^2$ or $\sigma_R = 0.247\,931\ldots L$.

It is interesting to note that as $L_1 \to \infty$, i.e. we have a semi-infinite strip, the mean value behaves as

$$\langle R\rangle \to \frac{L_1}{3} \tag{30}$$

i.e. it tends to infinity, but as expected is always less than the diagonal.

4. Simulations

The origin of the probability distribution discussed above stems from a problem arising in neutron transport in spatially stochastic media. In that problem, we assume that there is a container filled with a moderating and absorbing medium. Embedded in this medium are lumps of fissile material positioned randomly. The random position of the lump centroid is chosen by a random number generator. In our case, the Cartesian coordinates defined by the container, which is usually a cubic box, are assumed to be uniformly distributed. More precisely, if the box is of side L, then the coordinate (x_i, y_i, z_i) which defines the position of the ith lump, is chosen in accordance with equation (2), i.e. uniformly distributed in the range $(0, L)$. In practice, because the lumps are of finite size (we assume they are spheres), this range is curtailed to $(a, L-a)$, where a is the sphere radius. We further note that the finite size of the spheres also modifies the probability distribution because it is necessary to exclude the case of two or more spheres overlapping. We now describe how we choose the positions of the spheres from the random Cartesian positions (x_i, y_i, z_i).

First, we assume that all the spheres are of the same size; this is not essential but simplifies the problem. If the box is a cube of side L and the spheres are of radius a, then the box is divided into N^3 cells where $N = \mathrm{int}(L/2a)$. Then a sphere can fall in any one of these cells and we neglect small deviations due to a non-integral number of spheres lying in the box. Two matters must be considered, however:

(1) only one sphere is allowed in a cell and once the cell is occupied all other spheres are excluded from it;
(2) a method is needed to ensure that each cell has an equal chance of containing a sphere.

Condition (1) is achieved by a selection algorithm which removes a cell from consideration once it has been occupied. Condition (2) is achieved by 'unwrapping' the cells so that they become a linear chain of cells each characterized by a Cartesian coordinate. Thus, if there are N^3 cells and N_p spheres, we select N_p random numbers between 0 and N^3, bearing in mind the exclusion principle discussed above. Once all the spheres have been placed, the integer defining their position in the chain is associated with a prescribed Cartesian coordinate and hence we have the actual physical position within the box. In the limit of very small spheres, this selection procedure approaches the theoretical distribution derived above. For finite size spheres, there will be some deviation due to the discrete positioning that arises from being restricted to a cell. Our simulations, which will be described below, will allow us to assess the effect of such packing on the theoretical distribution, although that is not the prime purpose of this paper.

5. Numerical results

We note that the theoretical curve defined by equation (19) describes a universal function of R/L, and is the probability distribution of inter-particle distances for infinitesimally small spheres.

For the purposes of calculation, we set $L = 30$ units; the number of spheres and their sizes will be varied. As an illustration of $G(x)$, we show this universal function in figure 1 for the range $0 < x < \sqrt{3}$, where as explained above $\sqrt{3}$ is the maximum corner-to-corner distance in a cube of unit side.

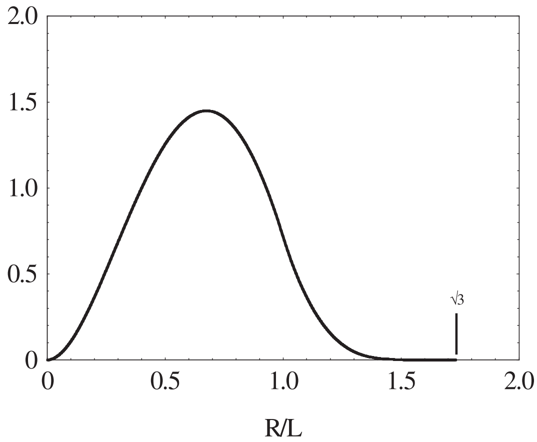

Figure 1. Analytical probability distribution $P(R/L)$.

It is interesting to note that at the higher end, the distribution drops to very small values well below $\sqrt{3}$. This implies that the chance of getting very large separations is very small; intuitively one can see why this is.

