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A generating function for the second moment of the distinct number of sites visited by an n-step lattice random walk

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Abstract. We derive a generating function for the second moment of the distinct number of sites visited by an n-step lattice random walk. The formalism allows us to find asymptotic forms for the second moment as previously given in the mathematical literature using much more complicated techniques. The general technique can, in principle, be utilized in a derivation of higher moments.

1. Introduction

The number of distinct sites visited by a n-step random walk on a lattice has been the subject of investigation, both rigorous and heuristic, since being suggested as being of theoretical interest by Dvoretzky and Erdös [1]. Since that time this random variable, to be denoted by R_n, has come to play an increasingly important role in a number of applications in physics and chemistry. In particular it plays a significant role in the trapping problem, in which one seeks to find the survival probability of a single random walker on a lattice with a concentration of randomly placed trapping sites [2]. In the simplest version of this problem each site of a translationally-invariant lattice is designated as a trap with probability c. Let S_n be the probability that an initially randomly placed random walker survives for n or more steps in such a field of traps. Then S_n is related to R_n and c by

$$S_n = \langle (1-c)^{R_n} \rangle \tag{1}$$

in which the brackets indicate an average over all random n-step random walks and all possible placements of traps. Equation (1) states that in order for the random walk to survive for n steps each lattice point visited by the random walk must not have been a trap.

Because R_n is a non-Markovian random variable even for simple random walks the analysis required to determine its properties presents considerable difficulties. One property of this random variable whose asymptotic form is relatively straightforward to calculate is the first moment, $\langle R_n \rangle$, since a generating function for this quantity

$$R_1(z) = \sum_{n=0}^{\infty} \langle R_n \rangle z^n \tag{2}$$

is easily found [3, 4] and Tauberian methods can be applied to the resulting function to derive asymptotics. However, a determination of the higher moments of R_n generally poses much more challenging problems. Jain and Pruitt have calculated asymptotic forms of the second moment in different dimensions using a somewhat complicated analysis [5, 6] and Torney later studied properties of this same variable in two dimensions using a combination of analytical and numerical methods [7]. As shown by Zumofen and Blumen, moments of R_n can be used to generate successively more accurate approximations to the survival probability in the trapping problem, S_n, that are useful at times at which S_n takes on values meaningful in physical applications [8, 9]. This is in contrast to mathematically rigorous asymptotic results [10], which are generally found to be usable when S_n is of the order of 10^{-13} or less depending on the formulation of the trapping model [11, 12].

In this paper we derive a generating function for $\langle R_n^2 \rangle$. The general technique used here can be systematized and extended to the calculation of higher moments as well. However, the resulting calculation becomes algebraically, but not conceptually, more complicated than the one for the second moment. As will be seen, the derivation is based on probability distributions for random walks conditioned to avoid a single site, while the analogous derivation of generating functions for higher moments requires the use of similar distributions for random walks conditioned on the avoidance of several sites. The theory of random walks that are so conditioned has been developed in [13, 14].

2. General formalism

Let $I_n(\boldsymbol{r})$ denote an indicator variable associated with site $\boldsymbol{r}$ at step n, which is to say that

$$I_n(\boldsymbol{r}) = \begin{cases} 0 & \text{if } \boldsymbol{r} \text{ has not been reached by step } n \\ 1 & \text{if } \boldsymbol{r} \text{ has been reached by step } n. \end{cases} \tag{3}$$

The random variable R_n can be represented in terms of the $I_n(\boldsymbol{r})$ as

$$R_n = \sum_{\boldsymbol{r}} I_n(\boldsymbol{r}) \tag{4}$$

so that the quantity of interest in the present exposition is

$$\langle R_n^2 \rangle = \sum_{\boldsymbol{r}} \sum_{\boldsymbol{r}'} \langle I_n(\boldsymbol{r}) I_n(\boldsymbol{r}') \rangle = \sum_{\boldsymbol{r}} \sum_{\boldsymbol{r}'} G_n(\boldsymbol{r}, \boldsymbol{r}'). \tag{5}$$

