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The Theory of Ordered Spans of Unrestricted Random Walks

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The spans of an n-step random walk on a simple cubic lattice are the sides of the smallest rectangular box, with sides parallel to the coordinate axes, that contains the random walk. Daniels first developed the theory in outline and derived results for the simple random walk on a line. We show that the development of a more general asymptotic theory is facilitated by introducing the spectral representation of step probabilities. This allows us to consider the probability density for spans of random walks in which all moments of single steps may be infinite. The theory can also be extended to continuous-time random walks. We also show that the use of Abelian summation simplifies calculation of the moments. In particular we derive expressions for the span distributions of random walks (in one dimension) with single step transition probabilities of the form $P(j) \sim 1/j^{1+\alpha}$, where $0 < \alpha < 2$. We also derive results for continuous-time random walks in which the expected time between steps may be infinite.

KEY WORDS: Random walks; ordered spans; stable distributions; Abelian summation.

1. INTRODUCTION

Daniels[(1)] appears to have been the first to investigate what he termed the "extent," and what we will term the span, of a random walk. The spans of an

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n-step random walk are defined to be the sides of the smallest (rectangular) box with sides parallel to the coordinate axes that entirely contains the random walk. Kuhn[2,3] studied the same problem for continuous diffusion, in the context of polymer configurations. Daniels' and Kuhn's studies were followed by that of Feller,[4] who discussed the case of the one-dimensional random walk in greater detail. Feller's work was extended by Zaharov and Sarmonov,[5] and Rubin[6] has studied the same problem for the unrestricted random walk in the context of the configurations of polymer chains. Most recently Rubin and Mazur[7] have obtained results on the properties of spans for both the unrestricted and the self-avoiding random walk. Properties of the ordered spans can be used as an alternative characterization of asymmetries in random walks to that proposed by Solč and Stockmayer[8] and studied further by Solč.[9] In a symmetric random walk the statistical properties of any one span are clearly the same as those for any other span. However, when the spans are ordered from smallest to greatest, the statistical properties of these ordered spans do differ; e.g., the expected value of the smallest span is obviously smaller than that of the largest one.

In this paper we develop the theory of spans for unrestricted lattice random walks, both in discrete and continuous time in any number of dimensions. The present development allows for a simple derivation of asymptotic results (for large numbers of steps or at large time) and permits us to consider approximate calculation of the span distribution for random walks in which individual jump probabilities may have infinite variances.

2. EXACT EXPRESSIONS FOR THE SPAN DISTRIBUTION

We begin by deriving several exact representations for the span distribution that are useful in different circumstances. Consider a lattice random walk in n dimensions characterized by the single-step probabilities $\{p(\mathbf{j})\} = \{p(j_1, j_2,..., j_n)\}$. The function $p(\mathbf{j})$ gives the probability of the random walker making a displacement j in a single step. We further define the structure factor $\lambda(\boldsymbol{\theta})$ by

$$\lambda(\boldsymbol{\theta}) = \sum_{j_1=-\infty}^{\infty} \sum_{j_2=-\infty}^{\infty} \cdots \sum_{j_n=-\infty}^{\infty} p(\mathbf{j}) \exp(i\mathbf{j}\cdot\boldsymbol{\theta}) \tag{1}$$

where $\boldsymbol{\theta} = (\theta_1, \theta_2,..., \theta_n)$. The state probability for the random walk, that is, the probability that the random walker is at position r after m steps, is given in terms of $\lambda(\theta)$ as

$$U_m(\mathbf{r}) = \frac{1}{(2\pi)^n} \int_{-\pi}^{\pi} \cdots \int \lambda^m(\boldsymbol{\theta}) \exp(-i\mathbf{r}\cdot\boldsymbol{\theta})\, d^n\boldsymbol{\theta} \tag{2}$$

We show, following Daniels,[1] that the distribution of spans can be expressed in terms of the $U_m(\mathbf{r})$. The use of the spectral representation in Eq. (2) allows us to find alternative and more convenient representations.

Let $p_r(\mathbf{m})$ be the probability that at step r the span in direction i is m_i, $i = 1, 2, \ldots, n$. This is the desired distribution. Let $F_r(\mathbf{m})$ be the total number of ways that an r-step random walk can be characterized by the span vector $\mathbf{m}$. A straightforward extension of the argument given by Daniels can be used to establish the relation

$$p_r(\mathbf{m}) = \Delta^2_{m_1}\Delta^2_{m_2}\cdots\Delta^2_{m_1}F_r(\mathbf{m}) \tag{3}$$

between $F_r(\mathbf{m})$ and $p_r(\mathbf{m})$ so that $p_r(\mathbf{m})$ can be found from $F_r(\mathbf{m})$. In this last equation Δ^2 is just the second difference operator; $\Delta^2 g(m) = g(m+2) - 2g(m+1) + g(m)$. Thus, we must find $F_r(\mathbf{m})$. For this purpose we introduce functions $f_r(\boldsymbol{\lambda}; \mathbf{m})$, the number of random walks in which, for $j = 1, 2, \ldots, n$, the jth coordinate has remained in the interval $(-\lambda_j, m_j - \lambda_j)$ during all r steps. Then $F_r(\mathbf{m})$ can be expressed as

$$F_r(\mathbf{m}) = \sum_{\lambda_1=1}^{m_1-1} \cdots \sum_{\lambda_n=1}^{m_n-1} f_r(\boldsymbol{\lambda}; \mathbf{m}) \tag{4}$$

Now the $f_r(\boldsymbol{\lambda}; \mathbf{m})$ can be written in terms of the state probabilities at step r of a random walk in the presence of absorbing barriers at $-\boldsymbol{\lambda}$ and $\mathbf{m} - \boldsymbol{\lambda}$. Let the $u_r(\mathbf{k}; \mathbf{m})$ be these probabilities, which are defined to satisfy

$$u_r(-\boldsymbol{\lambda}; \mathbf{m}) = u_r(\mathbf{m} - \boldsymbol{\lambda}; \mathbf{m}) = 0 \tag{5}$$

The $f_r(\boldsymbol{\lambda}; \mathbf{m})$ can be written in terms of the u_r as

$$f_r(\boldsymbol{\lambda}; \mathbf{m}) = \sum_{k_1=-\lambda_1}^{m_1-\lambda_n} \cdots \sum_{k_n=-\lambda_n}^{m_1-\lambda_n} u_r(\mathbf{k}; \mathbf{m}) \tag{6}$$

It is the $u_r(\mathbf{k}; \mathbf{m})$ that are most easily expressed in terms of the unrestricted probabilities, the $U_r(\mathbf{k})$.