We have noted from our simulations that the results do not depend on the number of spheres used; thus whether we use two spheres or 100 spheres leads to the same distribution. In practice, using one simulation of 100 spheres is the same as using 50 simulations of two spheres. Indeed, if the cube contained N_c cells and we chose $N_p = N_c$ spheres we would only need one simulation to obtain the distribution because all the inter-particle distances would be known in a deterministic sense. The total number of links between the centres of N_p spheres is $N_p(N_p - 1)/2$, which is the number of separation distances for each realization. If $N_p = N_c$ then clearly $N_p(N_p - 1)/2$ covers all possible links between cells as well as between spheres.

However, in practice, for a sphere of unit diameter and a cube of 30 units side, that would mean running the code for 27 000 spheres, which is beyond the memory capabilities of most personal computers.

In figures 2 and 3 we show the simulations for sphere diameters of 0.5, 1, 2, 3, 5 units. The full curve is the analytical form as shown in figure 1, and the symbols denote the frequency of occurrence of a separation distance in a 'bin' of width $D = 2a$ from D up to $\sqrt{3}L - D$. Clearly, the values for $D = 0.5$ fall very close to the analytical curve. As the sphere size increases, the

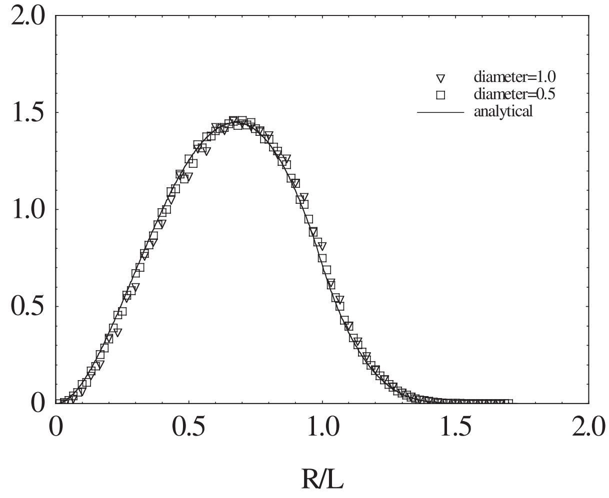

Figure 2. Probability distribution $P(R/L)$ for 100 spheres.

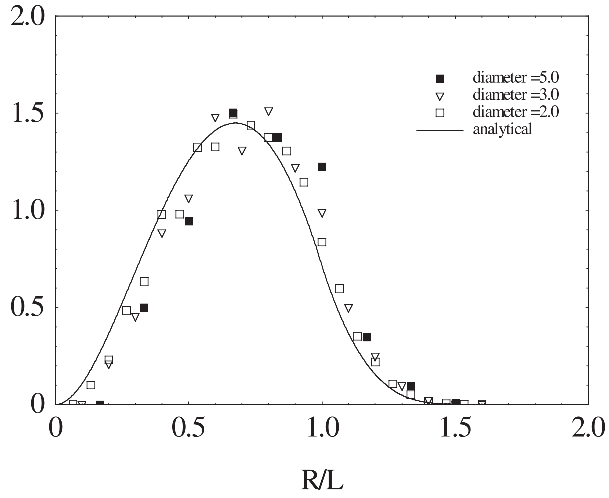

Figure 3. Probability distribution $P(R/L)$ for 100 spheres.

Table 1. Statistical parameters of the distribution.

N_{cell}	D	$\langle R\rangle/L$	σ_R/L
∞	0	0.661 707	0.249 29
216 000	0.5	0.670 3	0.249 1
27 000	1	0.679 4	0.248 7
3 375	2	0.698 2	0.247 2
1 000	3	0.718 0	0.245 3
216	5	0.759 5	0.237 6

'envelope' of the symbols moves to the right and the 'mesh' size becomes coarse. The general behaviour of the curves can be seen clearly in table 1, where we show the mean values and standard deviations for increasing sphere size.

All simulations were carried out using 10^5 random numbers. The entry in table 1 for $D = 0$ corresponds to the analytical case and we note how the average value of the separation distance moves towards higher values as the sphere size increases. This is self-evident from the figures. We also note that the standard deviation decreases very slightly.

