Expected number of distinct sites visited by N random walks in the presence of an absorbing boundary

2003 J. Phys. A: Math. Gen. 36 8367

(http://iopscience.iop.org/0305-4470/36/31/302)

J. Phys. A: Math. Gen. **36** (2003) 8367–8372 PII: S0305-4470(03)62694-6

Expected number of distinct sites visited by *N* random walks in the presence of an absorbing boundary

Hernán Larralde[1] **and George H Weiss**[2]

[1] Centro de Ciencias Físicas, UNAM, Av. Universidad s/n Col. Chamilpa 62210, Cuernavaca Mor., Mexico
[2] Center for Information Technology, National Institutes of Health, Bethesda, MD 20892, USA

Received 23 April 2003
Published 23 July 2003
Online at stacks.iop.org/JPhysA/36/8367

Abstract
In earlier work we have studied the expected number of distinct sites (ENDS) visited by N random walkers in time t on a translationally invariant lattice. Optical applications suggest the interest in analysing the same problem for a semi-infinite lattice in three dimensions bounded by a plane of absorbing sites. We here study this problem, showing a multiplicity of time regimes, and at the longest times showing that the ENDS is proportional to $N\sqrt{t}$ where t is the time. In the absence of a boundary the comparable result is proportional to Nt. Thus, the boundary effect eliminates approximately $\sqrt{t}$ random walks.

PACS number: 05.40.Fb

1. Introduction

Many properties of lattice random walks have been studied since the pioneering initial investigation by Polyá [1]. The overwhelming majority of these use the assumption that the random walk takes place in a translationally invariant space [2, 3]. However, there are applications which involve boundaries whose effects cannot be neglected. An example of such a system arises in analysing optical techniques applied in a biomedical setting [4–6], the analysis being based on the theory of lattice random walks [7, 8]. This theory has proved to be useful in reducing optical data from experiments [4–6]. In such experiments tissue is irradiated by a laser beam, and either the reflected or the transmitted light is used for diagnostic purposes based on optical parameters of the tissue. The main feature of optical measurements is that they are non-invasive. Therefore, the information is embodied in the variations of the light intensity at the boundary. Accordingly, the interface or boundary is an important component of the physical system.

We have recently calculated the expected volume visited by N identical Wiener sausages in the presence of a planar absorbing boundary [9], thus generalizing an analysis of the volume generated by a single Wiener sausage moving in an unbounded space [12]. The lattice analogue to this system is the expected number of distinct sites visited by N lattice random walks in time t on an unbounded lattice [11]. This function will be termed the ENDS. The ENDS visited by a single random walker, in time t, in the presence of an absorbing boundary, has been suggested as a measure of the region visited by photons in measurements of optical parameters [10].

In this paper we evaluate the ENDS visited by N random walkers in the presence of an absorbing boundary in one and three dimensions as a function of time, for N large. The analysis in these cases will be seen to be similar to that for N Wiener sausages whose centres diffuse in a continuum. Although the time-dependent behaviour both in the lattice and continuum cases will be seen to have the same mathematical structure, there seems to be no unique prescription for extending the continuum results to those for a lattice. The new feature in the present paper is a study of the competition between the increase in the ENDS visited by the N random walkers and the decrease in the number of random walkers due to the absorbing boundary.

2. One dimension

In one dimension, due to the simple geometry, the ENDS is essentially equal to the span of the diffusion process. The formalism for this is quite similar to that used to analyse the expected volume generated by N Wiener sausages, as in [9]. Let $\langle L_N(t|x_0)\rangle$ be the ENDS at time t for a random walker initially at x_0. Then, at the very earliest times, this function is proportional to t since no sites have been visited earlier. In the remaining time regimes we have

$$\langle L_N(t|x_0)\rangle \approx \begin{cases} (4/e)\sqrt{2\pi Dt \ln N} & \sqrt{Dt} \ll x_0 \\ [4Dt\ln(Nx_0/\sqrt{4Dt})]^{1/2} & x_0 \ll \sqrt{Dt} \ll Nx_0 \\ Nx_0 \ln\left(\frac{\sqrt{4Dt}}{Nx_0}\right) & Nx_0 \ll \sqrt{Dt}. \end{cases} \tag{2.1}$$

The result in the regime $\sqrt{Dt} \ll x_0$ has the same dependence on N and t as given in [10] because in that time span the random walkers have not had time to reach the absorbing point. At the very longest times $\langle L_N(t|x_0)\rangle$ is dramatically slowed, increasing only logarithmically as a function of time because of the depletion of random walkers at the absorbing point.