According to the definition in equation (3) the quantity $I_n(\boldsymbol{r}) I_n(\boldsymbol{r}') = 1$ if both $\boldsymbol{r}$ and $\boldsymbol{r}'$ have been visited by step n and $= 0$ otherwise. Thus $G_n(\boldsymbol{r}, \boldsymbol{r}') \equiv \langle I_n(\boldsymbol{r}) I_n(\boldsymbol{r}') \rangle$ is the probability that the random walk has reached both $\boldsymbol{r}$ and $\boldsymbol{r}'$ by step n. Our object will be to calculate a generating function for $\langle R_n^2 \rangle$. This function, defined analogously to equation (2), will be denoted by $R_2(z)$ and, according to the relation in equation (5), can be represented in terms of the generating function of the $G_n(\boldsymbol{r}, \boldsymbol{r}')$ as

$$R_2(z) = \sum_{\boldsymbol{r}} \sum_{\boldsymbol{r}'} \hat{G}(\boldsymbol{r}, \boldsymbol{r}'; z) \tag{6}$$

where $\hat{G}(\boldsymbol{r}, \boldsymbol{r}'; z)$ is the generating function of the $G_n(\boldsymbol{r}, \boldsymbol{r}')$ with respect to n. In the analysis to follow only the case of a symmetric random walk on a translationally-invariant lattice will be considered, although it is not difficult to generalize the analysis to allow for asymmetric transition probabilities for random walks on such lattices.

We start by recalling some of the common probabilities and their associated transforms to be used in the subsequent analysis. Let $p(\boldsymbol{j})$ denote the probability of a displacement equal to $\boldsymbol{j}$ in a single step, let $p_n(\boldsymbol{r}|\boldsymbol{0})$ be the probability that the random walker is at $\boldsymbol{r}$ at step n given that it was initially at $\boldsymbol{j} = \boldsymbol{0}$, and let $f_n(\boldsymbol{r}|\boldsymbol{0})$ be the probability that it is at $\boldsymbol{r}$ for the first time at step n with the same initial position. A crucial role in the analysis will be played by the generating functions for these probabilities with respect to n. These will be denoted by $\hat{p}(\boldsymbol{r}; z|\boldsymbol{0})$ and $\hat{f}(\boldsymbol{r}; z|\boldsymbol{0})$ respectively, which are defined by

$$\hat{p}(\boldsymbol{r}; z|\boldsymbol{0}) = \sum_{n=0}^{\infty} p_n(\boldsymbol{r}|\boldsymbol{0}) z^n \qquad \hat{f}(\boldsymbol{r}; z|\boldsymbol{0}) = \sum_{n=0}^{\infty} f_n(\boldsymbol{r}|\boldsymbol{0}) z^n. \tag{7}$$

These are related by

$$\hat{f}(\boldsymbol{r}; z|\boldsymbol{0}) = \begin{cases} \hat{p}(\boldsymbol{r}; z|\boldsymbol{0})/\hat{p}(\boldsymbol{0}; z|\boldsymbol{0}) & \boldsymbol{r} \neq \boldsymbol{0} \\ 1 - 1/\hat{p}(\boldsymbol{0}; z|\boldsymbol{0}) & \boldsymbol{r} = \boldsymbol{0} \end{cases} \tag{8}$$

[3,4]. Define the characteristic function $\hat{p}(\boldsymbol{\theta})$ by $\hat{p}(\boldsymbol{\theta}) = \sum_{\boldsymbol{j}} p(\boldsymbol{j}) \exp(\mathrm{i}\boldsymbol{j} \cdot \boldsymbol{\theta})$. The generating function $\hat{p}(\boldsymbol{r}; z|\boldsymbol{0})$ can then be represented in integral form as

$$\hat{p}(\boldsymbol{r}; z|\boldsymbol{0}) = \frac{1}{(2\pi)^D} \int \cdots \int \frac{\mathrm{e}^{-\mathrm{i}\boldsymbol{r}\cdot\boldsymbol{\theta}}}{1 - z\hat{p}(\boldsymbol{\theta})} \, \mathrm{d}^D\theta \tag{9}$$

where D is the number of dimensions.

