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# Random distance distribution for spherical objects: general theory and applications to physics

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## Abstract

A formalism is presented for analytically obtaining the probability density function,  $P_n(s)$ , for the random distance  $s$  between two random points in an  $n$ -dimensional spherical object of radius  $R$ . Our formalism allows  $P_n(s)$  to be calculated for a spherical  $n$ -ball having an arbitrary volume density, and reproduces the well-known results for the case of uniform density. The results find applications in geometric probability, computational science, molecular biological systems, statistical physics, astrophysics, condensed matter physics, nuclear physics and elementary particle physics. As one application of these results, we propose a new statistical method derived from our formalism to study random number generators used in Monte Carlo simulations.

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(Some figures in this article are in colour only in the electronic version)

## 1. Introduction

In two recent papers [1, 2], geometric probability techniques were developed to calculate the functions  $P_3(s)$  which describe the probability density of finding a random distance  $s$  separating two random points distributed in a uniform sphere and in a uniform ellipsoid. As discussed in [1–17], these results are of interest as tools in mathematical physics, and have numerous applications in other fields as well. Specifically, it was demonstrated in [1–5] that knowing the random distance distribution in a spherical object greatly facilitates the calculation of self-energies for spherical matter distributions arising from electromagnetic, gravitational or weak interactions.

As an example we calculate the total electrostatic energy  $W_3$  of a collection of  $Z$  charges uniformly distributed within the same spherical volume of radius  $R$ . For illustrative purposes,

we assume that  $Z$  is a large number. For each pair of charges the potential energy due to the Coulomb interaction in Gaussian units is

$$V_3 = \frac{e^2}{r_{12}} = \frac{e^2}{|\vec{r}_2 - \vec{r}_1|} \quad (1)$$

where  $e$  is the elementary charge,  $\vec{r}_1$  ( $\vec{r}_2$ ) is the coordinate of the first (second) charge. The total Coulomb energy  $W_3$  can then be expressed as

$$\begin{aligned} W_3 &= \frac{1}{2} \rho^2 \int r_1^2 dr_1 \int \sin \theta_1 d\theta_1 \int d\phi_1 \int r_2^2 dr_2 \int \sin \theta_2 d\theta_2 \int \frac{1}{r_{12}} d\phi_2 \\ &= \frac{Z^2}{2} \times \frac{6 e^2}{5 R} \end{aligned} \quad (2)$$

where  $\rho = 3Ze/4\pi R^3$  (see [18]). We note that equation (2) requires evaluating a six-dimensional integral, and using the addition theorem for spherical harmonics [19]

$$P_l(\cos \gamma) = \frac{4\pi}{2l+1} \sum_{m=-l}^l (-1)^m Y_l^m(\theta_1, \phi_1) Y_l^{-m}(\theta_2, \phi_2). \quad (3)$$

Alternatively, we can use the probability density function  $P_3(s)$  [6] giving the random distance distribution for a sphere with a uniform density to calculate  $W_3$ . For a collection of  $Z$  charges there are  $Z(Z-1)/2$  such pairs, and hence the total Coulomb energy  $W_3$  is

$$W_3 = \frac{Z(Z-1)}{2} \int_0^{2R} P_3(s) \frac{e^2}{s} ds = \frac{Z(Z-1)}{2} \times \frac{6 e^2}{5 R} \simeq \frac{Z^2}{2} \times \frac{6 e^2}{5 R} \quad (4)$$

where

$$P_3(s) = 3 \frac{s^2}{R^3} - \frac{9 s^3}{4 R^4} + \frac{3 s^5}{16 R^6}. \quad (5)$$

We note that by using geometric probability techniques we can simplify the expression for  $W_3$  from a six-dimensional non-trivial integral (2) to a one-dimensional elementary integral (4). Generalizing to  $n$ -dimensions, a calculation of the electrostatic energy  $W_n$  for a collection of  $Z$  charges uniformly distributed within the same  $n$ -dimensional spherical volume of radius  $R$  can be greatly simplified by utilizing the  $n$ -dimensional random distance distribution. This reduces the complexity of calculating  $W_n$  from a  $2n$ -dimensional intractable integral involving  $n$ -dimensional spherical harmonics to a simple one-dimensional integral.

The probability density function  $P_n(s)$  for the distribution of the random distance  $s$  between two random points in a uniform spherical  $n$ -ball is well known. Hence the object of the present paper is to generalize the results of [9–11] to the case of an arbitrarily non-uniform density distribution by using a new method which we present below. Note that the sample space  $\mathbf{B}_n$  for the random points is a spherical  $n$ -ball of radius  $R$  defined as

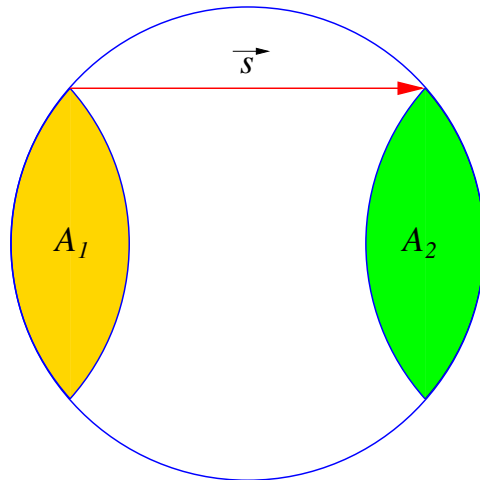
$$\mathbf{B}_n = \{(x_1, x_2, \dots, x_n) \in \mathbf{R}^n : x_1^2 + x_2^2 + \dots + x_n^2 \leq R^2\} \quad (6)$$

where

$$\mathbf{R}^n = \{\mathbf{x} : \mathbf{x} = (x_1, x_2, \dots, x_n)\} \quad (7)$$

represents  $n$ -dimensional Euclidean space.

To illustrate our formalism, we begin by deriving the probability density function (PDF) for a spherical  $n$ -ball with a uniform density distribution, and compare our results with those obtained earlier by other means [9–11]. We then extend this technique to a spherical  $n$ -ball with an arbitrary density distribution, and this leads to a general-purpose master formula for  $P_n(s)$  given in equation (39). The outline of this paper is as follows. In section 2 we present



**Figure 1.** The locus of points in a circle separated by a vector  $\vec{s} = s\hat{x}$ . For each random point  $\vec{r}_1$  in  $A_1$ , there is a unique random point  $\vec{r}_2$  in  $A_2$  such that  $\vec{s} = \vec{r}_2 - \vec{r}_1$ .

our formalism and illustrate it by rederiving the well-known results for a circle and for a sphere of uniform density. In section 3 we extend this formalism to the case of non-uniform but spherically symmetric density. In section 4 we develop the formalism for the most general case of an arbitrary density distribution. In section 5 we present some applications of our results including a new proposed computational scheme for testing random number generators (RNG) used in Monte Carlo simulations.