The $u_r(\mathbf{k}; \mathbf{m})$ are solutions to a linear difference equation characterizing the random walk, subject to the boundary conditions in Eq. (5). Let us construct such a solution in terms of the unrestricted solutions, the $U_r(\mathbf{k})$. Daniels gave a solution by means of images. We will give one by an algebraic technique. Let us first assume that the random walk is symmetric, which implies that $U_r(\mathbf{k})$ is invariant to a change in sign of any of the k_j. Then consider the properties of the function

$$G_r(\mathbf{k}; \mathbf{m}) = \sum_{j_1=-\infty}^{\infty} \cdots \sum_{j_n=-\infty}^{\infty} U_r(\mathbf{k} + 2\mathbf{j}\cdot\mathbf{m}) \tag{7}$$

The first property of interest is that $G_r(\mathbf{k}; \mathbf{m})$ is invariant to a change in sign of any $\mathbf{k}_j$, and the second is that $G_r(\mathbf{k}; \mathbf{m})$ is periodic in the k_i, the period being $2m_i$, $i = 1, 2, \ldots, n$. Let L_j be an operator on the k that increases the argument k_j by $2\lambda_j$. Then we assert that the $u_r(\mathbf{k}; \mathbf{m})$ are given by

$$u_r(\mathbf{k}; \mathbf{m}) = (1 - L_1)(1 - L_2)\cdots(1 - L_n)G_r(\mathbf{k}; \mathbf{m}) \tag{8}$$

For example, in two dimensions

$$\begin{aligned} u_r(\mathbf{k}; \mathbf{m}) = {} & G_r(k_1, k_2) - G_r(k_1 + 2\lambda_1, k_2) - G_r(k_1, k_2 + 2\lambda_2) \\ & + G_r(k_1 + 2\lambda_1, k_2 + 2\lambda_2) \end{aligned} \tag{9}$$

where we have suppressed the m's in G_r. It is easily verified from this expression for two dimensions that the $u_r(\mathbf{k}; \mathbf{m})$ satisfy the absorbing boundary conditions, and since the G's are linear combinations of solutions to the equations describing the kinetics of the random walk, the $u_r(\mathbf{k}; \mathbf{m})$ likewise satisfy these equations. The conclusion for general n follows by an inductive argument. It is also easily verified that the expression for the $u_r(\mathbf{k}; \mathbf{m})$ in Eq. (8) is valid without any restriction to symmetric random walks. Unless otherwise stated, we restrict ourselves to the case of symmetric random walks.

When Eqs. (3)–(8) are combined we find that $F_r(\mathbf{m})$ can be expressed as

$$\begin{aligned} F_r(\mathbf{m}) = {} & \sum_{j_1=-\infty}^{\infty} \cdots \sum_{j_n=-\infty}^{\infty} \sum_{\lambda_1=0}^{m_1} \cdots \sum_{\lambda_n=0}^{m_n} \sum_{y_1=0}^{m_1} \cdots \sum_{y_n=0}^{m_n} (-1)^{j_1+j_2+\cdots+j_n} \\ & \times U_r(y_1 - \lambda_1 + j_1 m_1, y_2 - \lambda_2 + j_2 m_2, \ldots, y_n - \lambda_n + j_n m_n) \end{aligned} \tag{10}$$

generalizing Daniels' result to $n > 1$. A much more useful expression for $p_r(\mathbf{m})$, the span distribution, can be derived by substituting the integral representation of $U_r(\mathbf{k})$ given in Eq. (2) into this last equation. The finite sums can be evaluated in closed form, leading to the expression for $F_r(\mathbf{m})$:

$$F_r(\mathbf{m}) = \frac{1}{(2\pi)^n} \int_{-\pi}^{\pi} \cdots \int \lambda^r(\boldsymbol{\theta}) \prod_{s=1}^{n} V(m_s, \theta_s) d^n\boldsymbol{\theta} \tag{11}$$

where

$$V(m, \theta) = \frac{1 - \cos[(m + 1)\theta]}{1 - \cos\theta} \sum_{j=-\infty}^{\infty} (-1)^j \cos(jm\theta) \tag{12}$$

The sum in this last equation can and will be interpreted in terms of generalized functions.[10] To go from $F_r(\mathbf{m})$ to $p_r(\mathbf{m})$, one needs to take second differences as in Eq. (3). Since the V's factor in Eq. (11), we may take each second difference separately to find, finally, that

$$p_r(\mathbf{m}) = \frac{1}{\pi^n} \int_{-\pi}^{\pi} \cdots \int \lambda^r(\boldsymbol{\theta}) \prod_{s=1}^{n} W(m_s, \theta_s) d^n\boldsymbol{\theta} \tag{13}$$

in which

$$W(m, \theta) = \cot^2(\theta/2) \sum_{j=-\infty}^{\infty} (-1)^{j+1}(1 - \cos j\theta) \cos[j(m + 1)\theta] \tag{14}$$

The n-dimensional generalization of Rubin's[6] expression for $p_r(m)$ can be derived from Eq. (11) by using the identity

$$\sum_{j=-\infty}^{\infty} (-1)^j \cos(jx) = \sum_{l=-\infty}^{\infty} \delta((x/2\pi) - l + \tfrac{1}{2}) \tag{15}$$

to find that

$$p_r(\mathbf{m}) = \prod_{s=1}^{n} \left\{ \Delta_{m_s}^2 \left[\frac{1}{m_s} \sum_{l_s} \cot^2\left(\frac{\pi(l_s + \frac{1}{2})}{m_s} \right] \right) \right\} \times \lambda^r \left(\frac{2\pi(l_1 + \frac{1}{2})}{m_1}, \frac{2\pi(l_2 + \frac{1}{2})}{m_2}, \ldots, \frac{2\pi(l_n + \frac{1}{2})}{m_n} \right) \tag{16}$$

where the sums over l are over all integers such that the arguments are < 1 in absolute value.

