Descriptive parameter for photon trajectories in a turbid medium

Amir H. Gandjbakhche[1] and George H. Weiss[2]
[1]Laboratory of Integrative and Medical Biophysics, National Institute of Child Health and Human Development, National Institutes of Health, Bethesda, Maryland 20892
[2]Mathematical and Statistical Computing Laboratory, Center for Information Technology, National Institutes of Health, Bethesda, Maryland 20892

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In many applications of laser techniques for diagnostic or therapeutic purposes it is necessary to be able to characterize photon trajectories to know which parts of the tissue are being interrogated. In this paper, we consider the cw reflectance experiment on a semi-infinite medium with uniform optical parameters and having a planar interface. The analysis is carried out in terms of a continuous-time random walk and the relation between the occupancy of a plane parallel to the surface to the maximum depth reached by the random walker is studied. The first moment of the ratio of average depth to the average maximum depth yields information about the volume of tissue interrogated as well as giving some indication of the region of tissue that gets the most light. We have also calculated the standard deviation of this random variable. It is not large enough to qualitatively affect information contained in the first moment.

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I. INTRODUCTION

There is a lively and growing interest in developing techniques for measuring optical parameters in tissue for possible diagnostic purposes. Useful summaries of the current state in both theory and experiment are to be found in Refs. [1–6] as well as in several meeting Proceedings devoted to the subject, cf, for example, Refs. [4] and [5]. In all of these applications it is necessary to characterize photon trajectories in order to specify the regions of tissue that are being interrogated.

Optical spectroscopy is based on information obtained from highly scattered diffusive photons. Because of the diffusion photon trajectories can only be known in a statistical sense. Theoretical models are therefore required to translate experimental data into usable information. In this paper, we describe features that characterize photon trajectories in a continuous wave (cw) experiment. The tissue is modelled as a semi-infinite medium with uniform optical properties. A crude characterization of the region being probed can be given in terms of at least two parameters, which can be calculated by random walk or diffusion theory. These are the maximum depth to which an eventually detected photon has penetrated into the tissue. An expression for this parameter is derived in Ref. [7]. The second is the average depth probed by a photon that eventually reaches the surface at a specified distance from the point at which it originally enters the tissue [12,13].

In this paper, we combine these calculations by calculating the joint distribution of the mean depth of penetration and the maximum penetration depth of photons re-emitted from the tissue surface to determine what can be learned from those photons re-emitted at the surface. Our development is based on the lattice random theory as first applied to this problem in Ref. [7] and thereafter also framed and analyzed in terms of the continuous-time random walk (CTRW), [8], analyzed in [9]. The advantage in using this formalism in the present instant is that it allows one to find exact results for parameters of physical interest. It has also been shown to yield results that, except at very short times, are close to those of the discrete-time random walk or diffusion approaches.

II. DESCRIPTION OF THE MODEL

The tissue is modelled as a semi-infinite simple cubic lattice bounded by a planar interface, the coordinate of an arbitrary point being $\mathbf{r}=(x,y,z)$, where x, y, and z are integers. The planar surface or interface is assumed to consist only of trapping points, and is specified by $z=0$. Points in the interior of the tissue correspond to $z>0$.

Tissues generally scatter light strongly in the forward direction. The effects of anisotropy can be incorporated in random walk or diffusion models by using scaling relationships described in Refs. [10] and [11]. Conversion of the dimensionless coordinate $\mathbf{r}$ to a physical coordinate $\overline{\mathbf{r}}$ is expressed in terms of the transport-corrected scattering coefficient, $\mu_s'=\mu_s(1-g)$, where $g=\langle\cos\theta\rangle$, θ being the scattering angle, as $\overline{\mathbf{r}}=\mathbf{r}\sqrt{2}/\mu_s'$ [10,11]. Absorption in the interior of the medium will be assumed to follow Beer's law so that the probability that the random walk makes a single step without being absorbed is equal to $\exp(-\nu)$ where $\nu=\mu_a/\mu_s'$. The parameter μ_a is the absorption coefficient. Typical values of ν in human tissue in NIR are generally quite small, being of the order of 0.01.