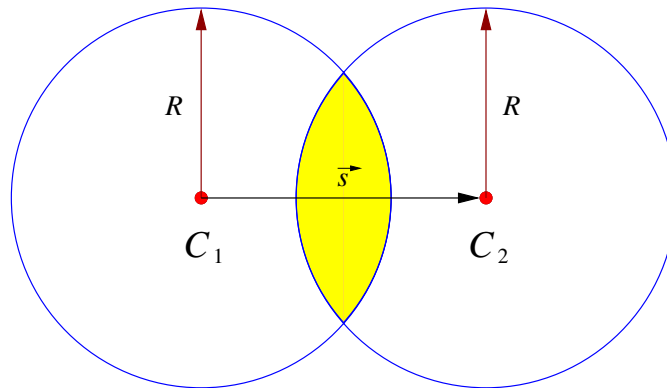
## 2. Uniform density distributions

In this section we illustrate our formalism by deriving the PDF for a circle of radius  $R$  having a spatially uniform density characterized by a density function  $\rho$ , where  $\rho$  is an arbitrary constant. For two points randomly sampled inside the circle located at  $\vec{r}_1$  and  $\vec{r}_2$  measured from the centre, define a random vector  $\vec{s} = \vec{r}_2 - \vec{r}_1$  and a random distance  $s = |\vec{s}|$ , where  $0 \leq s \leq 2R$ . To simplify the discussion, we translate the centre of the circle to the origin so that the equation for the circle is  $x^2 + y^2 = R^2$ . It is sufficient to consider initially those vectors  $\vec{s}$  which are aligned in the positive  $\hat{x}$  direction, since rotational symmetry can eventually be used to extend our results to those vectors  $\vec{s}$  with arbitrary orientations. We begin by identifying those pairs of points,  $\vec{r}_1$  and  $\vec{r}_2$ , which satisfy  $\vec{s} = s\hat{x}$ . One set of random points for  $\vec{r}_1$  is located in  $A_1$  and the other set of random points for  $\vec{r}_2$  is located in  $A_2$  as shown in figure 1. We observe that  $A_2$  is the overlap area between the original circle  $C_1$  and an identical circle  $C_2$  whose centre is shifted from  $(0, 0)$  to  $(|\vec{s}|, 0)$  as shown in figure 2. Since the areas of  $A_1$  and  $A_2$  are equal, it follows that the probability density of finding a given  $s = |s\hat{x}|$  in a circle of uniform density is proportional to the area of  $A_2$ :

$$\int_{s-R}^{\frac{s}{2}} dx \int_{-\sqrt{R^2-(x-s)^2}}^{\sqrt{R^2-(x-s)^2}} dy + \int_{\frac{s}{2}}^R dx \int_{-\sqrt{R^2-x^2}}^{\sqrt{R^2-x^2}} dy. \quad (8)$$

Using rotational symmetry, this result can be applied to any orientation of  $\vec{s}$ , where  $0 \leq \phi \leq 2\pi$ , and hence the probability density  $P_2(s)$  for a circle of uniform density can be factorized as

$$P_2(s) = 2\pi s \times f(s) \quad (9)$$



**Figure 2.** The probability density that two random points are separated by a random distance  $|s\hat{x}|$  in a circle of radius  $R$  is proportional to the shaded area given by the overlap of  $C_1$  and  $C_2$ , where  $C_1$  is  $x^2 + y^2 = R^2$  and  $C_2$  is  $(x - s)^2 + y^2 = R^2$ .

where  $f(s)$  is a function to be determined and is proportional to expression (8). If we impose the normalization requirement

$$\int_0^{2R} P_2(s) ds = 1 \quad (10)$$

we then have

$$P_2(s) = \frac{2\pi s \int_{\frac{s}{2}}^R dx \int_{-\sqrt{R^2-x^2}}^{\sqrt{R^2-x^2}} dy}{\int_0^{2R} \left( 2\pi s \int_{\frac{s}{2}}^R dx \int_{-\sqrt{R^2-x^2}}^{\sqrt{R^2-x^2}} dy \right) ds} \quad (11)$$

$$= \frac{2s}{R^2} - \frac{s^2}{\pi R^4} \sqrt{4R^2 - s^2} - \frac{4s}{\pi R^2} \sin^{-1}(s/2R). \quad (12)$$

Equation (12) is identical to the results obtained in [9, 10] by other means.

The conclusion that emerges from this formalism is that the probability density of finding two random points separated by a random vector  $\vec{s}$  in a circle of uniform density can be derived by simply calculating the overlap region of that circle with an identical circle obtained by shifting the centre from the origin to  $\vec{s}$ . In the following discussion, we show that this result generalizes to higher dimensions and provides a simple way of calculating  $P_n(s)$  for  $n \geq 3$ .

For a given  $\vec{s}$  sampled from a uniform sphere, we select the positive  $\hat{z}$  direction and study the distribution of the random vectors  $\vec{s}$  in this direction. It then follows that the probability density of finding  $s\hat{z}$  is proportional to