One can also find the generalization of these results to continuous-time random walks[11] quite simply. A continuous-time random walk is one in which the time between successive steps is a random variable with probability density function $\psi(t)$. Let $\psi^*(s)$ be the Laplace transform of $\psi(t)$, let $p(\mathbf{m}; t)$ be the distribution of spans at time t, and let $p^*(\mathbf{m}; s)$ be the Laplace transform of this function. Since the Laplace transform of the probability that exactly r steps have been taken is

$$[\psi^*(s)]^r[1 - \psi^*(s)]/s$$

we can combine this expression with that given in Eq. (13) to find that

$$p^*(\mathbf{m}; s) = \frac{1}{\pi^n} \frac{1 - \psi^*(s)}{s} \int_{-\pi}^{\pi} \cdots \int \frac{\prod_l W(m_l, \theta_l)}{1 - \psi^*(s)\lambda(\boldsymbol{\theta})} d^n\boldsymbol{\theta} \tag{17}$$

The above expressions for $p_r(m)$ are all exact, involving no approximations. We now consider the asymptotic properties of $p_r(\mathbf{m})$ and $p(\mathbf{m}; t)$ that are a consequence of their representations in terms of the structure functions $\lambda(\boldsymbol{\theta})$. For the random walks of interest here $|\lambda(\boldsymbol{\theta})| < 1$ for $\theta \neq 0$ and $\lambda(0) = 1$, so that the asymptotic behavior of $p_r(m)$ for large r is determined by the behavior of the integrand in Eq. (13) in a neighborhood of the origin. A first step in determining the asymptotic behavior is to expand $W(m, \theta)$ for small $|\theta|$. From the definition in Eq. (14) we find that

$$\begin{aligned} W(m, \theta) &\sim \left(\frac{4}{\theta^2} - \frac{2}{3} + \frac{\theta^2}{60} + \cdots \right) \sum_{j=-\infty}^{\infty} (-1)^{j+1} j^2 \left(\frac{\theta^2}{2} - \frac{j^2\theta^4}{24} + \cdots \right) \\ &\quad \times \cos[j(m+1)\theta] \\ &\sim 2 \sum_{j=-\infty}^{\infty} (-1)^{j+1} j^2 \cos[j(m+1)\theta] \\ &\quad - \frac{\theta^2}{3} \sum_{j=-\infty}^{\infty} (-1)^{j+1}(2j^2 + j^4) \cos[j(m+1)\theta] + \cdots \end{aligned} \tag{18}$$

When this expansion is substituted into Eq. (13) and account taken of the definition of state probabilities in Eq. (2), we find that

$$p_r(\mathbf{m}) \sim 8^n \sum_{j_1=1}^{\infty} \sum_{j_2=1}^{\infty} \cdots \sum_{j_n=1}^{\infty} (-1)^{j_1+j_2+\cdots+j_n+n} j_1^2 j_2^2 \cdots j_n^2$$
$$\times \left[U_r(j_1(m_1+1),\ldots,j_n(m_n+1)) \right.$$
$$\left. + \frac{1}{6}\sum_{i=1}^{n} (j_i^2+2) \frac{\partial^2 U_r(\mathbf{k})}{\partial k_i^2} \bigg|_{k_1=j_1(m_1+1);k_2=j_2(m_2+1),\ldots,k_n=j_n(m_n+1)} + \cdots \right] \tag{19}$$

That is to say, the asymptotic properties of the $p_r(\mathbf{m})$ can be found in terms of the state probabilities, the $U_r(\mathbf{k})$.

3. PROPERTIES OF THE SPAN DISTRIBUTION IN ONE DIMENSION

The simplest results are those for the one-dimensional symmetric random walk. Let us first assume that all of the low-order moments are finite, i.e.,

$$\sum_{j=-\infty}^{\infty} j^2 p(j) = \sigma^2 < \infty, \qquad \sum_{j=-\infty}^{\infty} j^4 p(j) = \nu^4 < \infty \tag{20}$$

so that

$$\lambda^r(\theta) = \exp[r \ln \lambda(\theta)] \sim \exp\left(-\frac{r\theta^2\sigma^2}{2}\right)\left[1 + \frac{r\theta^4}{24}(\nu^4 - 3\sigma^4) + \cdots\right] \tag{21}$$

Therefore by a familiar asymptotic argument[11] we can write

$$U_r(k) \sim \frac{1}{(2\pi r\sigma^2)^{1/2}} \exp\left(-\frac{k^2}{2r\sigma^2}\right)\left\{1 + \frac{1}{8r}\left(\frac{\nu^4}{\sigma^4} - 3\right)\left[1 - \frac{2k^2}{r\sigma^2} + \frac{k^4}{3r^2\sigma^4}\right] + O\left(\frac{1}{r^2}\right)\right\} \tag{22}$$

Notice that all of the terms in square brackets must be retained for consistency because k^2 can be $O(r)$. The lowest order term is obtained by substituting this last expression into Eq. (19) and is

$$p_r(m) \sim \frac{8}{(2\pi r\sigma^2)^{1/2}} \sum_{j=1}^{\infty} (-1)^{j+1} j^2 \exp\left(-\frac{j^2(m+1)^2}{2r\sigma^2}\right) \tag{23}$$

in the case of a symmetric random walk. When the random walk is asymmetric such that the expected value of a single step is μ, then Eq. (23) is to be replaced by

$$p_r(m) \sim \frac{8}{(2\pi r\sigma^2)^{1/2}} \sum_{j=1}^{\infty} (-1)^{j+1} j^2 \exp\left\{-\frac{1}{2r\sigma^2}[j(m+1) - r\mu]^2\right\} \tag{23a}$$

which is equivalent to centering the density given in Eq. (23) around $r\mu$.