The calculation of $G_n(\boldsymbol{r}, \boldsymbol{r}')$ is based on a decomposition which expresses the fact that if both $\boldsymbol{r}$ and $\boldsymbol{r}'$ have been occupied by step n and $\boldsymbol{r} \neq \boldsymbol{r}'$ then either $\boldsymbol{r}$ was reached first and then $\boldsymbol{r}'$ was reached or else the points were reached in the opposite order. Consider the first of these possibilities, and let $g_m(\boldsymbol{r}|\boldsymbol{r}')$ be the probability that the random walk reaches $\boldsymbol{r}$ for the first time at step m starting from $\boldsymbol{0}$ before having reached $\boldsymbol{r}'$ by that time. The function $G_n(\boldsymbol{r}, \boldsymbol{r}')$ can be written in terms of these probabilities as

$$G_n(\boldsymbol{r}, \boldsymbol{r}') = \begin{cases} \displaystyle\sum_{m=0}^{n} \sum_{j=0}^{m} [g_j(\boldsymbol{r}'|\boldsymbol{r}) f_{m-j}(\boldsymbol{r}|\boldsymbol{r}') + g_j(\boldsymbol{r}|\boldsymbol{r}') f_{m-j}(\boldsymbol{r}'|\boldsymbol{r})] & \boldsymbol{r} \neq \boldsymbol{r}' \\ \displaystyle\sum_{m=0}^{n} f_m(\boldsymbol{r}|\boldsymbol{0}) & \boldsymbol{r} = \boldsymbol{r}'. \end{cases} \tag{10}$$

To simplify notation we define the function

$$J_m(\boldsymbol{r}, \boldsymbol{r}') = \begin{cases} \displaystyle\sum_{j=0}^{m} [g_j(\boldsymbol{r}'|\boldsymbol{r}) f_{m-j}(\boldsymbol{r}|\boldsymbol{r}') + g_j(\boldsymbol{r}|\boldsymbol{r}') f_{m-j}(\boldsymbol{r}'|\boldsymbol{r})] & \boldsymbol{r} \neq \boldsymbol{r}' \\ f_m(\boldsymbol{r}|\boldsymbol{0}) & \boldsymbol{r} = \boldsymbol{r}' \end{cases} \tag{11}$$

so that

$$G_n(\boldsymbol{r}, \boldsymbol{r}') = \sum_{m=0}^{n} J_m(\boldsymbol{r}, \boldsymbol{r}') \tag{12}$$

which can be inserted into the relation in equation (5) to yield an expression for $\langle R_n^2 \rangle$.

Further simplification is possibly by introducing generating functions with respect to n. In order to find such generating functions we must derive the generating function for the $g_n(\boldsymbol{r}'|\boldsymbol{r})$. This may be found either by making use of the formalism developed in [13] or [14], or by a direct approach, which is the one to be used here. We may immediately write

$$g_n(\boldsymbol{r}'|\boldsymbol{r}) = f_n(\boldsymbol{r}'|\boldsymbol{0}) - \sum_{j=0}^{n} g_j(\boldsymbol{r}|\boldsymbol{r}') f_{n-j}(\boldsymbol{r}'|\boldsymbol{r}) \tag{13}$$

with a similar equation holding when $\boldsymbol{r}$ and $\boldsymbol{r}'$ are interchanged. The relation in equation (13) follows by noting that the first-passage time probability for reaching $\boldsymbol{r}'$ at step n conditional on not having passed through $\boldsymbol{r}$ is found by subtracting from the unrestricted first-passage time probability the contributions from all of those random walks which reach $\boldsymbol{r}$ before reaching r'. Equation (13) and its conjugate are simplified when expressed in terms of generating functions with respect to n. Let $\hat{g}(r'; z|r)$ denote the generating function that corresponds to $g_n(r'|r)$. The various generating functions satisfy a set of linear simultaneous equations which are

