Number of distinct sites visited by a random walker trapped by an absorbing boundary

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The number of distinct sites visited by a lattice random walker is a subject of continuing interest in both mathematics and physics. All previous investigations have used the assumption that the lattice is unbounded. An assessment of the amount of tissue interrogated by a photon in reflectance measurements for diagnostic purposes suggests analyzing properties of the average number of distinct sites visited by a random walker trapped by an absorbing plane at time t. We show that for sufficiently large t this number is the same as the average number of distinct sites visited for this time when the surface is not present. A more complete analysis is possible for a random walk on a line terminated by an absorbing point.

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I. INTRODUCTION

Techniques for estimating optical parameters in human tissue for diagnostic purposes are being widely explored, because of potential hazards associated with the modalities based on other forms of radiation. Good descriptions of a sampling of experimental techniques used for this purpose are suggested in [1–3]. Many theoretical approaches to this problem have been used, requiring varying degrees of mathematical and numerical sophistication in their implementation. These include transport theory, diffusion theory, and the theory of lattice random walks, which may be characterized as a discrete version of diffusion theory. The latter theory [4,5] has been successfully applied to the analysis of a large number of data sets, by Gandjbakhche and his collaborators [6]. In the class of models to be discussed here, the tissue is often modeled as a semi-infinite medium whose interface is represented by an absorbing plane since penetration depths are generally of the order of millimeters when near-infrared radiation is used.

An important requirement in the measurement of optical parameters is the ability to characterize the extent to which tissue has been interrogated by photons. One approach to characterizing the interrogated region has recently been reported in [7]. The calculation in that reference, based on the continuous-time random walk (CTRW) [8], applied to the problem at hand [9], produced an exact expression for the average value of the ratio $z_{\rm av}/z_{\rm max}$, where $z_{\rm av}$ is the average depth of penetration by a photon and $z_{\rm max}$ is the maximum depth of penetration. In this paper we suggest an alternative characterization of the volume probed by a photon. Our analysis will again be based on properties of a lattice CTRW in three dimensions. Specifically, we study the expected number of distinct sites visited by the random walk (which is the surrogate for a photon), conditioned on its being absorbed by the surface at a target site at a specific time. Our suggested analysis can also be extended to the case of photons traversing a finite slab, which models so-called transillumination experiments.

We parenthetically remark that statistical properties of the number of distinct sites visited on a lattice have heretofore only been studied in the case of translational invariance, i.e., an unbounded space. Recently, the effects of an absorbing boundary on the average volume of a Wiener sausage have been analyzed [10]. The Wiener sausage is a continuum analog of the random walk. There, in contrast to the present work, they analyzed properties of Wiener sausages for trajectories that have not been absorbed. This work focuses on absorbed trajectories, which are closer to the optical application.

II. GENERAL FORMALISM

The tissue will be modeled in terms of a semi-infinite simple cubic lattice bounded by a plane consisting of trapping points. A point in the lattice will be denoted by $\mathbf{r}=(\boldsymbol{\rho},z)$, where $\boldsymbol{\rho}=(x,y)$ and x, y, and z are integers. The absorbing surface is defined to be $z=0$, and the interior points correspond to $z>0$ so that the range of variables is $z\geqslant 0$ and $-\infty\leqslant x,y\leqslant\infty$. If μ_s' is the transport-corrected scattering coefficient, the actual physical coordinate $\mathbf{r}$ is found to equal $\mathbf{r}\sqrt{2}/\mu_s'$ [11]. We consider a Markovian nearest-neighbor continuous-time random walk with the average time between successive steps equal to k^{-1}, where k is the step frequency. Without loss of generality we can set $k=1$. The propagator for this model in an unbounded space is known to be [8] $G_{\rm un}(\mathbf{r},t)=\exp(-t)I_x(t/3)I_y(t/3)I_z(t/3)$, where $I_m(u)$ is a modified Bessel function of order m and argument u [12].

