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Random Flights in Euclidean Space. I. General Analysis and Results for Flights with Prescribed Hit Expectance Density About the Origin

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We consider the problem of random flights in Euclidean space defined by a series of displacements, $\mathbf{r}_i$, the magnitude and direction of each being independent of all the preceding ones. The displacements are not restricted to prescribed lattice sites. We begin with some new results generalizing a well-known lattice-walk relation between the probability of return to the origin and the expected number of times the origin is visited in the course of a random walk. We go on to consider flights for which the hit expectancy is prescribed within a hypersphere of radius R centered at the flight origin. For uniform hit expectance density (i.e., hit expectancy proportional to volume size) within the sphere, we solve the problem in three and five dimensions for a certain class of displacement probability densities that are prescribed only for displacement distances r greater than R. For each such displacement probability $\tau(\mathbf{r})$, we find both the value of the hit expectance density and the form of the displacement probability density for $r < R$ that are dictated by the constraint of uniform hit expectance density within the sphere of radius R. In an appendix, we show the way the common appearance of integral equations of Ornstein–Zernike type in problems of random flight, liquid and lattice-gas structure, and percolation theory yield certain corresponding results in all three areas.

KEY WORDS: Random walks; prescribed return expectance; Ornstein–Zernike equation in random walks theory.

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1. INTRODUCTION

This paper reports the first of a series of investigations we have made into the properties of random walks (in Euclidean space) that are not restricted to regular lattice sites. Subsequent work, concerned with both more general random-flight properties as well as a specific subclass of random walks with orientational dependence, will be considered in future articles.

Consider a point particle in a d-dimensional Euclidean space. At time t_0 its initial position is at the origin. At subsequent times $t_1, t_2, \ldots, t_n$ it undergoes displacements $\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_n$ so that at time t_n its position is

$$\mathbf{R}_n = \sum_{i=1}^{n} \mathbf{r}_i \tag{1.1}$$

This equation defines a random flight (or random walk) if the sequence of jumps $\{\mathbf{r}_i\}$ are mutually independent random variables with probability density functions $\tau_i(\mathbf{r}_i)$, each having the property that $\tau_i(\mathbf{r})\,d\mathbf{r}$ is the probability that $\mathbf{r}_i$ lies in the interval $(\mathbf{r}, \mathbf{r} + d\mathbf{r})$.

The problem of random flights has a long and interesting history, both as a purely mathematical problem in probability theory[1] and as a model for various physical and chemical processes.[2,3] [3] A large proportion of the effort in this field has been expended on the problem, first introduced by Polya,[6] in which the points $\mathbf{r}_i$ are confined to a countable number of discrete positions in the d-dimensional space, usually a regular lattice.[4,5] The term random walk has come to be almost synonymous with the lattice problem; to emphasize that our interest in this paper is in the continuum problem (where the $\mathbf{r}_i$ are not confined to a set of discrete points), we shall use the term random flights. For convenience, we shall refer to the object executing the random flight as the random jumper, and the individual displacements in the random flights as jumps. In all the subsequent analysis, we consider $\tau_i = \tau$.

Typically in a random flight problem in Euclidean space one begins with a prescribed jump probability density $\tau(r_i)$ associated with the series of jumps, $\mathbf{r}_i$, $i = 1, 2, \ldots,$ the magnitude and direction of each being independent of all the preceding ones. One is then often interested in such quantities as the probability $w_n(\mathbf{r})\,d\mathbf{r}$ that the position of a particle describing such a flight lies in the volume element $d\mathbf{r}$ centered at $\mathbf{r}$ after n jumps. Chandrasekhar[7] has reviewed a number of classic examples of this problem, which dates back to the work of Lord Rayleigh.[8] More recent

[3] A number of excellent surveys of results on random walks and related problems on periodic lattices have been written by E. W. Montroll; see, for example, Ref. 4. In this connection see also the beautiful article by Kasteleyn, Ref. 5.

research on random flights not restricted to a regular lattice has been done mainly in the context of its application to the polymer chain problem. Such work, through 1970, is summarized nicely by Yamakawa.[3]

We begin in Section 2 by considering some expressions that generalize the well-known lattice-walk relation between the probability of return to the origin and the expected number of times the origin is visited during the course of a random walk. In the subsequent sections, we focus on a problem somewhat different from the usual random-flight problem considered in Refs. 7 and 3. We contemplate a random flight in which $\tau(\mathbf{r}_i)$ is not fully prescribed but instead $N(V)$, the number of visits of the object in flight within a sphere of volume V (and radius R) about the origin, is prescribed by requiring that the hit expectance density $e(\mathbf{r})$, defined in Eq. (2.4) below, be constant within the sphere. We have

$$N(V) = 1 + E(V) \tag{1.2}$$

[counting the object's presence at the origin before the flight begins as the first visit, which accounts for the 1 in (1.2)] where $E(V)$ is given by

$$E(V) = \int_V e(\mathbf{r})\, d\mathbf{r} \tag{1.3}$$

Thus for constant $e(\mathbf{r})$ inside the sphere

$$e(\mathbf{r}) = \epsilon, \qquad |\mathbf{r}| < R \tag{1.4}$$

we have, in d dimensions,

$$E(V) = \epsilon V(d, R) \tag{1.5}$$

where $V(d, R)$ is the volume of the d-dimensional hypersphere of radius R.

The jumps we shall consider here will be those of random direction so that $\tau(\mathbf{r}_i)$ depends only on $|\mathbf{r}_i|$, which we denote as r_i. If we prescribe $E(V)$ by (1.5), with ϵ an undetermined constant, it becomes clear in the development given below that we can only hope to formulate a well-posed problem if we prescribe $\tau(r_i)$ only for $r_i > R$.

Perhaps the simplest such prescription is to limit each jump r_i to be less than or equal to R so that

$$\tau(r_i) = 0 \qquad \text{for} \quad r_i > R \tag{1.6}$$

The problem defined by (1.4) and (1.6) is as follows: are there any real nonnegative values of ϵ such that real nonnegative $\tau(r_i)$ satisfying (1.6) can be found? As we shall show below, the answer is "yes" in three and five dimensions (which are the only dimensions in which we have analyzed this question).

We can go beyond the above result as follows: in three dimensions, the "Yukawa" function

$$\tau(r_i) = K r_i^{-1} \exp[-z(r_i - R)], \qquad K \geqslant 0, \quad z \geqslant 0 \tag{1.7}$$

is a very natural jump probability to consider in the classical random flight problem, because it leads to a generating function for the $w_n(r)$ and a hit expectance density $e(r)$ that are also both of Yukawa form. We have therefore considered the prescribed hit expectancy problem defined by (1.4) along with

$$\tau(r) = K r^{-1} \exp[-z(r - R)], \qquad r > R \tag{1.8}$$

We find that for some but not all prescribed K and z there exist $\epsilon(K, z)$ and $\tau(r)$ for $r > R$ that are consistent with (1.4) and (1.8) with both ϵ and $\tau(r)$ nonnegative.

Two key equations in our analysis [(2.7) and (2.12a)] prove to be of "Ornstein–Zernike" form. We show in an appendix how the common appearance of such equations here, as well as in liquid and lattice-gas theory and in percolation theory, yield certain closely corresponding results in all these areas.

2. SOME GENERAL CONSIDERATIONS

2.1. Definitions

We begin by considering the function $\tau(\mathbf{r})$, the jump probability density in d dimensions. It is defined as follows:

$$\tau(\mathbf{r})d\mathbf{r} = \text{probability of the jumper making a jump from the origin to within the volume element } d\mathbf{r} \text{ centered on the point } \mathbf{r} \tag{2.1}$$

As it is a probability density, it satisfies the normalization

$$\int \tau(\mathbf{r})\, d\mathbf{r} = 1 \tag{2.2}$$

where the integral in (2.2) is over all space. Here, we shall consider only cases for which

$$\tau(\mathbf{r}) = \tau(r) \tag{2.3}$$

with $r = |\mathbf{r}|$.

Another function of key interest is $e(\mathbf{r})$, the hit expectance density at the point $\mathbf{r}$. It is defined in such a way that

$$1 + E(V) = \int_V \left[\delta(\mathbf{r}) + e(\mathbf{r}) \right] d\mathbf{r}$$

$$= \text{expected number of times that the volume } V \text{ enclosing the origin is visited by the jumper during a random flight of arbitrary length} \tag{2.4}$$

The delta function corresponds to the contribution of a jumper who makes no jumps, i.e., who remains at the origin. The $E(V)$ is the "hit expectancy," i.e., the expected number of times the volume is visited once the jumper has left the origin.

For a random jumper executing jumps according to a probability density satisfying (2.3)

$$e(\mathbf{r}) = e(r) \tag{2.5}$$

In general, $e(\mathbf{r})$ is related to $\tau(\mathbf{r})$ as follows:

$$e(\mathbf{r}) = \tau(\mathbf{r}) + \tau * e(\mathbf{r}) \tag{2.6a}$$

$$= \tau(\mathbf{r}) + \int d\mathbf{s}\, \tau(\mathbf{s}) e(\mathbf{r} - \mathbf{s}) \tag{2.6b}$$

where the asterisk in (2.6a) denotes the Fourier convolution displayed explicitly in (2.6b). The integral in (2.6b) is over all d-dimensional space. For spherically symmetric τ and e, (2.6) may be written as

$$e(r) = \tau(r) + \int d\mathbf{s}\, \tau(s) e(|\mathbf{r} - \mathbf{s}|) \tag{2.7}$$

The origin of Eqs. (2.6) can be easily seen from the following considerations. The probability density for the position of the jumper after n steps, $w_n(\mathbf{r})$, is given by (see, for example, Chandrasekhar[7])

$$\begin{aligned} w_1(\mathbf{r}) &= \tau(\mathbf{r}) \\ w_n(\mathbf{r}) &= \tau * w_{n-1}(\mathbf{r}) \end{aligned} \tag{2.8}$$

so that $w_n(\mathbf{r})$ is the n-fold Fourier convolution of $\tau(\mathbf{r})$ with itself. Equation (2.6) may be written in terms of the $w_n(\mathbf{r})$ as

$$e(\mathbf{r}) = \sum_{n=1}^{\infty} w_n(\mathbf{r}) \tag{2.9}$$

so that it is clear that $e(\mathbf{r})$ enumerates all possible n-step jumps, $n = 1, 2, \ldots,$ that land the jumper at the point r.

2.2. Generating Functions

An important concept in stochastic processes is that of the generating function. In the random flights considered here, the natural generating function to consider is $e(\mathbf{r}, t)$, the generating function for the n-jump probability densities $w_n(\mathbf{r})$, which is defined by

$$e(\mathbf{r}, t) = \sum_{n=1}^{\infty} t^{n-1} w_n(\mathbf{r}) \tag{2.10}$$

where t is an arbitrary parameter. There are two important properties to note about $e(\mathbf{r}, t)$, viz.,

$$w_{n+1}(\mathbf{r}) = \frac{1}{n!} \frac{\partial^n}{\partial t^n} e(\mathbf{r}, t)\bigg|_{t=0} \tag{2.11a}$$

$$e(\mathbf{r}) = e(\mathbf{r}, t = 1) \tag{2.11b}$$

It is interesting to note that an integral equation for $e(\mathbf{r}, t)$ can be formulated as

$$e(\mathbf{r}, t) = \tau(\mathbf{r}) + t \int d\mathbf{s}\, \tau(\mathbf{s}) e(\mathbf{r} - \mathbf{s}, t) \tag{2.12a}$$

which, on Fourier transforming can be written as

$$\hat{e}(\mathbf{k}, t) = \hat{\tau}(\mathbf{k}) + t\hat{\tau}(\mathbf{k})\hat{e}(\mathbf{k}, t) \tag{2.12b}$$

where $\hat{e}(\mathbf{k}, t)$ and $\hat{\tau}(\mathbf{k})$ are the Fourier transforms of $e(\mathbf{r}, t)$ and $\tau(\mathbf{r})$, respectively. Equations (2.12) are similar in functional form to the Ornstein–Zernike equation that arises in the statistical theory of fluids and is discussed in the Appendix. For each of the random flights discussed in this paper, $\hat{e}(\mathbf{k}, t)$ can be calculated trivially from (2.12b) and $\hat{\tau}(\mathbf{k})$. For the random flight considered in Section 3, Case 2, $e(\mathbf{r}, t)$ can be obtained in closed form, allowing $w_n(\mathbf{r})$ to be determined for arbitrarily large n by repeated application of (2.11a).

2.3. Probability of Return to a Volume Enclosing the Origin

For random walks (i.e., random flights on a lattice), the jump *probability density* $\tau(\mathbf{r})$ is replaced by the jump probability $T(\mathbf{r}_i)$, the *probability* of jumping to the lattice point $\mathbf{r}_i$; similarly, the n-jump *probability density* $w_n(\mathbf{r})$ and the generating function $e(\mathbf{r}, t)$ are replaced by $W_n(\mathbf{r}_i)$, the *probability* of being at the lattice point $\mathbf{r}_i$ after n jumps, and $E(\mathbf{r}_i, t)$, the generating function for these probabilities. Clearly, $E(\mathbf{r}_i) = E(\mathbf{r}_i, t = 1)$ is the expected number of times that the lattice point $\mathbf{r}_i$ is visited during the course of a random walk. The lattice problem may be formally developed as a continuum problem using the continuum notation. To see the connection between the lattice probabilities and the continuum probability densities, consider a lattice to be a collection of points $\mathbf{r}_i$, $i = 1, 2, \ldots,$ and let V_i be a small volume containing the lattice point $\mathbf{r}_i$ and no other lattice point. For a random flight on a lattice, we then have the following relations between the two descriptions:

$$\tau(\mathbf{r}) = \sum_{i=1}^{\infty} T(\mathbf{r}_i)\delta(\mathbf{r} - \mathbf{r}_i) \tag{2.13a}$$

$$T(\mathbf{r}_i) = \int_{V_i} \tau(\mathbf{r})\, d\mathbf{r} \tag{2.13b}$$

Analogous relations hold between each of the quantities $W_n(\mathbf{r}_i), E(\mathbf{r}_i, t)$, $E(\mathbf{r}_i)$ and their counterparts $w_n(\mathbf{r}), e(\mathbf{r}, t), e(\mathbf{r})$.