When r is large and m is $O(r^{1/2})$ or less, the series in Eq. (23) converges poorly, and it is convenient to make a Poisson transformation[10] to speed convergence. For convenience we neglect the difference between $m + 1$ and m, which is of no consequence for large m. We then find, in terms of the variable $x = m/(\sigma\sqrt{r})$,

$$\sigma\sqrt{r}p_r(m) \sim \frac{8}{x^3} \sum_{n=0}^{\infty} \left[\frac{(2n+1)^2\pi^2}{x^2} - 1\right] \exp\left(-\frac{\pi^2(2n+1)^2}{2x^2}\right) \tag{24}$$

with the corresponding cumulative distribution

$$P_r(m) \sim \int_0^x p_r(u)\,du = \frac{8}{\pi^2} \sum_{n=0}^{\infty} \frac{1}{(2n+1)^2} \left[1 + \frac{\pi^2(2n+1)^2}{x^2}\right] \times \exp\left(-\frac{\pi^2(2n+1)^2}{2x^2}\right) \tag{25}$$

Another expression useful for large x can be derived by directly integrating Eq. (23):

$$P_r(m) \sim 1 + 2 \sum_{j=1}^{\infty} (-1)^j j \operatorname{erfc}(jx) \tag{26}$$

where

$$\operatorname{erfc}(z) = (2\pi)^{-1/2} \int_z^{\infty} \exp(-u^2/2)\,du \tag{27}$$

The sum in Eq. (26) is rapidly convergent for $x > 1$ and is even useful for small x when an Euler transformation[12] is applied to speed convergence.

Asymptotic values (for large r) of the moments of m are easily found by integrating with respect to $p_r(m)$ as given in Eq. (23). In this way we find that

$$\langle m \rangle \sim \int_0^{\infty} m p_r(m)\,dm = \sum_{j=1}^{\infty} (-1)^{j+1} j^2 \int_0^{\infty} m \exp\left(-\frac{j^2 m^2}{2r\sigma^2}\right) dm = \frac{8\sigma\sqrt{r}}{(2\pi)^{1/2}} \sum_{j=1}^{\infty} (-1)^{j+1} \tag{28}$$

The remaining sum will be interpreted in the sense of Abel summation,[13] which identifies the sum

$$S = \sum_{n=0}^{\infty} a_n \tag{29}$$

as

$$S = \lim_{x \to 1-} \sum_{n=0}^{\infty} a_n x^n \tag{30}$$

In this sense we see that

$$\sum_{j=1}^{\infty} (-1)^{j+1} = \lim_{x \to 1} \frac{x}{1+x} = \frac{1}{2} \tag{31}$$

so that

$$\langle m \rangle = (8r\sigma^2/\pi)^{1/2} \tag{32}$$

in agreement with Daniels.[1] The corresponding expression for the variance is

$$\sigma^2(r) = \langle m^2 \rangle - \langle m \rangle^2 \sim 4r\sigma^2\left(\ln 2 - \frac{2}{\pi}\right) \sim 0.226r\sigma^2 \tag{33}$$

Higher order corrections can be found and are $O(1/r)$ with respect to the first term.

A similar argument can be given for the one-dimensional continuous-time random walk when the mean time between steps is finite. We specifically require the assumption that

$$T = \int_0^{\infty} t\psi(t)\, dt \tag{34}$$

is finite so that for small $|s|$ we can expand $\psi^*(s)$ as $\psi^*(s) = 1 - sT + O(sT)$. The small-$|s|$ behavior of $p^*(m; s)$ is required for the behavior of $p(m; t)$ at large t/T. It follows from Eq. (17) that, to lowest order in sT,

$$p^*(m; s) \sim \frac{T}{\pi} \int_{-\pi}^{\pi} \frac{W(m, \theta)\, d\theta}{1 - (1 - sT)\lambda(\theta)} \tag{35}$$

Also, at large t/T only the lowest order terms in θ can be used in this representation and the range of the integral can be extended to $(-\infty, \infty)$. In this way we find for the symmetric random walk

$$p^*(m, s) \sim \frac{2}{\pi} \sum_{j=1}^{\infty} (-1)^{j+1} j^2 \int_{-\infty}^{\infty} \frac{\cos[j(m+1)\theta]\, d\theta}{s + (\sigma^2\theta^2/(2T^2))} \tag{36}$$

If we invert this term by term, we find that

$$p(m, t) \sim 8\left(\frac{T}{2\pi\sigma^2 t}\right)^{1/2} \sum_{j=1}^{\infty} (-1)^{j+1} j^2 \exp\left(-\frac{j^2(m+1)^2 T}{2\sigma^2 t}\right) \tag{37}$$

This expression has the same form as the asymptotic result for $p_r(m)$ given in Eq. (23), when r is replaced by t/T. Higher order terms can be calculated by retaining higher powers of θ. Parenthetically, we note that when $\psi(t)$ is negative exponential,

$$\psi(t) = (1/T)\exp(-t/T) \tag{38}$$

the exact expression for $p(m, t)$ is

$$p(m, t) = \frac{1}{\pi}\int_{-\pi}^{\pi} W(m, \theta)\exp\left\{-\frac{t}{T}[1 - \lambda(\theta)]\right\} d\theta \tag{39}$$

and a complete expansion in terms of t/T is easily found. The leading term is given in Eq. (37), and correction terms are $O(T/t)$.