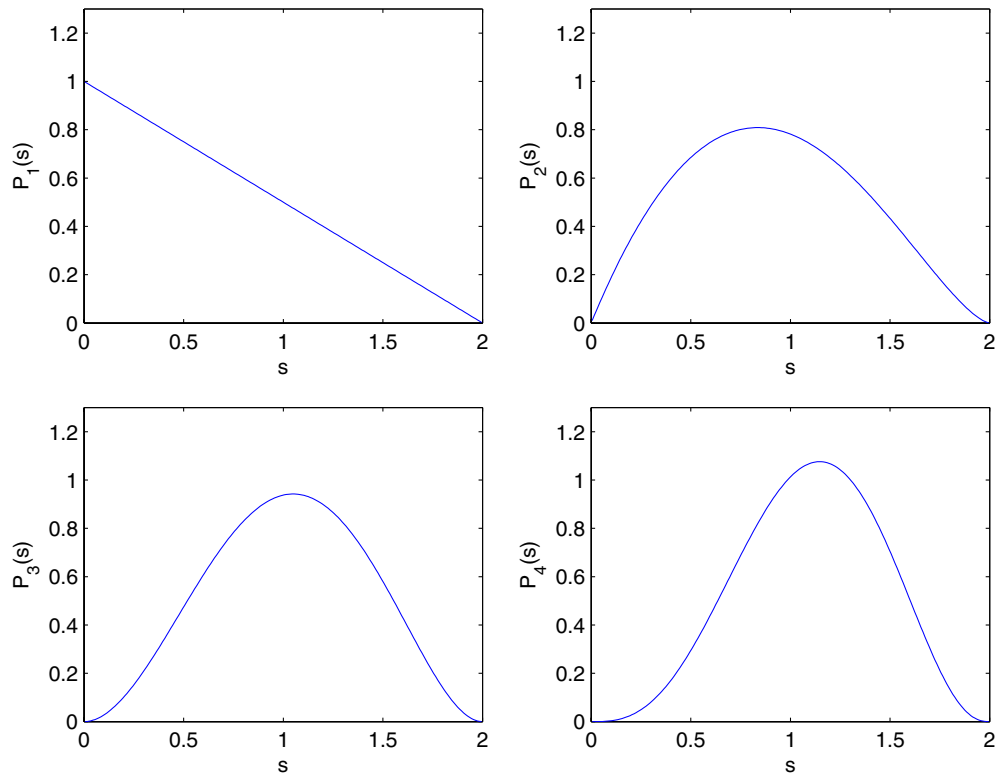
$$\int_{s-R}^{\frac{s}{2}} dz \int_{-\sqrt{R^2-(z-s)^2}}^{\sqrt{R^2-(z-s)^2}} dx \int_{-\sqrt{R^2-(z-s)^2-x^2}}^{\sqrt{R^2-(z-s)^2-x^2}} dy + \int_{\frac{s}{2}}^R dz \int_{-\sqrt{R^2-z^2}}^{\sqrt{R^2-z^2}} dx \int_{-\sqrt{R^2-z^2-x^2}}^{\sqrt{R^2-z^2-x^2}} dy. \quad (13)$$

In a three-dimensional space, we note that the direction of the random vector  $\vec{s}$  can have the following range:  $0 \leq \theta \leq \pi$  and  $0 \leq \phi \leq 2\pi$ . From the previous discussion, we thus arrive at the following expression for a sphere with a uniform density distribution:

$$P_3(s) = \frac{4\pi s^2 \left( \int_{\frac{s}{2}}^R dz \int_{-\sqrt{R^2-z^2}}^{\sqrt{R^2-z^2}} dx \int_{-\sqrt{R^2-z^2-x^2}}^{\sqrt{R^2-z^2-x^2}} dy \right)}{\int_0^{2R} 4\pi s^2 \left( \int_{\frac{s}{2}}^R dz \int_{-\sqrt{R^2-z^2}}^{\sqrt{R^2-z^2}} dx \int_{-\sqrt{R^2-z^2-x^2}}^{\sqrt{R^2-z^2-x^2}} dy \right) ds} \quad (14)$$

$$= 3 \frac{s^2}{R^3} - \frac{9}{4} \frac{s^3}{R^4} + \frac{3}{16} \frac{s^5}{R^6}. \quad (15)$$

The result in equation (15) agrees exactly with the expression obtained previously in [6–11].



**Figure 3.** Plots of  $P_1(s)$ ,  $P_2(s)$ ,  $P_3(s)$  and  $P_4(s)$  for a uniform density distribution. Note that in all cases  $\int_0^{2R} P_n(s) ds = 1$ .

The present formalism can be readily generalized to express  $P_n(s)$  for a sphere of uniform density in  $n$ -dimensions as

$$P_n(s) = \frac{s^{n-1} \int_{s/2}^R dx_n \int_{-\sqrt{R^2-x_n^2}}^{\sqrt{R^2-x_n^2}} dx_1 \cdots \int_{-\sqrt{R^2-x_n^2-\cdots-x_{n-2}^2}}^{\sqrt{R^2-x_n^2-\cdots-x_{n-2}^2}} dx_{n-1}}{\int_0^{2R} \left( s^{n-1} \int_{s/2}^R dx_n \int_{-\sqrt{R^2-x_n^2}}^{\sqrt{R^2-x_n^2}} dx_1 \cdots \int_{-\sqrt{R^2-x_n^2-\cdots-x_{n-2}^2}}^{\sqrt{R^2-x_n^2-\cdots-x_{n-2}^2}} dx_{n-1} \right) ds} \quad (16)$$

We find that if  $n$  is an even number, then

$$P_n(s) = \frac{n \times s^{n-1}}{R^n} \left[ \frac{2}{\pi} \cos^{-1}(s/2R) - \frac{s}{\pi} \sum_{k=1}^{\frac{n}{2}} \frac{(n-2k)!!}{(n-2k+1)!!} (R^2 - s^2/4)^{\frac{n-2k+1}{2}} R^{2k-2-n} \right] \quad (17)$$

where  $0! = 0!! = 1$ . If  $n$  is an odd number, then

$$P_n(s) = \frac{n \times s^{n-1}}{R^n} \frac{n!!}{(n-1)!!} \sum_{k=0}^{\frac{n-1}{2}} \frac{(-1)^k}{2k+1} \frac{\left(\frac{n-1}{2}\right)!}{k! \left(\frac{n-1}{2} - k\right)!} [1 - (s/2R)^{2k+1}]. \quad (18)$$

The functional forms of equation (16) for  $n = 1, 2, 3$  and  $4$  are shown in figure 3.

The cumulative distribution function (CDF) [20] for  $P_n(s)$  is given by

$$\begin{aligned} D_n(x) &= \int_0^x P_n(s) ds \\ &= \frac{x^n}{R^n} - \frac{B_\alpha\left(\frac{1}{2}, \frac{n}{2} + \frac{1}{2}\right)}{B\left(\frac{1}{2}, \frac{n}{2} + \frac{1}{2}\right)} \frac{x^n}{R^n} + 2^n \frac{B_\alpha\left(\frac{n}{2} + \frac{1}{2}, \frac{n}{2} + \frac{1}{2}\right)}{B\left(\frac{1}{2}, \frac{n}{2} + \frac{1}{2}\right)} \end{aligned} \quad (19)$$

where  $0 \leq x \leq 2R$ ,  $\alpha = x^2/4R^2$  and  $B_\alpha$  is the incomplete beta function.