We derive an expression for the average number of distinct sites visited by a random walker, initially at the point $\mathbf{r}_0=(\mathbf{0},z_0)$, conditional on being absorbed at a target site $\mathbf{R}=(\boldsymbol{\rho}_{\rm f},0)$ at time t. This number is equal to the average number of distinct sites visited by trajectories, initially at $\mathbf{r}_0$, that are at the site $\mathbf{r}_{\rm f}=(\boldsymbol{\rho}_{\rm f},1)$ at time t. The fraction of these trajectories is the propagator $G(\mathbf{r}_{\rm f},t|\mathbf{r}_0)$. The average number of distinct sites visited by these trajectories will be denoted by $\langle N(t|\mathbf{r}_0)\rangle_{\mathbf{r}_{\rm f}}$, where the summation is over trajectories that are at $\mathbf{r}_{\rm f}$ at time t. If we let $\overline{N}(t|\boldsymbol{\rho}_{\rm f}|z_0)$ be the average number of distinct sites visited by trajectories trapped at $\mathbf{R}$ at time t, then we have the relation

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$$\overline{N}(t|\boldsymbol{\rho}_{\rm f}|z_0)=\frac{\langle N(t|\mathbf{r}_0)\rangle_{\mathbf{r}_{\rm f}}}{G(\mathbf{r}_{\rm f},t|\mathbf{r}_0)}. \tag{2.1}$$

A formal expression for the number of distinct sites visited by a trajectory W_t defined in terms of the position of the random walker at times $t'\leqslant t$, $\{\mathbf{r}_{W_t}(t')\}$, can be written using an indicator function $I(\mathbf{r}|W_t)$ defined by $I(\mathbf{r}|W_t)=1$ if $\mathbf{r}_{W_t}(t')=\mathbf{r}$, $t'\leqslant t$ and $=0$ otherwise. The number of sites visited by the trajectory is $N(W_t)=\Sigma_{\mathbf{r}}I(\mathbf{r}|W_t)$. Averaging both sides of this definition over trajectories conditioned on $\mathbf{r}(0)=\mathbf{r}_0$ and $\mathbf{r}(t)=\mathbf{r}_{\rm f}$, we obtain

$$\langle N(t|\mathbf{r}_0)\rangle_{\mathbf{r}_{\rm f}}=\langle N(W_t)\rangle_{\mathbf{r}_{\rm f}}=\sum_{\mathbf{r}}\langle I(\mathbf{r}|W_t)\rangle_{\mathbf{r}_{\rm f}}, \tag{2.2}$$

which requires calculating the function $\langle I(\mathbf{r}|W_t)\rangle_{\mathbf{r}_{\rm f}}$. This function can be expressed in terms of the probability density for the first time that the random walk reaches site $\mathbf{r}$, $f(\mathbf{r},t|\mathbf{r}_0)$. The required relation is

$$\langle I(\mathbf{r}|W_t)\rangle_{\mathbf{r}_{\rm f}}=\int_0^t G(\mathbf{r}_{\rm f},t-\tau|\mathbf{r})|f(\mathbf{r},\tau|\mathbf{r}_0)d\tau. \tag{2.3}$$

Substituting this into Eq. (2.2), we can write

$$\langle N(t|\mathbf{r}_0)\rangle_{\mathbf{r}_{\rm f}}=\int_0^t\sum_{\mathbf{r}} G(\mathbf{r}_{\rm f},t-\tau|\mathbf{r})f(\mathbf{r},\tau|\mathbf{r}_0)d\tau. \tag{2.4}$$

The Laplace transform of the function $f(\mathbf{r},t|\mathbf{r}_0)$ will be denoted by $\hat{f}(\mathbf{r},s|\mathbf{r}_0)$, and can be expressed in terms of transforms of the propagator as [8],

$$\hat{f}(\mathbf{r},s|\mathbf{r}_0)=\frac{\hat{G}(\mathbf{r},s|\mathbf{r}_0)}{\hat{G}(\mathbf{r},s|\mathbf{r})}, \quad \mathbf{r}\neq\mathbf{r}_0. \tag{2.5}$$

Using the method of images, we can express $\hat{G}(\mathbf{r},s|\mathbf{r})$ in terms of Laplace transforms of the propagator for a random walk, initially at the origin, on an unbounded lattice $\hat{G}_{\rm un}(\mathbf{r},s)$ as

$$\hat{G}(\mathbf{r},s|\mathbf{r})=\hat{G}((\boldsymbol{\rho},z);s|(\boldsymbol{\rho},z))=\hat{G}_{\rm un}((\mathbf{0},0);s)-\hat{G}_{\rm un}((\mathbf{0},2z);s). \tag{2.6}$$

We take advantage of the fact that the second term on the right-hand side of Eq. (2.6) is small when compared to the first term, which allows us to write $\hat{G}(\mathbf{r},s|\mathbf{r})\approx\hat{G}_{\rm un}((\mathbf{0},0);s)$. Thus, we have

$$\hat{f}(\mathbf{r},s|\mathbf{r}_0)\approx\frac{\hat{G}(\mathbf{r},s|\mathbf{r}_0)}{\hat{G}_{\rm un}(\mathbf{0};s)}. \tag{2.7}$$

