ARTICLES

Expected number of sites visited by a constrained *n*-step random walk

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We develop a formalism based on generating functions for calculating the expected number of sites visited by a lattice random walk constrained to visit a fixed point at the *n*th step. Explicit results are given in the large-n limit when the target point is not too far from the origin.

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I. INTRODUCTION

There have been a number of investigations of the sometimes striking effects of constraints on the properties of random walks [1-9]. The analyses of constrained random walks are motivated by applications in polymer physics and, more generally, in chemical physics [10,11]. A simple constraint whose effects have been studied is that of requiring the random walk to reach a specified site **v** at step n [8,9]. One effect of this type of constraint is that the average displacement at step $j \leq n$ is equal to \mathbf{v}/n , independent of any property of the probability distribution for a single step of the random walk [8]. This is true, for example, even when the probability distribution of a single step of the unconstrained walk has no finite moments.

A property of lattice random walks whose analysis presents a considerable mathematical challenge, as well as finding many physical applications, is the number of distinct sites visited by an n-step random walk [12]. This random variable will be denoted by R_n . Finding even an asymptotic distribution for this random variable requires quite sophisticated mathematical methods [13-15]. As a consequence, very few results related to this class of problems are known at this time. However, it is sometimes true that a particular physical application requires knowing less information than is contained in the full probability distribution. Many investigators have focused their attention on determining properties of just the first moment $\langle R_n \rangle$. At this level the problem is formally simple since the generating function for $\langle R_n \rangle$ can be found. Making use of this generating function, the application of Tauberian methods is then able to provide information about the large-*n* limit of $\langle R_n \rangle$. Unfortunately this approach is unavailable for higher moments since the corresponding generating functions have not been determined except for a recently calculated one for $\langle R_n^2 \rangle$ [16]. Nevertheless, the average number of distinct sites visited by an *n*-step random walk is interesting, for example, because it can be used to generate a lowest order approximation to the so-called trapping problem [12], as was first suggested by Rosenstock [17]. The approach to such problems based on a cumulant expansion was discussed

by Zumofen and Blumen [18,19].

In this paper we derive some specific asymptotic results for $\langle R_n \rangle$ for constrained random walks in different dimensions. This is relatively straightforward because, just as is true for the unconstrained random walk, it is possible to find an explicit generating function for this variable. It should be noted that this problem has been considered earlier from a somewhat more abstract point of view [9], but no explicit results were generated there.

II. GENERAL FORMALISM

Let $p(\mathbf{r})$ be the probability that the displacement in a single step of the unconstrained random walk is equal to \mathbf{r} , and let $p_n(\mathbf{r})$ be the probability that such a random walker, initially at the origin, is at \mathbf{r} at step n. The first-passage time probability $f_j(\mathbf{r})$ is defined as the probability that the random walk, in the absence of constraints, visits \mathbf{r} for the first time at step j. Let $g(\mathbf{r}|\mathbf{v},n)$ be the joint probability that the random walk visits \mathbf{r} for the first time at step j. Let $g(\mathbf{r}|\mathbf{v},n)$ be the joint probability that the random walk visits \mathbf{r} for the first time at step n. This function can be written in terms of those for the unconstrained walk as

$$g(\mathbf{r}|\mathbf{v},n) = \sum_{j=0}^{n} f_j(\mathbf{r}) p_{n-j}(\mathbf{v}-\mathbf{r}) .$$
(1)

This implies that the expected number of distinct sites visited by an n-step random walk constrained as described earlier is equal to

$$\langle R_n(\mathbf{v}) \rangle = \frac{\sum_{\mathbf{r}} g(\mathbf{r}|\mathbf{v},n)}{p_n(\mathbf{v})} = \frac{S_n(\mathbf{v})}{p_n(\mathbf{v})},$$
 (2)

in which $S_n(\mathbf{v})$ is the sum over \mathbf{r} appearing in the numerator. It does not seem possible to find a generating function for $\langle R_n(\mathbf{v}) \rangle$ directly because *n* appears both in the numerator and denominator of this expression. However, since Eq. (1) is a convolution, it is possible to derive a generation function for $S_n(\mathbf{v}) = p_n(\mathbf{v}) \langle R_n(\mathbf{v}) \rangle$. Large-*n* approximations can then be obtained by means of a Tauberian theorem. When the second moment of individual displacements of the random walk is finite, one can complete the calculation in the large-*n* limit by inserting the

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Gaussian approximation for $p_n(\mathbf{v})$.