If we drop the assumption that the mean time between steps is finite, replacing it by the assumption that $\psi^*(s)$ has the expansion

$$\psi^*(s) = 1 - (sT)^\alpha + O(sT) \tag{40}$$

for $|sT|$ small and $\alpha < 1$, then the expression in Eq. (36) is replaced by

$$p^*(m, s) \sim \frac{2}{\pi}\sum_{n=0}^{\infty}(-1)^{j+1}j^2 s^{\alpha-1}\int_{-\infty}^{\infty}\frac{\cos[j(m+1)\theta]\,d\theta}{s^\alpha + (\sigma^2\theta^2/(2T^\alpha))} \tag{41}$$

The inversion with respect to time of each term in the sum can be expressed in terms of a stable distribution, as Shlesinger[14] and Tunaley[15] have demonstrated. If we define $B_\alpha(z)$ to be the Mittag–Leffler function

$$B_\alpha(z) = \sum_{n=0}^{\infty}\frac{(-1)^n z^{\alpha n}}{\Gamma(\alpha n + 1)} \tag{42}$$

then $p(m, t)$ takes the form

$$p(m, t) \sim \frac{2}{\pi}\sum_{j=1}^{\infty}(-1)^{j+1}j^2\int_{-\infty}^{\infty} B_\alpha\left[\left(\frac{\sigma|\theta|}{2}\right)^{2/\alpha}\frac{t}{T}\right]\cos[j(m+1)\theta]\,d\theta \tag{43}$$

An alternative form of this expression can be derived by making use of an identity cited by Feller.[16] This result can be written in terms of the stable distribution $F_\alpha(z)$, whose Laplace transform is

$$\int_0^\infty [\exp(-sz)]\,dF_\alpha(z) = \exp(-s^\alpha) \tag{44}$$

This identity, attributed to H. Pollard, states that the Laplace transform of the distribution

$$G_\alpha(\beta; z) = 1 - F_\alpha(\beta/z^{1/\alpha}) \tag{45}$$

with respect to z, is $B_\alpha(\beta s^{1/\alpha})$. If we insert this representation of $B_\alpha(z)$ into

Eq. (43), the integration with respect to θ can be performed, leading to the final expression

$$p(m, t) \sim \frac{1}{\sigma}\left(\frac{8}{\pi}\right)^{1/2}\int_0^\infty \left\{\sum_{j=1}^{\infty}(-1)^{j+1}j^2 \exp\left(-\frac{j^2(m+1)^2}{2\sigma^2x^2}\right)\right\}\frac{\partial}{\partial x}G_\alpha\left(\frac{t}{T}, x^2\right)dx \tag{46}$$

The asymptotic results given to this point all use the assumptions enumerated in Eq. (20), as do the analyses of earlier authors. It is of some interest to present some generalizations whose validity does not require the existence of the moments of jump probabilities. We start with a particular case for which results are available in closed form. Let

$$p(j) = \frac{3}{\pi^2}\frac{1}{j^2}, \qquad j = \pm 1, \pm 2, \ldots \tag{47}$$

Then $\lambda(\theta)$ can be represented in the neighborhood of the origin as

$$\lambda(\theta) \sim 1 - (3\theta/\pi) \tag{48}$$

neglecting a term proportional to θ^2. The lowest order term in $p_r(m)$ will be obtained from the first term in the expansion given in Eq. (19), for which we need an expression for $U_r(k)$ valid for large k. But this is easily found to be

$$U_r(k) \sim \frac{1}{\pi}\int_0^\infty e^{-3r\theta/\pi}\cos(k\theta)\,d\theta = \frac{3r}{\pi^2k^2 + 9r^2} \tag{49}$$

Hence the formal expression for the asymptotic $p_r(m)$ is

$$\begin{aligned} p_r(m) &\sim 24r\sum_{j=1}^{\infty}(-1)^{j+1}\frac{j^2}{9r^2 + \pi^2j^2(m+1)^2} \\ &= \frac{24r}{\pi^2(m+1)^2}\sum_{j=1}^{\infty}(-1)^{j+1}\left[1 - \frac{9r^2}{9r^2 + \pi^2j^2(m+1)^2}\right] \end{aligned} \tag{50}$$

The first sum can be evaluated by Abelian summation and the second is convergent in the usual sense and can be evaluated in closed form. By combining the two results we find that

$$p_r(m) \sim \frac{36r^2}{\pi^2(m+1)^3}\operatorname{cosech}\frac{3r}{m+1} \tag{51}$$

For r fixed and m large this probability goes like

$$p_r(m) \sim 12r/\pi^2m^2 \tag{52}$$

which implies that $\langle m\rangle$ does not exist since $p_r(m)$ has too long a tail. In order to compare the properties of $p_r(m)$ with and without finite variances, i.e., Eqs. (23) and (51), we calculate $\langle m^{1/2}\rangle$ for both distributions.

In the case of the finite variance distribution we find that

$$\langle m^{1/2}\rangle \sim \frac{8}{(2\pi r\sigma^2)^{1/2}} \sum_{j=1}^{\infty} (-1)^{j+1} j^2 \int_0^{\infty} m^{1/2} \exp\left(-\frac{j^2 m^2}{2r\sigma^2}\right) dm$$
$$= \frac{4}{\sqrt{\pi}} (2r\sigma^2)^{1/4} \Gamma\left(\frac{3}{4}\right) \sum_{j=1}^{\infty} (-1)^{j+1} \sqrt{j} \tag{53}$$