$$\begin{aligned}\hat{g}(r'; z|r) &= \hat{f}(r'; z|0) - \hat{g}(r; z|r')\hat{f}(r'; z|r)\\ \hat{g}(r; z|r') &= \hat{f}(r; z|0) - \hat{g}(r'; z|r)\hat{f}(r; z|r')\end{aligned} \tag{14}$$

which are readily solved, yielding

$$\hat{g}(r'; z|r) = \frac{\hat{f}(r'; z|0) - \hat{f}(r'; z|r)\hat{f}(r; z|0)}{1 - \hat{f}(r'; z|r)\hat{f}(r; z|r'0)} \tag{15}$$

and $\hat{g}(r; z|r) = \hat{f}(r; z|0)$.

It is evident from equations (5) and (12) that the key quantity in the calculation of the generating function of the $\langle R_n^2\rangle$ is the set of functions $\{G_n(r, r')\}$. As mentioned, our analysis will be restricted to the most interesting case of the isotropic random walk, since, with this restriction, the first-passage time probabilities for the unrestricted random walk will be symmetric in their arguments, i.e. $f_n(r|r') = f_n(r'|r)$. The generating function corresponding to equation (11) leads to the result

$$\hat{G}(r, r'; z) = \frac{\hat{f}(r; z|r')[\hat{f}(r; z|0) + \hat{f}(r'; z|0)]}{1 + \hat{f}(r; z|r')} \tag{16}$$

and

$$\hat{G}(r, r; z) = \hat{f}(r; z|0). \tag{17}$$

If we define the function

$$C_n = \sum_{r}\sum_{r'} J_n(r, r') \tag{18}$$

and an associated generating function $C(z)$ then the combination of equations (16) and (17), together with the assumed isotropy of the random walk, implies the result

$$C(z) = \sum_{r} \hat{f}(r; z|0) + 2\sum_{r}\sum_{r'\neq r} \frac{\hat{f}(r; z|r')\hat{f}(r; z|0)}{1 + \hat{f}(r; z|r')}. \tag{19}$$

We next observe that for the isotropic random walk the function $f_n(r|r')$ depends on its arguments only through the difference $\rho = r - r'$. Hence equation (19) is equivalent to

$$\begin{aligned}C(z) &= \sum_{r} \hat{f}(r; z|0)\left\{1 + 2\sum_{\rho\neq 0} \frac{\hat{f}(\rho; z|0)}{1 + \hat{f}(\rho; z|0)}\right\}\\ &= 2\left\{\sum_{r} \hat{f}(r; z|0)\left[\sum_{\rho} \frac{\hat{p}(\rho; z)}{\hat{p}(0; z) + \hat{p}(\rho; z)}\right]\right\}.\end{aligned} \tag{20}$$

This can be simplified slightly by observing that the generating function for the expected number of sites visited by an n-step random walk defined in equation (2) can be expressed in terms of the $\hat{f}(r; z|0)$ as

$$\sum_{r} \hat{f}(r; z|0) = R_1(z) = \frac{z}{(1-z)^2\hat{p}(0; z)}. \tag{21}$$

Thus, according to equations (6) and (20) we have

$$R_2(z) = \frac{2z}{(1-z)^2\hat{p}(0; z)}\left[\sum_{\rho} \frac{\hat{p}(\rho; z)}{\hat{p}(0; z) + \hat{p}(\rho; z)}\right]. \tag{22}$$

This is the central relation in our analysis, which will be the basis of our calculation of the asymptotic form of $\langle R_n^2 \rangle$.

3. One dimension

The crucial quantity in the calculation of $\langle R_n^2 \rangle$ is the sum in square brackets in equation (22), which we denote by $I(z)$. In order to find the leading term in the asymptotic expansion of the second moment of R_n we apply a Tauberian theorem to the generating function in equation (22). For this purpose it suffices to replace the sum in the definition of

$$I(z) = \sum_{\rho} \frac{\hat{p}(\rho; z)}{\hat{p}(0; z) + \hat{p}(\rho; z)} \tag{23}$$