3. Three dimensions

We will see that the mathematical development in three dimensions is closely related to that used in [9]. To define the coordinates we assume that the random walk is performed in a half space defined by $-\infty \leqslant x, y \leqslant \infty$ and $0 \leqslant z \leqslant \infty$, the plane $z = 0$ being an absorbing boundary. The function required, the ENDS at time t, is then denoted by $\langle L_N(t|\mathbf{r}_0)\rangle$ where $\mathbf{r}_0$ is the initial position for all of the N random walkers. By convention the initial position is taken equal to $\mathbf{r}_0 = (0, 0, z_0)$.

Let $\Gamma(\mathbf{r}; t|\mathbf{r}_0)$ be the probability that $\mathbf{r}$ has not been visited by time t. The definitions in the previous paragraph allow us to express $\langle L_N(t|\mathbf{r}_0)\rangle$ as

$$\langle L_N(t|\mathbf{r}_0)\rangle = \sum_{z=0}^{\infty} \sum_{x,y=-\infty}^{\infty} [1 - \Gamma^N(\mathbf{r}; t|\mathbf{r}_0)] \approx \int_0^\infty \mathrm{d}z \iint_{-\infty}^{\infty} [1 - \Gamma^N(\mathbf{r}; t|\mathbf{r}_0)]\,\mathrm{d}x\,\mathrm{d}y \tag{3.1}$$

where we have passed to the continuum limit to replace the sum by a more convenient integral representation. This is consistent with our later use of the Gaussian approximation to the propagator. We follow the analysis in [10] by defining a generating function with respect to N:

$$\begin{aligned}\hat{L}(\varepsilon; t|\mathbf{r}_0) &= \sum_{N=0}^{\infty} \langle L_N(t|\mathbf{r}_0)\rangle (1-\varepsilon)^N \\ &\approx \frac{1}{\varepsilon}\int_0^{\infty} \mathrm{d}z \iint_{-\infty}^{\infty} \left[\frac{1-\Gamma(\mathbf{r}; t|\mathbf{r}_0)}{1-\Gamma(\mathbf{r}; t|\mathbf{r}_0)+\varepsilon\Gamma(\mathbf{r}; t|\mathbf{r}_0)}\right] \mathrm{d}x\,\mathrm{d}y \\ &= \frac{1}{\varepsilon}\int_0^{\infty} \mathrm{d}z \iint_{-\infty}^{\infty} \frac{\Omega(\mathbf{r}; t|\mathbf{r}_0)}{\varepsilon+\Omega(\mathbf{r}; t|\mathbf{r}_0)}\,\mathrm{d}x\,\mathrm{d}y = \frac{1}{\varepsilon} I(\varepsilon, t)\end{aligned} \tag{3.2}$$

in which

$$\Omega(\mathbf{r}; t|\mathbf{r}_0) = \frac{1-\Gamma(\mathbf{r}; t|\mathbf{r}_0)}{\Gamma(\mathbf{r}; t|\mathbf{r}_0)}. \tag{3.3}$$

In equation (3.2) $I(\varepsilon, t)$ is seen to be a three-dimensional integral. Later we will show that because of radial symmetry in any (x, y) plane it can be reduced to a one-dimensional integral.

It is clear, from the second line in equation (3.2), that in the limit $\varepsilon \to 0$, both $I(\varepsilon, t)$ and the multiplicative factor $(1/\varepsilon)$ diverge. By the application of a Tauberian theorem [13], it can be shown that an expansion of $\hat{L}(\varepsilon; t|\mathbf{r}_0)$ around $\varepsilon = 0$ furnishes information about the large-N behaviour of $\langle L_N(t|\mathbf{r}_0)\rangle$. Hence we investigate the behaviour of $I(\varepsilon, t)$ in the neighbourhood of the singularity. This is determined by the behaviour of the integral at large r, in which limit $\Omega(\mathbf{r}; t|\mathbf{r}_0)$ goes to 0. In this limit $\Gamma(\mathbf{r}; t|\mathbf{r}_0) \approx 1$ allowing us to approximate $\Omega(\mathbf{r}; t|\mathbf{r}_0)$ by

$$\Omega(\mathbf{r}; t|\mathbf{r}_0) \approx 1 - \Gamma(\mathbf{r}; t|\mathbf{r}_0) \tag{3.4}$$

which is the form to be used in our later analysis.