We summarize three important representations for the probability density function  $P_n(s)$  for a spherical  $n$ -ball of radius  $R$  with a uniform density distribution as follows:

1. *Integral representation:*

$$P_n(s) = \frac{s^{n-1} \int_{\frac{s}{2}}^R (R^2 - x^2)^{\frac{n-1}{2}} dx}{\frac{1}{2^n} B\left(\frac{n}{2} + \frac{1}{2}, \frac{1}{2}\right) R^{2n}}. \quad (20)$$

2. *Generating function representation:*

$$P_n(s) = \frac{s^{n-1} \frac{1}{n!} \left(\frac{\partial}{\partial h}\right)_{h=0}^n \frac{1}{\sqrt{1-h^2}} \left[ \sin^{-1} h - \sin^{-1} \left( \frac{2h - \sqrt{4-s^2}}{2-h\sqrt{4-s^2}} \right) \right]}{\frac{1}{2^n} B\left(\frac{n}{2} + \frac{1}{2}, \frac{1}{2}\right)} \quad (21)$$

where  $|h| < 1$  and  $R = 1$ . We note that one can obtain a number of identities and recursion relations for  $P_n(s)$  from the generating function representation in equation (21).

3. *Hypergeometric function representation:*

$$P_n(s) = \frac{2n}{B\left(\frac{n}{2} + \frac{1}{2}, \frac{1}{2}\right)} \left[ {}_2F_1(a, b, c, \alpha) R - \frac{s}{2} {}_2F_1(a, b, c, \beta) \right] \frac{s^{n-1}}{R^{n+1}} \quad (22)$$

where  $a = 1/2$ ,  $b = 1/2 - n/2$ ,  $c = 3/2$ ,  $\alpha = 1$ ,  $\beta = s^2/4R^2$  and  ${}_2F_1(\dots)$  is the hypergeometric function [19]. Note that we can obtain the orthogonality relations for  $P_n(s)$  from the hypergeometric function representation as shown in equation (22).

In [5] additional identities and recursion relations for  $P_n(s)$  are discussed in greater detail.

### 3. Spherically symmetric density distributions

In this section we extend the previous results to the case of a circle with a variable (but spherically symmetric) density characterized by a density function  $\rho(r)$ . Following the derivation presented in the previous section, we note that for any random vector  $\vec{s} = s\hat{x}$  if the second random point  $\vec{r}_2$  carries the density information  $\rho(x, y)$ , then the first random point  $\vec{r}_1$  should have the density information  $\rho(x - s, y)$ . It then follows that  $P_2(s)$  can be expressed as

$$P_2(s) = \frac{s \int_{\frac{s}{2}}^R dx \int_{-\sqrt{R^2-x^2}}^{\sqrt{R^2-x^2}} \rho(x-s, y) \times \rho(x, y) dy}{\int_0^{2R} \left( s \int_{\frac{s}{2}}^R dx \int_{-\sqrt{R^2-x^2}}^{\sqrt{R^2-x^2}} \rho(x-s, y) \times \rho(x, y) dy \right) ds} \quad (23)$$

A general formula for  $P_n(s)$  for an  $n$ -dimensional spherical ball of radius  $R$  having a spherically symmetric density can be derived, and we find that

$$P_n(s) = \frac{s^{n-1} \int_{\frac{s}{2}}^R dx_n \int_{-\sqrt{R^2-x_n^2}}^{\sqrt{R^2-x_n^2}} dx_1 \cdots \int_{-\sqrt{R^2-x_n^2-x_1^2-\cdots-x_{n-1}^2}}^{\sqrt{R^2-x_n^2-x_1^2-\cdots-x_{n-1}^2}} \rho_1 \times \rho_2 dx_{n-1}}{\int_0^{2R} \left( s^{n-1} \int_{\frac{s}{2}}^R dx_n \int_{-\sqrt{R^2-x_n^2}}^{\sqrt{R^2-x_n^2}} dx_1 \cdots \int_{-\sqrt{R^2-x_n^2-x_1^2-\cdots-x_{n-1}^2}}^{\sqrt{R^2-x_n^2-x_1^2-\cdots-x_{n-1}^2}} \rho_1 \times \rho_2 dx_{n-1} \right) ds} \quad (24)$$

where

$$\begin{aligned} \rho_1 &= \rho(x_1, x_2, \dots, x_n - s) \\ \rho_2 &= \rho(x_1, x_2, \dots, x_n). \end{aligned} \tag{25}$$

Some analytical results for a sphere with various spherically symmetric density distributions can be found in [5].

As an application of equation (24) we consider the case of an  $n$ -dimensional spherical space of radius  $R \rightarrow \infty$  with a Gaussian density given by

$$\rho_n(r) = \frac{N}{(2\pi)^{\frac{n}{2}} \sigma^n} e^{-\frac{1}{2} \frac{r^2}{\sigma^2}} \tag{26}$$

where

$$N = \lim_{R \rightarrow \infty} n \frac{\pi^{\frac{n}{2}}}{\Gamma(\frac{n}{2} + 1)} \int_0^R \rho_n(r) r^{n-1} dr. \tag{27}$$

In equation (27)  $r$  is measured from the centre, and the integral is over all space. The PDF for an  $n$ -dimensional spherical Gaussian space can then be obtained as

$$P_n(s) = \frac{s^{n-1} e^{-\frac{s^2}{4\sigma^2}}}{2^{n-1} \Gamma(\frac{n}{2}) \sigma^n}. \tag{28}$$

Finally, we note that the maximum probability density, denoted by  $s_{\max}$ , occurs at

$$s_{\max} = \sqrt{2(n-1)}\sigma. \tag{29}$$

#### 4. Arbitrary density distributions

We consider in this section the probability density functions for a spherical  $n$ -ball having an arbitrary density characterized by a density function  $\rho$ . We begin with a circle and use the conventional notation for polar coordinates:  $x = r \cos \phi$  and  $y = r \sin \phi$ . In a two-dimensional space, the random vector  $\vec{s}$  can be characterized by an angle  $\phi$  in the range  $0 \leq \phi \leq 2\pi$ . Associate each random unit vector  $\hat{s}(\phi)$  with a rotation operator  $\mathcal{R}$  such that

$$|\hat{x}\rangle = \mathcal{R}|\hat{s}(\phi)\rangle. \tag{30}$$

To ensure that the product of  $\rho(\vec{r}_1)$  and  $\rho(\vec{r}_2)$  maintains the correct density information, we use a  $2 \times 2$  matrix

$$R_{2 \times 2}(\phi) = \begin{bmatrix} \cos \phi & -\sin \phi \\ \sin \phi & \cos \phi \end{bmatrix} \tag{31}$$

to characterize this particular operator  $\mathcal{R}$  such that

$$\rho(x, y) \longrightarrow \rho(\cos \phi x - \sin \phi y, \sin \phi x + \cos \phi y). \tag{32}$$

Note that  $R_{2 \times 2}(\phi)$  is an orthogonal matrix which satisfies  $R_{2 \times 2}^{-1}(\phi) = R_{2 \times 2}^T(\phi)$  and its determinant is +1, where  $T$  denotes the transpose.