For random walks, there is a well-known result[4,5,9] that permits the probability of return to the origin, $P(\mathbf{0})$, to be calculated in terms of $E(\mathbf{r}_i, t = 1) = E(\mathbf{r}_i)$

$$P(\mathbf{0}) = \frac{E(\mathbf{0})}{1 + E(\mathbf{0})} \tag{2.14}$$

For nearest-neighbor walks [i.e., $T(\mathbf{r}_i) = 0$ except for the $\mathbf{r}_i$ that are nearest neighbors of the origin] it is well known[2] that $E(\mathbf{0})$ is infinite in one and two dimensions, and is finite in three and higher dimensions. (Reference 2 also contains generalizations of this result.) Thus, a return to the origin is certain in one and two dimensions.

We shall now derive the continuum analogue of the result (2.14). Our ultimate aim is to calculate $P(V)$, the probability of returning to a volume V which encloses the origin. To calculate this quantity, it is convenient to introduce a new quantity $f_n(V; \mathbf{r}_1, \mathbf{r}_2)$ (noting that the subscripts here do not refer to lattice positions) defined as follows:

$f_n(V; \mathbf{r}_1, \mathbf{r}_2)\, d\mathbf{r}_2$ = probability that a jumper, starting at the point $\mathbf{r}_1$, lands within volume element $d\mathbf{r}_2$ of $\mathbf{r}_2$ (enclosed in V) after n jumps, such that this is the first time that the volume V is entered during the course of the n jumps. (2.15)

In (2.15), V is a convex, closed volume, and the point $\mathbf{r}_1$ may be contained in V. The quantity $P(V)$ is clearly given by

$$P(V) = \sum_{n=1}^{\infty} \int f_n(V; \mathbf{0}, \mathbf{r})\, d\mathbf{r} \tag{2.16}$$

so that in order to calculate $P(V)$ a prescription for calculating $f_n(V; \mathbf{0}, \mathbf{r})$ must be given.

Consider $w_n(\mathbf{r})$, the n-jump probability density. Clearly, $w_n(\mathbf{r})$ for $r \in V$ does not equal $f_n(V; \mathbf{0}, \mathbf{r})$ since $w_n(\mathbf{r})$ contains contributions from flights that begin at the origin and terminate within the volume V with the termination point of the flight being the first, second, . . . , nth time that the volume V is entered during the course of the flight. There is a clear relationship between the two functions, however, since an arbitrary flight of n steps that terminates in the volume V can be broken up into two parts: the first part of i steps which terminates at a point $\mathbf{r}_1 \in V$, this being the first time that the volume V is entered during the course of the flight, and the remaining part of $n - i$ steps which begins at $\mathbf{r}_1$ and terminates at $\mathbf{r} \in V$. This will be the case for i between 1 and $n - 1$; the last possibility is that the termination point $\mathbf{r}$ of the walk is the first time that the volume V is entered. Thus, we may write

$$\begin{aligned} w_n(\mathbf{r}) = \int_V f_1(V; \mathbf{0}, \mathbf{r}_1) w_{n-1}(\mathbf{r} - \mathbf{r}_1)\, d\mathbf{r}_1 + \cdots \\ + \int_V f_{n-1}(V; \mathbf{0}, \mathbf{r}_1) w_1(\mathbf{r} - \mathbf{r}_1)\, d\mathbf{r}_1 + f_n(V; \mathbf{0}, \mathbf{r}) \end{aligned} \tag{2.17}$$

Summing the terms on the left- and right-hand sides of (2.17) over n yields the following integral equation:

$$e(\mathbf{r}) = p(V; \mathbf{0}, \mathbf{r}) + \int_V p(V; \mathbf{0}, \mathbf{r}_1) e(\mathbf{r} - \mathbf{r}_1)\, d\mathbf{r}_1 \tag{2.18}$$

where $e(\mathbf{r})$ is the hit expectancy density and $p(V; \mathbf{0}, \mathbf{r})$ is defined as

$$p(V; \mathbf{0}, \mathbf{r}) = \sum_{n=1}^{\infty} f_n(V; \mathbf{0}, \mathbf{r}) \tag{2.19}$$

Note that (2.16) can be rewritten in terms of the function $p(V; \mathbf{0}, \mathbf{r})$ as

$$P(V) = \int_V p(V; \mathbf{0}, \mathbf{r})\, d\mathbf{r} \tag{2.20}$$

A detailed examination of (2.20) reveals that, in the case of a random walk on a lattice, $P(V)$ reduces to the expression for $P(\mathbf{0})$ given in (2.14) above if the volume V contains only one lattice point (the origin). In addition, if $e(\mathbf{r} - \mathbf{r}_1)$ is constant ($= \epsilon$) for all $\mathbf{r}, \mathbf{r}_1 \in V$, then (2.20) yields the particularly simple form

$$P(V) = \frac{\epsilon V}{1 + \epsilon V} \tag{2.21}$$

for $P(V)$, which bears a close resemblance to (2.14). If $\tau(\mathbf{r})$, $e(\mathbf{r})$, and V are spherically symmetric, then $p(V; \mathbf{0}, \mathbf{r})$ will be also.

For a given $e(\mathbf{r})$, (2.18) is solved by a simple numerical procedure. For the random flights considered in this paper, $P(V)$ will be calculated for the volume V defined by $\{\mathbf{r} : |\mathbf{r}| \leqslant 1/2\}$; that is, a ball of unit diameter enclosing the origin.

Interestingly, if the limit $V \to R^n$ is taken, then $p(V; \mathbf{0}, \mathbf{r})$ is related to $e(\mathbf{r})$ in the same way that $\tau(\mathbf{r})$ is related to $e(\mathbf{r})$ [cf. (2.6)], thus implying by uniqueness that $p(R^n; \mathbf{0}, \mathbf{r}) = \tau(\mathbf{r})$. A moment of reflection reveals that this must indeed be the case, since $\tau(\mathbf{r})$ is, by definition, the probability density of hitting the point $\mathbf{r}$ so that volume R^n is being entered for the first time during the random flight.

As in the case of the $w_n(\mathbf{r})$, we can define a generating function for the $f_n(V; \mathbf{0}, \mathbf{r})$, denoted by $p(V; \mathbf{0}, \mathbf{r}, t)$, which is related to the $f_n(V; \mathbf{0}, \mathbf{r})$ in the same way that $e(\mathbf{r}, t)$ is related to the $w_n(\mathbf{r})$ [cf. Eq. (2.10)] and moreover reduces to $p(V; \mathbf{0}, \mathbf{r})$ at $t = 1$. From (2.17) and the definitions of the two generating functions, we conclude that they are related by the following integral equation:

$$e(\mathbf{r}, t) = p(V; \mathbf{0}, \mathbf{r}, t) + t \int_V p(V; \mathbf{0}, \mathbf{r}_1, t) e(\mathbf{r} - \mathbf{r}_1, t)\, d\mathbf{r}_1 \tag{2.22}$$

Equations (2.12) and (2.22) suggest a natural sequence to be used in finding the generating functions we have introduced. First, (2.12a) can be used to obtain $e(\mathbf{r}, t)$ from $\tau(\mathbf{r})$, and this $e(\mathbf{r}, t)$ can be used in (2.22) to obtain $p(V; \mathbf{0}, \mathbf{r}, t)$. In the case in which $\tau(\mathbf{r})$ is initially not fully prescribed, but $e(\mathbf{r})$ is given for $|\mathbf{r}| < R$ by Eq. (1.4) and $\tau(\mathbf{r})$ is given for $|\mathbf{r}| > R$ by Eq. (1.6), then (2.6) can first be used to find $\tau(\mathbf{r})$ for all $\mathbf{r}$ as discussed in the following sections.

3. THREE-DIMENSIONAL RANDOM FLIGHTS

Taking Fourier transforms of both sides of (2.6) yields, upon rearrangement,

$$\hat{e}(\mathbf{k}) = \frac{\hat{\tau}(\mathbf{k})}{1 - \hat{\tau}(\mathbf{k})} \tag{3.1}$$

where the symbol $\hat{f}(\mathbf{k})$ is used to denote the Fourier transform of the function $f(\mathbf{r})$, viz.,

$$\hat{f}(\mathbf{k}) = \int d\mathbf{r} \exp(i\mathbf{k} \cdot \mathbf{r}) f(\mathbf{r}) \tag{3.2}$$

Note that if $f(\mathbf{r}) = f(r)$ then $f(\mathbf{k}) = f(k)$, $k = |\mathbf{k}|$. [From this point onward in this paper, we shall assume that $\tau(\mathbf{r}) = \tau(r)$, and so from (2.5) $e(\mathbf{r}) = e(r)$ as well.] The relation (3.1) makes it clear that if $\tau(r)$ is prescribed for all r, then $e(r)$ is immediately determined via $\hat{e}(k)$.

We use the term "free random flight" (FRF) to refer to a random flight problem defined by a fully prescribed jump probability $\tau(r)$—that is, a random flight problem in which $\tau(r)$ is given for all r. We shall refer to a random flight problem in which $\tau(r)$ and $e(r)$ are prescribed on complimentary domains as a constrained random flight (CRF) since we may view the prescription of $e(r)$ on some domain as a constraint on the form of $\tau(r)$ on that same domain. In Section 3.1, we describe two FRFs in three dimensions, and in Section 3.2 we formulate CRFs that are characterized by using functional forms for $\tau(r)$ for $r > 1$ that coincide with those discussed in Section 3.1. In Section 3.2, we additionally solve the CRFs formulated there using a Wiener–Hopf factorization technique. Thus, the impact of the constraint on the probability of return to the vicinity of the origin, $P(V)$, and on the asymptotic form of $e(r)$ can be determined.

3.1. The Free Random Flight (FRF) in Three Dimensions

Case 1. The Simplest FRF. The classic FRF problem in three dimensions can be defined by a spherically symmetric jump probability given by

$$\tau(r) = \frac{1}{4\pi}\delta(r-1) \tag{3.3}$$

where $\delta(r)$ is the one-dimensional Dirac delta function. Physically, this corresponds to jumps that are random in direction and of length 1 (in suitably chosen units). For this problem, as noted above, it is straightforward to calculate $e(r)$. For $\tau(r)$ given by (3.3), $\hat{\tau}(k)$ is given by

$$\hat{\tau}(k) = \frac{\sin k}{k} \tag{3.4}$$

and $\hat{e}(k)$ follows immediately from (3.1). Although $e(r)$ is most readily obtained by numerical Fourier inversion of $\hat{e}(k)$, a number of its analytic properties may be easily found:

i. From the exact analytic forms of $w_n(r)$,[3,7] it is clear that $e(r)$ contains a delta function located at $r = 1$ [given by (3.3)] and is discontinuous at $r = 2$ with discontinuity $1/(16\pi)$. Apart from this, $e(r)$ is a continuous function.

ii. It is easily verified that

$$\hat{e}(k) \to \frac{6}{k^2} O(k^0), \qquad k \to 0 \tag{3.5}$$

Consequently, $e(r)$ is long-ranged and its asymptotic form is given by

$$e(r) \to \frac{3}{2\pi}\frac{1}{r}, \qquad r \to \infty \tag{3.6}$$

Combining (3.4) and (3.1), a formal expression for $e(r)$ may be obtained as the inverse Fourier transform of $\hat{e}(k)$. The function $e(r)$, obtained by performing this inversion numerically, is shown in Fig. 1.

We solve (2.18) for $p(V; \mathbf{0}, \mathbf{r})$ and perform the integral in (2.20), using standard numerical techniques, yielding

$$P(V) = 0.204 \tag{3.7}$$

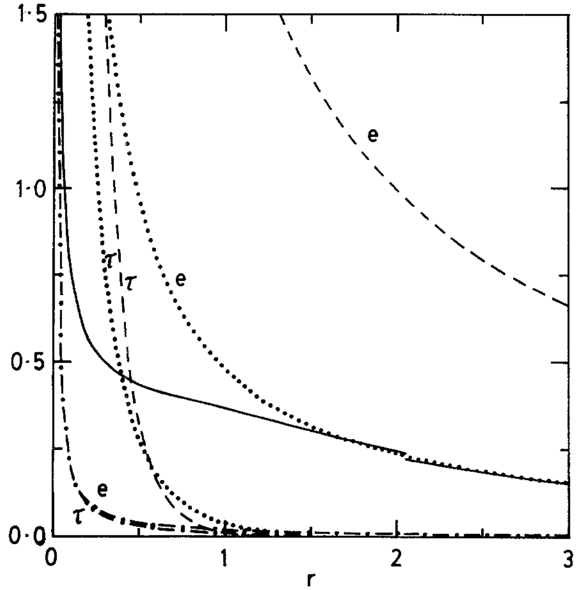

Fig. 1. The jump probability density $\tau(r)$ and the hit expectance density $e(r)$ for the FRF problems considered in Section 3.1. The solid curve exhibits $e(r)$ for the FRF considered in Case 1 with $\tau(r)$ given by (3.3). The other results are for the FRF with $\tau(r)$ given by (3.10), and both $e(r)$ (labeled by the symbol e) and $\tau(r)$ (labeled by the symbol τ) are shown for $z = 1/2$ (-·-·-), $z = 6^{1/2}$(· · ·) and $z = 5$ (- - -).

As expected, $P(V)$ is less than unity, indicating that in this three-dimensional continuum flight return to the vicinity of the origin is not assured. This is a well-known result, although the dependence of the return probability on dimensionality is most often discussed in the context of lattice walks.

