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Abstract. The probability density and distribution function of the sum of N isotropic random vectors is studied for the general case in which the probability density of the lengths of the individual vectors vanishes identically outside a finite interval. The probability density function is expressed in a Fourier sine series whose coefficients are the sampled values of the characteristic function. Typical numerical calculations are summarized in graphical form for the case where the lengths of the vectors obey a rectangular probability density. Sampling expansions are also developed for the moments and the distribution function.

1. Introduction

The problem of isotropic random flights, besides being interesting in its own right, has numerous applications in the physical sciences (Barber and Ninham 1970, Flory 1969). In the now standard situation each random vector is taken to be an independent random variable having *fixed* length and random orientation (isotropic). Under these circumstances, the determination of the probability density of such finite sums of random vectors follows a standard formal procedure. The characteristic function for an individual vector is evaluated and since the vectors are independent random variables, the characteristic function of the sum is the product of the characteristic functions. Having determined the total characteristic function one merely takes its Fourier transform to obtain the probability density of the sum in the form of an infinite integral possessing a rapidly oscillating integrand. Such an integral does not lend itself to explicit general evaluation or numerical computation.

Should the lengths of the vectors also be random variables, then the situation is decidely unfavourable because the characteristic function of the sum is generally a product of complicated integrals. Obviously the computational problem is orders of magnitude more involved than in the simple fixed-length case should one attempt brute force.

The purpose of the present paper is twofold. First, to present a computational scheme based upon the sampling theorem for the evaluation of the probability density directly in terms of sampled values of the total characteristic function. This method is ideally suited to automatic computation and is capable of reasonable accuracy (4 or 5 digits) with little effort. Second, to utilize this scheme to study the problem of chains of vectors each vector having random length.

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2. Formal solution

The length of the chain is given by the vector

$$\boldsymbol{R}_N = \sum_{n=1}^{N} \boldsymbol{r}_n, \tag{1}$$

where the $\boldsymbol{r}_n$ are statistically independent vectors having isotropic probability density functions

$$W(\boldsymbol{r}_n) = W(\theta_n)W(\phi_n)W(|\boldsymbol{r}_n|) = \frac{1}{4\pi^2}W(r_n) \tag{2}$$

where $r_n \equiv |\boldsymbol{r}_n|$. We leave $W(r_n)$, the probability density function of the length of $\boldsymbol{r}_n$, unspecified at present.

The characteristic function of $W_n(r)$ is

$$A_n(\rho) = \int_{-\infty}^{\infty} W(\boldsymbol{r}_n)\exp(\mathrm{i}\boldsymbol{\rho}\,.\,\boldsymbol{r})\,\mathrm{d}\boldsymbol{r} = \int_0^{\infty} r^2 W(r_n)\left(\frac{\sin \rho r}{\rho r}\right)\mathrm{d}r \tag{3}$$

where $\rho \equiv |\boldsymbol{\rho}|$. Since the individual vectors are statistically independent, the characteristic function of their sum is the product of their characteristic functions

$$A_N(\rho) = \prod_{n=1}^{N} A_n(\rho). \tag{4}$$

Consequently the probability density function of the total sum is

$$W_N(\boldsymbol{R}) = \frac{1}{(2\pi)^3}\int_{-\infty}^{\infty} A_N(\boldsymbol{\rho})\exp(-\mathrm{i}\boldsymbol{\rho}\,.\,\boldsymbol{R})\,\mathrm{d}\boldsymbol{\rho} = \frac{1}{2\pi^2 R}\int_0^{\infty} A_N(\rho)\rho\sin R\rho\,\mathrm{d}\rho \tag{5}$$

where $R \equiv |\boldsymbol{R}|$.

Rather than deal with W_N itself, we choose to work with a scalar quantity, the radial density function

$$f_N(R) = 4\pi R^2 W_N(\boldsymbol{R}) \tag{6}$$

which is the probability that R assumes a given magnitude irrespective of the direction of the chain displacement vector $\boldsymbol{R}$.