6. Conclusions and discussion

The problem of the distribution of distance in a hypercube has been studied by a number of workers (Hammersley 1950, 1951a, b, Kendall and Moran 1963, Lord 1954). However, the cases of the rectangular box and the rectangle have not hitherto been solved. Even the hypersphere cases have not been evaluated using the Dirac delta function approach described above. Thus, for completeness, we describe in the appendix how we can also solve the problem for a sphere and a one-dimensional rod.

The present problem arose from the author's interest in neutron transport in spatially stochastic media. In a new approach to this problem, a method was developed in which fissile lumps were distributed at random in a neutron moderator. The Cartesian coordinates of the lumps were chosen such that they fell uniformly over the volume of the moderator. If the system contained N lumps, this procedure necessitated sampling $3N$ random numbers to locate all the lumps. However, in some of the problems considered, it was not the absolute position that was needed but the inter-particle distance R. Thus by sampling from $p(R)$ instead of $p(x, y, z)$, we could reduce the computational time considerably. This was the rationale behind the present investigation.

During the course of the work, we noted that our problem was not a new one. Indeed, the ideas could be traced back to Crofton who published on these matters in 1877. His work is referenced in Kendall and Moran (1963). The inter-particle separation problem had also been developed by contributors to Monte Carlo methods with particular emphasis on neutron and gamma ray transport (Hammersley and Handscomb 1964). However, a search of the literature indicated that the case of the rectangular box had not been solved and, moreover, in evaluating the box case, we were able to introduce yet another mathematical device to solve the problem, involving the Fourier representation of the Dirac delta function.

As a practical matter, the problem we met in the context of neutron transport theory, required that the lumps (in our case spheres) never overlap. This required the cell structure described above and the need to exclude particles from a cell once it had been occupied. There is also the matter of using finite-size cells which modifies the theoretical distribution which is for points, i.e. spheres of vanishingly small radius. For the case of points there is clearly no correlation between sphere positions, by definition and by virtue of equation (4). However, for finite spheres, some correlation occurs and although we have been unable to find an analytical form for the modified inter-particle distribution function, table 1 and figure 2 show how the size of the sphere influences the distribution.

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Appendix

A.1. Probability of a given separation distance in a sphere

If we consider two points r_1 and r_2 in a sphere of radius a, where the centre of the sphere is the origin of coordinates, then the probability that the two points appear at random within the sphere is

$$p\,(r_1, \vartheta_1, r_2, \vartheta_2) = \frac{9}{4a^6} r_1^2 \sin\vartheta_1 r_2^2 \sin\vartheta_2 \tag{A1}$$

where

$$\int_0^a \mathrm{d}r_1 \int_0^a \mathrm{d}r_2 \int_0^\pi \mathrm{d}\vartheta_1 \int_0^\pi \mathrm{d}\vartheta_2\, p\,(r_1, \vartheta_1, r_2, \vartheta_2) = 1. \tag{A2}$$

The separation distance R between the points r_1 and r_2 is

$$R = \sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos(\vartheta_1 - \vartheta_2)}. \tag{A3}$$

But because this depends only on the difference $\vartheta_1 - \vartheta_2$, we may modify equation (A1) to

$$p\,(r_1, r_2, \vartheta) = \frac{9}{2a^6} r_1^2 r_2^2 \sin\vartheta. \tag{A4}$$

The probability of finding a separation distance R per unit interval is therefore

$$P(R) = \frac{9}{2a^6} \int_0^a \mathrm{d}r_1\, r_1^2 \int_0^a \mathrm{d}r_2\, r_2^2 \int_0^\pi \mathrm{d}\vartheta \sin\vartheta\, \delta\left(R - \sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos\vartheta}\right) \tag{A5}$$

where we have introduced a factor of two to account for the fact that integration over ϑ is $(0, \pi)$ rather than $(0, 2\pi)$.