Case 2. FRF with Jump Probability Density of Yukawa Form. As noted in the Introduction, a natural jump probability to consider in the FRF problem is the Yukawa function

$$\tau(r) = \frac{K}{r}\exp\left[-z(r-1)\right] \tag{3.8}$$

If (3.8) is the prescribed form of $\tau(r)$ for all r, then the normalization of $\tau(r)$ requires that

$$K = \frac{z^2}{4\pi}\exp(-z)$$

so that

$$\tau(r) = \frac{z^2}{4\pi} \frac{\exp(-zr)}{r} \tag{3.9}$$

is an appropriate jump probability for use in the FRF problem. The Fourier transform of (3.9) is easily taken and $\hat{e}(k)$ calculated from (3.1) as

$$\hat{e}(k) = \frac{z^2}{k^2}$$

Thus, the form of $e(r)$ can be found analytically for all r as

$$e(r) = \frac{z^2}{4\pi} \frac{1}{r} \tag{3.10}$$

Note that z is unconstrained (except that $z > 0$). The functions $e(r)$ and $\tau(r)$ are shown in Fig. 1 for various values of z, including $z = 6^{1/2}$, the value that causes the $e(r)$ of (3.10) to match the asymptotic form of the FRF problem considered as Case 1 above. Notice that on the scale of Fig. 1, $\tau(r)$ and $e(r)$ are very similar for $z = 1/2$; in addition, although $\tau(r)$ for $z = 6^{1/2}$ and $z = 5$ are similar, the corresponding $e(r)$ differ considerably in magnitude.

Using the analytic expression (3.12) for $e(r)$, $p(V; \mathbf{0}, \mathbf{r})$ and $P(V)$ are calculated numerically from (2.18) and (2.20), the results for $P(V)$ being given in Fig. 12. (This figure is discussed in greater detail in Section 3.2, Case 3.) Interestingly, if $z \to \infty$, $P(V) \to 1$. This limit corresponds to a jump probability that is simply a delta function at the origin.

For any finite z, $P(V) < 1$ and, as for the FRF considered in Case 1 above, return to the volume V is not assured. Note that z functions as an inverse range parameter for the jump probability density; the greater the range of the latter, the lower the probability of return to the neighborhood of the origin.

The Fourier transform $\hat{e}(k,t)$ of the generating function $e(r,t)$ discussed in Section 2.2 is given by [see Eqs. (2.12)]

$$\hat{e}(k,t) = \frac{z^2}{(1-t)z^2 + k^2}$$

the inverse transform of which is obtained trivially as

$$e(r,t) = \frac{z^2}{4\pi} \frac{e^{-z(1-t)^{1/2}r}}{r} \tag{3.11}$$

This expression enables the $w_n(r)$ to be obtained for arbitrarily large n by repeated application of (2.11a). The results for $n = 1, \ldots, 5$ are given in Table I. To our knowledge, the FRF problem with jump probability (3.9) has not previously been considered in detail [in contrast to the FRF

Table I. The n-Jump Probability Densities $w_n(r)$, $n = 1$ to 5, for the FRF with Jump Probability of Yukawa form[a]

n	$w_n(r)$
1	$\frac{z^2}{4\pi}\frac{\exp(-zr)}{r}$
2	$\frac{z^3}{8\pi}\exp(-zr)$
3	$\frac{z^3(1+zr)}{32\pi}\exp(-zr)$
4	$\frac{z^3(3+3zr+z^2r^2)}{192\pi}\exp(-zr)$
5	$\frac{z^3(15+15zr+6z^2r^2+z^3r^3)}{1536\pi}\exp(-zr)$

[a] See Section 3.1, Case 2 of the text for details.

problems with the $\tau(r)$ considered in Case 1 above and with $\tau(r)$ of Gaussian form].

3.2. The Constrained Random Flight (CRF) in Three Dimensions

Suppose we wish to prescribe the hit expectance density on a sphere about the origin, which we take here to be of unit radius without loss of generality. It is clear that $\tau(r)$ can itself then only be prescribed outside the unit sphere. Let us therefore contemplate the problem defined by the conditions

$$\begin{aligned} \tau(r) &= f_1(r), \qquad r > 1 \\ e(r) &= f_2(r), \qquad r < 1 \end{aligned} \tag{3.12}$$

where f_1 and f_2 are known, nonnegative functions. An appropriate technique for the solution of the problem posed in (3.12) is the Wiener–Hopf technique.[9]

In the following sections we consider various problems for odd dimensionalities of the form (3.12) with $e(r)$ restricted to be a constant for $r < 1$.

Case 1. Jump Probability Density of Finite Range. We begin with an $f_1(r)$ of the simplest possible form, $f_1(r) = 0$, a property shared by the first of the two FRFs discussed in Section 3.1. The problem at hand is thus defined by

$$\begin{aligned} \tau(r) &= 0, \qquad r > 1 \\ e(r) &= \epsilon, \qquad r < 1 \end{aligned} \tag{3.13}$$

For technical convenience we initially assume that the normalization condition (2.2) is replaced by the condition

$$\int \tau(r)\, d\mathbf{r} = 1 - \alpha^2, \qquad \alpha > 0 \tag{3.14}$$

and we will subsequently take the limit $\alpha \to 0$, recovering (2.2), once our analysis is complete. The reason for doing so is that for $\alpha = 0$, $e(r)$ is long-ranged, which renders (2.6) a singular integral equation. Although this presents no difficulty in principle,[4] we find it more convenient to perform our analysis off $\alpha = 0$, taking the limit $\alpha \to 0$ in our final equations.

The method used is an adaptation of that introduced by Baxter[11] for the analytic solution of similar problems that arise in the statistical theory of fluids. (A discussion of the relation between the present analysis and the statistical mechanical problem is given in the Appendix.) We rewrite (3.1) in the form

$$[1 + \hat{e}(k)][1 - \hat{\tau}(k)] = 1 \tag{3.15}$$

For $\hat{e}(k)$ satisfying (3.13), $1 + \hat{e}(k)$ has no poles in some strip $|\mathrm{Im}(k)| < \xi$ where $\xi > 0$. Hence, $1 - \hat{\tau}(k)$ has no zeros in the strip and is positive. Consider the function

$$\hat{A}(k) = 1 - \hat{\tau}(k) \tag{3.16}$$

As a result of the above comments, $\log A(k)$ is analytic in the strip $|\mathrm{Im}(k)| < \xi$. Moreover, since $\tau(r)$ is finite ranged, it follows that

$$\hat{\tau}(k) \sim \frac{\exp(ik)}{k} \tag{3.17}$$

and so for real k, $\hat{\tau}(k) \to 0$ as $|k| \to \infty$. In fact, $\hat{\tau}(k) \to 0$ for $|k| \to \infty$ in the upper-half k-plane.

Choosing a rectangular contour Γ within the strip $|\mathrm{Im}(k)| < \xi$ and enclosing the real k axis, the Cauchy residue theorem states that

$$\log \hat{A}(k) = \int_{\Gamma} \frac{\log \hat{A}(z)\, dz}{z - k} \tag{3.18}$$

The contour Γ is shown in Fig. 2 in which the contours Γ_i, $i = 1, \ldots, 4$ are defined. From (3.17), the integrals along Γ_2 and Γ_4 are zero. Hence,

$$\log \hat{A}(k) = \int_{\Gamma_1} \frac{\log \hat{A}(z)\, dz}{z - k} + \int_{\Gamma_3} \frac{\log \hat{A}(z)\, dz}{z - k} \tag{3.19}$$

[4] Standard techniques for dealing with such singularities are discussed at length in Noble.[9]

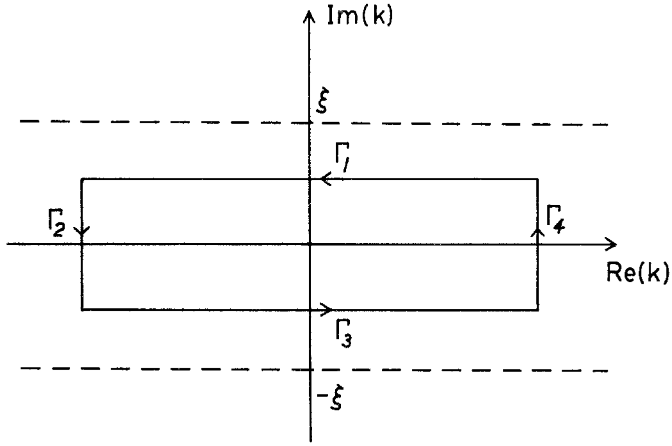

Fig. 2. The contour Γ used in (3.20), noting that $\Gamma = \Gamma_1 + \Gamma_2 + \Gamma_3 + \Gamma_4$. Note that the Re($k$) is infinite along Γ_2 and Γ_4.

if we define

$$\log \hat{Q}(k) = \int_{\Gamma_3} \frac{\log \hat{A}(z)\, dz}{z - k} \tag{3.20}$$

then we find the following:

i. $\log \hat{Q}(k)$ is analytic and has no poles in the upper half-plane;

ii. $$\int_{\Gamma_1} \frac{\log \hat{A}(z)\, dz}{z - k} = \log \hat{Q}(-k)$$

Thus, within the strip $|\mathrm{Im}(k)| < \xi$.

$$\hat{A}(k) = \hat{Q}(k)\, \hat{Q}(-k) \tag{3.21}$$

Here $\hat{Q}(k)$ is regular and has no poles in the upper half-plane. This completes the constructive splitting characteristic of the Wiener–Hopf technique.[10]

Consider the functions $\hat{e}(k)$ and $\hat{\tau}(k)$ more closely. It is straightforward to show that, by choosing the z axis of the coordinate system to lie along $\mathbf{k}$,

$$\hat{e}(k) = 4\pi \int_0^\infty dr\, E(r) \cos kr \tag{3.22}$$

where

$$E(r) = \int_r^\infty dt\, t e(t) \tag{3.23}$$

Thus, $\hat{e}(k)$ [and similarly $\hat{\tau}(k)$] can be written as the one-dimensional Fourier transforms of the functions $E(r)$ and $T(r)$, where

$$\begin{aligned} T(r) &= \int_r^1 dt\, t\tau(r), \qquad r<1 \\ &= 0, \qquad\qquad\quad r>1 \end{aligned} \tag{3.24}$$

We now proceed with the factorization. Since $\hat{Q}(k) \to 1$ as $|k| \to \infty$ in the upper half-plane, define a function $Q(r)$ by

$$\hat{Q}(k) = 1 - 2\pi \int_{-\infty}^{\infty} dr \exp(ikr) Q(r) \tag{3.25}$$

The inverse of (3.25) is given by

$$2\pi Q(r) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \exp(-ikr)\left[1 - \hat{Q}(k)\right] \tag{3.26}$$

For $r < 0$, the integral in (3.26) may be closed around the upper half-plane where $\hat{Q}(k)$ has no poles and the integral along the semicircular arc is zero [from (3.17)]. Thus,

$$Q(r) = 0 \qquad r < 0 \tag{3.27}$$

For $r \geqslant 1$, the integral in (3.26) can be closed around the lower half-plane where the analytic continuation of $\hat{Q}(k)$, $\hat{A}(k)/\hat{Q}(-k)$, must be used. Since $\hat{Q}(-k)$ has no zeros in the lower half-plane, $\hat{A}(k)$ is analytic for all k and the integral on the semicircular arc is zero, then

$$Q(r) = 0, \qquad r \geqslant 1 \tag{3.28}$$

Equation (3.25) becomes

$$\hat{Q}(k) = 1 - 2\pi \int_0^1 dr \exp(ikr) Q(r) \tag{3.29}$$

We now need only find the equations for $T(r)$ and $E(r)$ in terms of $Q(r)$. We begin by writing (3.1), (3.16), and (3.21) as

$$\hat{Q}(k)\left[1 + \hat{e}(k)\right] = 1/\hat{Q}(-k) \tag{3.30}$$

$$1 - \hat{\tau}(k) = \hat{Q}(k)\,\hat{Q}(-k) \tag{3.31}$$

Multiplying both sides of these equations by $\exp(-ikr)$ and integrating over k yields

$$E(r) = Q(r) + 2\pi \int_0^1 dt\; Q(t) E(|r-t|), \qquad r > 0 \tag{3.32}$$

$$T(r) = Q(r) - 2\pi \int_r^1 dt\; Q(t) Q(t-r), \qquad 0 < r < 1 \tag{3.33}$$

[Note that the right-hand side of (3.30) evaluates to zero by closure around the lower half-plane.] Differentiating (3.32) and (3.33), we obtain the desired equations

$$re(r) = -Q'(r) + 2\pi\int_0^1 dt\ Q(t)(r-t)e(|rt|), \qquad r > 0 \tag{3.34}$$

$$r\tau(r) = -Q'(r) + 2\pi\int_r^1 dt\ Q'(t)Q(t-r), \qquad 0 < r < 1 \tag{3.35}$$

Note that from (3.14), (3.16), and (3.21)

$$1 - \hat{\tau}(0) = \alpha^2 = \hat{A}(0) = [\hat{Q}(0)]^2 \tag{3.36}$$

Our interest is in the limit $\alpha = \hat{Q}(0) \to 0$. From this point on, we assume that this limit has been taken.