Let the propagator, the probability that a single random walker is at $\mathbf{r}$ at time t, be denoted by $p(\mathbf{r};t|\mathbf{r}_0)$, let its Laplace transform be denoted by $\hat{p}(\mathbf{r}; s|\mathbf{r}_0)$, where s is the transform parameter and let $f(\mathbf{r};t|\mathbf{r}_0)$ be the probability density for the first-passage time to $\mathbf{r}$, its transform being denoted by $\hat{f}(\mathbf{r}; s|\mathbf{r}_0)$. The function $\Gamma(\mathbf{r}; t|\mathbf{r}_0)$ is related to $f(\mathbf{r}; t|\mathbf{r}_0)$ by

$$\Gamma(\mathbf{r}, t|\mathbf{r}_0) = 1 - \int_0^t f(\mathbf{r}, \tau|\mathbf{r}_0)\,\mathrm{d}\tau \tag{3.5}$$

so that the transform $\hat{\Gamma}(\mathbf{r};s|\mathbf{r}_0)$ is

$$\hat{\Gamma}(\mathbf{r};s|\mathbf{r}_0) = \frac{1}{s}[1-\hat{f}(\mathbf{r}; s|\mathbf{r}_0)] = \frac{1}{s}\left[1 - \frac{\hat{p}(\mathbf{r}; s|\mathbf{r}_0)}{\hat{p}(\mathbf{r};s|\mathbf{r})}\right]. \tag{3.6}$$

In writing the last relation on the right-hand side we have made use of a standard relation in random walk theory which expresses the generating function for first-passage times in terms of that for the propagators [2, 3]. The last equation is quite difficult to work with because $\mathbf{r}$ appears both in the numerator and denominator. Fortunately, to a good approximation, the denominator equation (3.6) can be simplified.

In expressing the propagator and accounting for the presence of the absorbing plane we will write the propagator in terms of the propagator in free space, which we denote by $p^{(F)}(\mathbf{r}; t|\mathbf{r}_0)$. It follows that:

$$p(\mathbf{r}; t|\mathbf{r}) = p^{(F)}(0, 0, 0; t|\mathbf{0}) - p^{(F)}(0, 0, 2z; t|\mathbf{0}). \tag{3.7}$$

When z gets large the first term in this relation is much greater than the second. Hence, to a good approximation, the second term in the last equation can be dropped. The validity of this approximation has been checked by simulations. In consequence, the spatial dependence disappears in the denominator of equation (3.6). This, in effect, linearizes the $\hat{\Gamma}(\mathbf{r};s|\mathbf{r}_0)$ as a function of $\mathbf{r}$. This can be shown in detail for a nearest-neighbour CTRW model on a simple cubic lattice in which the pausing time density is a negative exponential, $\psi(t) = e^{-t}$, and for which the propagator is known to be [2],

$$p^{(F)}(\mathbf{r}, t|\mathbf{r}_0) = e^{-t} I_{x-x_0}\left(\frac{t}{3}\right) I_{y-y_0}\left(\frac{t}{3}\right) I_{z-z_0}\left(\frac{t}{3}\right). \tag{3.8}$$

The relations cited in equations (3.1)–(3.6), except for the use of a continuum approximation, are all exact. We derive approximations to the large-t, large-N limits of the integral representation in equation (3.1). In the large-t limit we can invoke the central limit theorem to approximate to the propagator:

$$p(\mathbf{r}, t|\mathbf{r}_0) \approx \left(\frac{3}{2\pi t}\right)^{3/2} \exp\left(-\frac{3\rho^2}{2t}\right)\left[\exp\left(-\frac{3(z-z_0)^2}{2t}\right) - \exp\left(-\frac{3(z+z_0)^2}{2t}\right)\right] \tag{3.9}$$

where $\rho^2 = x^2 + y^2$. The method of images allows the assertion that in three dimensions $\Omega(\mathbf{r}; t|\mathbf{r}_0)$ takes the form

$$\Omega(\mathbf{r}; t|\mathbf{r}_0) = \frac{\operatorname{erfc}\left(\sqrt{\frac{3[\rho^2+(z-z_0)^2]}{2t}}\right)}{\sqrt{\rho^2+(z-z_0)^2}} - \frac{\operatorname{erfc}\left(\sqrt{\frac{3[\rho^2+(z-z_0)^2]}{2t}}\right)}{\sqrt{\rho^2+(z+z_0)^2}} \tag{3.10}$$

which shows explicitly that $\Omega(\mathbf{r}; t|\mathbf{r}_0)$ is radially symmetric in any x, y plane. Because of this symmetry the integral with respect to x and y can, to a good approximation, be reduced to a single integral.