The diffusion process will be modelled in terms of an isotropic CTRW in which steps are allowed to nearest-neighbors only. That is to say, a step can only be made to a particular one of the six adjacent sites with a probability equal to 1/6. The times between successive steps by the random walker will be assumed to be identically distributed random variables whose properties are described by the probability density

$$\psi(t)=ke^{-kt}, \tag{2.1}$$

so that the mean time between successive steps is $\langle t\rangle = 1/k$. Henceforth, we work in terms of dimensionless times by setting $\tau = kt$, or equivalently by setting $k=1$. The motion of the random walker is described by a propagator $p(\mathbf{r};\tau|\mathbf{r}_0;0)$ which is the probability that a random walker is at $\mathbf{r} = (x,y,z)$ at time τ if it was initially at $\mathbf{r}_0 = (x_0,y_0,z_0)$. Since it will be assumed that any plane parallel to the surface of the lattice is translationally invariant, the propagator satisfies the property

$$p(\rho,z;\tau|\rho_0,z_0;0) = p(\rho-\rho_0,z;\tau|0,z_0;0), \tag{2.2}$$

where $\rho = (x,y)$ is any point in a plane parallel to the interface. The advantage of working with the CTRW is that the propagator for the nearest-neighbor random walk on an infinite lattice (that is, a boundary-free lattice) and the negative exponential interjump density is known exactly [9]. It is

$$p(\mathbf{r};\tau|\mathbf{r}_0;0) = \frac{e^{-(1+\nu)\tau}}{6} I_{x-x_0}\left(\frac{\tau}{3}\right) I_{y-y_0}\left(\frac{\tau}{3}\right) I_{z-z_0}\left(\frac{\tau}{3}\right), \tag{2.3}$$

where $I_m(u)$ is a modified Bessel function of the first kind [14]. The effects of simple boundaries, e.g., reflecting or absorbing planes, are readily calculated in terms of these propagators for motion in free space.

Let $z_{\max}$ denote the (random) maximum depth of penetration of the photon, or random walk into the medium, and let z_{av} be the average depth of a single trajectory conditioned on eventually reaching the interface, independent of the location of the absorbing point. This parameter will be calculated from the mean occupancy of level z. By the terminology "occupancy of level z" we mean the fraction of time spent by the random walk at depth z before reaching the absorbing surface. The event "absorption at the interface $(z=0)$" will be denoted by the letter A. The initial position of the random walker is set at one lattice site below the surface, $(\mathbf{0},1) = (0,0,1)$ where the lattice spacing is of the order of a scattering length.

An outline of our later calculations is as follows: In the following section, we calculate

$$g(L|A) = \Pr\{z_{\max} < L|A\}, \tag{2.4}$$

which is defined as the probability that the maximum depth is equal to L, conditional on eventual absorption at $z=0$. This quantity is calculated by inserting a perfectly absorbing plane at $z=L$, which has the effect of removing all photons that would have penetrated to a depth of L or greater. In Sec. 4 we calculate the relative occupancy of the depth z, for $z_{\max} < L$ and conditioned on eventual absorption of the photon at the interface. This, in turn, will allow us to to find the conditional first moment, $\langle z_{\mathrm{av}}|z_{\max} < L,A\rangle$ which we interpret as the mean depth conditional on the maximum depth being less than L and on ultimate absorption at $z=0$.

Let the relative occupancy of the depth be $\vartheta(L',L|A)$. This function is the fraction of time spent at $z=L'$ when the maximum depth is exactly equal to L, conditioned on absorption at the interface. When $\vartheta(L',L|A)$ is known, the average depth is calculated as

$$\langle z_{\mathrm{av}}, z_{\max} = L|A\rangle = \frac{\sum_{L'=1}^{L} L'\,\vartheta(L',L|A)}{\sum_{L'=1}^{L} \vartheta(L',L|A)}, \tag{2.5}$$

This is a conditional average but can be converted into a joint average and probability by multiplying Eqs. (2.4) and (2.5) together; that is

$$\langle z_{\mathrm{av}}, z_{\max} < L|A\rangle = \langle z_{\mathrm{av}}|z_{\max} < L,A\rangle g(L|A). \tag{2.6}$$