The analysis thus far has been perfectly general but we now place a restriction on $W(r_n)$ and require that it vanish identically when r exceeds a fixed *finite* value, say β_n:

$$W(r_n) \equiv 0 \qquad r > \beta_n. \tag{7}$$

Such a requirement is a perfectly reasonable one for the class of physical problems in which we are interested; after all individual bond lengths of the freely-rotating polymer chain are finite. Since $W(r_n)$ vanishes identically outside a compact region, its Fourier transform, the characteristic function $A_n(\rho)$, is therefore a bandlimited function. Now the products of bandlimited functions are also bandlimited functions so that $A_N(\rho)$ is bandlimited with

$$f_N(R) \equiv 0 \qquad R > R_N \equiv \sum_{n=1}^{N} \beta_n. \tag{8}$$

This suggests that we employ a sampling theorem to evaluate $f_N(R)$ in terms of sampled values of $A_N(\rho)$ in place of direct evaluation of equation (5).

Let us write our basic equations in the form

$$f_N(R)R^{-1} = \frac{2}{\pi}\int_0^{\infty} (\rho A_N(\rho)) \sin R\rho \, \mathrm{d}\rho \tag{9}$$

$$\rho A_N(\rho) = \int_0^{R_N} (f_N(R)R^{-1}) \sin \rho R \, \mathrm{d}\rho \tag{10}$$

and expand $(f_N(R)R^{-1})$ in the fundamental interval $(0, R_N)$:

$$f_N(R)R^{-1} \begin{cases} = \sum_{m=1}^{\infty} f_m \sin(m\pi R/R_N), & 0 \leqslant R \leqslant R_N \\ = 0, & \text{elsewhere.} \end{cases} \tag{11}$$

The Fourier coefficients f_m can be written directly in terms of the *sampled* values of $A_N(\rho)$ by virtue of equation (10):

$$f_m = \frac{2}{R_N}\int_0^{R_N} (f_N(R)R^{-1}) \sin(m\pi R/R_N) \, \mathrm{d}R = \frac{2}{R_N}\left(\frac{m\pi}{R_N}\right) A_N\left(\frac{m\pi}{R_N}\right). \tag{12}$$

Consequently

$$f_N(R) \begin{cases} = 2\left(\frac{R}{R_N}\right) \sum_{m=1}^{\infty} \left(\frac{m\pi}{R_N}\right) A_N\left(\frac{m\pi}{R_N}\right) \sin\left(\frac{m\pi R}{R_N}\right), & 0 \leqslant R \leqslant R_N \\ = 0, & \text{elsewhere.} \end{cases} \tag{13}$$

The smoother $f_N(R)$, the more rapid is the convergence of its Fourier series expansion.

Since $f_N(R)$ must integrate to unity we have a convenient check on the magnitude of $A_N(m\pi/R_N)$:

$$\int_0^{\infty} f_N(R) \, \mathrm{d}R = \int_0^{R_N} f_N(R) \, \mathrm{d}R = 1 \tag{14}$$

which implies

$$\sum_{m=1}^{\infty} (-1)^{m+1} A_N(m\pi/R_N) = \tfrac{1}{2}. \tag{15}$$

The radial distribution function $F_N(R')$, which is the probability that $R' < R_N$, is

$$F_N(R') = \int_0^{R'} f_N(R) \, \mathrm{d}R. \tag{16}$$

Upon performing the required manipulations, we have

$$F_N(R') \begin{cases} = \frac{R'\sqrt{2\pi}}{R_N} \sum_{m=1}^{\infty} \left(\frac{m\pi R'}{R_N}\right)^{1/2} A_N\left(\frac{m\pi}{R_N}\right) \mathrm{J}_{3/2}\left(\frac{m\pi R'}{R_N}\right), & R' < R_N \\ = 1, \quad R' > R_N \end{cases} \tag{17}$$

where $\mathrm{J}_{3/2}(x)$ is the Bessel function of order $\frac{3}{2}$.

The moments of the radial density function are also easily obtained in terms of the sampling series coefficients

$$E_N(R^k) \equiv \int_0^{R_N} f_N(R)R^k \, \mathrm{d}R = \frac{2}{R_N}\sum_{m=1}^{\infty} \left(\frac{R_N}{m\pi}\right)^k A_N\left(\frac{m\pi}{R_N}\right) g_m(k) \tag{18}$$

where $k = 1, 2, \ldots,$ and

$$g_m(k) \equiv \int_0^{m\pi} x^{k+1} \sin x \, \mathrm{d}x.$$

Since $g_m(k)$ is independent of $f_N(R)$, the moments can be calculated without the necessity of resorting to new integrations each time k is changed. The first few $g_m(k)$ are:

$$\begin{aligned} g_m(1) &= (-1)^{m+1}\{(m\pi)^2 - 2\} - 2 \\ g_m(2) &= (-1)^{m+1}\{(m\pi)^3 - 6m\pi\} \\ g_m(3) &= (-1)^{m+1}\{(m\pi)^4 - 120(m\pi)^2 + 24\} + 24 \\ g_m(4) &= (-1)^{m+1}\{(m\pi)^5 - 20(m\pi)^3 + 120m\pi\}. \end{aligned} \tag{20}$$