by an integral, at the same time replacing the factor z by a variable $e^{-\varepsilon} \approx 1 - \varepsilon$, where the limit $z \to 1$ is obviously equivalent to the limit $\varepsilon \to 0$. This replacement is equivalent to considering the generating function as a Laplace transform. The small-ε form of $\hat{p}(\rho; z)$ is known to be

$$\hat{p}(\rho; z) \approx \frac{1}{\sigma\sqrt{2\varepsilon}} \exp\left(-\frac{|\rho|\sqrt{2\varepsilon}}{\sigma}\right) \tag{24}$$

which allows us to write as an approximation

$$R_2(z) \approx \frac{\sigma\sqrt{8}}{\varepsilon^{3/2}} \int_{-\infty}^{\infty} \frac{d\rho}{1 + \exp(|\rho|\sqrt{2\varepsilon}/\sigma)} = \frac{4\sigma^2 \ln(2)}{\varepsilon^2}. \tag{25}$$

This relation implies the asymptotic behaviour

$$\langle R_n^2 \rangle \approx 4\sigma^2 n \ln(2) \tag{26}$$

which, when combined with the asymptotic expression for $\langle R_n \rangle$ [4], implies that the asymptotic form of the variance associated with R_n is

$$\sigma^2(R_n) \approx 4\sigma^2 \left(\ln(2) - \frac{2}{\pi}\right) n. \tag{27}$$

This can be found otherwise, since in one dimension the variable R_n is just the span of the random walk [16, 17].

4. Two dimensions

The same basic technique can be used to find the lowest order term in the large-n approximation to $\langle R_n^2 \rangle$. The crux of the calculation is that of finding the analytic behaviour of $I(z)$ which is defined in terms of $p(\rho; z)$ analogous to the one-dimensional result given in equation (23). As in one dimension singular behaviour of $p(\rho; z)$ arises from the singularity of the integrand of equation (9) at $\boldsymbol{\theta} = \mathbf{0}$.

We consider only the completely isotropic random walk for which, in the neighbourhood of the origin, the generating function $\hat{p}(\boldsymbol{\theta})$ can be approximated by

$$\hat{p}(\boldsymbol{\theta}) \approx 1 - \tfrac{1}{2}\sigma^2[\theta_1^2 + \theta_2^2] = 1 - \tfrac{1}{2}\sigma^2\theta^2. \tag{28}$$

The singular behaviour of $\hat{p}(\mathbf{0}; z)$ is therefore found to be

$$\hat{p}(\mathbf{0}; z) \approx \frac{1}{4\pi^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{d\theta_1\, d\theta_2}{\varepsilon + \frac{1}{2}\sigma^2\theta^2} \approx \frac{1}{2\pi\sigma^2} \ln\left(\frac{1}{\varepsilon}\right) \tag{29}$$

where, as before, $\varepsilon = 1 - z$ and, as shown in [4],

$$\hat{p}(\rho; z) \approx \frac{1}{\pi\sigma^2} K_0\left(\frac{\rho}{\sigma}\sqrt{2\varepsilon}\right) \qquad \rho \neq 0. \tag{30}$$

Thus, the function $I(z)$ is approximately given by

$$I(z) \approx \sum_{\rho} \frac{K_0((\rho/\sigma)\sqrt{2\varepsilon})}{\frac{1}{2}\ln(1/\varepsilon) + K_0((\rho/\sigma)\sqrt{2\varepsilon})} \approx \frac{\pi\sigma^2}{\varepsilon} \int_0^\infty \frac{\xi K_0(\xi)}{\frac{1}{2}\ln(1/\varepsilon) + K_0(\xi)}\, d\xi. \tag{31}$$

Since $\lim_{\xi\to\infty} K_0(\xi) = 0$ we can drop the Bessel function term in the denominator of the integral in comparison with the logarithmic term and evaluate the resulting integral exactly to find, as a final result, the approximation

$$I(z) \approx \frac{2\pi\sigma^2}{\varepsilon \ln(1/\varepsilon)}. \tag{32}$$

On combining this relation with equations (22) and (29) we find

$$R_2(z) \approx \frac{8\pi^2\sigma^4}{(1-z)^3 \ln^2(1/(1-z))}. \tag{33}$$

The use of a Tauberian theorem then allows us to infer that the first term in the asymptotic expression for $\langle R_n^2 \rangle$ is

$$\langle R_n^2 \rangle \approx 4\pi^2\sigma^4 \frac{n^2}{\ln 2n}. \tag{34}$$

It can be shown by similar techniques that the correction term to this result is $O[1/\ln(n)]$, and it is further known that $\sigma^2(R_n) \propto n^2/\ln^4(n)$ [6].