This, in turn, can be converted into an expression for the joint average depth and probability that $z_{\max}=L$, through the identity

$$\langle z_{\mathrm{av}}|z_{\max} = L,A\rangle = \langle z_{\mathrm{av}},|z_{\max} < L+1,A\rangle - \langle z_{\mathrm{av}},|z_{\max} < L,A\rangle \tag{2.7}$$

III. MAXIMUM DEPTH

In this section, we derive an expression for $g(L|A)$ as defined in Eq. (2.4). The probability that the maximum depth is exactly equal to L and that the photon reaches the surface is then expressed as

$$\phi(L|A) = g(L+1|A) - g(L|A). \tag{3.1}$$

Thus, only a knowledge of the function $g(L|A)$ is required to calculate the function $\phi(L|A)$. To ensure satisfaction of the requirement that $L_{\max} < L$ it is necessary to make $z=L$ an absorbing boundary.

The joint probability density that the random walker reaches the surface $z=0$ at time τ and that the maximum depth is less than L has been shown in Ref. [9] to be

$$v(L;\tau|A) = \frac{e^{-\nu\tau}}{3L} \sum_{j=1}^{L} \exp\left[-\frac{2\tau}{3}\sin^2\left(\frac{\pi j}{2L}\right)\right] \sin^2\left(\frac{\pi j}{L}\right). \tag{3.2}$$

Hence, it follows that the joint probability that the interface is reached at some time by a random walk in which the maximum penetration depth is less than L is

$$g(L,A) = \int_0^\infty v(L;\tau|A)\,d\tau = \frac{1}{L} \sum_{j=1}^{L} \frac{\sin^2\left(\frac{\pi j}{L}\right)}{\left[3\nu + 2\sin^2\left(\frac{\pi j}{2L}\right)\right]}. \tag{3.3}$$

A quantity of greater interest than $g(L,A)$ is the conditional, rather than the joint, probability that $z_{\max} < L$, conditioned on eventual absorption at the surface. This can be expressed in terms of the joint probability that $z_{\max}$ is less than L and that the particle eventually reaches the interface, $g(L,A)$, as

$$g(L|A) = \frac{g(L,A)}{g(\infty,A)}, \tag{3.4}$$

where the denominator is the probability of eventual absorption at the interface. This can be calculated as

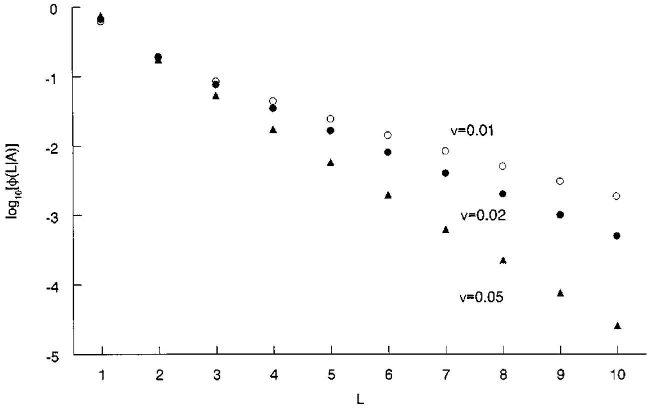

FIG. 1. Curves of $\log_{10}[\phi(L|A)]$ for several values of the internal absorption parameter, ν. These show that the maximum depth tends to remain within three lattice spacings of the surface over the range of values of ν that are physiologically realistic.