3. Fixed lengths

If the lengths are taken to be fixed quantities β_n then

$$W(r_n) = \frac{1}{r^2}\delta(r - \beta_n) \tag{21}$$

with the result that the characteristic function becomes

$$A_n(\rho) = \frac{\sin \beta_n \rho}{\beta_n \rho} \tag{22}$$

so that the radial density function reads

$$f_N(R) = \frac{2R}{\pi} \int_0^{\infty} \rho \sin R\rho \prod_{n=1}^{N} \frac{\sin \beta_n \rho}{\beta_n \rho} \, \mathrm{d}\rho. \tag{23}$$

This is the integral solution originally obtained by Rayleigh (1919). Even this case has not been studied when $\beta_1 \neq \beta_2 \neq \ldots \neq \beta_N$.

However Rayleigh evaluated the integral explicitly for $N = 2, 3, 4, 6$ in the special case of equal lengths. It was left to Treloar (1946) to obtain an exact solution of equation (3.3) *for equal lengths*. His solution, although simple looking, is relatively difficult to evaluate because $f_N(R)$ undergoes discontinuous changes in slope in the fundamental interval $(0, R_N)$, the number of changes depending on N. Furthermore $f_N(R)$ is expressed in terms of polynomials in R with a different polynomial in each subinterval between discontinuities in slope. For example

$$f_5(R) \begin{cases} = (16\beta^5)^{-1}(5\beta^5 R^2 - R^4), & R \epsilon I_1 \\ = (48\beta^5)^{-1}(-5\beta^3 R + 30\beta^2 R^2 - 15\beta R^3 + 2R^4), & R \epsilon I_2 \\ = (96\beta^5)^{-1}(125\beta^3 R - 75\beta^2 R^2 + 15\beta R^3 - R^4), & R \epsilon I_3 \end{cases} \tag{24}$$

where I_1 is the interval $(0 \leqslant R \leqslant \beta)$, I_2 is $(\beta \leqslant R \leqslant 3\beta)$, and I_3 is $(3\beta \leqslant R \leqslant 5\beta)$. The complexity and number of these polynomials increases with N.

This fact lead Jerrigan and Flory (1969) to evaluate the integral in equation (23) by quadrature, again for equal displacement lengths. No details of the actual integration procedure are given in their paper but the fact that equation (23) has an infinite interval of integration *and* a rapidly fluctuating integrand mitigates against any reasonable accuracy unless a very high order quadrature formula is employed.

We have calculated $f_N(R)$ for equal displacement lengths using the sampled series representation with fifteen terms in the series. The numerical results for $N = 2, 3, \ldots, 8$ were checked against the explicit expressions obtained by Vincenz and Bruckshaw (1946) who were unaware of Treloar's previous solution. Reference is made to figure 1 of their paper for curves of $f_N(R)$. For some further work on this special case, see the two recent papers by Dvorak (1972a, b).

Even though we take unequal displacements, the resultant behaviour of $f_N(R)$ is qualitatively similar to that of equal displacement lengths *provided* $N \geqslant 4$ (see figure 1 for a typical situation). The case $N = 2\,(\beta_1 \geqslant \beta_2)$ was given by Rayleigh and is

$$f_2(R)\begin{cases} = 0, & 0 < R < \beta_1 - \beta_2 \\ = \dfrac{R}{\beta_1\beta_2}, & \beta_1 - \beta_2 < R < \beta_1 + \beta_2 \\ = 0, & R > \beta_1 + \beta_2 . \end{cases} \tag{25}$$