To analyze the behavior of the expected number of distinct sites visited by random walkers that escape at long times, we approximate to $\hat{G}_{\rm un}(\mathbf{0};s)$ by setting $s=0$. This allows us to find the large-time behavior of $f(\mathbf{r},t|\mathbf{r}_0)$, given by

$$f(\mathbf{r},t|\mathbf{r}_0)\approx\frac{G(\mathbf{r},t|\mathbf{r}_0)}{\hat{G}_{\rm un}(\mathbf{0};0)}. \tag{2.8}$$

Substituting this into Eq. (2.4) and using the relation $G(\mathbf{r}_{\rm f},t|\mathbf{r}_0)=\Sigma_r G(\mathbf{r}_{\rm f},t-\tau|\mathbf{r})G(\mathbf{r},\tau|\mathbf{r}_0)$, one finds $\langle N(t|\mathbf{r}_0)\rangle_{\mathbf{r}_{\rm f}}\approx tG(\mathbf{r}_{\rm f},t|\mathbf{r}_0)/\hat{G}_{\rm un}(\mathbf{0},0)$. To finish the calculation of the long-time behavior of the average number of distinct sites visited by trajectories that are trapped at time t, we then substitute $\langle N(t|\mathbf{r}_0)\rangle_{\mathbf{r}_f}$ into the definition of $\overline{N}(t|\boldsymbol{\rho}_{\rm f}|z_0)$ in Eq. (2.1) to finally find

$$\overline{N}(t|\boldsymbol{\rho}_{\rm f}|z_0)\approx t/\hat{G}_{\rm un}(\mathbf{0},0). \tag{2.9}$$

This is one of the main results of our paper. It shows that $\overline{N}(t|\boldsymbol{\rho}_{\rm f}|z_0)$ depends neither on the initial distance from the absorbing plane z_0, nor on the position of the trapping site $\mathbf{R}=(\boldsymbol{\rho}_{\rm f},0)$. Moreover, it is identical to the result in the absence of any boundary [8].

Equation (2.9) predicts a linear dependence of $\overline{N}(t|\boldsymbol{\rho}_{\rm f}|z_0)$ on time with the slope $[\hat{G}_{\rm un}(\mathbf{0},0)]^{-1}=[\int_0^\infty \exp(-t)I_0^3(t/3)dt]^{-1}\approx 0.6596$. To check the validity of the result in Eq. (2.9), we ran simulations consisting of 30 000 random walks, each starting from $\mathbf{r}_0=(0,0,z_0)$ for two initial locations, $z_0=10$ and 15. The slope estimated from the simulations agreed with the theoretically predicted value to within 2%.

III. THE ONE-DIMENSIONAL CASE

It is interesting to consider properties of the expected number of distinct sites visited on a line terminated by an absorbing point because, in contrast to three dimensions, an exact solution can be found. In the linear random walk, the function $N(t|x_0)$ coincides with the span when the lattice spacing is used as a unit of length. With this in mind, we analyze the span for trajectories that originate from $x_0>0$ and are trapped at the origin at time t. Notice that for these trajectories the span coincides with the maximal deviation from the origin and, therefore, exceeds x_0. For simplicity, we approximate the random walk by a diffusion process.

To calculate the probability density for the span, we insert a second absorbing point at $L>x_0$ that ensures that any random walker trapped at $x=0$ cannot reach $x=L$. Let $g_L(x,t|x_0)$ be the corresponding propagator. It satisfies the diffusion equation

$$\frac{\partial g_L}{\partial t}=D\frac{\partial^2 g_L}{\partial x^2}, \tag{3.1}$$

where D is the diffusion constant. This equation is to be solved subject to the initial condition $g_L(x,0|x_0)=\delta(x-x_0)$ and boundary conditions $g_L(0,t|x_0)=g_L(L,t|x_0)=0$. The flux into the origin by trajectories whose span is less than L will be denoted by $J_L(t|x_0)$, and is related to the propagator by $J_L(t|x_0)=D\partial g_L(x,t|x_0)/\partial x|_{x=0}$. The fraction of trajectories escaping at $x=0$ between times t and $t+dt$, whose span is less than L, is $J_L(t|x_0)dt$. The fraction of the trajectories with a span between L and $L+dL$, trapped between t and $t+dt$, is given by

$$[J_{L+dL}(t|x_0)-J_L(t|x_0)]dt \approx \frac{\partial J_L(t|x_0)}{\partial L}dL\,dt. \tag{3.2}$$

The total fraction of trajectories trapped by the absorbing point at the origin between t and $t+dt$ is $J_\infty(t|x_0)dt$, where $J_\infty(t|x_0)$ is the flux in the absence of a second boundary.