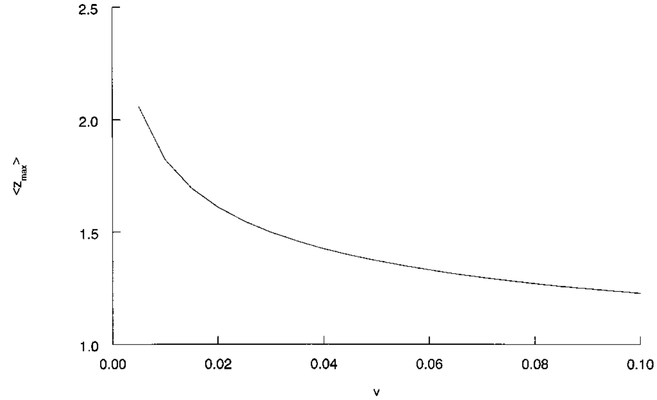

FIG. 2. A curve of $\langle z_{\max}\rangle$ plotted against υ. One sees a relatively rapid falloff of this parameter to unity with increasing values of the absorption parameter. It is obvious that when the absorption parameter is infinite $z_{\mathrm{av}}=1/2$ since in this case the photon only samples $z=1$ once and is then absorbed at the surface.

$$
\begin{aligned}
g(\infty,A) &= \lim_{L\to\infty}\frac{1}{L}\sum_{j=1}^{L}\frac{\sin^2\left(\dfrac{\pi j}{L}\right)}{\left[3\nu+2\sin^2\left(\dfrac{\pi j}{2L}\right)\right]} \\
&= \frac{1}{\pi}\int_0^{\pi}\frac{\sin^2\theta}{[3\nu+1-\cos\theta]}d\theta \\
&= 1+3\nu-\sqrt{6\nu+9\nu^2}. \qquad (3.5)
\end{aligned}
$$

Figure 1 shows points of the logarithm of the probability that the the maximum depth reached by the photon, $\log_{10}[\phi(L|A)]$, plotted as a function of L for different values of ν. Because of the rapid decrease of this function evident from this figure one sees that the penetration by the random walker of the semi-infinite medium is essentially confined to the first three lattice sites in the z direction (i.e., $3\sqrt{2}/\mu_s'$) when the dimensionless absorption parameter ν has physiologically realistic values. Significant differences appear only at larger values of L where the probabilities are quite small.

The average value of $z_{\max}$ can be found by multiplying Eq. (3.1) by L and summing. A consequence of the property $\lim_{L\to\infty} g(L|A)=1$ is that

$$
\langle z_{\max}\rangle=\sum_{L=1}^{\infty}[1-g(L|A)]. \qquad (3.6)
$$

A plot of $\langle z_{\max}\rangle$ as a function of ν, shown in Fig. 2, emphasizes the fact that the maximum depth of penetration, as measured in lattice spacings, is very close to 1 except at very small values of ν. Higher moments of $z_{\max}$ can also be represented as an infinite series similar to that in Eq. (3.6).

IV. AVERAGE PENETRATION

We next define and calculate a measure of the the average penetration depth, conditioned on a finite maximum depth. In calculating this function, we follow the analysis in Ref. [12] by identifying the average penetration depth with the occupancy at a given depth, that is, the relative fraction of time a given depth is occupied during the course of the random walk, [8]. The difference between the average penetration depth as calculated here, and that in Ref. [12], is that we now condition the average depth on the existence of a maximum. As a final step we perform the average over all values of the maximum.

Let $p_L(\rho,z;t|\rho_0,z_0;t_0)$ be the probability that a photon that is at site (ρ_0,z_0) at t_0 and is at (ρ,z) at time t with both $z=0$ and $z=L$ being absorbing planes. It is therefore the propagator under the condition that $z_{\max}<L$. The propagator under the condition that $z_{\max}=L$ is

$$
\begin{aligned}
q_L(\rho,z;t|\rho_0,z_0;t_0) &= p_{L+1}(\rho,z;t|\rho_0,z_0;t_0) \\
&\quad - p_L(\rho,z;t|\rho_0,z_0;t_0). \qquad (4.1)
\end{aligned}
$$

The probability that the random walker is at depth z at time ξ, later reaching the interface at time $\tau\geqslant\xi$ at the surface point $\rho=(x,y)$, was shown in Ref. [13] to have the form

$$
\begin{aligned}
U_{\xi,\tau}(z|\rho;L) &= \frac{e^{-\nu\tau}}{6}\sum_{\rho'}\int_{\xi}^{\tau}e^{-(\tau-\tau')}q_L(\rho',z;\xi|0,1;0) \\
&\quad\times q_L(\rho-\rho',z;\tau'-\xi|0,1;0)\,d\tau'. \qquad (4.2)
\end{aligned}
$$