To proceed with our calculations it will be convenient to recall a few results from the theory of random walks in free space that are not constrained. The generating function for the single-step generating functions, the $p(\mathbf{j})$ with respect to \mathbf{j} will be denoted by $\hat{p}(\boldsymbol{\theta})$, which is defined by

$$\hat{p}(\boldsymbol{\theta}) = \sum_{\mathbf{r}} p(\mathbf{r}) e^{i\mathbf{r}\cdot\boldsymbol{\theta}} .$$
(3)

The generating function of the set of functions $p_n(\mathbf{r})$ with respect to *n* will be denoted by $\hat{p}(\mathbf{r};z)$, the exact expression being

$$\hat{p}(\mathbf{r};z) = \frac{1}{(2\pi)^D} \int_{-\pi}^{\pi} \cdots \int \frac{e^{i\theta \cdot \mathbf{r}}}{1 - z\hat{p}(\theta)} d^D \theta , \qquad (4)$$

where D is the number of dimensions. We observe, from Eq. (2), that the generating function with respect to n of $S_n(\mathbf{v})$ can be written as a product of the individual transforms, which is to say

$$\sum_{n=0}^{\infty} S_n(\mathbf{v}) z^n = \hat{f}(\mathbf{r}; z) \hat{p}(\mathbf{v} - \mathbf{r}; z) .$$
(5)

Continuing the calculation by taking the generating function with respect to v and denoting the result by $\overline{S}(\theta;z)$, we find from Eq. (2) the relation

$$\overline{S}(\boldsymbol{\theta};z) = \overline{f}(\boldsymbol{\theta};z)\overline{p}(\boldsymbol{\theta},z) .$$
(6)

An expression for the function $\overline{p}(\theta;z)$ is obtained by summing Eq. (4) over all r, and making use of the identity

$$\sum_{\mathbf{r}} e^{i\boldsymbol{\theta}\cdot\mathbf{r}} = (2\pi)^D \delta(\boldsymbol{\theta}) \ . \tag{7}$$

In this way we find that

$$\overline{p}(\boldsymbol{\theta}; z) = [1 - z \widehat{p}(\boldsymbol{\theta})]^{-1} .$$
(8)

The function $\overline{f}(\theta;z)$ is found through the use of the formulas

$$\hat{f}(\mathbf{r};z) = \begin{cases} \frac{\hat{p}(\mathbf{r};z)}{\hat{p}(\mathbf{0};z)}, & \mathbf{r} \neq \mathbf{0} \\ \frac{1-\hat{p}(\mathbf{0};z)}{\hat{p}(\mathbf{0};z)}, & \mathbf{r} = \mathbf{0} \end{cases}$$
(9)

[20]. On multiplying both sides of this relation by $exp(i\theta \cdot \mathbf{r})$ and summing over all \mathbf{r} , one finally has

$$\widehat{f}(\boldsymbol{\theta}; z) = \frac{z \widehat{p}(\boldsymbol{\theta})}{\widehat{p}(\mathbf{0}; z) [1 - z \widehat{p}(\boldsymbol{\theta})]} .$$
(10)

Hence it follows that

$$\overline{S}(\boldsymbol{\theta};z) = \frac{z\widehat{p}(\boldsymbol{\theta})}{\widehat{p}(\mathbf{0};z)[1-z\widehat{p}(\boldsymbol{\theta})]^2} = \frac{1}{\widehat{p}(\mathbf{0};z)} \left[\frac{1}{\{1-z\widehat{p}(\boldsymbol{\theta})\}^2} - \frac{1}{\{1-z\widehat{p}(\boldsymbol{\theta})\}} \right], \quad (11)$$

which is the starting point for our analysis. An alternative expression is found by noting that

$$\widehat{S}(\boldsymbol{\theta};z) = \frac{z}{\widehat{p}(\mathbf{0};z)} \frac{\partial}{\partial z} \left[\frac{1}{1 - z \widehat{p}(\boldsymbol{\theta})} \right].$$
(12)