5. Three dimensions

In the case of three dimensions, since $\hat{p}(\rho; 1)$ is finite we expect the generating function $I(z)$ to diverge at $z = 1$. The form of this divergence can be determined by noting the inequality

$$|\hat{p}(\boldsymbol{r}; z)| < |\hat{p}(\mathbf{0}; z)| \qquad \boldsymbol{r} \neq \mathbf{0} \tag{35}$$

that follows directly from the integral representation of $\hat{p}(\boldsymbol{r}; z)$. This observation allows us to expand the sum for $I(z)$ as

$$I(z) = \frac{1}{2} + \sum_{\rho}{}' \left\{ \frac{\hat{p}(\rho; z)}{\hat{p}(\mathbf{0}; z)} - \left[\frac{\hat{p}(\rho; z)}{\hat{p}(\mathbf{0}; z)}\right]^2 + \left[\frac{\hat{p}(\rho; z)}{\hat{p}(\mathbf{0}; z)}\right]^3 + \cdots \right\} \tag{36}$$

where the prime indicates that the term $\rho = \mathbf{0}$ is to be omitted. The factor of $\frac{1}{2}$ on the right-hand side of the equation does not contribute to the singular behaviour of $I(z)$. Therefore, only the first three terms in brackets need be considered in the remainder of our calculation as it can be shown that the quartic term in the expansion is not singular. The first sum can be evaluated exactly since $\sum_{\boldsymbol{r}} p_n(\boldsymbol{r}) = 1$, thereby yielding a contribution equal to

$$\sum_{\rho \neq \mathbf{0}} \frac{\hat{p}(\rho; z)}{\hat{p}(\mathbf{0}; z)} = \frac{z}{(1-z)\hat{p}(\mathbf{0}; z)}. \tag{37}$$

The remaining sums can only be evaluated approximately by replacing the sums by integrals, which suffices to find at least the leading term in the expansion of $I(z)$ in the neighbourhood of $z = 1$. For this purpose we need to find an approximation to $\hat{p}(\rho; z)$ in that neighbourhood. To do so we write

$$\begin{aligned}\hat{p}(\rho; z) &= \hat{p}(\rho; 1) + [\hat{p}(\rho; z) - \hat{p}(\rho; 1)] \equiv \hat{p}(\rho; 1) - \Delta\hat{p}(\rho; z)\\ &= \hat{p}(\rho; 1) - \frac{(1-z)}{(2\pi)^3}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\frac{\hat{p}(\theta)\mathrm{e}^{-\mathrm{i}\rho\cdot\theta}}{[1-\hat{p}(\theta)][1-z\hat{p}(\theta)]}\,\mathrm{d}^3\theta.\end{aligned} \tag{38}$$

The second term on the right-hand side is a singular function of $\varepsilon = 1 - z$ in the limit $\varepsilon \to 0$. The form of the singularity will be determined for isotropic unbiased random walks whose steps have finite second moments. In this case the function $\hat{p}(\theta)$ has an expansion around the origin whose first two terms are

$$\hat{p}(\theta) \approx 1 - \tfrac{1}{2}\sigma^2[\theta_1^2 + \theta_2^2 + \theta_3^2] = 1 - \tfrac{1}{2}\sigma^2\theta^2. \tag{39}$$