The formally divergent series can be evaluated by Abelian summation as shown in the appendix. In that sense we obtain the result

$$\sum_{j=1}^{\infty} (-1)^{j+1} \sqrt{j} = \frac{1}{\sqrt{\pi}} \int_0^{\infty} \frac{t^{-1/2} e^t}{(e^t + 1)^2}\, dt = 0.3801+ \tag{54}$$

so that

$$\langle m^{1/2}\rangle \sim 0.7031 \sigma^{1/2} r^{1/4} \tag{55}$$

On the other hand, for the model whose single-step jump probabilities are given by Eq. (47) the asymptotic behavior of $\langle m^{1/2}\rangle$ is

$$\langle m^{1/2}\rangle \sim \frac{36\sqrt{r}}{\pi^2} \int_0^{\infty} \frac{1}{x^{5/2}} \frac{dx}{\sinh(3/x)} = \frac{12}{\pi^2} \left(\frac{r}{3}\right)^{1/2} \int_0^{\infty} \frac{y^{1/2}}{\sinh y}\, dy$$
$$= \frac{12}{\pi^{3/2}} \frac{1}{3^{1/2}} \left(1 - \frac{1}{2^{3/2}}\right) \zeta\left(\frac{3}{2}\right) r^{1/2} = 2.101 r^{1/2} \tag{56}$$

where $\zeta(3/2)$ is a Riemann zeta function. Thus the values of $\langle m^{1/2}\rangle$ show a different dependence on r, as expected.

A different tack is required to find the asymptotic form for $p_r(m)$ for the single-step jump probability

$$p(j) = \frac{1}{2\zeta(1+\alpha)} \frac{1}{|j|^{1+\alpha}} \tag{57}$$

where $0 < \alpha < 2$. For the purpose of calculating $p_r(m)$ we substitute the integral representation of $U_r(j(m+1))$ into the lowest order approximation in Eq. (21) and interchange orders of summation and integration, finding

$$p_r(m) \sim \frac{2}{\pi} \int_{-\pi}^{\pi} \lambda^r(\theta) \left(\sum_{j=-\infty}^{\infty} (-1)^{j+1} j^2 \cos[j(m+1)\theta] \right) d\theta \tag{58}$$

But the identity in Eq. (15) implies that

$$\sum_{j=-\infty}^{\infty} (-1)^{j+1} j^2 \cos(jx) = \sum_{l=-\infty}^{\infty} \frac{d^2}{dx^2}\, \delta\left(\frac{x}{2\pi} - l - \frac{1}{2}\right) \tag{59}$$

When this identity is substituted into Eq. (58) and the integrals evaluated, the following answer is obtained:

$$p_r(m) \sim \frac{8}{(m+1)^3} \sum_{l \geq 0} \frac{d^2}{d\theta^2} [\lambda^r(\theta)]_{\theta = 2\pi[l + (1/2)]/(m+1)} \tag{60}$$

where the upper limit of the sum must be set equal to ∞ to be consistent with the use of the small-θ approximation [cf. Eqs. (61) and (64)]. One can show that the expression in Eq. (60) is asymptotically normalized. For this purpose we use the form of $\lambda(\theta)$ valid for small, positive θ

$$\lambda(\theta) \sim 1 - b\theta^{\alpha} \tag{61}$$

where b is the constant[17]

$$b = \frac{\pi}{2\sin(\pi\alpha/2)} \frac{1}{\zeta(1+\alpha)\Gamma(1+\alpha)} \tag{62}$$

so that for large r

$$\lambda^{r}(\theta) \sim \exp(-rb\theta^{\alpha}) \tag{63}$$

The value of b is valid for $p(j)$ given exactly by Eq. (57). When $p(j)$ is only asymptotic to $1/|j|^{1+\alpha}$ the expressions we derive below are still valid but the parameter b then depends on the detailed form of $p(j)$. For convenience we set

$$g(\theta) = (d^2/d\theta^2)[\exp(-rb\theta^{\alpha})] \tag{64}$$

Then, if we ignore the difference between $m + 1$ and m, we have

$$\begin{aligned}\int_0^\infty p_r(m)\,dm &\sim 8\int_0^\infty \frac{1}{m^3}\sum_{l=0}^{\infty} g\left[\frac{2\pi}{m}\left(l+\frac{1}{2}\right)\right] dm \\ &= \frac{2}{\pi^2}\int_0^\infty vg(v)\,dv \sum_{l=0}^{\infty}\frac{1}{(l+\frac{1}{2})^2} = \int_0^\infty vg(v)\,dv\end{aligned} \tag{65}$$

This then implies that

$$\int_0^\infty p_r(m)\,dm = \int_0^\infty \theta(d^2/d\theta^2)[\exp(-rb\theta^{\alpha})]\,d\theta = 1 \tag{66}$$

where the last result follows from an integration by parts.

A second representation of $p_r(m)$ given in Eq. (60) can be given as an integral over the probability density of a stable process[16] of order α. Let $f_\alpha(t)$ be this density defined so that

$$\int_0^\infty e^{-st} f_\alpha(t)dt = \exp(-s^{\alpha}) \tag{67}$$

The function $d^2[\lambda^r(\theta)]/d\theta^2$ in Eq. (64) is therefore

$$\frac{d^2[\lambda^r(\theta)]}{d\theta^2} = (rb)^{2/\alpha}\int_0^\infty t^2 f_\alpha(t)\exp[-(rb)^{1/\alpha}\theta t]\,dt \tag{68}$$

and the resulting sum is just a geometric series. An evaluation of the series of exponentials yields

$$\sum_{l=0}^{\infty} \exp\left(-\frac{2\pi(rb)^{1/\alpha}t(l+\frac{1}{2})}{m+1}\right) = \frac{1}{2}\operatorname{cosech}\left(\frac{\pi(rb)^{1/\alpha}t}{m+1}\right) \tag{69}$$

or

$$p_r(m) \sim \frac{4}{m^3}(rb)^{2/\alpha}\int_0^{\infty} t^2 f_\alpha(t)\operatorname{cosech}\left(\frac{\pi(rb)^{1/\alpha}t}{m}\right) dt \tag{70}$$

neglecting the difference between m and $m+1$. Except for the cases[18] $\alpha = 1/2$ and 1, the evaluation of $f_\alpha(t)$ is a matter of some difficulty. When $\alpha = 1$ this expression can be shown to reduce to Eq. (51).