This expression for $\overline{S}(\theta;z)$ can be inverted with respect to θ , leading to

$$\widehat{\mathbf{S}}(\mathbf{v};z) = \frac{z}{\widehat{p}(\mathbf{0};z)} \frac{\partial}{\partial z} \widehat{p}(\mathbf{v};z)$$
(13)

or

$$\widehat{\mathbf{S}}(\mathbf{v};z) = \frac{z}{(2\pi)^D \widehat{p}(\mathbf{0};z)} \int_{-\pi}^{\pi} \cdots \int \frac{\widehat{p}(\boldsymbol{\theta})e^{-i\mathbf{v}\cdot\boldsymbol{\theta}}}{[1-z\widehat{p}(\boldsymbol{\theta})]^2} d^D\boldsymbol{\theta} .$$
(14)

Since singularities occur only when z is equal to 1 the leading order terms in the large-n limit can be found from the first term on the right-hand side of Eq. (11). Thus, the lowest order in an asymptotic expansion of $S_n(\mathbf{v})$ is related to the singular behavior of

$$\widehat{S}(\mathbf{v};z) \sim \frac{1}{(2\pi)^D \widehat{p}(\mathbf{0};z)} \int_{-\pi}^{\pi} \cdots \int \frac{e^{-i\mathbf{v}\cdot\boldsymbol{\theta}}}{[1-z\widehat{p}(\boldsymbol{\theta})]^2} d^D \boldsymbol{\theta} \quad (15)$$

in the limit $z \rightarrow 1$.

III. ASYMPTOTIC PROPERTIES

A. One dimension

The results up to Eq. (13) are exact. In order to obtain asymptotic results we will pass to the limit $z \rightarrow 1$, which generally corresponds to the singular behavior of the generating function, which enables us to make use of Tauberian methods. Referring to the integral representation of $\hat{p}(j;z)$ in Eq. (4) we see that the denominator of the integral vanishes when z=1 and $\theta=0$. In assessing the singular behavior we need only examine the behavior of the integrand in the neighborhood of the origin in θ space. Let σ^2 be the variance associated with a single step of the unconstrained random walk, assumed to be finite. If we measure distances in units of σ , then $\hat{p}(\theta)$ can be expanded around $\theta=0$ as

$$\hat{p}(\theta) \sim 1 + i\mu\theta - \frac{\theta^2}{2} , \qquad (16)$$

where μ is the value of the bias also scaled by σ . Since our primary interest is in the contribution to the integral from the neighborhood of the origin, we can also extend the limits on the integral to $\pm \infty$. Thus the leading term from which asymptotic behavior may be inferred can be expressed as

$$\widehat{S}(v;z) \sim \frac{1}{2\pi \widehat{p}(0;z)} \int_{-\infty}^{\infty} \frac{e^{-iv\theta}}{\left[1-z-i\mu\theta+\frac{\theta^2}{2}\right]^2} d\theta , \quad (17)$$

in which v is taken as a scaled variable.

Both the integral shown and $\hat{p}(0;z)$ may be found by using essentially the same technique. We integrate the integral shown in detail. To evaluate the integral in Eq. (17) we can exponentiate the denominator of the integrand by making use of the identity $u^{-2} = \int_0^\infty \xi e^{-u\xi} d\xi$. This gives rise to the representation

$$I = \frac{1}{2\pi} \int_{0}^{\infty} \xi e^{-(1-z)\xi} d\xi \int_{-\infty}^{\infty} \exp\left\{i(\mu\xi - iv)\phi - \frac{\xi\phi^{2}}{2}\right\} d\phi$$
$$= \frac{|v|}{2(1-z) + \mu^{2}} \left[1 + \frac{1}{u\sqrt{2(1-z) + \mu^{2}}}\right]$$
$$\times \exp\{\mu v - |v|\sqrt{2(1-z) + \mu^{2}}\}.$$
(18)