Since the singular behaviour is due to the behaviour of the denominator of the integrand in equation (38) in the neighbourhood of the origin we can substitute equation (39) into that equation, at the same time extending the limits of integration to $(-\infty, \infty)$. The resulting integrals can be evaluated in closed form, leading to the result

$$\Delta\hat{p}(\rho; z) \approx \frac{1}{2\pi\sigma^2\rho}\left[1 - \exp\left(-\frac{\rho}{\sigma}\sqrt{2\varepsilon}\right)\right] \approx \frac{1}{\pi\sigma^3}\sqrt{\frac{\varepsilon}{2}} \tag{40}$$

in which $\rho = (\rho\cdot\rho)^{1/2}$. Hence we can write

$$\hat{p}(\rho; z) \approx \hat{p}(\rho; 1) - \frac{1}{\pi\sigma^3}\sqrt{\frac{\varepsilon}{2}} \approx \hat{p}(\rho; 1)\exp\left\{-\frac{1}{\pi\sigma^3\hat{p}(\rho; 1)}\sqrt{\frac{\varepsilon}{2}}\right\}. \tag{41}$$

As will be seen, the behaviour of the function $\hat{p}(\rho; z)$ required for calculating the singularity of $I(z)$ is the behaviour of $\hat{p}(\rho; z)$ at large values of the distance ρ. In this limit we have the approximation

$$\hat{p}(\rho; 1) \approx \frac{2}{(2\pi)^3\sigma^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{\mathrm{e}^{-\mathrm{i}\rho\cdot\theta}}{\theta^2}\,\mathrm{d}^3\theta = \frac{1}{2\pi\sigma^2\rho} \tag{42}$$

which implies the approximation

$$\hat{p}(\rho; z) \approx \frac{1}{2\pi\sigma^2\rho}\exp\left[-\frac{\rho}{\sigma}\sqrt{2\varepsilon}\right] \tag{43}$$

which will be used in our subsequent development.

The formula in equation (43) is the form which will be used in evaluating the remaining sums in equation (36). To do so we approximate the sum by a triple integral ranging over the entire space:

$$\sum_{\rho}{}'[\hat{p}(\rho; z)]^2 \approx \frac{1}{(2\pi\sigma^2)^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{1}{\rho^2}\exp\left[-\frac{2\rho}{\sigma}\sqrt{2\varepsilon}\right]\mathrm{d}^3\rho. \tag{44}$$

If ε is set equal to 0 the resulting integral on the right-hand side diverges. A transformation of the triple integral to spherical coordinates allows a simplification in that the integrals over the angles can be evaluated exactly, leaving us with the single integral

$$\sum_{\rho}{}'[\hat{p}(\rho; z)]^2 \approx \frac{1}{\pi\sigma^4}\int_0^{\infty}\exp\left[-\frac{2\rho}{\sigma}\sqrt{2\varepsilon}\right]\mathrm{d}\rho = \frac{1}{\pi\sigma^3\sqrt{8\varepsilon}}. \tag{45}$$

A calculation of the sum over the third power of $\hat{p}(\rho; z)$ is similar but there is a slight additional complication. We have

$$\sum_{\rho}{}'[\hat{p}(\rho; z)]^3 \approx \frac{1}{(2\pi\sigma^2)^3}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{1}{\rho^3}\exp\left[-\frac{3\rho}{\sigma}\sqrt{2\varepsilon}\right]\mathrm{d}^3\rho. \tag{46}$$

At this point an exact transformation to spherical coordinates would again allow an exact evaluation of the angular integrals but the final integral with respect to ρ diverges at both $\rho = 0$ and $\rho = \infty$ in the limit $\varepsilon = 0$ because of the ρ^3 term in the denominator of equation (46). The singularity at $\rho = 0$ is apparent rather than real, since the term $\rho = 0$ does not appear in the original sum. Consequently we can eliminate the effect of the singularity at the origin by setting the lower limit of integration to a value other than 0, noting that the remaining integral still diverges when ε is set equal to 0 since the integrand behaves as $1/\rho$ as $\rho \to \infty$. Since there is no contribution to singular behaviour attributable to the behaviour of the integrand in the small-ρ regime we may set the lower limit of the integral with respect to ρ to be $\rho = 1$ which yields the approximation

$$\sum_{\rho}{}'[\hat{p}(\rho; z)]^3 \approx \frac{1}{2\pi^2\sigma^6}\int_1^{\infty}\frac{\exp[-(3\rho/\sigma)\sqrt{2\varepsilon}]}{\rho}\,d\rho \approx \frac{1}{4\pi^2\sigma^6}\ln\left(\frac{1}{\varepsilon}\right). \tag{47}$$