Using these functions, we introduce the probability density for the span of a diffusing particle, initially at x_0, that escapes at time t, $w(L|t|x_0)$. The probability $w(L|t|x_0)dL$ is the fraction of trajectories escaping between t and $t+dt$, whose span is between L and $L+dL$, out of the total number of trajectories that escape between t and $t+dt$. This probability is given by the ratio of the fraction in Eq. (3.2) to $J_\infty(t|x_0)dt$. This leads to

$$w(L|t|x_0)=\frac{1}{J_\infty(t|x_0)}\frac{\partial J_L(t|x_0)}{\partial L}. \tag{3.3}$$

The function $w(L|t|x_0)$ is properly normalized, satisfying $\int_{x_0}^{\infty}w(L|t|x_0)dL=1$. Thus, the flux $J_L(t|x_0)$ is the function from which all properties can be calculated. Specifically, the average span for trajectories escaping at time t is

$$\overline{L}(t|x_0)=\int_{x_0}^{\infty}Lw(L|t|x_0)dL=\frac{1}{J_\infty(t|x_0)}\int_{x_0}^{\infty}L\frac{\partial J_L(t|x_0)}{\partial L}dL. \tag{3.4}$$

A relatively easy way to do the calculations is in terms of the Laplace transform with respect to t. If we let $a=(s/D)^{1/2}$, the transform of $J_L(t|x_0)$ is found to be $\hat{J}_L(s|x_0)=\cosh(ax_0)-\sinh(ax_0)\coth(aL)$, so that

$$\int_{x_0}^{\infty}L\frac{\partial \hat{J}_L(s|x_0)}{\partial L}dL=x_0e^{-ax_0}+\frac{\sinh(ax_0)}{a}\ln\left[\frac{1}{1-e^{-2ax_0}}\right]. \tag{3.5}$$

An expression for the flux $J_\infty(t|x_0)$, required for the denominator term in Eqs. (3.3) and (3.4), is

$$J_\infty(t|x_0)=\frac{x_0}{\sqrt{4\pi Dt^3}}\exp\left(-\frac{x_0^2}{4Dt}\right). \tag{3.6}$$

Using the results in Eqs. (3.5) and (3.6), we can write the average span as

$$\overline{L}(t|x_0)=x_0+\frac{1}{J_\infty(t|x_0)}\mathcal{L}^{-1}\left\{\frac{\sinh(ax_0)}{a}\ln\left[\frac{1}{1-e^{-2ax_0}}\right]\right\}, \tag{3.7}$$

where $\mathcal{L}^{-1}\{\}$ denotes the inverse Laplace transform of the function in brackets. We use this expression to evaluate the long- and short-time behaviors of $\overline{L}(t|x_0)$. At long times one finds

$$\overline{L}(t|x_0)\approx\sqrt{\pi Dt}, \quad Dt \gg x_0^2, \tag{3.8}$$

which is independent of x_0, as might be expected. In the opposite limit, one finds

$$\overline{L}(t|x_0)\approx x_0+\frac{Dt}{x_0}, \quad x_0^2 \gg Dt. \tag{3.9}$$

It is also possible to expand and invert the transform in Eq. (3.7) to find a solution valid for all times, and expressed in terms of an infinite series. One can also find a solution in terms of an infinite series for the probability density $w(L|t|x_0)$.

It is interesting to compare the long-time behavior of the span given in Eq. (3.8) to the span on an unbounded line. In this case, the average span is known exactly, and is given by $\overline{L}_{\mathrm{un}}(t)=4\sqrt{Dt/\pi}$ [13]. A comparison of the two results shows that the ratio $\overline{L}(t|x_0)/\overline{L}_{\mathrm{un}}(t)$ approaches $\pi/4$ as $t\to\infty$. In contrast, in three dimensions the ratio approaches unity.

In conclusion, we have obtained a seemingly paradoxical result that in three or more dimensions the boundary has no effect on the asymptotic behavior of the expected number of distinct sites visited by a random walker before trapping. It remains an open question as to whether or not the asymptotic distribution remains a Gaussian in three or more dimensions, as proved in [14] for an unbounded random walk, but we conjecture that this is indeed the case.

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