A similar derivation can be used to prove that

$$\hat{p}(0;z) \sim \frac{1}{\sqrt{2(1-z)+\mu^2}}$$
 (19)

To find the asymptotic form of the inverse of S(v;n) in the limit $n \to \infty$, we consider $\hat{S}(v;z)$ to be a Laplace transform by setting $z = e^{-s}$ and taking the limit $s \to 0$. The resulting transform can be inverted exactly, and after dividing by

$$p_n(v) \sim \frac{1}{\sqrt{2\pi n}} \exp\left[-\frac{(v-n\mu)^2}{2n}\right]$$
(20)

as in Eq. (2), we find, as the asymptotic result

$$\langle R_n(v) \rangle \sim |v| + \left[\frac{\pi n}{2} \right]^{1/2} \exp\left[\frac{v^2}{2n} \right] \operatorname{erfc}\left[\frac{|v|}{\sqrt{2n}} \right].$$
 (21)

The first somewhat surprising result is that the bias parameter μ does not appear in the expression just shown. Thus the function $\langle R_n(v) \rangle$, just as the mean displacement in a single step of the constrained random walk, depends only on the location of the target site and on no other property of the underlying displacement probability $p(\theta)$ [8]. We do not anticipate that this will also be true for higher moments of $R_n(v)$, but proving this to be the case presents quite difficult problems.

To examine the properties of $\langle R_n(v) \rangle$ as given in Eq. (21), we note that two regimes can be identified, according to whether $v^2 \ll n$ or $v^2 \gg n$. In the first case we have the expansion

$$\langle R_n(v) \rangle \sim \left[\frac{\pi n}{2} \right]^{1/2} \left\{ 1 + \frac{v^2}{2n} + \cdots \right\}.$$
 (22)

To lowest order in *n* the expected number of distinct sites visited is proportional to $n^{1/2}$ just as for the unconstrained walk. In the second case in which the random walk is relatively stretched one expects that

$$\langle R_n(v) \rangle \sim |v| ,$$
 (23)

so that the feature that determines the behavior of $\langle R_n(v) \rangle$ to leading order in this case is just the amount by which the random walk is stretched. We remark that, while the central-limit theorem implies that $p_n(v)$ is approximately Gaussian, this is generally valid only in the neighborhood of the peak and not in the tails. It would

therefore be wrong to calculate corrections to Eq. (23) by dividing by a Gaussian approximation for $p_n(\mathbf{v})$ without invoking further properties of this function.

Note finally that the preceding calculations have all been made in terms of scaled coordinates, which is equivalent to setting $\sigma = 1$. Taking the actual value of σ into account requires multiplying Eq. (21) by that value.

B. Two dimensions

In two and three dimensions we will deal only with the isotropic random walk in which case $\hat{p}(\theta)$ is approximated in the neighborhood of the origin as

$$\hat{p}(\boldsymbol{\theta}) \sim 1 - \frac{\theta^2}{2}, \quad \theta^2 = \theta_1^2 + \theta_2^2, \quad (24)$$

where we again measure distances in units of σ . Because the central-limit theorem does not, in general, furnish information about the behavior of $p_n(\mathbf{v})$ in the tails of the distribution, we consider only the close-in regime defined by $v^2 \ll n$, where $v = (\mathbf{v} \cdot \mathbf{v})^{1/2}$. Our analysis will be based on the expression for $\hat{S}(\mathbf{v};z)$ in Eq. (15). We first present a heuristic argument that demonstrates that our formalism leads to the known result for $\langle R_n \rangle$ in the lowest order of approximation. This requires determining the behavior of both the integral in Eq. (15) and the function $\hat{p}(\mathbf{0};z)$ in the limit $z \rightarrow 1$. The behavior of $p(\mathbf{0};z)$ in the limit $z \rightarrow 1$, or equivalently $\varepsilon \rightarrow 0$, is found by focusing on the singular behavior of the integral representation in the neighborhood of $\theta_1 = \theta_2 = 0$,