The last step in our derivation of the singular behaviour of $I(z)$ is that of finding a correction term to $\hat{p}(\mathbf{0}; z)$ in the neighbourhood of $z = 1$. Since the calculation is similar to that required in the more general case we present only the final result, which is

$$\hat{p}(\mathbf{0}; z) \approx \hat{p}(\mathbf{0}; 1) - \frac{1}{\pi\sigma^3}\sqrt{\frac{\varepsilon}{2}}. \tag{48}$$

On combining equations (37) and (43)–(48) according to equation (36) we find

$$I(z) \approx \frac{1}{(1-z)\hat{p}(\mathbf{0}; 1)} + \frac{1}{\pi\sigma^3[\hat{p}(\mathbf{0}; 1)]^2\sqrt{8(1-z)}} + \frac{1}{4\pi^2\sigma^6[\hat{p}(\mathbf{0}; 1)]^3}\ln\left(\frac{1}{1-z}\right). \tag{49}$$

Hence, if we make use of equation (22) we find that the most singular terms in the expansion of $R_2(z)$ are

$$R_2(z) \approx \frac{2}{(1-z)^2[\hat{p}(\mathbf{0}; 1)]^2}\left\{\frac{1}{1-z} + \frac{3}{2^{3/2}\pi\sigma^3\hat{p}(\mathbf{0}; 1)\sqrt{1-z}} + \frac{1}{4\pi^2\sigma^6[\hat{p}(\mathbf{0}; 1)]^2} \times \ln\left(\frac{1}{1-z}\right) + \cdots\right\}. \tag{50}$$

This translates, in the time domain, to the following lowest-order terms in an asymptotic expansion of $\langle R_n^2\rangle$:

$$\langle R_n^2\rangle \approx \frac{n^2}{[\hat{p}(\mathbf{0}; 1)]^2} + \frac{1}{\sigma^3[\hat{p}(\mathbf{0}; 1)]^3}\left(\frac{2n}{\pi}\right)^{3/2} + \frac{1}{2\pi^2\sigma^6[\hat{p}(\mathbf{0}; 1)]^4}n\ln(n) + \cdots. \tag{51}$$

On the other hand, the asymptotic expansion of $\langle R_n\rangle$ is, to second order,

$$\langle R_n\rangle \approx \frac{n}{\hat{p}(\mathbf{0}; 1)} + \frac{(2n)^{1/2}}{\pi^{3/2}\sigma^3[\hat{p}(\mathbf{0}; 1)]^2} + \cdots. \tag{52}$$

This implies that the lowest order term in the asymptotic variance is

$$\sigma^2(n) \approx \frac{1}{2\pi^2\sigma^3[\hat{p}(\mathbf{0}; 1)]^4}n\ln(n) + \cdots \tag{53}$$

which agrees with the earlier result in [6]. It is also known from that reference that the asymptotic distribution of R_n is Gaussian so that the combination of equations (52) and (53) suffices to specify the asymptotic probability density of R_n, although no information is available about the order of magnitude of n required to make this a useful approximation. In four or more dimensions $\sigma^2(n) \propto n$ to lowest order.

6. Discussion

The significance of our analysis is not in being able to rederive results already in the mathematical literature. Rather it is in the fact that we have been able to use techniques based on generating functions, which are otherwise widely utilized by physicists to solve problems in the theory of Markovian random walks [15]. Clearly, it is possible in principle to extend the present analysis to derive large-n approximations to higher moments, albeit at the expense of very much more tedious algebra and analysis. We are presently engaged in generalizing our analysis to the study of $\langle R_n^2 \rangle$ for one-dimensional random walks with jump probabilities asymptotic to stable-law probabilities.

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