We can then express  $P_2(s)$ , for a circle with an arbitrary density distribution, as

$$P_2(s) = \frac{s \int_0^{2\pi} d\phi \int_{s/2}^R dx \int_{-\sqrt{R^2-x^2}}^{\sqrt{R^2-x^2}} \rho(x', y') \times \rho(x'', y'') dy}{\int_0^{2R} \left( s \int_0^{2\pi} d\phi \int_{s/2}^R dx \int_{-\sqrt{R^2-x^2}}^{\sqrt{R^2-x^2}} \rho(x', y') \times \rho(x'', y'') dy \right) ds} \tag{33}$$

where

$$\begin{aligned} \rho(x', y') &= \rho(\cos \phi(x - s) - \sin \phi y, \sin \phi(x - s) + \cos \phi y) \\ \rho(x'', y'') &= \rho(\cos \phi x - \sin \phi y, \sin \phi x + \cos \phi y). \end{aligned}$$



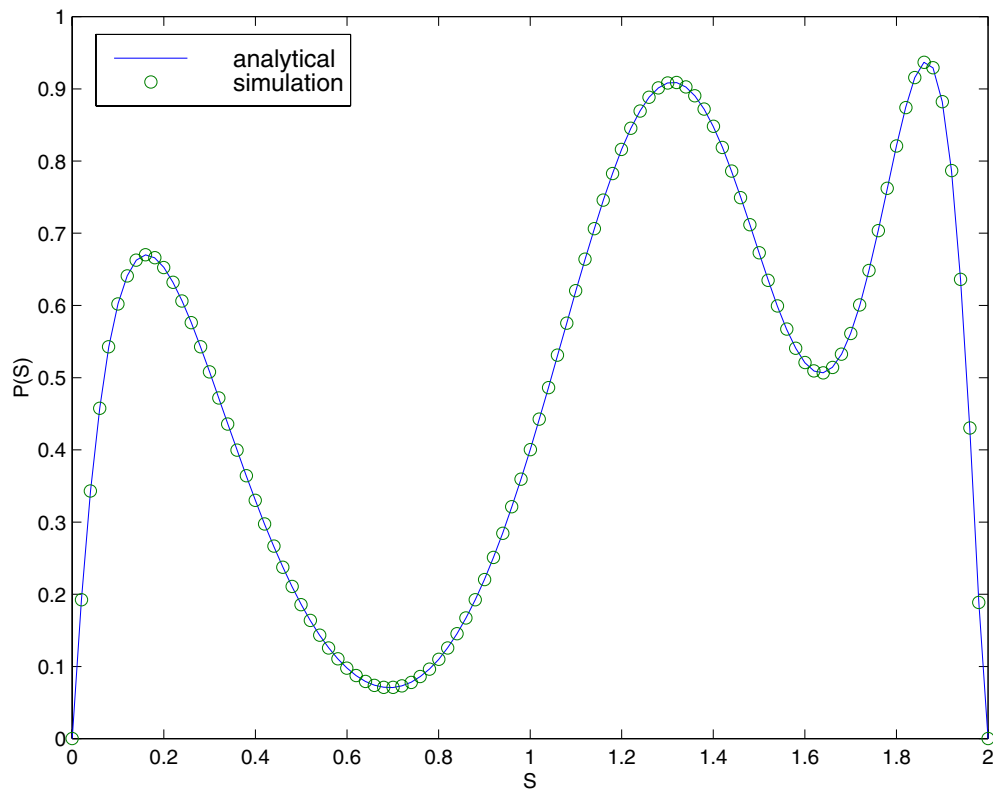


Figure 4. Plot of  $P_2(s)$  as a function of  $s$  for the case  $R = 1$  and  $\rho(x, y) \propto x^4 y^4$ .

Figure 4 exhibits  $P_2(s)$  when  $R = 1$  and illustrates the agreement between the Monte Carlo simulation and the analytical result when  $\rho(x, y) \propto x^4 y^4$ .

The preceding discussion can be generalized to the case of a spherical  $n$ -ball with an arbitrary density. We define the following  $n$ -dimensional spherical coordinates [21] as

$$\begin{aligned}
 x_1 &= r \sin \theta_{n-2} \sin \theta_{n-3} \cdots \sin \theta_2 \sin \theta_1 \cos \phi \\
 x_2 &= r \sin \theta_{n-2} \sin \theta_{n-3} \cdots \sin \theta_2 \sin \theta_1 \sin \phi \\
 &\vdots \\
 x_i &= r \sin \theta_{n-2} \sin \theta_{n-3} \cdots \sin \theta_{i-1} \cos \theta_{i-2} \\
 &\vdots \\
 x_{n-1} &= r \sin \theta_{n-2} \cos \theta_{n-3} \\
 x_n &= r \cos \theta_{n-2}.
 \end{aligned} \tag{34}$$

where  $\theta_i \in [0, \pi]$  and  $\phi \in [0, 2\pi]$ . We associate each random unit vector  $\hat{s}(\theta_1, \dots, \phi)$  with a rotation operator  $\mathcal{R}$  such that

$$|\hat{x}_n\rangle = \mathcal{R}|\hat{s}(\theta_1, \dots, \phi)\rangle. \tag{35}$$

The  $n \times n$  matrix representation for the rotation operator  $\mathcal{R}$  in equation (35) can be expressed as

$$R_{n \times n}(\theta_{n-2}, \dots, \theta_1, \phi) = R_{n \times n}(\phi) \times R_{n \times n}(\theta_1) \times \cdots \times R_{n \times n}(\theta_{n-2}) \tag{36}$$

where  $n \geq 3$ . The various matrices on the right-hand side of equation (36) are defined as follows:

1.  $R_{n \times n}(\phi)$ : The matrix elements are  $a_{11} = \cos \phi, a_{12} = -\sin \phi, a_{21} = \sin \phi, a_{22} = \cos \phi$ ; for  $i \in [1, 2]$  and  $j \in [3, n]$   $a_{ij} = 0$ ; for  $i \in [3, n]$  and  $i \in [1, 2]$   $a_{ij} = 0$ ; for  $i \in [3, n]$  and  $j \in [3, n]$   $a_{ij} = \delta_{ij}$ .
2.  $R_{n \times n}(\theta_1)$ : The matrix elements are  $a_{11} = \cos \theta_1, a_{12} = 0, a_{13} = \sin \theta_1, a_{21} = 0, a_{22} = 1, a_{23} = 0, a_{31} = -\sin \theta_1, a_{32} = 0, a_{33} = \cos \theta_1$ ; for  $i \in [1, 3]$  and  $j \in [4, n]$   $a_{ij} = 0$ ; for  $i \in [4, n]$  and  $j \in [1, 3]$   $a_{ij} = 0$ ; for  $i \in [4, n]$  and  $j \in [4, n]$   $a_{ij} = \delta_{ij}$ .
3.  $R_{n \times n}(\theta_k)$  and  $k \in [2, n - 3]$ : The matrix elements are  $a_{k+1, k+1} = \cos \theta_k, a_{k+1, k+2} = \sin \theta_k, a_{k+2, k+1} = -\sin \theta_k, a_{k+2, k+2} = \cos \theta_k$ ; for  $i \in [1, k]$  and  $j \in [1, k]$   $a_{ij} = \delta_{ij}$ ; for  $i \in [k + 3, n]$  and  $j \in [k + 3, n]$   $a_{ij} = \delta_{ij}$ ; for  $i \in [1, k]$  and  $j \in [k + 1, n]$   $a_{ij} = 0$ ; for  $i \in [k + 1, n]$  and  $j \in [1, k]$   $a_{ij} = 0$ ; for  $i \in [k + 1, k + 2]$  and  $j \in [k + 3, n]$   $a_{ij} = 0$ ; for  $i \in [k + 3, n]$  and  $j \in [k + 1, k + 2]$   $a_{ij} = 0$ .
4.  $R_{n \times n}(\theta_{n-2})$ : The matrix elements are  $a_{n-1, n-1} = \cos \theta_{n-2}, a_{n-1, n} = \sin \theta_{n-2}, a_{n, n-1} = -\sin \theta_{n-2}, a_{n, n} = \cos \theta_{n-2}$ ; for  $i \in [1, n - 2]$  and  $j \in [1, n - 2]$   $a_{ij} = \delta_{ij}$ ; for  $i \in [1, n - 2]$  and  $j \in [n - 1, n]$   $a_{ij} = 0$ , for  $i \in [n - 1, n]$  and  $j \in [1, n - 2]$   $a_{ij} = 0$ .

Note that all the matrices in equation (36) are orthogonal and their determinants are +1. The matrix elements for  $R_{n \times n}(\theta_{n-2}, \dots, \theta_1, \phi)$  can be summarized as follows:

1. The matrix elements for the first column are  $a_{11} = \cos \theta_1 \cos \phi, a_{21} = \cos \theta_1 \sin \phi, a_{31} = -\sin \theta_1$ , and for  $i \in [4, n]$   $a_{i1} = 0$ .
2. The matrix elements for the second column are  $a_{12} = -\sin \phi, a_{22} = \cos \phi$ , and for  $i \in [3, n]$   $a_{i2} = 0$ .
3. The matrix elements for the  $j$ th column where  $j \in [3, n - 1]$  are  $a_{j+1, j} = -\sin \theta_{j-1}$ ; for  $i \in [j + 2, n]$   $a_{ij} = 0$ , and for  $i \in [1, j]$   $a_{ij} = \cos \theta_{j-1} \times x_i$ , where  $x_i = \hat{r} \times \hat{x}_i$  and  $x_i$  is the  $i$ th Cartesian coordinate component for a unit vector  $\hat{r}$  in  $j$ -dimensions. For example,

$$\begin{aligned} a_{14} &= \cos \theta_3 \sin \theta_2 \sin \theta_1 \cos \phi \\ a_{24} &= \cos \theta_3 \sin \theta_2 \sin \theta_1 \sin \phi \\ a_{34} &= \cos \theta_3 \sin \theta_2 \cos \theta_1 \\ a_{44} &= \cos \theta_3 \cos \theta_2. \end{aligned}$$

4. The matrix elements for the  $n$ th column are for  $i \in [1, n]$   $a_{in} = x_i$ , where  $x_i = \hat{r} \times \hat{x}_i$  and  $x_i$  is the  $i$ th Cartesian coordinate component for a unit vector  $\hat{r}$  in  $n$ -dimensions.

Additionally, it is convenient to define the following transforms:

$$x'_i = \sum_{j=1}^n a_{ij}(x_j - \delta_{jn}s) \tag{37}$$

$$x''_i = \sum_{j=1}^n a_{ij}x_j \tag{38}$$

where  $a_{ij}$  are the matrix elements for  $R_{n \times n}(\theta_{n-2}, \dots, \theta_1, \phi)$  defined in equation (36). The master equation for  $P_n(s)$  for a spherical  $n$ -ball with an arbitrary density characterized by a density function  $\rho(\mathbf{x}) = \rho(x_1, x_2, \dots, x_n)$  can then be formulated as

$$P_n(s) = \frac{s^{n-1} \times \mathbf{F}_n(x, \theta)}{\int_0^{2R} [s^{n-1} \times \mathbf{F}_n(x, \theta)] ds} \tag{39}$$

where

$$\begin{aligned} \mathbf{F}_n(x, \theta) = & \int_0^\pi \sin^{n-2} \theta_{n-2} d\theta_{n-2} \int_0^\pi \sin^{n-3} \theta_{n-3} d\theta_{n-3} \cdots \\ & \times \int_0^\pi \sin \theta_1 d\theta_1 \int_0^{2\pi} d\phi \int_{s/2}^R dx_n \int_{-\sqrt{R^2-x_n^2}}^{\sqrt{R^2-x_n^2}} dx_1 \cdots \\ & \times \int_{-\sqrt{R^2-x_n^2-\cdots-x_{n-2}^2}}^{\sqrt{R^2-x_n^2-\cdots-x_{n-2}^2}} \rho(\mathbf{x}') \times \rho(\mathbf{x}'') dx_{n-1} \end{aligned}$$

and

$$\rho(\mathbf{x}') = \rho(x'_1, x'_2, \dots, x'_n) \quad \rho(\mathbf{x}'') = \rho(x''_1, x''_2, \dots, x''_n)$$

where  $x'_i$  and  $x''_i$  are defined in equations (37) and (38).