Equation (60) also allows us to find the asymptotic form for $p_r(m)$ for r large and m of the order of $r^{1/\alpha}$ or greater. For this purpose we convert the sum of Eq. (60) to an integral by the Euler–Maclaurin formula,[12] finding

$$\begin{aligned} p_r(m) &\sim \frac{4}{\pi m^2}\int_{\pi/m}^{\infty} g(\theta)\, d\theta + \frac{4}{m^3} g\left(\frac{\pi}{m}\right) \\ &\sim \frac{4rb\alpha(2-\alpha)}{m^{1+\alpha}} \exp\left[-rb\left(\frac{\pi}{m}\right)^{\alpha}\right] \end{aligned} \tag{71}$$

valid for $0 < \alpha < 2$. In continuous time, when the mean time between steps T is finite, the result analogous to the last equation can be obtained by replacing r by t/T.

4. SPAN DISTRIBUTIONS IN HIGHER DIMENSIONS

General expressions for the multidimensional span density are given in Eq. (13) for discrete time and in Eq. (19) for continuous time. The multidimensional theory is complicated by the fact that at sufficiently short time $p_r(\mathbf{m})$ does not factor in the m_i. We will show that when the transition probabilities all satisfy the finiteness conditions

$$\sigma_l^2 = \sum_{j_1=-\infty}^{\infty} \cdots \sum_{j_n=-\infty}^{\infty} j_l^2 p(\mathbf{j}) < \infty \tag{72}$$

the span density is asymptotically factorable, so that important properties of $p_r(\mathbf{m})$ can be determined from the one-dimensional $p_r(\mathbf{m})$. Before we demonstrate this asymptotic separability, it is interesting to point out that in at least one case initial separability implies separability at all times. More precisely, we show, for a particular class of random walks in continuous time, that

$$p(\mathbf{m}; 0) = \prod_{i=1}^{n} p_i(m_i; 0) \tag{73}$$

implies that

$$p(\mathbf{m}; t) = \prod_{i=1}^{n} p_i(m_i; t) \tag{74}$$

Two conditions are required: that the time between successive steps have a negative exponential distribution, Eq. (38), and that the structure function be separable in the θ's, that is to say,

$$\lambda(\boldsymbol{\theta}) = \lambda_1(\theta_1) + \lambda_2(\theta_2) + \cdots + \lambda_n(\theta_n) \tag{75}$$

When these conditions are fulfilled, $p(\mathbf{m}; t)$ can be expressed as

$$p(\mathbf{m}; t) = e^{-t/T} \prod_{l=1}^{n} \frac{1}{\pi} \int_{-\pi}^{\pi} W(m_l, \theta) e^{t\lambda_l(\theta)/T} \, d\theta \tag{76}$$

for $t > 0$, which is the form given in Eq. (74).

When these special conditions do not hold, separability can be demonstrated only in the asymptotic sense and only under some such assumption as that of Eq. (72). More precisely, if we assume that the following moments are finite,

$$\begin{aligned} \sigma_l^2 &= \sum_{j_1=-\infty}^{\infty} \cdots \sum_{j_n=-\infty}^{\infty} j_l^2 p(\mathbf{j}) \\ \nu_l^4 &= \sum_{j_1=-\infty}^{\infty} \cdots \sum_{j_n=-\infty}^{\infty} j_l^4 p(\mathbf{j}) \\ \rho_{lm}^4 &= \sum_{j_1=-\infty}^{\infty} \cdots \sum_{j_n=-\infty}^{\infty} j_l^2 j_m^2 p(\mathbf{j}) \end{aligned} \tag{77}$$

we can write, analogous to Eq. (22) for one dimension

$$\begin{aligned} U_r(\mathbf{k}) \sim \frac{1}{(2\pi r)^{n/2}} &\left\{ \exp\left[-\frac{1}{2r} \left(\frac{k_1^2}{\sigma_1^2} + \frac{k_2^2}{\sigma_2^2} + \cdots + \frac{k_n^2}{\sigma_n^2} \right) \right] \right\} \\ &\times \left[1 + \frac{1}{8r} \sum_{l=1}^{n} \left(\frac{\nu_l^4}{\sigma_l^4} - 3 \right) \left(1 - \frac{2k_l^2}{r\sigma_l^2} + \frac{1}{3} \frac{k_l^4}{r^2 \sigma_l^4} \right) \right. \\ &\left. + \frac{1}{4r} \sum_l \sum_m{}' \left(\frac{\rho_{lm}^4}{\sigma_l^2 \sigma_m^2} - 1 \right) \left(1 - \frac{k_l^2}{r\sigma_l^2} \right) \left(1 - \frac{k_m^2}{r\sigma_m^2} \right) + O\left(\frac{1}{r^2} \right) \right] \end{aligned} \tag{78}$$

where the prime on the last sum indicates that the term $l = m$ is omitted. If we let $q_r(j; m)$ be the distribution in Eq. (23) with $\sigma = \sigma_j$, then the lowest approximation to $p_r(\mathbf{m})$ is just

$$p_r(\mathbf{m}) = q_r(1; m_1) q_r(2; m_2) \cdots q_r(n; m_n) \tag{79}$$

That is, the joint distribution of spans can, in this case, be calculated by assuming that the spans are independent random variables.