This relation says that the random walker, initially at the point (0,1), later reached the point (ρ',z) at time ξ, from which it moved to the point $(\rho, 1)$ at time τ'. As its final step it moved to the surface $z=0$ at time $\tau\geqslant\tau'$. While Eq. (4.2) was derived for motion in a semi-infinite space in Ref. [9], its extension to allow for motion in a slab is straightforward. The expected, or local, time spent at z at time τ is found by integrating Eq. (4.2) with respect to ξ. If this quantity is denoted by $T(\tau;z|\rho;L)$ then

$$
T(\tau;z|\rho;L)=\int_0^{\tau}U_{\xi,\tau}(z|\rho;L)\,d\xi. \qquad (4.3)
$$

The expected amount of time spent at z, conditioned on both the eventual absorption at the surface at the point ρ and on the maximum penetration depth being less than L is

$$E(z|\rho;L)=\int_0^\infty T(\tau;z|\rho;L)\,d\tau, \tag{4.4}$$

This is a Laplace transform of $T(\tau;z|\rho;L)$ with the Laplace parameter set equal to 0. The function $E(z|\rho;L)$ is not itself of direct interest, but rather its sum over all points on the surface

$$E(z;L)=\sum_\rho E(z|\rho;L) \tag{4.5}$$

is. It is useful to interpret this as a two-dimensional Fourier series evaluated at the origin in two-dimensional Fourier space because, when the sum over ρ is taken, the formula in Eq. (4.2) is a convolution in the two-dimensional space.

Let $\hat{U}_{\xi,s}(z|\omega;L)$ be the joint Fourier-Laplace transform defined by

$$\hat{U}_{\xi,s}(z|\omega;L)=\int_0^\infty e^{-s\tau}d\tau\int U_{\xi,\tau}(z|\rho;L)e^{i\omega\cdot\rho}d^2\rho. \tag{4.6}$$

This transform can be expressed in terms of the joint transform of the propagator that appears in Eq. (4.2). It is not difficult to show that

$$\hat{U}_{\xi,s}(z|\omega;L)=\frac{1}{6(s+\nu+1)}\hat{q}_L^2(\omega,z;s+\nu|0,1;0), \tag{4.7}$$

where $\hat{q}_L(\omega,z;s+\nu|0,1;0)$ is the joint transform of $q_L(\rho,z;\tau|0,1;0)$. As in earlier work we identify the distribution of the average depth with the occupancy (or local time, [15]) of the random walk, i.e., it is the fraction of time spent at depth z before absorption at the interface $z=0$. Recall that $\vartheta(L',L|A)$ is the relative occupancy of level L' when the maximum depth is equal to L, conditional on eventual absorption at the surface $z=0$. The expression for this function is

$$\vartheta(L',L|A)=\frac{\hat{q}_L^2(0,L';\nu|0,1;0)}{\sum_{z=1}^{L}\hat{q}_L^2(0,z;\nu|0,1;0)},\quad L'<L, \tag{4.8}$$

so that the mean depth calculated when $z_{\max}=L$ is

$$\langle z_{\rm av}(L|A)\rangle=\frac{\sum_{z=1}^{L} z\hat{q}_L^2(0,z;\nu|0,1;0)}{\sum_{z=1}^{L}\hat{q}_L^2(0,z;\nu|0,1;0)}. \tag{4.9}$$

Notice that $\langle z_{\rm av}(L|A)\rangle$ is necessarily greater than 1 since we have used integer depths in our calculations. However, when ν is very large, detected photons tend to be those that return immediately to the interface. Under these conditions the average depth is 1/2. It is therefore reasonable to define the average depth in terms of the depth in terms of the halfway point between the integer depths. This leads to the formula