The sampled series representation for this case is not particularly useful because $f_2(R)$ is discontinuous giving rise to a Gibbs phenomena if we attempt numerical computation. The reason that $f_2(R)$ is zero for $\beta_1 \neq \beta_2$ is obvious. When $N = 3$ the author has attempted an explicit solution but was only able to derive one for the case

$$\beta_1 + \beta_2 + \beta_3 \geqslant \beta_1 + \beta_2 - \beta_3 \geqslant \beta_1 - \beta_2 + \beta_3 \geqslant -\beta_1 + \beta_2 + \beta_3;$$

it is:

$$f_3(R)\begin{cases} = \dfrac{R^2}{2\beta_1\beta_2\beta_3}, & 0 < R \leqslant B_1 \\ = \dfrac{R(R-\beta_1+\beta_2+\beta_3)}{4\beta_1\beta_2\beta_3}, & B_1 \leqslant R \leqslant B_2 \\ = \dfrac{R}{2\beta_1\beta_2}, & B_2 \leqslant R \leqslant B_3 \\ = \dfrac{R(\beta_1+\beta_2+\beta_3-R)}{4\beta_1\beta_2\beta_3}, & B_3 \leqslant R \leqslant B_4 \end{cases} \tag{26}$$

where

$$B_1 \equiv -\beta_1 + \beta_2 + \beta_3, \qquad B_2 \equiv \beta_1 - \beta_2 + \beta_3$$
$$B_3 \equiv \beta_1 + \beta_2 - \beta_3, \qquad B_4 \equiv \beta_1 + \beta_2 + \beta_3 .$$

Thus $f_3(R)$ is continuous in the basic interval but possesses three discontinuities in slope when $\beta_1 \neq \beta_2 \neq \beta_3$ compared to only one when $\beta_1 = \beta_2 = \beta_3$. However only two of these discontinuities in slope are strong (see figure 2). The sampled series representation of $f_3(R)$ was also employed as a numerical check with excellent results.

It is in the calculation of the radial distribution function $F_N(R')$ that the power of the sampled series representation is displayed. Even in the simple case of equal lengths for which we have explicit formulae it is not a simple feat to work through the integration of all the sets of polynomials over all the necessary subintervals. However the calculation according to equation (17) is carried out *independently* of the subintervals between discontinuities in slope. Furthermore since the series for $F_N(R)$ is an integrated version of the series for $f_N(R)$ it converges more rapidly than that of $f_N(R)$.

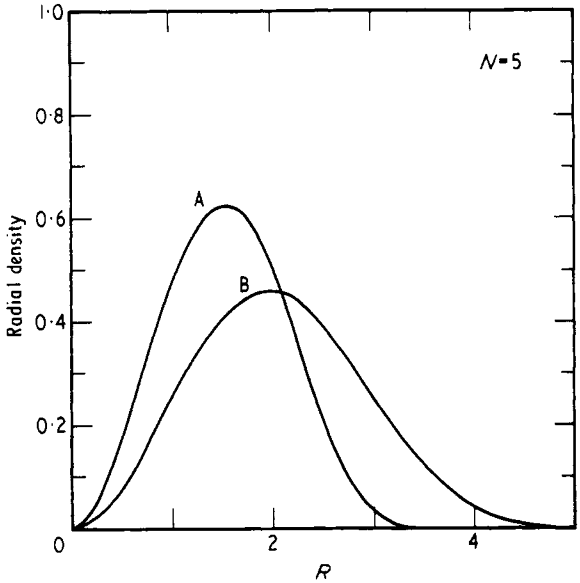

Figure 1. Radial density $f_5(R)$ for chain of five vectors of fixed length: curve A $\beta_1 = \beta_2 = 1$, $\beta_3 = \beta_4 = \beta_5 = 0{\cdot}5$; curve B $\beta_1 = \ldots = \beta_5 = 1$.

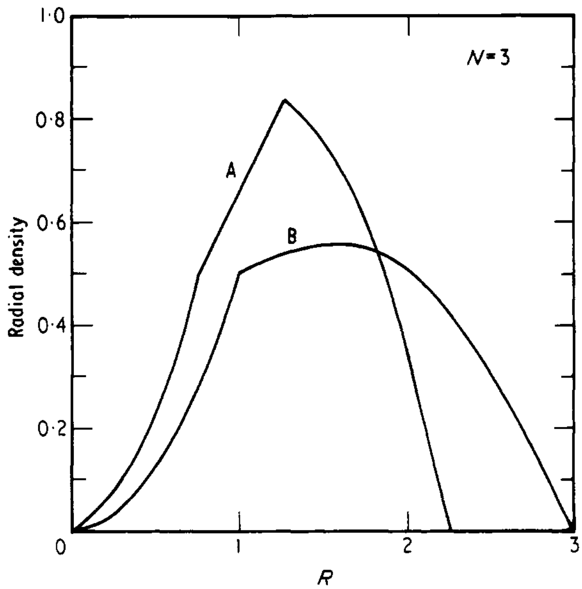

Figure 2. Radial density $f_3(R)$ for chain of three vectors of fixed length: curve A $\beta_1 = 1$, $\beta_2 = 0{\cdot}75$, $\beta_3 = 0{\cdot}50$; curve B $\beta_1 = \beta_2 = \beta_3 = 1$.