In the large-t limit further simplification of equation (3.10) is possible. To effect this simplification we change variables in equation (3.2) by defining $\rho = \alpha\sqrt{t}$, $z = \beta\sqrt{t}$. This transforms the expression for $\Omega(\mathbf{r}; t|\mathbf{r}_0)$ to

$$\Omega(\mathbf{r}; t|\mathbf{r}_0) = \frac{1}{\sqrt{t}}\left\{\frac{\operatorname{erfc}\left(\sqrt{\frac{3}{2}\left[\alpha^2+\left(\beta-\frac{z_0}{\sqrt{t}}\right)^2\right]}\right)}{\sqrt{\alpha^2+\left(\beta-\frac{z_0}{\sqrt{t}}\right)^2}} - \frac{\operatorname{erfc}\left(\sqrt{\frac{3}{2}\left[\alpha^2+\left(\beta+\frac{z_0}{\sqrt{t}}\right)^2\right]}\right)}{\sqrt{\alpha^2+\left(\beta+\frac{z_0}{\sqrt{t}}\right)^2}}\right\}. \tag{3.11}$$

In the limit $t \gg z_0^2$ $\Omega(\mathbf{r}; t|\mathbf{r}_0)$ will be approximated by expanding it in powers of $z_0/\sqrt{t}$, retaining only the lowest order term. This can be found by differentiating equation (3.11) with respect to t and integrating the result. This procedure leads to

$$\Omega(\mathbf{r}; t|\mathbf{r}_0) \approx \frac{2z_0\beta}{t}\left[\sqrt{\frac{6}{\pi}}\frac{\exp\left(-\frac{3(\alpha^2+\beta^2)}{2}\right)}{\alpha^2+\beta^2} + \frac{\operatorname{erfc}\left(\sqrt{\frac{3(\alpha^2+\beta^2)}{2}}\right)}{(\alpha^2+\beta^2)^{3/2}}\right] \qquad t \to \infty \tag{3.12}$$

in which the time and space variables decouple.

One also sees that the bracketed terms in equation (3.12) depend only on the radial coordinate $\rho = (\alpha^2 + \beta^2)^{1/2}$, i.e. $\Omega(\mathbf{r}; t|\mathbf{r}_0)$ can be expressed as $(2z_0\beta/t)V(\rho)$ so that

$$I(\varepsilon, t) \approx 2z_0 t^{3/2} \int_0^\infty d\beta \int_0^\infty \frac{V(\rho)}{2z_0\beta V(\rho) + \varepsilon t}\alpha\, d\alpha \tag{3.13}$$

where $V(\rho)$ is, according to equation (3.12),

$$V(\rho) = \sqrt{\frac{6}{\pi}}\frac{\exp\left(-\frac{3\rho^2}{2}\right)}{\rho^2} + \frac{\operatorname{erfc}\left(\rho\sqrt{\frac{3}{2}}\right)}{\rho^3}. \tag{3.14}$$

Since the ranges of α and β are both $(0, \infty)$ we can introduce polar coordinates by writing $\alpha = \rho\cos\theta$ and $\beta = \rho\sin\theta$. The integral over θ can be evaluated exactly. In this way the double integral in equation (3.13) reduces to the single integral

$$I(\varepsilon, t) \approx t^{3/2} \int_0^\infty \rho^2 \left[1 - \frac{\varepsilon t}{2z_0\rho F(\rho)} \ln\left\{1 + \frac{2z_0\rho F(\rho)}{\varepsilon t}\right\}\right] d\rho. \tag{3.15}$$

The parameter ε that appears in equation (3.2) is small. It will be treated as a Laplace transform parameter. In light of this observation we may eliminate ε by inverting the transform using the result

$$\mathcal{L}^{-1}\left\{\ln\left[1+\frac{2z_0\rho V(\rho)}{\varepsilon t}\right]\right\} = \frac{1}{N}\left[1-\exp\left(-\frac{2z_0\rho V(\rho)N}{t}\right)\right] \tag{3.16}$$

which immediately leads to an integral representation for $\langle L_N(t|\mathbf{r}_0)\rangle$ having the form

$$\langle L_N(t|\mathbf{r}_0)\rangle \approx t^{3/2}\int_0^\infty \rho^2\left[1-\frac{t}{2z_0\rho V(\rho)N}\left\{1-\exp\left(-\frac{2z_0\rho V(\rho)N}{t}\right)\right\}\right]\mathrm{d}\rho. \tag{3.17}$$

We write this relation as $\langle L_N(t|\mathbf{r}_0)\rangle \approx t^{3/2}I(\xi)$ where $I(\xi)$ is the integral on the right-hand side of equation (3.17) and ξ is the combination $\xi = t/(2z_0N)$. Properties of this integral have been derived in [9] so that we need only translate the results so as to apply to the present problem.