To complete the solution of the problem posed in (3.13), we must determine the function $Q(r)$. Consider (3.34) for $0 < r < 1$: from (3.13) we have

$$r\epsilon = -Q'(r) + 2\pi\int_0^1 dt\ Q(t)(r-t)\epsilon \tag{3.37}$$

which is a Fredholm integral equation of the first kind with degenerate kernel. The solution is given by

$$Q'(r) = ar + b \tag{3.38}$$

where a and b, determined by substitution into (3.37), are given by

$$a = \epsilon\left[-1 + 2\pi\int_0^1 dt\ Q(t)\right] \tag{3.39a}$$

$$b = -\epsilon 2\pi\int_0^1 dt\, tQ(t) \tag{3.39b}$$

From (3.39a) and (3.29), we see that

$$a = \epsilon\alpha = 0 \tag{3.40}$$

by normalization. Thus, using the conditions (3.27) and (3.28), (3.38) yields

$$\begin{aligned} Q(r) &= b(r-1), \qquad && 0 \leqslant r \leqslant 1 \\ &= 0 && \text{elsewhere} \end{aligned} \tag{3.41}$$

The parameter b may be determined by substituting (3.41) into (3.39a) and (3.40). We find that

$$b = -1/\pi \tag{3.42}$$

The value of ϵ is then found by substituting (3.41) and (3.42) into (3.39b), yielding

$$\epsilon = 3/\pi \tag{3.43}$$

The function $\tau(r)$ may then be obtained from (3.35) as

$$\tau(r) = \frac{1}{\pi} r, \qquad 0 \leqslant r \leqslant 1$$
$$= 0 \qquad \text{elsewhere} \tag{3.44}$$

Since ϵ and $\tau(r)$ are manifestly nonnegative, we have found by construction a solution to our random flight problem.

The function $e(r)$ may be found for $r > 1$ analytically by a zone-by-zone analysis of (3.34) as a difference-differential equation [see the discussion following Eq. (3.47) below], or numerically using standard techniques. In Fig. 3, we plot the functions $\tau(r)$ and $e(r)$ obtained above, with the results for the free random flight included for comparison.

An analysis of the large-r behavior of $e(r)$ (similar to that given in Section 3.1 above) yields

$$e(r) \to \frac{9}{4\pi} \frac{1}{r}, \qquad r \to \infty \tag{3.45}$$

In common with the free random flight, $e(r)$ is long-ranged; however, we note that the amplitude of the decay for the random flight constrained by (3.13) is larger than that in the free random flight case.

The discontinuity in $e(r)$, which occurs at $r = 1$, is given by

$$e(1^+) = e(1^-) - 1/\pi \tag{3.46}$$

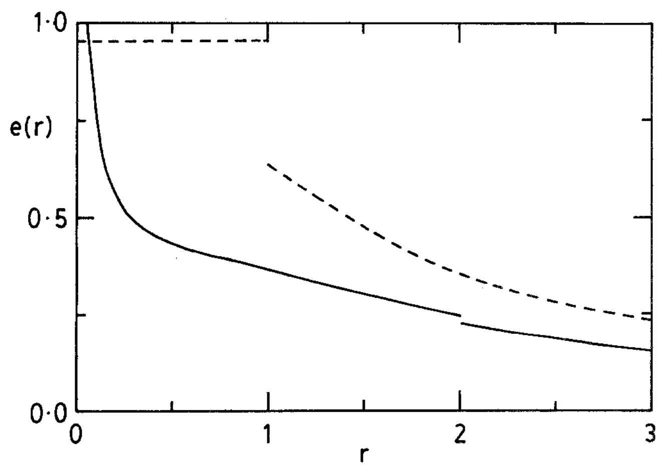

Fig. 3. The hit expectance density $e(r)$ for the CRF considered in Section 3.1, Case 1 [the problem defined by (3.13)] is shown as the dashed curve. The corresponding result for the FRF with $\tau(r)$ given by (3.3) is given by the solid curve and is included for comparison.

Since $e(r)$ is constant for $r < 1$, then for any $\mathbf{r}_1, \mathbf{r}_2 \in V$, the ball of diameter 1 enclosing the origin, $|\mathbf{r}_2 - \mathbf{r}_1| \leqslant 1$ so that $e(|\mathbf{r}_2 - \mathbf{r}_1|)$ is constant over V. Thus, $P(V)$ is given by (2.21) which, combined with (3.45) yields

$$P(V) = 1/3 \tag{3.47}$$

Note that this is larger than $P(V)$ for the random flight discussed in Section 3.1, Case 1, indicating that the constraint of constant hit expectance density inside the unit sphere increases the probability of return to the volume V.

Although we have found it most convenient to find $e(r)$ numerically, we indicate briefly one method by which a closed form analytic expression for $e(r)$ can be obtained. Consider the function $f(r) = re(r)$; for $r > 1$, (3.34) may be written as

$$f(r) = 2\pi \int_0^1 dt\; Q(t) f(r - t) \tag{3.48}$$

Using the functional form (3.43) for $Q(r)$ and differentiating twice, we obtain the following delay-differential equation for $f(r)$:

$$f''(r) - 2f'(r) + 2f(r) = 2f(r - 1) \tag{3.49}$$

A standard technique for such equations[12] is to solve (3.49) iteratively in the domains $I_n = \{r : n \leqslant r \leqslant n + 1\}$, $n = 1, 2, 3, \ldots,$ as ordinary inhomogeneous differential equations. As an example, consider $r \in I_1$. The function $f(r - 1)$ is known trivially in this case $[= \epsilon(r - 1)]$ and the solution of (3.49) is immediate. This yields

$$e(r) = \frac{3}{\pi}\frac{1}{r} - \frac{1}{\pi}\frac{e^{-(r-1)}}{r}\left[\cos(r - 1) + \sin(r - 1)\right], \qquad 1 \leqslant r \leqslant 2$$

after the boundary conditions [the value of $f(r)$ and $f'(r)$ at $r = 1$] are applied. Clearly, this method may be repeated to obtain an analytic formula for $e(r)$ at larger r, although the algebra involved quickly becomes tedious.

Case 2. Jump Probability Density of Yukawa Form Beyond $r = 1$**.** Consider now the case where $f_1(r)$ is taken to be of Yukawa form for $r > 1$, viz.,

$$\tau(r) = \frac{K}{r}\exp\left[-z(r - 1)\right], \qquad r > 1 \tag{3.50a}$$

$$= \epsilon, \qquad r < 1 \tag{3.50b}$$

At this point, the parameters K and z are regarded as arbitrary positive numbers.

Equation (3.50b) may be written as

$$\tau(r) = \tau_0(r) + \frac{K}{r}\exp[-z(r-1)], \qquad r > 0 \tag{3.51}$$

where

$$\tau_0(r) = 0, \qquad r > 1 \tag{3.52}$$

Thus, the Fourier transform of $\tau(r)$, $\hat{\tau}(k)$, is given by

$$\hat{\tau}(k) = \hat{\tau}_0(k) + \frac{4\pi K e^z}{z^2 + k^2}, \qquad |\mathrm{Im}(k)| < z \tag{3.53}$$

The Wiener–Hopf factorization formally proceeds as before, although we note that the contour used in (3.18) must lie inside $|\mathrm{Im}(k)| < z$ as well as $|\mathrm{Im}(k)| < \xi$. With this proviso, we find that, as before,

$$\hat{A}(k) = 1 - \hat{\tau}(k) = \hat{Q}(k)\,\hat{Q}(-k) \tag{3.54}$$

where $\hat{Q}(k)$ is regular, has no zeros in the upper half-plane, and is related to a real space function $Q(r)$ by (3.25) and (3.26). The latter function has the property

$$Q(r) = 0, \qquad r < 0 \tag{3.55}$$

derived in the same way as (3.27). For $r > 1$, we close the integral in (3.26) around the lower half-plane where we must use the analytic continuation of $1 - \hat{Q}(k)$, $\hat{A}^{\dagger}(k)/\hat{Q}(-k)$. Here, $\hat{A}^{\dagger}(k)$ is itself the analytic continuation of $\hat{A}(k)$ into the lower half-plane. We find that

$$Q(r) = \beta \exp[-z(r-1)], \qquad r > 1 \tag{3.56}$$

where

$$\beta = \frac{K}{z\hat{Q}(iz)} \tag{3.57}$$

This differs from (3.28) due to the contribution from the pole in $\hat{A}^{\dagger}(k)$ in the lower half-plane at $k = -iz$.

It is convenient to define a function $Q_0(r)$ by

$$Q(r) = Q_0(r) + \beta \exp[-z(r-1)], \qquad r > 0 \tag{3.58}$$

where

$$Q_0(r) = 0, \qquad r \geqslant 0 \tag{3.59}$$

Thus, (3.57) may be written as

$$\pi\beta^2 e^z - z\beta\left[1 - 2\pi\int_0^1 dr\, \exp(-zr) Q_0(r)\right] + K = 0 \tag{3.60}$$

The equations relating $e(r)$ and $\tau(r)$ to $Q(r)$, (3.34) and (3.35), become for the present problem

$$re(r) = -Q'(r) + 2\pi\int_0^\infty dt\ Q(t)(r-t)e(|r-t|), \qquad r \geqslant 0 \quad (3.61)$$

$$r\tau(r) = -Q'(r) + 2\pi\int_r^\infty dt\ Q'(t)Q(t-r), \qquad r \geqslant 0 \quad (3.62)$$

To determine $Q_0(r)$, we consider (3.61) on the domain $0 < r < 1$ where $e(r)$ is known, finding

$$Q_0'(r) = ar + b + \beta dz \exp[-z(r-1)] \tag{3.63}$$

where

$$a = \epsilon\left[-1 + 2\pi\int_0^1 dt\ Q_0(t) + \frac{2\pi\beta e^z}{z}\right] \tag{3.64}$$

$$b = \epsilon\left[-2\pi\int_0^1 dt\, tQ_0(t) - \frac{2\pi\beta e^z}{z^2}\right] \tag{3.65}$$

$$d = 1 - \frac{2\pi}{z}\tilde{g}(z) \tag{3.66}$$

Here, $\tilde{g}(s)$ is the Laplace transform of $rg(r)$, where $g(r)$ is defined by

$$\tau(r) = \epsilon + g(r) \tag{3.67}$$

so that, explicitly,

$$\tilde{g}(s) = \int_0^\infty \exp(-sr) rg(r)\, dr \tag{3.68}$$

As before, the parameter a is related to α by

$$a = \alpha\epsilon \tag{3.69}$$

and so, by normalization, $a = 0$. Combining (3.63) and (3.59), we find

$$Q_0(r) = b(r-1) + \beta d\{1 - \exp[-z(r-1)]\} \tag{3.70}$$

The condition $a = 0$ yields the following result for b [when (3.70) is substituted into (3.64)]:

$$b = b_0 + b_1\beta + b_2\beta d \tag{3.71}$$

where

$$b_0 = -\frac{1}{\pi}, \qquad b_1 = \frac{2e^z}{z}, \qquad b_2 = \frac{2e^z}{z}\begin{bmatrix} -1 & 0 \\ 1 & 1 \end{bmatrix} \tag{3.72}$$

Here, we have introduced the following notation: the function

$$f(r) = \sum_{i=1}^{m}\sum_{j=1}^{n} a_{ij} r^{j-1} \exp[-(i-1)z] \tag{3.73}$$

is represented by the matrix A given by

$$[A]_{ij} = a_{ij} \tag{3.74}$$

The equation for b, (3.63), yields the following expression for ϵ:

$$\epsilon = \frac{3\left\{1 - \frac{2\pi e^z}{z}\beta - \frac{2\pi e^z}{z}\begin{bmatrix} -1 & 0 \\ 1 & 1 \end{bmatrix}\beta d\right\}}{\pi\left\{1 - \frac{2\pi e^z}{z^2}\begin{bmatrix} -3 & 1 \end{bmatrix}\beta - \frac{\pi e^z}{z^2}\begin{bmatrix} 6 & -2 & 0 \\ -6 & -4 & -1 \end{bmatrix}\beta d\right\}} \tag{3.75}$$

Note that $K = 0$ implies that $\beta = 0$, and ϵ reduces to the value found for the CRF with finite-ranged jump probability discussed in Case 1 above. There is no guarantee that the ϵ given by (3.75) is nonnegative for a given pair of K and z, so that it is not yet clear whether a solution to the problem as posed has been found.

Using (3.70), (3.60) may be written more explicitly as

$$\pi\beta^2 e^z\left[1 - d(1 - e^{-z})^2\right] - z\beta + K + b\frac{2\pi}{z}\begin{bmatrix} 1 & -1 \\ -1 & 0 \end{bmatrix}\beta = 0 \tag{3.76}$$

We require one further equation to completely determine both β and d. The second equation comes from considering (3.61) for $r > 1$ and writing it in terms of $g(r)$. It is found that

$$\begin{aligned} rg(r) &= b + \beta dz \exp\left[-z(r-1)\right] \\ &\quad + 2\pi\int_0^r dt\ Q(t)(r-t)g(r-t), \qquad r \geqslant 1 \end{aligned} \tag{3.77}$$

Note that, comparing (3.50a) and (3.67),

$$g(r) = 0, \qquad r < 1 \tag{3.78}$$

Multiplying both sides of (3.77) by $\exp(-sx)$ and integrating from 1 to ∞ yields

$$\tilde{g}(s) = \left(\frac{b}{s} + \frac{\beta dz}{z+s}\right)e^{-s} + 2\pi\tilde{Q}(s)\,\tilde{g}(s) \tag{3.79}$$

where $\tilde{g}(s)$ is defined in (3.60) and $\tilde{Q}(s)$ is the Laplace transform of $Q(r)$. Noting that

$$\hat{Q}(is) = 1 - 2\pi\tilde{Q}(s) \tag{3.80}$$

(3.79) can be written as

$$\tilde{g}(s) = \left(\frac{b}{s} + \frac{\beta dz}{z+s}\right)e^{-s}/\hat{Q}(is) \tag{3.81}$$

In particular,

$$\tilde{g}(s) = \left(\frac{b}{z} + \frac{\beta d}{2}\right)e^{-z}/\hat{Q}(iz) \tag{3.82}$$

which, making use of (3.57), may be written as

$$\tilde{g}(z) = \left(\frac{b}{z} + \frac{\beta d}{2}\right)e^{-z}\frac{z\beta}{K} \tag{3.83}$$

Expressing $\tilde{g}(z)$ in terms of d [using (3.66)], (3.83) becomes

$$2\pi e^{-z}g\beta^2 + (\pi e^{-z}\beta^2 + Kz)\beta d - Kz\beta = 0 \tag{3.84}$$