This brings us to the practical problem of ascertaining the number of terms in the sampled series representation to achieve a prescribed accuracy. Unfortunately only the global error can be specified not the local error since we are dealing with Fourier series. Equation (15) is a constraint upon the sampled values of A_N and can serve as a reasonable indicator of the global error. This point is illustrated in table 1 where we list the numerical values of A_N for $N = 3, 4$ and equal unit lengths. Only the first few terms are of any real consequence. The last three figures in each column represent the number of terms that are summed in equation (15).

Table 1. Numerical values of the first nine sampled values of A_N for $N = 3, 4$ where all displacement lengths are unity

m	$N = 3$	$N = 4$
1	0·565596	0·657023
2	0·070699	0·164256
3	0·000000	0·008111
4	−0·008837	0·000000
5	−0·004525	0·001051
6	0·000000	0·002028
7	0·001649	0·000274
8	0·001115	0·000000
9	0·000000	0·000100
S(3)	0·494897	0·500878
S(5)	0·499209	0·501929
S(9)	0·499753	0·500275

4. Random lengths

We are particularly interested in the case where each random length obeys a rectangular density:

$$W(r_n)\begin{cases} = \dfrac{1}{r^2(\beta_n-\alpha_n)}, & \alpha_n \leqslant r \leqslant \beta_n \\ = 0, & \text{elsewhere} \end{cases} \tag{27}$$

where β_n is *finite*. Consequently the characteristic function of the nth vector, by virtue of equation (3), becomes

$$A_n(\rho) = \frac{1}{\beta_n-\alpha_n}\int_{\alpha_n}^{\beta_n} \frac{\sin \rho r}{\rho r}\,\mathrm{d}r = \frac{\mathrm{Si}(\beta_n\rho)-\mathrm{Si}(\alpha_n\rho)}{\beta_n-\alpha_n} \tag{28}$$

where $\mathrm{Si}(x)$ is the sine integral of argument x. As $\alpha_n \to \beta_n$ then $A_n(\rho)$ tends to the expression given in equation (22) for fixed length. Since $A_n(\rho)$ is a bandlimited function, we can apply the formulae derived in § 2.

Before presenting any numerical results for this case let us look at the asymptotic behaviour of $f_N(R)$ as N is taken to be very large. The main contribution to the integral on the right-hand side of equation (5) comes from $A_n(\rho)$ evaluated in the vicinity of the origin. Now when ρ is made very small in equation (28), it is a simple matter to prove

$$A_n(\rho) \sim 1 - \frac{(\alpha_n^2+\alpha_n\beta_n+\beta_n^2)\rho^2}{18} + \mathrm{O}(\rho^4) \sim \exp\left(-\frac{(\alpha_n^2+\alpha_n\beta_n+\beta_n^2)\rho^2}{18}\right) \tag{29}$$

so that

$$A_N(\rho) \sim \exp\left(-\frac{\rho^2}{18}\sum_{n=1}^{N}(\alpha_n^2+\alpha_n\beta_n+\beta_n^2)\right). \tag{30}$$

To evaluate $f_N(R)$, we merely substitute equation (30) into equation (9), the final result is

$$f_N(R) \sim \left(\frac{2}{\pi}\right)^{1/2} \frac{R^2}{\sigma^3} \exp\left(-\frac{R^2}{2\sigma^2}\right) \tag{31}$$

where

$$\sigma^2 \equiv \tfrac{1}{9} \sum_{n=1}^{N} (\alpha_n^2 + \alpha_n\beta_n + \beta_n^2). \tag{32}$$

This is the well known Maxwell density function.