$$p(\mathbf{0};z) \sim \frac{1}{2\pi^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{d\theta_1 d\theta_2}{2\varepsilon + \theta_1^2 + \theta_2^2}$$
$$= \frac{1}{2\pi^2} \int_{0}^{\infty} e^{-2e\xi} \left\{ \int_{-\pi}^{\pi} e^{-\xi\theta^2} d\theta \right\}^2 d\xi , \qquad (25)$$

which has the form of a Laplace transform. The limit of this transform at small ε can be determined from the behavior of the integrand of this transform in the limit $\xi \rightarrow \infty$, i.e.,

$$\int_{-\pi}^{\pi} e^{-\xi\theta^2} d\theta \sim \int_{-\infty}^{\infty} e^{-\xi\theta^2} d\theta = \sqrt{\pi/\xi} , \qquad (26)$$

where the limits of the integral can be extended to $\pm \infty$ because the main contribution comes from the neighborhood of $\theta = 0$. Application of an Abelian theorem for Laplace transforms [21,22] to Eq. (25) using the result in Eq. (26) then indicates that

$$p(\mathbf{0};z) \sim \frac{1}{2\pi} \ln \left[\frac{1}{\varepsilon} \right]$$
 (27)

A similar argument, based on Eq. (15) can be used to calculate the behavior of $S(\mathbf{v};z)$ in the limit $z \rightarrow 1$. We write

$$\widehat{S}(\mathbf{v};z) \sim \frac{1}{2\pi \ln(1/\varepsilon)} \int_{0}^{\infty} \xi \, e^{-e\xi} d\xi \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \exp\left[-\frac{\xi}{2} [\theta_{1}^{2} + \theta_{2}^{2}] - i\mathbf{v} \cdot \boldsymbol{\theta}\right] d\theta_{1} d\theta_{2}$$
$$= \frac{1}{\ln(1/\varepsilon)} \int_{0}^{\infty} \exp\left[-\varepsilon \xi - \frac{v^{2}}{2\xi}\right] d\xi = \frac{v}{\ln(1/\varepsilon)} \left[\frac{2}{\varepsilon}\right]^{1/2} K_{1}(v\sqrt{2\varepsilon}) , \qquad (28)$$

where $K_1(z)$ is a modified Bessel function of order 1 and where we have assumed that $v \neq 0$. The extension to v=0is straightforward. The relation in Eq. (28) can therefore be expressed in terms of a slowly varying function L(z)[21,22] as

$$\widehat{S}(\mathbf{v};z) \sim \frac{1}{\varepsilon} L \left[\frac{1}{\varepsilon} \right],$$
 (29)

where the specific form of the function $L(1/\epsilon)$ is found from Eq. (29) to be

$$L(1/\varepsilon) = \frac{v\sqrt{2\varepsilon}}{\ln(1/\varepsilon)} K_1(v\sqrt{2\varepsilon}), \quad v \neq 0$$
(30)

and $L(1/\varepsilon)=1$ when v=0. The fact that $L(1/\varepsilon)$ in Eq. (30) is slowly varying in the limit $\varepsilon \rightarrow 0$, can be verified by making use of the small-z expansion of the Bessel function $K_1(z) \sim (1/z) + (z/2) \ln(z/2)$.

The decomposition of $\hat{S}(\mathbf{v}; z)$ in Eq. (29) implies that in the limit $n \to \infty$ one has $S(\mathbf{v};n) \sim L(n) + nL'(n)$. After some element steps this translates into

$$S(\mathbf{v};n) \sim \frac{v}{\ln(n)} \left[\frac{2}{n}\right]^{1/2} \left\{ K_1 \left[v \left[\frac{2}{n}\right]^{1/2} \right] + \frac{v}{\sqrt{2n}} K_0 \left[v \left[\frac{2}{n}\right]^{1/2} \right] \right\}.$$
(31)

On making use of the small-z expansions of $K_0(z)$ and $K_{1}(z),$

$$K_0(z) \sim -\ln\left[\frac{z}{2}\right], \quad K_1(z) \sim \frac{1}{z} + \frac{z}{2}\ln\left[\frac{z}{2}\right], \quad (32)$$

together with the fundamental formula in Eq. (2), we finally find that in the regime defined by $v^2 \ll n$

$$\langle R_n(\mathbf{v}) \rangle \sim \langle R_n \rangle \left\{ 1 - \frac{v^4}{2n^2} \ln \left[\frac{v}{\sqrt{2n}} \right] + \cdots \right\},$$
 (33)

which again is an increasing function of v. In writing this relation we have neglected a term in brackets by invoking the assumption that $|\ln(v)| \ll \ln(n)$, which is based on fixing v and letting n become sufficiently large.