To do so, we define ρ^* to be the solution to the equation

$$\rho^* V(\rho^*) = \xi \tag{3.18}$$

where $V(\rho)$ is defined in equation (3.14). It is shown in [9] that $I(\xi)$ is, to a good approximation,

$$I(\xi) \approx \frac{(\rho^*)^3}{3} + \frac{1}{2\xi}\int_{\rho^*}^\infty \gamma^3 V(\gamma)\,\mathrm{d}\gamma. \tag{3.19}$$

Properties of the solution to equation (3.18) have been derived in [9] and yield the following results for $z_0 \ll N$

$$\langle L_N(t|\mathbf{r}_0)\rangle \approx \begin{cases} [t\ln(N/\sqrt{t})]^{3/2} & z_0^2 \gg t \\ [t\ln(z_0N/t)]^{3/2} & z_0N \gg t \gg z_0^2 \\ z_0N\sqrt{t} & t \gg z_0N \end{cases} \tag{3.20}$$

so that, at the longest times, the effect of the absorbing boundary appears in the final time regime. It changes the proportionality to t, which characterizes the three-dimensional random walk in the absence of boundaries, to proportionality to $t^{1/2}$. On the other hand, when N is large and $z_0 \gg N$ so that the initial position is far from the absorbing plane we have

$$\langle L_N(t|\mathbf{r}_0)\rangle \approx \begin{cases} [t\ln(2N/\sqrt{t})]^{3/2} & N^2 \gg t \\ Nt & z_0^2 \gg t \gg N^2. \\ z_0N\sqrt{t} & t \gg 4z_0^2 \end{cases} \tag{3.21}$$

At the very longest times the results in both cases, equations (3.20) and (3.21), coincide as physical intuition would dictate. The coefficients required in the last two equations can be calculated.

It has been shown that in a three-dimensional translational invariant space the variance of the ENDS for a single random walk is asymptotically proportional to $t\ln t$. Preliminary simulations suggest that this remains true when there are N random walks in the presence of the absorbing boundary. No results are yet available for the distribution in this case, which is known to be Gaussian for a single random walk in an unbounded space [14, 15].

Equations (2.1), (3.20) and (3.21) indicate the existence of three scaling regimes, similar to the situation on an unbounded lattice [10]. This is attributable to the initial condition which sets all of the random walkers at a single site. If there are several such sites we can anticipate that there could be more such regimes in time, depending on the relation between different initial positions and numbers of the random walkers and their relation to the absorbing boundary.

References

[1] Polyá G 1929 *Math. Ann.* **84** 149
[2] Weiss G H 1994 *Aspects and Applications of the Random Walk* (Amsterdam: North-Holland)
[3] Hughes B D 1995 *Random Walks and Random Environments* vols 1 and *2* (New York: Oxford University Press)
[4] Das B B, Liu F and Alfano R R 1997 *Rep. Prog. Phys.* **60** 227
[5] Hebden J C, Arridge S R and Delpy D T 1997 *Phys. Med. Biol.* **42** 841
[6] Arridge S R and Hebden J C 1997 *Phys. Med. Biol.* **42** 841
[7] Bonner R F, Nossal R J, Havlin S and Weiss G H 1987 *J. Opt. Soc. Am.* **4** 423
[8] Gandjbakhche A H and Weiss G H 1995 *Prog. Opt.* **34** 335
[9] Larralde H, Berezhkovskii A M and Weiss G H *Physica* A at press
[10] Larralde H, Berezhkovskii A M and Weiss G H 2002 *Phys. Rev.* E **66** 012901
[11] Larralde H, Trunfio P, Havlin S, Stanley H E and Weiss G H 1992 *Phys. Rev.* A **45** 7128
[12] Berezhkovskii A M, Makhnovskii Yu A and Suris R A 1989 *J. Stat. Phys.* **57** 333
[13] Feller W 1971 *An Introduction to Probability Theory and its Applications* vol 2 (New York: Wiley)
[14] Jain N C and Pruitt W E 1971 *J. Anal. Math.* **24** 369
[15] Jain N C and Pruitt W E 1971 *Proc. Sixth Berkeley Symp. on Probability and Statistics* (Berkeley, CA: University of California) p 131