The result in Eq. (79) for the finite variance case allows us to study

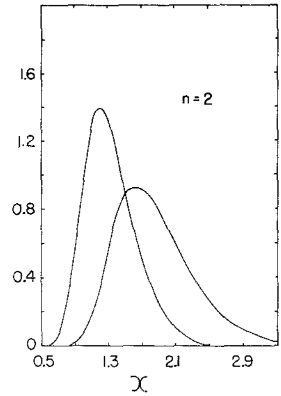

Fig. 1. Probability densities for the smaller and larger spans in two dimensions.

statistical properties of the ordered spans reasonably simply. If we assume that $\sigma_1 = \sigma_2 = \cdots = \sigma_n = \sigma$, then, in terms of the function $P_r(m)$ defined in Eq. (25), the probability density for the smallest and largest spans can be written, respectively, as

$$\begin{aligned} S_r(m) &= np_r(m)[1 - P_r(m)]^{n-1} \\ L_r(m) &= np_r(m)P_r^{n-1}(m) \end{aligned} \tag{80}$$

Formulas for the intermediate spans are also easy to write down. In Fig. 1 we have plotted $S_r(m)$ and $L_r(m)$ for $n = 2$. The probability density for the maximum is broader than that for the minimum, as might be expected on intuitive grounds. When n is increased, the probability density for the minimum narrows and becomes more and more concentrated at lower values of m. This is illustrated in Fig. 2. The distribution of the maximum span shifts to the right with increasing n and broadens. This is illustrated by the curves in Fig. 3.

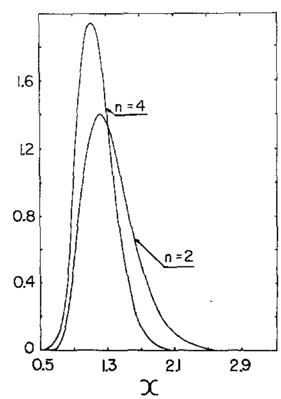

Fig. 2. Probability densities for the smallest span in two and four dimensions.

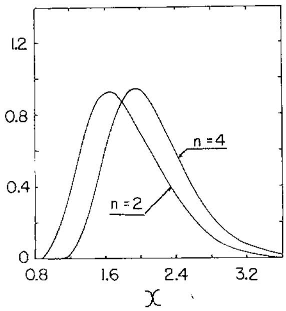

Fig. 3. Probability densities for the largest span in two and four dimensions.

To gain some idea of the variation of spans with time, we can calculate asymptotic moments of the expected largest and smallest span for an n-dimensional symmetric random walk using $p_r(m)$ from Eq. (23) and $P_r(m)$ from Eq. (25). We then have, for the averages of the smallest and largest spans, respectively,

$$\begin{aligned} \langle S(r)\rangle &\sim n\int_0^\infty mp_r(m)[1 - P_r(m)]^{n-1}\,dm = \int_0^\infty [1 - P_r(m)]^n\,dm \\ \langle L(r)\rangle &\sim n\int_0^\infty mp_r(m)P_r^{n-1}(m)\,dm = \int_0^\infty [1 - P_r^n(m)]\,dm \end{aligned} \tag{81}$$

where the second terms on the right-hand sides follow from the first by an integration by parts. The integrals can be evaluated numerically using the representation of $P_r(m)$ in Eq. (25), leading to results that are of the form $\langle S(r)\rangle = a_n\sigma\sqrt{r}$ and $\langle L(r)\rangle = b_n\sigma\sqrt{r}$ for large r. The constants a_n and b_n depend only on the dimension n and are given for several values of n in

Table I. Values for the Constants $a_n = S(r)/(\sigma\sqrt{r})$ and $b_n = L(r)/(\sigma\sqrt{r})$ for Different Values of n.

n	a_n	b_n
1	1.59577	1.59577
2	1.33530	1.85624
3	1.22675	2.00815
4	1.16347	2.11479
5	1.12059	2.19657
10	1.01335	2.44388
15	0.96403	2.58310
20	0.93343	2.67925
25	0.91178	2.75233

Table I. Clearly a_n must decrease to zero with increasing n, and b_n must increase with n to ∞. Asymptotic results for the distribution of the largest span in the limit of large n can be derived from the theory of order statistics.[19] This theory can also be used to furnish upper bounds on the spans when r is large enough so that Eq. (23) can be used and $\sigma_1 = \sigma_2 = \cdots = \sigma_n = \sigma$. As an example of the results that can be obtained, let S_n be the largest of n spans, for which the mean of a single span is given in Eq. (22), and the variance in Eq. (23). Then the inequality

$$\langle S(r)\rangle \leqslant \left[\left(\frac{8}{\pi}\right)^{1/2} + 2\left(\ln 2 - \frac{2}{\pi}\right)^{1/2} \frac{n-1}{(2n-1)^{1/2}}\right](r\sigma^2)^{1/2} \tag{82}$$

is valid. Similarly it can be shown that

$$\langle L(r)\rangle \geqslant \max\left\{0, \sigma\sqrt{r}\left[\left(\frac{8}{\pi}\right)^{1/2} - \left(\ln 2 - \frac{2}{\pi}\right)\frac{n-1}{(2n-1)^{1/2}}\right]\right\} \tag{83}$$

At sufficiently large values of n, the second term in the brackets goes negative.

In this paper we have dealt only with random walks on simple cubic lattices. The asymptotic theory that we have developed is valid for more general periodic lattices, but the correction terms necessarily depend on details of the lattice structure.

APPENDIX. EVALUATION OF THE SUM $S_\alpha = \sum_{j=1}^{\infty} (-1)^{j+1} j^\alpha$ FOR $0 < \alpha < 1$

In order to evaluate the sum S_α, we start from the representation

$$\frac{1}{j^{1-\alpha}} = \frac{1}{\Gamma(1-\alpha)}\int_0^\infty t^{-\alpha} e^{-jt}\, dt \tag{A.1}$$

so that

$$S_{\alpha-1}(x) = \sum_{j=1}^{\infty} (-1)^{j+1} \frac{x^j}{j^{1-\alpha}} = \frac{1}{\Gamma(1-\alpha)}\int_0^\infty t^{-\alpha} \frac{xe^{-t}}{(1+xe^{-t})}\, dt \tag{A.2}$$

From this result we have

$$S_\alpha = \lim_{x\to 1-} \frac{dS_{\alpha-1}}{dx} = \frac{1}{\Gamma(1-\alpha)}\int_0^\infty t^{-\alpha} \frac{e^{-t}}{(1+e^{-t})^2}\, dt \tag{A.3}$$

In particular $S_{1/2}$ is found to be that given in Eq. (54).

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