C. Three dimensions

Essentially the same techniques that were employed in the preceding section can be used to derive an expression for $\langle R_n(\mathbf{v}) \rangle$ in three dimensions. Our analysis is based on the approximation in Eq. (24) extended to allow for a third parameter, θ_3 . Let us return to Eq. (15), which is to be expanded in the neighborhood of z=1, or equivalently $\epsilon = 0$. In the calculations to follow it will shortly be seen that both of the terms in Eq. (11) contribute to $\langle R_n(\mathbf{v}) \rangle$ in the limit of large n. When z is set equal to 1 in the second of these terms the result is finite. It will be denoted by $K(\mathbf{v})$, which is therefore representable as

$$K(\mathbf{v}) = \frac{1}{(2\pi)^3} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{e^{-i\boldsymbol{v}\cdot\boldsymbol{\theta}}}{1-\hat{p}(\boldsymbol{\theta})} d^3\boldsymbol{\theta} .$$
(34)

It will also be necessary to calculate a correction term for the function $\hat{p}(0;z)$ beyond the constant $\hat{p}(0;1)$ in the limit $z \rightarrow 1$. To find this correction we write $\hat{p}(0;z) = \hat{p}(0;1) - [\hat{p}(0;1) - \hat{p}(0;z)]$. The term in brackets is easily seen to equal

$$\widehat{p}(\mathbf{0};1) - \widehat{p}(\mathbf{0};z) = \frac{\varepsilon}{(2\pi)^3} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{\widehat{p}(\boldsymbol{\theta})}{[1 - \widehat{p}(\boldsymbol{\theta})][1 - (1 - \varepsilon)\widehat{p}(\boldsymbol{\theta})]} d^3\boldsymbol{\theta} .$$
(35)

On expanding the integrand around $\theta = 0$ and converting the integrand to spherical coordinates we find

$$\widehat{p}(\mathbf{0};1) - \widehat{p}(\mathbf{0};z) \sim \frac{\varepsilon^{1/2}}{\pi^2} \int_0^\infty \frac{d\theta}{1 + \frac{\theta^2}{2}} = \frac{1}{\pi} \left[\frac{\varepsilon}{2}\right]^{1/2}.$$
 (36)

We next turn our attention to the singular contribution to $\hat{S}(\mathbf{v};z)$ in the neighborhood of z=1. The lowest order term in the analog of Eq. (28) is equal to

$$\hat{S}_{1}(\mathbf{v};z) \sim \frac{1}{(2\pi)^{3} \hat{p}(\mathbf{0};1)} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{e^{-i\mathbf{v}\cdot\boldsymbol{\theta}}}{\left[\epsilon + \frac{\theta^{2}}{2}\right]^{2}} d^{3}\boldsymbol{\theta}$$
$$= \frac{1}{2\pi \hat{p}(\mathbf{0};1)\sqrt{2\epsilon}} \exp(-v\sqrt{2\epsilon}) . \qquad (37)$$

If we regard ε as a Laplace transform, as is permissible in finding asymptotic behavior, we can invert the resulting transform, finding

$$\widehat{S}_{n,1}(\mathbf{v}) \sim \frac{1}{(2\pi)^{3/2} \widehat{p}(\mathbf{0}; 1) n^{1/2}} \exp\left[-\frac{v^2}{2n}\right] .$$
(38)

Hence, after dividing by $p_n(\mathbf{v})$, we find that the contribution from this term to $\langle R_n(\mathbf{v}) \rangle$ is

$$\langle R_n(\mathbf{v}) \rangle_1 \sim \frac{n}{\hat{p}(\mathbf{0};1)} \sim \langle R_n \rangle$$
 (39)

The lowest order of approximation to the dependence on v must therefore be due to the correction term in the expansion of $\hat{p}(0;z)$ around z=1 as well as from the constant indicated in Eq. (34).