Finally, we note that the formalism presented in this paper can be applied to an  $n$ -dimensional sphere (i.e. the boundary of a spherical  $n$ -ball) with an arbitrary surface density. Two random distance distributions including Euclidean distance and geodesic distance are discussed in [5, 22]. Specifically we will demonstrate the analytical solutions to Thomson's problem of finding the minimum energy configuration of unit charges on a spherical surface [23–31].

## 5. Applications

### 5.1. $m$ th moment of the distance

In some applications the  $m$ th moment of the distance, rather than the distance itself, is of interest. As an example, for a collection of nucleons interacting via simple harmonic oscillator potentials,  $\langle s^2 \rangle$  may be of interest rather than  $\langle s \rangle$  itself. We then calculate the  $m$ th moment  $\langle s^m \rangle$  for the case of a spherical  $n$ -ball of uniform density, where

$$\langle s^m \rangle = \int_0^{2R} s^m P_n(s) ds. \quad (40)$$

Using equation (20), the  $m$ th moment  $\langle s^m \rangle$  has the general form

$$\langle s^m \rangle = 2^{n+m} \left( \frac{n}{n+m} \right) \frac{B\left(\frac{n}{2} + \frac{1}{2}, \frac{n}{2} + \frac{1}{2} + \frac{m}{2}\right)}{B\left(\frac{n}{2} + \frac{1}{2}, \frac{1}{2}\right)} R^m \quad (41)$$

where  $B(p, q)$  is the beta function and  $m \geq -(n-1)$ .

Additionally,  $\langle s^m \rangle$  can be evaluated for a spherical space having a Gaussian density distribution where  $\rho \propto e^{-r^2/2\sigma^2}$ . From equation (28), we find

$$\langle s^m \rangle = \lim_{R \rightarrow \infty} \int_0^{2R} s^m P_n(s) ds = (2\sigma)^m \frac{\Gamma\left(\frac{n+m}{2}\right)}{\Gamma\left(\frac{n}{2}\right)}. \quad (42)$$

In some applications (such as in nuclear physics) involving low-energy interactions among nucleons the lower limit (zero) should be replaced by the hard-core radius  $r_c \cong 0.5 \times 10^{-13}$  cm [32]. In such cases the expressions for  $P_n(s)$  and  $\langle s^m \rangle$  can be expressed as follows:

$$P_n(s) = \frac{s^{n-1} \int_{\frac{s}{2}}^R (R^2 - x^2)^{\frac{n-1}{2}} dx}{C(2R, 0, n) - C(r_c, 0, n)} \quad (43)$$

and

$$\langle s^m \rangle = \int_{r_c}^{2R} s^m P_n(s) ds = \frac{H(R, r_c, m, n)}{H(R, r_c, 0, n)} \quad (44)$$

where

$$C(a, m, n) = \int_0^a s^{m+n-1} ds \int_{s/2}^R (R^2 - x^2)^{(n-1)/2} dx$$

and

$$H(R, r_c, m, n) = \frac{(2R)^{n+m}}{n+m} \left[ B\left(\frac{n}{2} + \frac{1}{2}, \frac{n}{2} + \frac{1}{2} + \frac{m}{2}\right) - B_x\left(\frac{n}{2} + \frac{1}{2}, \frac{n}{2} + \frac{1}{2} + \frac{m}{2}\right) \right] - \frac{r_c^{n+m}}{n+m} \left[ B\left(\frac{1}{2}, \frac{n}{2} + \frac{1}{2}\right) - B_x\left(\frac{1}{2}, \frac{n}{2} + \frac{1}{2}\right) \right] \tag{45}$$

with  $x = r_c^2/4R^2$  and  $m$  an integer. We note that equations (43) and (44) are the first known analytical results for  $P_n(s)$  and  $\langle s^m \rangle$  to incorporate the hard-core radius  $r_c$ .

### 5.2. Neutron star models

Another application of current interest is the self-energy of a neutron star arising from the exchange of  $\nu\bar{\nu}$  pairs [33–35]. Here we evaluate the probability density functions in three dimensions for neutron stars with a multiple-shell density distribution, which is what is typically assumed in neutron star models [36, 37]. For illustrative purposes, we discuss a spherically symmetric model with two spherical shells, each of uniform density, where for simplicity we assume shells of equal thickness. Some other multiple-shell models and their  $n$ -dimensional probability density functions can be found in [5].

For a two-shell model with a uniform density in each shell, define  $\rho = \rho_1$  for  $0 \leq r \leq R/2$  and  $\rho = \rho_2$  for  $R/2 \leq r \leq R$ , where  $\rho_1$  and  $\rho_2$  are arbitrary constants and  $r$  is measured from the centre of the neutron star. Using the preceding formalism we can show that  $P_3(s)$  has four different functional forms specified by four regions:

1.  $0 \leq s \leq \frac{1}{2}R$ :

$$P_3(s) = \frac{24(\rho_1^2 + 7\rho_2^2)s^2}{(\rho_1 + 7\rho_2)^2 R^3} - \frac{36(\rho_1^2 - 2\rho_1\rho_2 + 5\rho_2^2)s^3}{(\rho_1 + 7\rho_2)^2 R^4} + \frac{12(\rho_1^2 - 2\rho_1\rho_2 + 2\rho_2^2)s^5}{(\rho_1 + 7\rho_2)^2 R^6} \tag{46}$$

2.  $\frac{1}{2}R \leq s \leq R$ :

$$P_3(s) = -\frac{81(\rho_1 - \rho_2)\rho_2 s}{2(\rho_1 + 7\rho_2)^2 R^2} + \frac{24\rho_1 s^2}{(\rho_1 + 7\rho_2) R^3} - \frac{36\rho_1(\rho_1 + 3\rho_2)s^3}{(\rho_1 + 7\rho_2)^2 R^4} + \frac{12\rho_1^2 s^5}{(\rho_1 + 7\rho_2)^2 R^6} \tag{47}$$