If we introduce reduced variables $u = r_1/a$, $v = r_2/a$ and $\mu = \cos\vartheta$, we find that equation (A5) becomes

$$P(R) = \frac{9}{2a} \int_0^1 \mathrm{d}u\, u^2 \int_0^1 \mathrm{d}v\, v^2 \int_{-1}^1 \mathrm{d}\mu\, \delta\left(\frac{R}{a} - \sqrt{u^2 + v^2 - 2uv\mu}\right). \tag{A6}$$

Setting $R/a = \bar{R}$ and introducing the new variable t through

$$t = \sqrt{u^2 + v^2 - 2uv\mu} \tag{A7}$$

we can transform equation (A6) to give

$$P(R) = \frac{9}{2a} \int_0^1 \mathrm{d}u\, u \int_0^1 \mathrm{d}v\, v \int_{|u-v|}^{u+v} t\, \mathrm{d}t\, \delta\left(\bar{R} - t\right) \tag{A8}$$

which becomes

$$P(R) = \frac{9\bar{R}}{2a} \int_0^1 \mathrm{d}u\, u \int_0^1 \mathrm{d}v\, v \left[|u - v| < \bar{R} < u + v\right] \tag{A9}$$

where the quantity in square brackets indicates the limits on u and v introduced by the delta function. A careful examination of the area of integration shows that

$$\begin{aligned} \int_0^1 \mathrm{d}u\, u \int_0^1 \mathrm{d}v\, v[\cdots] &= \int_0^{1-\bar{R}} \mathrm{d}v\, v \int_{\bar{R}-v}^{\bar{R}+v} \mathrm{d}u\, u + \int_{1-\bar{R}}^{\bar{R}} \mathrm{d}v\, v \int_{\bar{R}-v}^{2\bar{R}-1} \mathrm{d}u\, u \\ &\quad + \int_{1-\bar{R}}^{\bar{R}} \mathrm{d}v\, v \int_{2\bar{R}-1}^{1} \mathrm{d}u\, u + \int_{\bar{R}}^{1} \mathrm{d}v\, v \int_{v-\bar{R}}^{1-\bar{R}} \mathrm{d}u\, u + \int_{\bar{R}}^{1} \mathrm{d}v\, v \int_{1-\bar{R}}^{1} \mathrm{d}u\, u. \end{aligned} \tag{A10}$$

These integrals are simple and the result is

$$P(R) = 12y^2(1 - y)^2(2 + y)^2 \tag{A11}$$

where $y = R/2a$. Clearly, $P(R) = 0$ outside the range $(0, 2a)$.

This result was obtained by Hammersley (1950) and Lord (1954) using different methods. Hammersley has also made similar calculations for infinite cylinders (1951a, b). The result for the cube as described in this paper is new. Problems of geometrical probability are discussed in detail in Kendall and Moran (1963).

The moments of the distribution can be calculated easily and we find

$$\frac{\langle R^n \rangle}{(2a)^n} = \frac{72}{(n+3)(n+4)(n+6)} \tag{A12}$$

leading to $\langle R \rangle = 0.5143\ldots(2a)$ and

$$\sigma_R = \frac{\sqrt{\langle R^2 \rangle - \langle R \rangle^2}}{\langle R \rangle} = 0.3664\ldots. \tag{A13}$$

These values are close to the normalized values for the box.

A.2. One-dimensional case

If we have two points, x_1 and x_2, uniformly distributed between $(0, a)$, then

$$p(x_1, x_2) = \frac{1}{a^2}. \tag{A14}$$

The separation distance is $s = |x_1 - x_2|$, hence

$$P(s) = \frac{1}{a^2} \int_0^a \mathrm{d}x_1 \int_0^a \mathrm{d}x_2\, \delta\,(s - |x_1 - x_2|) \tag{A15}$$

which after taking care of the area of integration becomes

$$\begin{aligned} P(s) &= \frac{1}{a^2} \int_0^a \mathrm{d}x_1\, \{[s < x_1 < a] + [0 < x_1 < a - s]\} \\ &= \frac{1}{a^2} \int_s^a \mathrm{d}x_1 + \frac{1}{a^2} \int_0^{a-s} \mathrm{d}x_1 = \frac{2}{a^2}(a - s). \end{aligned} \tag{A16}$$

We can verify that

$$\int_0^a \mathrm{d}s\, P(s) = 1$$

and also that $\langle s \rangle = a/3$, $\langle s^2 \rangle = a^2/6$ and hence

$$\sigma_s = \frac{a}{3\sqrt{2}}. \tag{A17}$$

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