Equations (3.76) and (3.84) must now be solved simultaneously. Solving (3.76) for βd, making use of (3.72), yields

$$\beta d = \frac{Ke^{-z} + De^{-z}\beta + E\beta^2}{F\beta} \tag{3.85}$$

$$D = \frac{1}{z}\begin{bmatrix} -2 & 2 & -1 \\ 2 & 0 & 0 \end{bmatrix} \tag{3.86}$$

$$E = \frac{\pi}{z^2}\begin{bmatrix} 4 & -4 & 1 \\ -4 & 0 & 0 \end{bmatrix} \tag{3.87}$$

$$F = \frac{\pi}{z^2}\begin{bmatrix} 4 & -4 & 1 \\ -8 & 0 & 2 \\ 4 & 4 & 1 \end{bmatrix} \tag{3.88}$$

Substituting for b and βd in (3.84) yields the following quartic equation for β:

$$\pi\beta^4 + X\beta^3 - 2\pi K\beta^2 + DK\beta + K^2 = 0 \tag{3.89}$$

where

$$X = \frac{1}{z}\begin{bmatrix} 2 & 0 & 0 \\ -2 & -2 & -1 \end{bmatrix} \tag{3.90}$$

and D is given by (3.86). There are four possible solutions to (3.89). An analysis of the small-K behavior of these solutions, labeled β_i, $i = 1, \ldots, 4$, reveals that

$$\beta_1 \to -\frac{1}{D}K + O(K^2), \qquad K \to 0 \tag{3.91}$$

$$\beta_{2,3} \to \pm(-D/X)^{1/2}K^{1/2} + O(K), \qquad K \to 0 \tag{3.92}$$

$$\beta_4 \to -\frac{X}{\pi^2} + O(K), \qquad K \to 0 \tag{3.93}$$

As $K \to 0$, the solution of this problem should approach that of the CRF with jump probability of finite range—that is, the problem considered above. Thus, as $K \to 0$, $\beta \to 0$ as well; this eliminates β_4 as the correct solution of the problem. In addition, D/X can be positive depending on the value chosen for z; this suggests that β_2 and β_3 are not generally acceptable as solutions to this problem. This leaves β_1 as the one acceptable solution, and all calculations presented use this root of the quartic (3.89).

The final quantity of interest is the functional form of $\tau(r)$ for $r \leqslant 1$. After some algebra, (3.62) yields the following functional form:

$$\tau(r) = \pi b^2 r + \left\{ K - \beta dz + 2\pi\beta d\left[\frac{(1-z)b}{z} + \frac{e^z}{2}\beta + \left(1 - \frac{e^z}{2}\right)\beta d\right]\right\} \times \frac{e^z[\exp(-zr) - 1]}{r} + 2\pi\beta(d-1)\left(\frac{b}{z} + \frac{\beta d}{2}\right)\frac{[\exp(-zr)-1]}{r} \tag{3.94}$$

The large-r asymptotic form of $e(r)$ is found to be

$$e(r) \to \frac{1}{4\pi\left\{\dfrac{\pi b}{3} - \dfrac{2\pi e^z}{z^2}\beta + \dfrac{2\pi e^z}{z^2}\begin{bmatrix} 2 & 0 & 0 \\ -2 & -2 & -1 \end{bmatrix}\beta d\right\}^2} \cdot \frac{1}{r}, \quad r \to \infty \tag{3.95}$$

and the discontinuity in $e(r)$ at $r = 1$ is given by

$$e(1^+) = e(1^-) + b + \beta dz \tag{3.96}$$

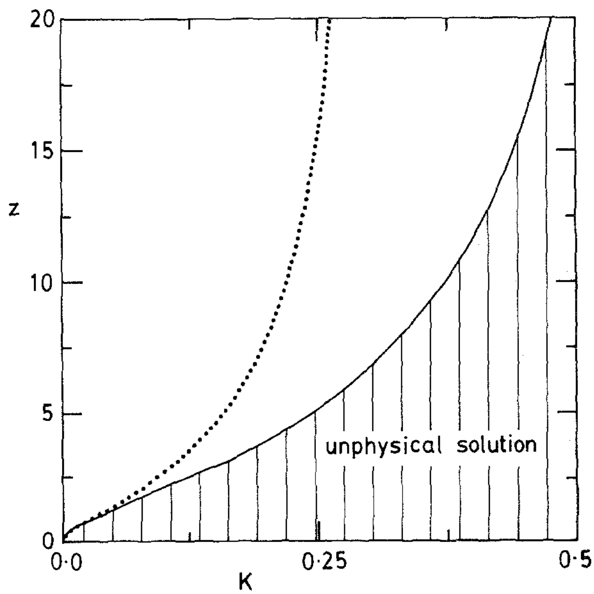

Fig. 4. The half-space in the (K, z) plane for which the CRF problem posed in (3.50) has "physically" acceptable solutions [i.e., the resulting $\tau(r)$ is nonnegative]. The set of (K, z) values for which $e(r)$ is continuous is shown as a dotted curve. A description of the latter problem is given in Section 3.2 (Case 3) of the text.

For arbitrary, nonnegative K and z it is not clear *a priori* whether a solution to the random flight problem posed in (3.50) exists, i.e., a solution to (2.6) such that the $\tau(r)$ and $e(r)$ which satisfy (3.50) are nonnegative for all r. [It is necessary and sufficient that $\tau(r)$ be nonnegative for all r.] To satisfy this requirement, it turns out that for any given value of K, z must exceed a minimum value $z_{\min}(K)$; otherwise, $\tau(r)$ is negative at small r. In Fig. 4, we exhibit a portion of the (K, z) half-space for which solutions of (3.50) are probabilistically, and hence "physically," acceptable [i.e., satisfy the nonnegativity condition $\tau(r) \geqslant 0$].

In Fig. 5, the parameter β is displayed as a function of K for various values of z. The dashed curve in this figure corresponds to the limit of acceptable solutions [i.e., solutions satisfying the condition $\tau(r) \geqslant 0$].

Figures 6 and 7 show the behavior of ϵ and $P(V)$, respectively, as a function of K for fixed values of z. At $K = 0$, the quantities reduce to their respective values for the CRF considered in Case 1 above. For fixed z, increasing K corresponds to loading more of the jump probability density outside the unit sphere centered on the origin; consequently, when z is held constant, the expectance density ϵ inside the unit sphere is a decreasing

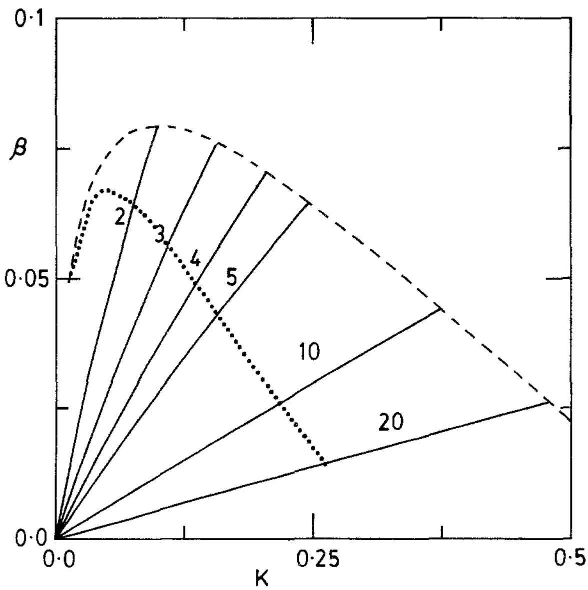

Fig. 5. Behavior of the parameter β, the solution of (3.89), as a function of K for various values of z. Each solid curve corresponds to the fixed value of z by which it is labeled. The dashed curve is the limit of acceptable solutions (cf. Fig. 4). The dotted curve is the locus of points along which $\tau(r)$ and $e(r)$ are continuous at $r = 1$.

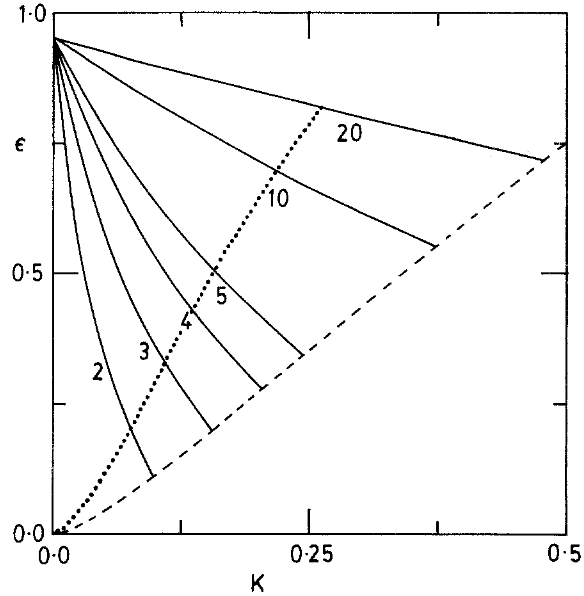

Fig. 6. Behavior of the parameter ϵ as a function of K for various values of z. The convention for the solid, dashed, and dotted lines is the same as that for Fig. 5.

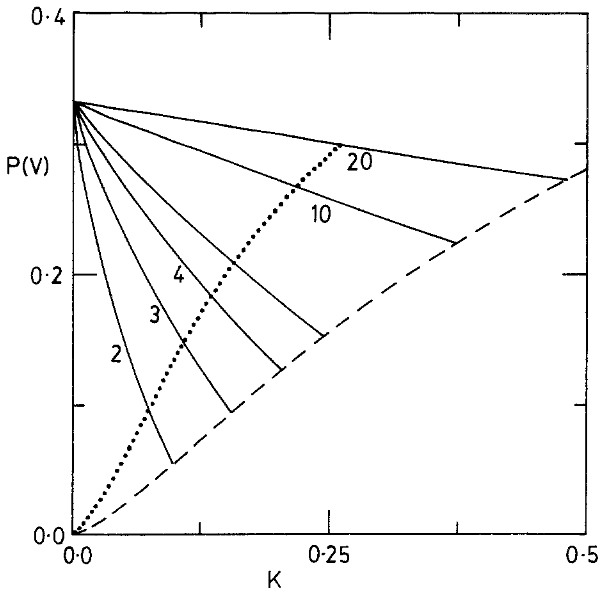

Fig. 7. The probability of return to the volume V, $P(V)$, shown as a function of K for various values of z. The convention used for the solid, dashed, and dotted curves is the same as that used in Fig. 5.

function of K. Similarly, the probability of returning to the volume V decreases as K is increased.

In Fig. 8, $\tau(r)$ is shown for a fixed value of z ($z = 3$) and various K. For this value of z, K must satisfy $K \leqslant 0.1558$ for the solution to be acceptable. The reader's attention is drawn to the value of $\tau(r)$ at the origin, which is initially zero at $K = 0$, increases to a maximum value, and then decreases, eventually becoming negative for $K > 0.1558$.

The hit expectance densities (corresponding to the jump probability densities of Fig. 8) are given in Fig. 9. It is interesting to note that, for K small, $e(1^+) < e(1^-)$, whereas for $K = 0.1558$, $e(1^+) > e(1^-)$. This suggests that, for a given z, there exists a value of $K = K(z)$ which causes $\tau(r)$, and so $e(r)$, to be continuous at $r = 1$. We now consider this problem in detail.

Case 3. Continuous Jump Probability Density of Yukawa Form Beyond $r = 1$. We consider the problem posed by Eqs. (3.50) with the additional constraint that $e(r)$ be continuous at $r = 1$. The solution is clearly obtained using the analysis given in Case 2 of the CRF given above,

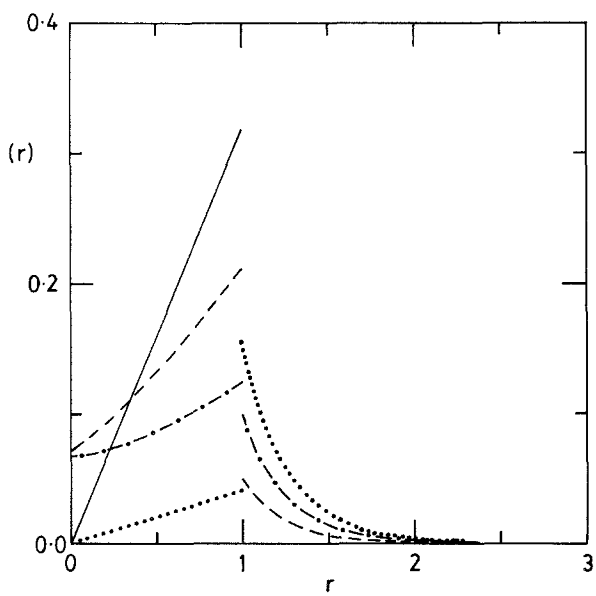

Fig. 8. The jump probability density $\tau(r)$ for the CRF considered in Case 2 of Section 3.2 with $z = 3$ and for $K = 0$ (——), $K = 0.05$ (- - -), $K = 0.1$ (-·-·-), and $K = 0.1558$ (· · ·).