3.  $R \leq s \leq \frac{3}{2}R$ :

$$P_3(s) = -\frac{81(\rho_1 - \rho_2)\rho_2 s}{2(\rho_1 + 7\rho_2)^2 R^2} + \frac{24(9\rho_1 - \rho_2)\rho_2 s^2}{(\rho_1 + 7\rho_2)^2 R^3} - \frac{36(5\rho_1 - \rho_2)\rho_2 s^3}{(\rho_1 + 7\rho_2)^2 R^4} + \frac{12(2\rho_1 - \rho_2)\rho_2 s^5}{(\rho_1 + 7\rho_2)^2 R^6} \tag{48}$$

4.  $\frac{3}{2}R \leq s \leq 2R$ :

$$P_3(s) = \frac{192\rho_2^2 s^2}{(\rho_1 + 7\rho_2)^2 R^3} - \frac{144\rho_2^2 s^3}{(\rho_1 + 7\rho_2)^2 R^4} + \frac{12\rho_2^2 s^5}{(\rho_1 + 7\rho_2)^2 R^6} \tag{49}$$

We observe that the probability density functions defined in adjacent regions are continuous across the boundaries separating the regions.

### 5.3. GRIP: a new computational test for randomness

Another interesting application of the present work is as a new test of random number generators used in a variety of stochastic simulations. Our statistical method follows by applying the probability density functions for the random distance distribution to evaluate the expectation values of the random inner product  $\vec{r}_{12} \cdot \vec{r}_{23}$ , where  $\vec{r}_{12} = \vec{r}_2 - \vec{r}_1$ ,  $\vec{r}_{23} = \vec{r}_3 - \vec{r}_2$ , and  $\vec{r}_1$ ,  $\vec{r}_2$  and  $\vec{r}_3$  are three random points independently sampled from a spherical  $n$ -ball. The quantity  $\langle \vec{r}_{12} \cdot \vec{r}_{23} \rangle_n$  is one of the geometric probability constants as discussed in [5]. It follows from the preceding formalism that for a spherical  $n$ -ball of radius  $R$  with a uniform density distribution,

$$\langle \vec{r}_{12} \cdot \vec{r}_{23} \rangle_n = -\frac{n}{n+2}R^2. \quad (50)$$

Note that

$$\lim_{n \rightarrow \infty} \langle \vec{r}_{12} \cdot \vec{r}_{23} \rangle_n = -R^2. \quad (51)$$

In a spherical Gaussian space where  $\rho \propto e^{-r^2/2\sigma^2}$  and  $R \rightarrow \infty$ ,

$$\langle \vec{r}_{12} \cdot \vec{r}_{23} \rangle_n = -n\sigma^2. \quad (52)$$

We refer to these tests as GRIP (geometric random inner product).

We now apply the GRIP test to check three popular random number generators frequently used in Monte Carlo simulations [38–42]. The random number generators tested are

1. RAN0 [39] which is a linear congruential generator and uses the following algorithm:

$$I_n = 16\,807 I_{n-1} \bmod m = 2^{31} - 1. \quad (53)$$

2. R31 [40] which uses the generalized feedback shift register (GFSR) method

$$x_n = x_{n-p} \oplus x_{n-q} \quad (54)$$

where  $p = 31$ ,  $q = 3$  and  $\oplus$  is the bitwise exclusive OR operator.

3. NWS [41, 42] which uses the nested Weyl sequence

$$Y_n = \{n\{n\alpha\}\} \quad (55)$$

where  $\{y\}$  is the fractional part of  $y$  and  $\alpha$  is an irrational number.

The results are shown in table 1. We have checked several initialization methods and the results are not affected. We note that the NWS generator using the nested Weyl sequence method fails to pass our randomness tests in all dimensions selected. Hence caution should be exercised in using this particular random number generator for Monte Carlo simulations, especially in molecular dynamics simulations. More numerical results for a variety of random number generators including the PSLQ algorithm using the binary digits of  $\pi$  [43], and other newly proposed computational methods, will be discussed in [44].

This series of geometric probability constants,  $\langle \vec{r}_{12} \cdot \vec{r}_{23} \rangle_n$ , can be added to the family of various computational tests for random number generators [38]. They can then serve to investigate the quality of random number generators for questions of randomness, especially in higher dimensions ( $n > 3$ ) where few results are currently available. The possibility that some random number generators such as NWS pass other tests but not ours, may indicate that the properties of random points in a sphere provide a more sensitive test of randomness than is otherwise available. These and other important issues will be discussed in greater detail in [44].

**Table 1.** Comparison of random number generators (RNG) with the exact results derived in this paper for  $\langle \vec{r}_{12} \cdot \vec{r}_{23} \rangle_n$ . The number of simulation samples in each case is  $N = 10^6$ . We note that the NWS generator fails to pass the new randomness test in all dimensions that we selected. See the text for further details.

RNG	$n = 3$	Result	$n = 5$	Result	$n = 10$	Result
RAN0	$-0.60037 \pm 0.00065$	Pass	$-0.71483 \pm 0.00059$	Pass	$-0.83310 \pm 0.00047$	Pass
R31	$-0.60028 \pm 0.00066$	Pass	$-0.71468 \pm 0.00058$	Pass	$-0.83229 \pm 0.00048$	Pass
NWS	$-0.64119 \pm 0.00071$	Fail	$-0.75427 \pm 0.00057$	Fail	$-0.85016 \pm 0.00049$	Fail
Exact	$-0.60000$		$-0.71429$		$-0.83333$	

## 6. Conclusions

A formalism has been presented in this paper for evaluating the analytical probability density function of the random distance distribution for a spherical  $n$ -ball with an arbitrary density distribution. We show that the random distance distribution technique can reduce otherwise difficult calculations from the complexity of  $2n$ -dimensional integrals to just a one-dimensional integral, even when the nucleon–nucleon hard-core radius  $r_c$  is included. Our formalism has applications to the currently active area of research surrounding string-inspired theories of higher dimensional physics, and has numerous potential applications to other fields as well. Specifically the results presented here are of interest in the context of recent work on the modifications to the Newtonian inverse-square law arising from the existence of extra spatial dimensions [45]. We have also presented a new computational method to test random number generators for studying random sequences used in Monte Carlo simulations.

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