If all the vectors possess the same length density functions, then $\alpha_n \equiv \alpha$, $\beta_n \equiv \beta$ and σ^2 becomes

$$\sigma^2 = \tfrac{1}{9}N(\alpha^2 + \alpha\beta + \beta^2). \tag{33}$$

Now if $\alpha \to \beta$, then $\sigma^2 = N\beta^2/3$ (known result for fixed equal lengths); however if $\alpha = 0$, then $\sigma^2 = N\beta^2/9$ which is three times smaller. This is simply a manifestation of the tendency of $f_N(R)$ to weigh against even moderately large lengths. Furthermore the approach to this limiting density is most rapid for $\alpha = 0$ as we will see from the numerical data; in fact, for a value of N as small as 4, $f_N(R)$ appears maxwellian for all practical purposes.

Because of the limitless combinations of parameters, we have confined our calculations to the special case of equal rectangular densities so that $\alpha_1 = \alpha_2 = \ldots = \alpha_N = \alpha$, $\beta_1 = \beta_2 = \ldots = \beta_N = \beta$, and taking $\beta = 1$ without any loss of generality. The final curves for $N = 3$, 6 are shown in figures 3, 4. The curves marked A correspond to $\alpha = 0$ and even for $N = 3$ the radial density looks maxwellian.

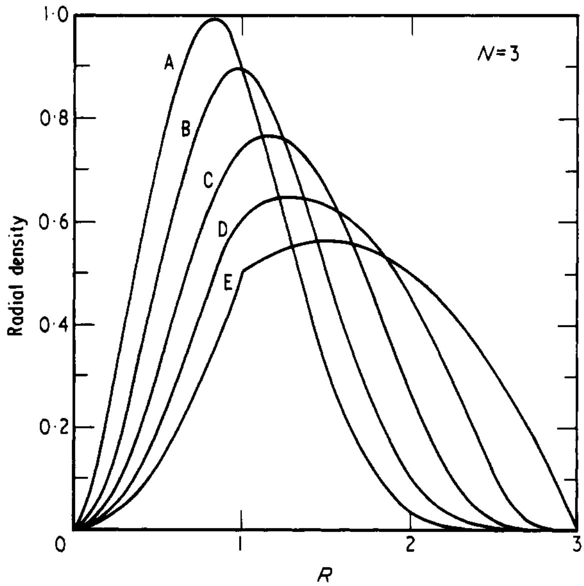

Figure 3. Radial density $f_3(R)$ for chain of three vectors having random lengths: curve A $\alpha = 0$, $\beta = 1$; curve B $\alpha = 0{\cdot}25$, $\beta = 1$; curve C $\alpha = 0{\cdot}50$, $\beta = 1$; curve D $\alpha = 0{\cdot}75$, $\beta = 1$; curve E $\alpha = 0{\cdot}99$, $\beta = 1$.

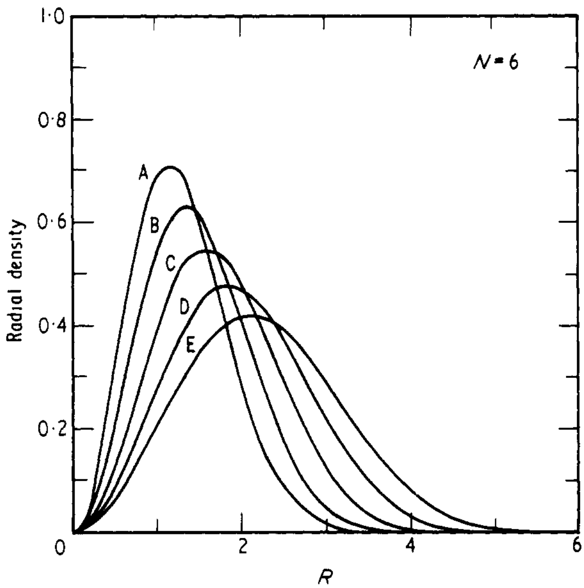

Figure 4. Radial density $f_6(R)$ for chain of six vectors having random lengths: curve A $\alpha = 0$, $\beta = 1$; curve B $\alpha = 0{\cdot}25$, $\beta = 1$; curve C $\alpha = 0{\cdot}50$, $\beta = 1$; curve D $\alpha = 0{\cdot}75$, $\beta = 1$; curve E $\alpha = 0{\cdot}99$, $\beta = 1$.

Since the present paper is concerned with general formalism, we do not feel it necessary to continue with examples. The mathematical procedure is now perfectly straightforward and the reader should have no difficulty working out any combinations of interest to him.

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