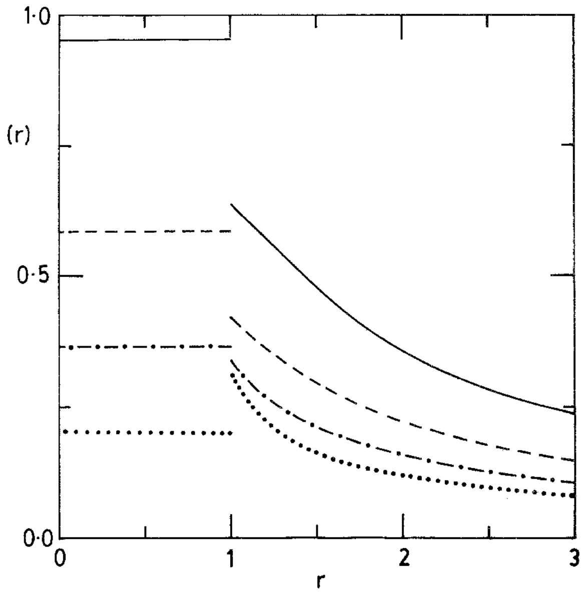

Fig. 9. The hit expectance density $e(r)$ for the CRF considered in Case 2 of Section 3.2 with $z = 3$ and for the same values of K as those displayed in Fig. 8.

the continuity condition yielding the constraint [see (3.96)]

$$b + \beta dz = 0 \tag{3.97}$$

For given z, we numerically determine $K = K(z)$ which causes (3.97) to be satisfied. In Fig. 4, the locus of (K, z) values for which (3.97) is satisfied is shown as a dotted curve; in Figs. 5–7, the corresponding points are also displayed.

In Figs. 10 and 11, the jump probability density and expectance density are shown for various values of z.

It is interesting to compare $P(V)$ for the CRF considered here with $P(V)$ for the FRF in which $\tau(r)$ is of Yukawa form over the whole range of r. This is done in Fig. 12, where $P(V)$ is plotted as a function of z for the two random flights. Whereas $P(V) \to 1$ as $z \to \infty$ in the FRF, $P(V)$ for the CRF does not. It appears that in the latter case, $P(V) \to 1/3$ as $z \to \infty$, which is consistent with the result for the CRF with jump probability density of finite range. However, this limit is not uniform, since the CRF with finite-ranged jump probability density is not continuous.

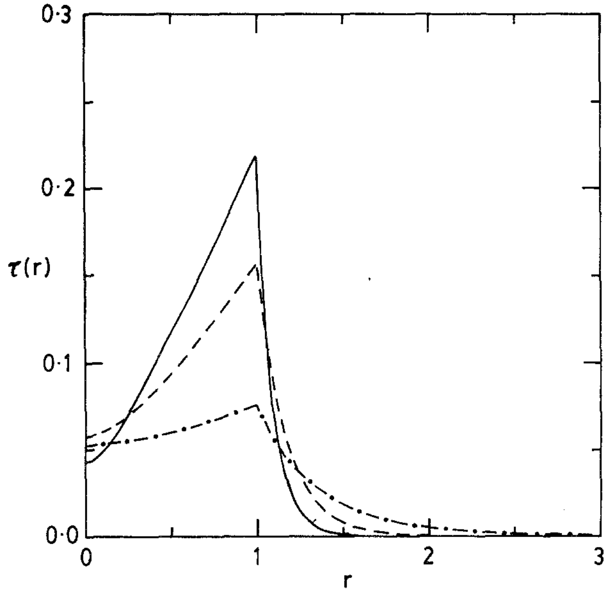

Fig. 10. The jump probability density $\tau(r)$ for the CRF considered in Case 3 of Section 3.2 for $z = 10$ (——), $z = 5$ (- - -) and $z = 2$ (-·-·-).

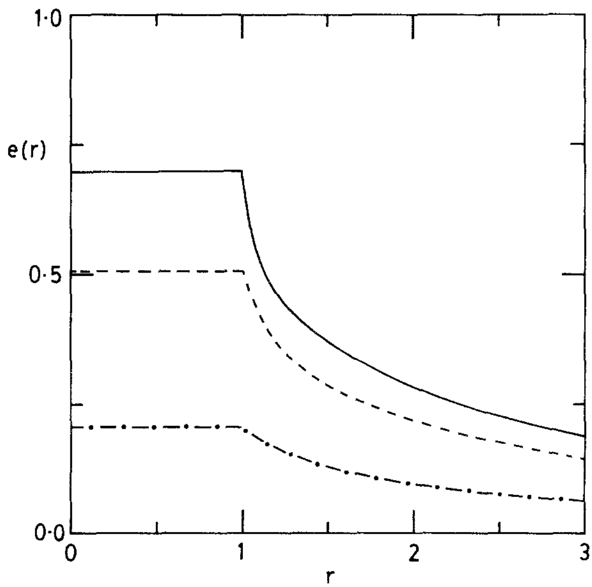

Fig. 11. The hit expectance density $e(r)$ for the CRF considered in Case 3 of Section 3.2 for the same values of z as those displayed in Fig. 10.

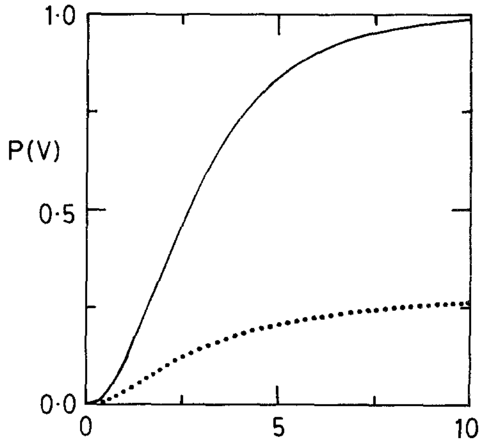

Fig. 12. The probability of return to the volume V, $P(V)$, as a function of z for the FRF in which $\tau(r)$ is of Yukawa form for all r (Case 2, Section 3.1) (——) and for the CRF in which $\tau(r)$ is continuous and of Yukawa form for $r \geqslant 1$ (Case 3, Section 3.2) (- - -).

4. FIVE-DIMENSIONAL RANDOM FLIGHTS

A point in five-dimensional space $(x_1, x_2, x_3, x_4, x_5)$ may be represented in five-dimensional spherical polar coordinates as $(r, \theta, \phi, \eta, \xi)$, where the two representations are related by

$$\begin{aligned} x_1 &= r\cos\theta, & 0 &\leqslant \theta \leqslant \pi \\ x_2 &= r\sin\theta\cos\phi, & 0 &\leqslant \phi \leqslant \pi \\ x_3 &= r\sin\theta\sin\phi\cos\eta, & 0 &\leqslant \eta \leqslant \pi \\ x_4 &= r\sin\theta\sin\phi\sin\eta\cos\xi, & 0 &\leqslant \xi \leqslant 2\pi \\ x_5 &= r\sin\theta\sin\phi\sin\eta\sin\xi \end{aligned} \tag{4.1}$$

The Jacobian of this transformation is given by

$$J = r^4 \sin^3\theta \sin^2\phi \sin\eta \tag{4.2}$$

and the element of solid angle $d\Omega$ satisfies

$$d\Omega = \sin^3\theta \sin^2\phi \sin\eta \, d\theta \, d\phi \, d\eta \, d\xi, \qquad \int d\Omega = \frac{8\pi^2}{3} \tag{4.3}$$

Thus, for a jump probability density $\tau(r)$ [note the implied spherical symmetry through the dependence of $\tau(r)$ only on $r = |\mathbf{r}|$] in five dimensions the normalization requirement becomes

$$\int \tau(r) \, d\mathbf{r} = \frac{8\pi^2}{3} \int \tau(r)^4 \, dr = 1 \tag{4.4}$$

4.1. The Free Random Flight (FRF) in Five Dimensions

Let us consider the situation in which the random jumper makes jumps in a random direction each of unit length. This is the five-dimensional analog of the problem considered in Case 1 of Section 3.1. The jump probability density $\tau(r)$ in the present case must be given by

$$\tau(r) = \frac{3}{8\pi^2}\delta(r-1) \tag{4.5}$$

where $\tau(r)$ is the one-dimensional Dirac delta function whose coefficient is determined by the normalization condition (4.4).

In five dimensions, the Fourier transform $\hat{f}(k)$ of a function $f(r)$ which depends only on $r = |\mathbf{r}|$ is given by

$$\hat{f}(k) = \frac{8\pi^2}{k}\int_0^\infty r^3 f(r) j_1(kr)\,dr \tag{4.6}$$

where $j_1(x)$ is the spherical Bessel function of order one, viz.,

$$j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x} \tag{4.7}$$

The inverse Fourier transform is given by

$$f(r) = \frac{1}{(2\pi)^5}\frac{8\pi^2}{r}\int_0^\infty k^3\hat{f}(k) j_1(kr)\,dk \tag{4.8}$$

Thus, the Fourier transform of $\tau(r)$ is given by

$$\hat{\tau}(k) = \frac{3}{k} j_1(k) \to 1 - \frac{k^2}{10} + O(k^4), \qquad k\to 0 \tag{4.9}$$

From (3.1), $\hat{e}(k)$ is given by

$$\hat{e}(k) = \frac{3j_1(k)}{k - 3j_1(k)} \to \frac{10}{k^2} + O(k^0), \qquad k\to 0 \tag{4.10}$$

From the asymptotic behavior of $\hat{e}(k)$ as $k\to 0$, we find that

$$e(r) \to \frac{5}{4\pi^2}\frac{1}{r^3} \cong 0.1267\frac{1}{r^3}, \qquad r\to\infty \tag{4.11}$$

The hit expectance density is shown in Fig. 13. It has very similar features to the corresponding curve in three dimensions: it diverges at the origin, a delta function at $r = 1$ and a small discontinuity at $r = 2$ that is too small to be resolved on the scale of Fig. 13.

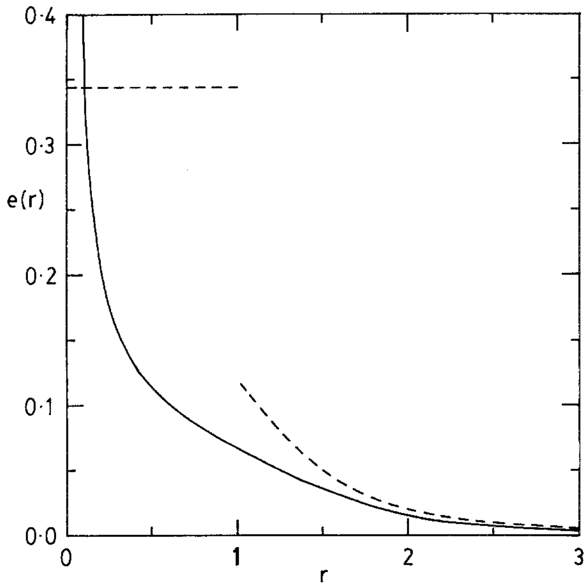

Fig. 13. The hit expectance density $e(r)$ for the FRF in five-dimensional Euclidean space considered in Section 4.1 (——) and for the CRF considered in Section 4.2 (- - -).

4.2. The Constrained Random Flight (CRF) in Five Dimensions

We now consider the simplest CRF in five dimensions in which the jump probability density is zero beyond $r = 1$, and the hit expectance density is constant for $r < 1$, viz.,

$$\tau(r) = 0, \qquad r > 1 \tag{4.12a}$$

$$e(r) = \epsilon, \qquad r < 1 \tag{4.12b}$$

As in Section 3.2, we seek a Wiener–Hopf factorization of the key equation (3.17). We use an adaptation of the method due to Freasier and Isbister[13] (in their study of the five-dimensional hard hypersphere fluid) which may be regarded as an extension of Baxter's formalism.[11] We first note that since

$$j_1(x) = -\frac{d}{dx} j_0(x) \tag{4.13}$$

$\hat{e}(k)$ may be written as

$$\hat{e}(k) = \frac{8\pi^2}{k} \int_0^\infty dr\, rE(r) \sin kr\, dr \tag{4.14}$$

where $E(r)$ is given by

$$E(r) = \int_r^\infty dt\, te(t) \tag{4.15}$$

Integrating again by parts, we obtain

$$\hat{e}(k) = 8\pi^2 \int_0^\infty dr\, \bar{E}(r) \cos kr \tag{4.16}$$

where

$$\bar{E}(r) = \int_r^\infty ds \int_s^\infty dt\, te(t) = \frac{1}{2}\int_r^\infty e(t)t(t^2 - r^2)\, dt \tag{4.17}$$

Similarly,

$$\hat{\tau}(k) = \frac{8\pi^2}{k}\int_0^1 dr\, rT(r) \sin kr = 8\pi^2 \int_0^1 dr\, r\bar{T}(r) \cos kr \tag{4.18}$$

where

$$\begin{aligned} T(r) &= \int_r^1 dt\, t\tau(t), \qquad 0 < r < 1 \\ &= 0, \qquad r > 1 \end{aligned} \tag{4.19}$$

$$\begin{aligned} \bar{T}(r) &= \frac{1}{2}\int_r^1 \tau(t)t(t^2 - r^2)\, dt, \qquad 0 < r < 1 \\ &= 0, \qquad r > 1 \end{aligned} \tag{4.20}$$

A Wiener–Hopf factorization may now be performed as in Section 3.2. We find that

$$1 - \hat{\tau}(k) = \hat{Q}(k)\,\hat{Q}(-k) \tag{4.21}$$

where $\hat{Q}(k)$ is regular and has no zeros in the upper half-plane. It is related to a real space function $Q(r)$ by

$$4\pi^2 Q(r) = \frac{1}{2\pi}\int_{-\infty}^\infty dk\, e^{-ikr}[1 - \hat{Q}(k)] \tag{4.22}$$

As in Section 3.2, it can be shown that

$$Q(r) = 0, \qquad r < 0, \qquad r \geqslant 1 \tag{4.23}$$

so that

$$\hat{Q}(k) = 1 - 4\pi^2 \int_0^1 dr\, e^{ikr} Q(r) \tag{4.24}$$

The real space relations between $Q(r)$ and $\tau(r)$ and $e(r)$ are given by

$$\bar{E}(r) = Q(r) + 4\pi^2 \int_0^1 dt\ Q(t)\bar{E}(|r-t|), \qquad r > 0 \tag{4.25}$$

$$\bar{T}(r) = Q(r) - 4\pi^2 \int_r^1 dt\ Q(t)Q(t-r), \qquad 0 < r \leqslant 1 \tag{4.26}$$

In view of (4.12b) and (4.17)

$$\bar{E}(r) = \frac{\epsilon}{8} r^4 + \left(-\frac{\epsilon}{4} - \frac{E_1}{2}\right) r^2 + \left(\frac{E_3}{2} - \frac{\epsilon}{8}\right), \qquad 0 < r < 1 \tag{4.27}$$

where

$$E_n = \int_0^\infty dt\, t^n e(t) \tag{4.28}$$

Substituting (4.27) into (4.25) for $0 < r < 1$ and differentiating three times, we obtain

$$Q'''(r) = ar + b \tag{4.29}$$

where

$$a = \epsilon\left[3 - 12\pi^2 \int_0^1 dt\ Q(t)\right] \tag{4.30}$$

$$b = \epsilon 12\pi^2 \int_0^1 dt\, tQ(t) \tag{4.31}$$

From (4.30) and (4.24)

$$a = 3\epsilon\alpha = 3\epsilon\hat{Q}(0) \tag{4.32}$$

where α is defined in (3.14). Consequently, as detailed in Section 3.2,

$$a = 0 \tag{4.33}$$

as a result of the normalization condition on the jump probability density $\tau(r)$.