Equation (36) implies that

$$\frac{1}{\hat{p}(\mathbf{0};z)} \sim \frac{1}{\hat{p}(\mathbf{0};1)} \left[1 + \frac{1}{\pi \hat{p}(\mathbf{0};1)} \left[\frac{\varepsilon}{2} \right]^{1/2} \right] . \tag{40}$$

Thus, there is a contribution to $\widehat{S}(\mathbf{v};z)$ which has the form

$$\widehat{S}_{2}(\mathbf{v};z) \sim \frac{1}{4\pi^{2}[\widehat{p}(\mathbf{0};1)]^{2}} \exp(-v\sqrt{2\varepsilon}) , \qquad (41)$$

which translates into

$$S_{n,2}(\mathbf{v}) \sim \frac{v}{8\pi^{5/2} [\hat{p}(\mathbf{0};1)]^2 n^{3/2}} \exp\left[-\frac{v^2}{2n}\right]$$
 (42)

or

$$\langle R_n(\mathbf{v}) \rangle_2 = \frac{1}{2^{3/2} \pi \hat{p}(\mathbf{0}; 1)} \langle R_n \rangle \frac{v}{n}$$
 (43)

The final contribution comes from the second term on the right-hand side of Eq. (11), together with the expansion of $1/\hat{p}(\mathbf{0};z)$ indicated in Eq. (40). In the transform domain the only term contributing to the asymptotic behavior is equal to

$$-\mathcal{L}^{-1}\left\{\frac{K(\mathbf{v})}{\pi[\hat{p}(\mathbf{0};1)]^2}\left(\frac{\varepsilon}{2}\right)^{1/2}\right\} = -\frac{K(\mathbf{v})}{(2\pi n)^{3/2}[\hat{p}(\mathbf{0};1)]^2},$$
(44)

which implies a contribution, to lowest order, to $\langle R_n(\mathbf{v}) \rangle$ of

$$\langle R_n(\mathbf{v}) \rangle_3 = -\langle R_n \rangle \frac{K(\mathbf{v})}{\hat{p}(\mathbf{0};1)n}$$
 (45)

The sum of the three contributions is

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$$\langle R_n(\mathbf{v}) \rangle \sim \langle R_n \rangle \left\{ 1 + \frac{1}{2^{3/2} \pi \hat{p}(\mathbf{0}; 1)} \frac{v}{n} - \frac{K(\mathbf{v})}{\hat{p}(\mathbf{0}; 1)n} + O\left[\frac{v^2}{n^2}\right] \right\}.$$

$$(46)$$

It can be remarked that since $K(\mathbf{v}) \neq 0$, $\langle R_n(\mathbf{v}) \rangle < \langle R_n \rangle$, in contrast to the result found in two dimensions. This difference is undoubtedly due to the fact that the three-dimensional random walk is transient rather than being recurrent, so that a random walk that returns to the origin at step *n* is more likely to have stayed in the neighborhood of its initial position than would be the case for a recurrent walk. An analysis of $\langle R_n(\mathbf{v}) \rangle$ at larger values of *v* requires a more detailed specification of the behavior of $p_n(\mathbf{v})$ in the regime in which the central-limit theorem provides no useful information.

It can be shown that the function $K(\mathbf{v})$ appearing in Eq. (46) decreases monotonically with v, so that the term in brackets is a monotonically increasing function of v. Hence, all of our results suggest that $\langle R_n(\mathbf{v}) \rangle$, viewed as a function of v, is monotonically increasing in this paper. While this property of monotonicity has not been proved rigorously, we believe it to be true, based on the consideration that "stretching" the random walk forces it to explore regions of space that it would otherwise tend not to visit in the absence of constraints. The validity of this conjecture remains a challenge for further investigation. An extension of our calculations to random walks in higher dimensions is straightforward and will not be described here.

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