Equation (4.29) may be integrated three times to yield

$$Q(r) = \frac{a}{24}(r^4 - 1) + \frac{b}{6}(r^3 - 1) + \frac{c}{2}(r^2 - 1) + d(r - 1), \qquad 0 < r \leqslant 1 \tag{4.34}$$

where c and d are constants to be determined. Note that the boundary condition on $Q(r)$ at $r = 1$ given in (4.23) has been applied.

Thus far, there are two equations for ϵ, b, c, and d: (4.30) and (4.31). A third equation comes from (4.26) which, on differentiating and making use of (4.20) yields

$$Q'(1) = 0 \tag{4.35}$$

The final equation comes from the differentiated form of (4.26) considered at $r = 0$:

$$\bar{T}'(r) = Q'(r) + 4\pi^2 Q(r)\, Q(0) + 4\pi^2 \int_r^1 dt\; Q(t) Q'(t-r)$$

When evaluated at $r = 0$, this becomes

$$Q'(0) + 2\pi^2 Q^2(0) = 0 \tag{4.36}$$

An expression for ϵ in terms of b, c, and d follows from (4.31):

$$\epsilon = \frac{-b}{\pi^2(\frac{3}{5}b + \frac{3}{2}c + 2d)} \tag{4.37}$$

The remaining equations—(4.30) [with (4.33)], (4.35), and (4.36)—result in the following explicit equations for b, c, and d:

$$\frac{3}{2}b + 4c + 6d = -\frac{3}{\pi^2} \tag{4.38}$$

$$\frac{b}{2} + c + d = 0 \tag{4.39}$$

$$d = -2\pi^2\left(\frac{b}{6} + \frac{c}{2} + d\right)^2 \tag{4.40}$$

From (4.38) and (4.39)

$$b = \frac{6}{\pi^2} + 4d, \qquad c = -\frac{3}{\pi^2} - 3d \tag{4.41}$$

which on substitution into (4.40) yields

$$d^2\frac{\pi^2}{18} + \frac{2}{3}d + \frac{1}{2\pi^2} = 0 \tag{4.42}$$

This is a quadratic equation for d, to which there are two solutions:

$$d_1 = \frac{-6 + 3\sqrt{3}}{\pi^2}, \qquad d_2 = \frac{-6 - 3\sqrt{3}}{\pi^2} \tag{4.43}$$

The second solution for d is found to give negative ϵ and so is not acceptable. Hence, d_1 is the correct root, and the complete solution is given by

$$b = \frac{-18 + 12\sqrt{3}}{\pi^2} \tag{4.44a}$$

$$c = \frac{15 - 9\sqrt{3}}{\pi^2} \tag{4.44b}$$

$$d = \frac{-6 + 3\sqrt{3}}{\pi^2} \tag{4.44c}$$

and

$$\epsilon = \frac{1}{\pi^2}(90 - 50\sqrt{3}) \cong 0.344 \tag{4.45}$$

Substituting (4.34) (with $a = 0$) into (4.26) and solving for $\tau(r)$, we obtain

$$\begin{aligned} \tau(r) &= \frac{3}{\pi^2}(4\sqrt{3} - 7)r^3 + \frac{9}{\pi^2}(2 - \sqrt{3})r, \qquad 0 < r \leqslant 1 \\ &= 0, \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad r > 1 \end{aligned} \tag{4.46}$$

which can be readily verified as satisfying the normalization condition (4.4).

An analysis of the small-k behavior of $e(k)$ shows that

$$\hat{e}(k) \to \frac{100}{(1 + \sqrt{3})^2} \frac{1}{k^2}, \qquad k \to 0 \tag{4.47}$$

so that

$$e(r) \to \frac{50}{4(1 + \sqrt{3})^2 \pi^2} \frac{1}{r^3} \approx 0.1697 \frac{1}{r^3}, \qquad r \to \infty \tag{4.48}$$

The $1/r^3$ decay in $e(r)$ for the CRF is the same as that of the FRF considered in Section 4.1 above, although the coefficient of the decay is different for the two random flights. The probability of return to the volume V, $P(V)$, is given by

$$P(V) = \frac{9 - 5\sqrt{3}}{15 - 5\sqrt{3}} \approx 0.0536 \tag{4.49}$$

5. CONCLUDING REMARKS

In this paper, we have considered the random flight problem in three and five dimensions. No solution to the CRF problem exists in one dimension. A Wiener–Hopf factorization technique can be applied to the problem as posed by Eqs. (1.4) and (1.6). However, the resulting ϵ is found to be purely imaginary. Another way of stating the nonexistence of a solution to this problem is the following: for random flights in which $\tau(r)$ is an even function of r and sufficiently short-ranged so that $\hat{\tau}(k)$ has a regular Taylor's expansion in k^2 for small k, it follows quite generally that $e(r)$ is infinite at the origin (as a simple asymptotic analysis will verify). Thus, one cannot expect to find a solution of the CRF problem in one dimension, at least for the short-ranged $\tau(r)$ we consider here.

We have not considered random flights in Euclidean spaces with even dimensionality since the Wiener–Hopf technique employed in this paper does not result in closed-form analytic solutions for $e(r)$ and $\tau(r)$ for such spaces. The primary reason that the Wiener–Hopf technique works in three and five dimensions follows from Eqs. (3.22) and (4.16), which demonstrate that the three- and five-dimensional Fourier transforms of a spherically symmetric function can be written as one-dimensional Fourier transforms of closely related functions; this is not the case for two-dimensional Fourier transforms (nor for even-dimensional Fourier transforms in general).

In future publications, we shall consider extensions of our analysis, and their application to various phenomena of physical interest. In particular, it appears that our analysis is applicable to a number of problems in the theory of dilute polymers, and to continuum models in percolation theory. We discuss the latter at the end of the appendix below. The most obvious application of our techniques to polymer problems is through the standard correspondence[3] between an n-step flight and a polymer chain of n-bonds connecting $n + 1$ units. In this regard, our analytic techniques extend to bond probability densities $\tau(\mathbf{r}_j - \mathbf{r}_{j-1}, \omega_j, \omega_{j-1})$ that depend upon orientations ω_j and ω_{j-1} of units j and $j - 1$ as well as the distance between them, $r_{j,j-1}$.

ACKNOWLEDGMENTS

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APPENDIX: THE UNDERLYING ORNSTEIN–ZERNIKE STRUCTURE OF PROBLEMS OF RANDOM FLIGHT, LATTICE-GAS AND LIQUID-STATE THEORY, AND PERCOLATION THEORY

There is a remarkable similarity between the generating function for an n-step random walk on a periodic lattice [the $E(\mathbf{r}, t)$ of Section 2.3] and the spin–spin correlation function of the spherical model (SM) of a ferromagnet[14] and its variants—the mean spherical model (MSM),[15] the Gaussian model (GM),[14] and the mean spherical approximation (MSA) and Gaussian approximation (GA) for the Ising model.[16] Moreover, the SM and its variants all have lattice-gas versions, in which the particle–particle correlation function also looks like $E(\mathbf{r}, t)$ except for trivial factors. This connection between these two-point correlation functions and $E(\mathbf{r}, t)$

has already been noted by a number of workers.[5] Here we shall make clear how the connection follows from the existence of an underlying equation of Ornstein–Zernike type in both the random walk (on a lattice) and lattice-gas problems. (We use lattice-gas language rather than spin–spin language to maximize correspondence between lattice systems and fluid results and we lean heavily on earlier work by one of us[(18)] in discussing the lattice gas.) We shall further discuss the connection between the generating function for a random flight *not* restricted to a lattice [the $e(\mathbf{r}, t)$ of this paper] and the two-particle correlation function for a fluid in the MSA. (The SM, GM, and MSM are not well defined for a fluid.) Here again the connection is via the fact that there is an equation of Ornstein–Zernike form underlying both the random-flight and fluid problems. Finally, we extend the connection induced by the Ornstein–Zernike equation to percolation theory and demonstrate an isomorphism between a particular random flight problem we have solved and a corresponding percolation problem.

In a fluid of monatomic particles, the two-particle correlation function $h(\mathbf{r}, \rho)$ and the direct correlation function $c(\mathbf{r}, \rho)$ are functions that are related by an Ornstein–Zernike equation—in fact, the *original* Ornstein–Zernike equation,[(19), 6]

$$h(\mathbf{r}, \rho) = c(\mathbf{r}, \rho) + \rho \int d\mathbf{s}\, c(\mathbf{s}, \rho) h(\mathbf{r} - \mathbf{s}, \rho) \tag{A.1a}$$

Here ρ is the expected number density of the fluid system, which we assume to be uniform and infinite in volume. The similarity between (A.1a) and (2.12a) is obvious. The differences are that $c(\mathbf{r}, \rho)$ in general depends nontrivially on ρ, while $\tau(r)$ is independent of t, and that $\int \tau(\mathbf{r})\, d\mathbf{r} = 1$ and $\tau(\mathbf{r}) \geqslant 0$ because $\tau(\mathbf{r})$ is a probability density whereas $c(\mathbf{r}, \rho)$ has no sign restriction and must satisfy $\int c(\mathbf{r})\, d\mathbf{r} = 1/\rho$ only at singular points associated with the existence of a phase transition. In the lattice-gas analog of (A.1a), the volume integral $\int d\mathbf{s}$ is simply replaced by (or interpreted as) a sum over all lattice sites. In Fourier space, (A.1a) becomes

$$\hat{h}(\mathbf{k}, \rho) = \hat{c}(\mathbf{k}, \rho) + \rho \hat{c}(\mathbf{k}, \rho) \hat{h}(\mathbf{k}, \rho) \tag{A.1b}$$

for both the fluid and lattice gas. In the fluid case, the Fourier transform is given by (3.2),

$$\hat{f}(\mathbf{k}) = \int d\mathbf{r}\, f(\mathbf{r}) \exp(i\mathbf{k} \cdot \mathbf{r})$$

[5] See, for example, Ref. 17.

[6] Equation (A.1) can be thought of as defining $c(\mathbf{r}, \rho)$ in terms of $h(\mathbf{r}, \rho)$. In the statistical theory of fluids one has an exact (but intractable) second independent relation among c, h, and the pair potential that has no counterpart in random flight theory. For quantitative fluid results, the second relation is typically replaced by a relatively simple approximation, such as Eq. (A.13).

while in the case of a lattice gas, one sums over all the vectors $\mathbf{r}$ corresponding to lattice sites instead of integrating, so that

$$\hat{f}(\mathbf{k}) = \sum_{\mathbf{r}} f(\mathbf{r})\exp(i\mathbf{k}\cdot\mathbf{r}) \tag{A.2}$$

In the lattice-gas case, we shall choose a simple hypercubic lattice in d dimensions as a concrete example. Then

$$f(\mathbf{r}) = (2\pi)^{-d}\int d\mathbf{k}\,\hat{f}(\mathbf{k})\exp(-i\mathbf{k}\cdot\mathbf{r}) \tag{A.3}$$

where the integration extends from $-\pi$ to π for each of the d components of the vector $\mathbf{k} = (x_1, \ldots, x_d)$. It immediately follows from (A.1) and (A.3) that

$$\frac{1}{(2\pi)^d}\int d\mathbf{k}\,\frac{\exp(-i\mathbf{k}\cdot\mathbf{r})}{1-\rho\hat{c}(\mathbf{k},\rho)} = \delta_{\mathbf{r},\mathbf{0}} + \rho h(\mathbf{r},\rho) \tag{A.4}$$

where $\delta_{\mathbf{r},\mathbf{0}}$ is a Kronecker delta.

Similarly, the corresponding relation between Fourier transforms of the lattice-walk generating function $E(\mathbf{r},t)$ and the single step probability $T(\mathbf{r})$ on the same lattice is given by

$$\frac{1}{(2\pi)^d}\int d\mathbf{k}\,\frac{\exp(-i\mathbf{k}\cdot\mathbf{r})}{1-t\hat{T}(\mathbf{k})} = \delta_{\mathbf{r},\mathbf{0}} + tE(\mathbf{r},t) \tag{A.5a}$$

which follows immediately from the lattice walk analog of (2.12a)

$$E(\mathbf{r},t) = T(\mathbf{r}) + t\sum_{\mathbf{s}} T(\mathbf{s})E(\mathbf{r}-\mathbf{s},t) \tag{A.5b}$$

which, like (2.12a), is of the Ornstein–Zernike form. The formal similarity between (A.4) and (A.5a), like that between (2.12a) and (A.1a), is clear. We shall next show that the differences one finds in functional forms between $c(\mathbf{r},\rho)$ and $T(\mathbf{r})$ do not destroy the essential correspondence between $E(\mathbf{r},t)$ and the $h(\mathbf{r},\rho)$ we are considering.

Although $T(\mathbf{r}) = 0$ for $\mathbf{r} = \mathbf{0}$ in the simple random walk (to which we restrict ourselves here), $c(\mathbf{r},\rho)$ at $\mathbf{r} = \mathbf{0}$ is not zero in the SM, MSM, GM, or MSA. Moreover, it is only at $\mathbf{r} = \mathbf{0}$ that the $c(\mathbf{r},\rho)$ is ρ dependent in the context of these descriptions of the lattice gas. For both these reasons, it is useful to decompose $c(\mathbf{r},\rho)$ into two terms,

$$\begin{aligned} c(\mathbf{r},\rho) &= c_0(\rho)\delta_{\mathbf{r},\mathbf{0}} + c^1(\mathbf{r}) \\ c^1(\mathbf{r}) &= c(\mathbf{r},\rho) \qquad \text{for} \quad \mathbf{r} \neq \mathbf{0} \\ c^1(\mathbf{r}) &= 0 \qquad\qquad \text{for} \quad \mathbf{r} = \mathbf{0} \end{aligned} \tag{A.6}$$

Then we can write (A.4) as

$$\frac{1}{(2\pi)^d}\int d\mathbf{k}\,\frac{\exp(-i\mathbf{k}\cdot\mathbf{r})}{1-z\hat{c}^1(\mathbf{k})}=\left(\frac{\rho}{z}\right)\left[\delta_{\mathbf{r},\mathbf{0}}+\rho h(\mathbf{r},\rho)\right] \tag{A.7a}$$

where (dropping the argument ρ of c_0 for notational simplicity)

$$z=\rho(1-\rho c_0)^{-1} \tag{A.7b}$$

In the SM and its variants, $c^1(\mathbf{r})$ can be identified with the pair potential $\phi(\mathbf{r})$ between particles on lattice sites displaced from one another by the vector $\mathbf{r}\neq 0$, divided by $k_B T$, where k_B is Boltzmann's constant, and T is the absolute temperature.[18] Thus

$$c^1(\mathbf{r})=-\phi(\mathbf{r})/k_B T, \qquad \mathbf{r}\neq\mathbf{0} \tag{A.8}$$

A typical $\phi(\mathbf{r})$ of interest is a nearest-neighbor interaction, such that $\phi(\mathbf{r})$ is nonzero only for $|\mathbf{r}|=1$, where it is ϕ_1, so that

$$\begin{aligned} c^1(\mathbf{r}) &= c_1 \qquad \text{for} \quad |\mathbf{r}|=1\\ &=0 \qquad \text{otherwise} \end{aligned} \tag{A.9}$$

$$c_1=-\phi_1/k_B T, \qquad \hat{c}^1(\mathbf{0})=2dc_1$$

In (A.5),

$$\hat{T}(\mathbf{0})=1 \tag{A.10}$$

because $T(\mathbf{r})$ is a probability, so $\sum_{\mathbf{r}} T(\mathbf{r})=1$. Thus, $t=1$ is a singular value of the integrand, at which $E(\mathbf{r},t)$ becomes infinite for $d=1$ and 2 and long-ranged for $d\geqslant 3$. [We recall that $E(\mathbf{r},1)$ is the expected number of visits to the lattice site described by vector $\mathbf{r}$.]

In (A.7), $\hat{c}(\mathbf{0})$ is not necessarily unity, but for $c^1(r)\geqslant 0$, an identical singularity will occur for z such that

$$1-z\hat{c}^1(\mathbf{0})=0 \tag{A.11}$$

This is associated with a phase transition of the model and the details vary among the models described by (A.7).[18] In the Gaussian approximation, for example, $c_0=(\rho-1)^{-1}$ so $z=\rho(1-\rho)$ and the singularity occurs when $\rho(1-\rho)\hat{c}^1(\mathbf{0})=1$ for all d. In the SM, MSM, and MSA, c_0 is instead determined by a "core condition"[18] $h(\mathbf{0},\rho)=-1$ which from (A.7) requires the satisfaction of

$$\frac{1}{(2\pi)^d}\int d\mathbf{k}\left[1-z\hat{c}^1(\mathbf{k})\right]=\rho(1-\rho)/z \tag{A.12}$$

This relation prevents (A.11) from being realized for nonzero temperature T when $d=1$ or 2. We refer to Ref. 18 for details but note here that despite the nonpositive value of $h(\mathbf{0},\rho)$ the full right-hand side of (A.7a) remains positive for all $\mathbf{r}$ when $\phi(r) \geqslant 0$ for the physically realizable range of ρ, $0 \leqslant \rho \leqslant 1$.

The upshot of the above analysis is that the left-hand sides of (A.5a) and (A.7a) can be identified as the same function if one identifies $T(\mathbf{r})$ with $c^1(\mathbf{r})/\hat{c}^1(\mathbf{0})$ and t with $z\hat{c}^1(\mathbf{0})$. We have thus shown how the Ornstein–Zernike structure induces a correspondence (but not quite an identity) between $E(\mathbf{r},t)$ and the lattice gas $h(\mathbf{r},\rho)$ for the models under consideration despite some differences between $T(\mathbf{r})$ and $c(\mathbf{r},\rho)$.

If we were looking at the case in which $c^1(\mathbf{r}) \leqslant 0$, the analysis would be different. For example, using (A.9) with $c_1 \leqslant 0$, we would find the integrand of (A.7a) becoming singular at $\mathbf{k} = (\pm\pi, \pm\pi, \ldots, \pm\pi)$, rather than at $\mathbf{k} = \mathbf{0}$, for physically realizable densities ρ. But if we let z be negative, corresponding to unphysical (negative) ρ, we would then again find a simple identity between the integrals of (A.7) and (A.5) for certain pairs of t and z. The $c^1(\mathbf{r}) \leqslant 0$ corresponds to a repulsive interaction between particles for $\mathbf{r} \neq \mathbf{0}$ in the SM and its variants. (In spin-system language, it corresponds to an antiferromagnetic exchange interaction.)

We return now to the fluid case, in which the mean spherical approximation[20] is typically of useful accuracy for hard-core molecules. Outside the core region, defined by the core diamater σ, one has the fluid analog of (A.8)

$$c(\mathbf{r},\rho) = -\phi(\mathbf{r})/k_B T \qquad \text{for} \quad r > \sigma, \tag{A.13}$$

while for $r < \sigma$, one has a core condition reflecting the impenetrability of hard core molecules,

$$h(\mathbf{r},\rho) = -1 \qquad \text{for} \quad r < \sigma \tag{A.14}$$

(We shall take the hard-core diameter to be unity without loss of generality). In contrast to the lattice-gas case, there is a lack of correspondence between the $h(\mathbf{r},\rho)$ in the MSA and the random flight $e(\mathbf{r},t)$ within the physically realizable range of ρ and T for $\phi(\mathbf{r})$ of interest. This is a result of the negative values that both $c(\mathbf{r},\rho)$ and $h(\mathbf{r},\rho)$ typically have over the whole range $0 \leqslant r \leqslant 1$, as well as the highly nontrivial ρ dependence that $c(\mathbf{r},\rho)$ typically assumes over this range, in contrast to the independence of $\tau(\mathbf{r})$ on t. One sees this already for the case of a hard-sphere fluid in which $\phi(r) = 0$ for $r > \sigma$, where (A.13) becomes (for hard spheres of unit diameter)

$$c(\mathbf{r},\rho) = 0 \qquad \text{for} \quad r > 1 \tag{A.15}$$

If one solves (A.1) with conditions (A.14) and (A.15) for *negative* (and hence unphysical) ρ, however, one finds a distinguished ρ value, $\rho = -3/\pi$, at which

$$1 - \rho \int c(\mathbf{r}, \rho)\, d\mathbf{r} = 0 \tag{A.16}$$

and for which $\rho h(\mathbf{r}, \rho)$ and $\rho c(\mathbf{r}, \rho)$ are *identical* to the $e(\mathbf{r}, 1)$ and $\tau(\mathbf{r})$ respectively, discussed in Case 1 of Section 3.2. Put another way, the solution of (A.1) subject to conditions (A.14), (A.15), and (A.16) is exactly equivalent to the solution of (2.7) subject to (2.2) and (3.13). In the first case, one finds a solution at $\rho = -3/\pi$. In the second case, equivalently, one finds the solution $\epsilon = 3/\pi$.

Similarly, one finds that each of the other cases we treat in which $e(\mathbf{r})$ is prescribed inside and $\tau(\mathbf{r})$ outside a unit ball corresponds exactly to a solution of (A.1) for the distinguished negative value of ρ that satisfies (A.16), subject to (A.14) and (A.13) for a prescribed $\phi(\mathbf{r})/k_B T$. These cases, which correspond to purely repulsive potentials in the MSA, are fluid generalizations of the lattice case in which $c^1(\mathbf{r}) \leqslant 0$, discussed between (A.12) and (A.13).

We shall end with one more remarkable application of the Ornstein–Zernike equation that leads again to our solution of (A.1) subject to conditions equivalent to (A.14), (A.15), and (A.16), but this time involves a physically realizable number density. It is an application to the theory of percolation and gelation and involves the pair connectedness function $P(\mathbf{r}, \rho)$ that yields the probability of finding two points displaced by $\mathbf{r}$ that are in the same connected cluster of particles. $P(\mathbf{r}, \rho)$ is related to a "direct" connectivity function $C^\dagger(\mathbf{r}, \rho)$, just as $h(\mathbf{r}, \rho)$ is related to $c(\mathbf{r}, \rho)$, by the Ornstein–Zernike equation (A.1). Moreover, the divergence of the mean cluster size is given by the condition

$$1 = \rho \int C^\dagger(\mathbf{r}, \rho)\, d\mathbf{r} \tag{A.17}$$

exactly analogous to the infinite compressibility condition (A.16). Condition (A.17) occurs at the percolation threshold (or gelation) density ρ_c. We refer readers to Coniglio *et al.*[(21)] for details of the general formalism.

Suppose the particles whose clustering properties we are considering are randomly overlapping spheres of unit diameter.[7] Using the obvious definition of connectedness for such particles (which is *not*, however, the connectedness criterion considered in Ref. 21), one can apply the MSA to this problem, which yields the boundary conditions

$$P(\mathbf{r}, \rho) = 1 \qquad \text{for} \quad r < 1 \tag{A.18}$$

$$C^\dagger(\mathbf{r}, \rho) = 0 \qquad \text{for} \quad r > 1 \tag{A.19}$$

Except for the change in sign in (A.18), this is the pair of conditions (A.14)

[7] See Ref. 22 for an analysis of this problem using series expansion.

and (A.15), respectively. The sign change maps solutions of (A.1) at $-\rho$ into solutions at ρ. Thus in the MSA, percolation occurs at a positive (and hence physically realizable) ρ_c of $3/\pi$ for overlapping spheres. The solution of this problem (off the percolation threshold as well as on it) and some of its immediate generalizations were first obtained by Chiew and Glandt, and we refer to their discussion[23] for details.

REFERENCES

1. F. Spitzer, *Principles of Random Walk* (Van Nostrand, Princeton, New Jersey, 1964).
2. M. N. Barber and B. W. Ninham, *Random and Restricted Walks* (Gordon and Breach, New York, 1970).
3. H. Yamakawa, *Modern Theory of Polymer Solutions* (Harper and Row, New York, 1970); see Chap. 2.
4. E. W. Montroll, in *Applied Combinatorial Mathematics*, E. F. Beckenback, ed. (Wiley, New York, 1964); and E. W. Montroll, *J. Soc. Indust. Appl. Math.* **4**:241 (1956).
5. P. W. Kasteleyn, in *Graph Theory and Theoretical Physics*, F. Harary, ed. (Academic Press, London, 1967).
6. G. Polya, *Math. Ann.* **84**:149 (1921).
7. S. Chandrasekhar, *Rev. Mod. Phys.* **15**:1 (1943).
8. Lord Rayleigh, *Phil. Mag.* **37**:321 (1919).
9. W. Feller, *An Introduction to Probability Theory and Its Applications*, Vol. 1 (John Wiley and Sons, New York, 1957).
10. B. Noble, *Methods Based on the Wiener–Hopf Technique* (Pergamon Press, London, 1958).
11. R. J. Baxter, *Aust. J. Phys.* **21**:563 (1968).
12. R. E. Bellman and K. L. Cooke, *Differential-Difference Equations* (Academic Press, New York, 1963).
13. B. C. Freasier and D. J. Isbister, *Mol. Phys.* **42**:927 (1981).
14. T. H. Berlin and M. Kac, *Phys. Rev.* **86**:821 (1952).
15. H. W. Lewis and G. H. Wannier, *Phys. Rev.* **88**:682 (1952); *Phys. Rev.* **90**:1131 (1953).
16. G. Stell, J. L. Lebowitz, S. Baer, and W. Theumann, *J. Math. Phys.* **7**:1532 (1966).
17. A. A. Maradudin, E. W. Montroll, G. H. Weiss, R. Herman, and H. W. Milnes, *Green's Functions for Monatomic Cubic Lattices* (Academie Royale de Belgique, Bruxelles, 1960); and G. Joyce, in *Phase Transitions and Critical Phenomena*, Vol. 2, C. Domb and M. S. Green, eds. (Academic Press, London, 1972).
18. G. Stell, *Phys. Rev.* **184**:135 (1969).
19. L. S. Ornstein and F. Zernike, *Proc. Acad. Sci. Amsterdam* **17**:793 (1914).
20. J. K. Percus and G. Yevick, *Phys. Rev.* **136**:290 (1964); J. L. Lebowitz and J. K. Percus, *Phys. Rev.* **144**:251 (1966).
21. A. Coniglio, U. De Angelis, and A. Forlani, *J. Phys. A.* **10**:1123 (1977).
22. S. W. Haan and R. Zwanzig, *J. Phys. A* **10**:1547 (1977).
23. Y. C. Chiew and E. D. Glandt, *J. Phys. A.* **16**:2599 (1983).