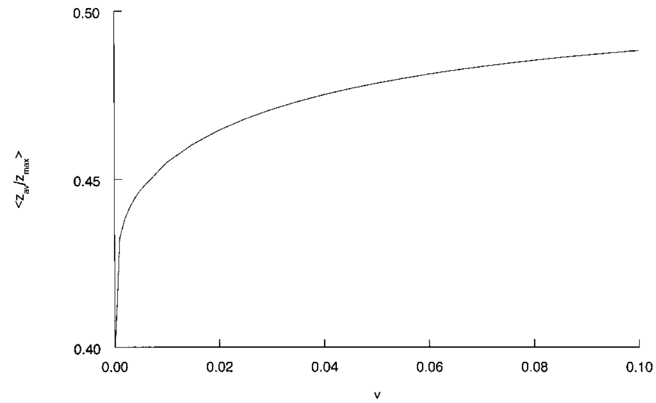

FIG. 3. A curve of $\langle z_{\rm av}/z_{\max}\rangle$ as a function of v. This function increases as a function of v, but only very gradually, except at the very smallest values of v.

$$\left\langle\frac{z_{\rm av}}{z_{\max}}\right\rangle=\sum_{L=1}^{\infty}\langle z_{\rm av}(L|A)\rangle\frac{\phi(L|A)}{L}-\frac{1}{2}. \tag{4.10}$$

The propagator needed to calculate $q_L(\rho,z;\tau|0,1;0)$ is found by placing an absorbing boundary at $z=L$. A slight modification of the argument in Ref. [9] allows us to express the propagator $p_L(\rho,z;\tau|0,1;0)$ as

$$p_L(\rho,z;\tau|0,1;0)=e^{-\tau}I_x\left(\frac{\tau}{3}\right)I_y\left(\frac{\tau}{3}\right)\times\sum_{l=-\infty}^{\infty}\left[I_{2lL+z-1}\left(\frac{\tau}{3}\right)-I_{2lL+z+1}\left(\frac{\tau}{3}\right)\right]. \tag{4.11}$$

By appealing to an argument similar to one found in Ref. [9] we can show that the sum over l in this last formula can be written as a finite series,

$$\sum_{l=-\infty}^{\infty}\left[I_{2lL+z-1}\left(\frac{\tau}{3}\right)-I_{2lL+z+1}\left(\frac{\tau}{3}\right)\right]=\frac{2}{L}\sum_{l=1}^{L}e^{(\tau/3)\cos(\pi l/L)}\sin\left(\frac{\pi l}{L}\right)\sin\left(\frac{\pi lz}{L}\right). \tag{4.12}$$

To get from Eq. (4.11) to Eq. (4.7) it is necessary to sum over all x and y which eliminates these parameters.

$$\sum_{x=-\infty}^{\infty}I_x\left(\frac{\tau}{3}\right)=e^{\tau/3}, \tag{4.13}$$

which then allows us to write

$$\hat{p}_L(0,z;\nu|0,1;0)=\frac{6}{L}\sum_{l=1}^{L}\frac{\sin\left(\frac{\pi l}{L}\right)\sin\left(\frac{\pi lz}{L}\right)}{3\nu+1-\cos\left(\frac{\pi l}{L}\right)}, \tag{4.14}$$

so that $\hat{p}_1(0,L;\nu|0,1;0)=0$. Substitution of this expression into Eq. (4.9) yields an exact representation for the mean value of z_{av} conditioned on eventual absorption at $z=0$ and a maximum penetration less than L [16].

Figure 3 contains a plot of the average of $\langle z_{av}/z_{max}\rangle$ as a function of ν. The standard deviation of z_{av}/z_{max} decreases as a function of ν as one expects since absorption tends to filter out the longer paths. The plot of $\langle z_{av}/z_{max}\rangle$ confirms the finding in Fig. 1 that the degree of penetration of the photon, measured in lattice spacings, is relatively shallow in the presence of even a small amount of internal absorption. This qualitative phenomenon can be explained by noting that when photons are close to the absorbing boundary fluctuations in their motion tends to remove them from the bulk, while photons near the maximum penetration depth are not similarly removed. Increasing the internal absorption only serves to ensure, with greater certainly, that z_{av} is approximately equal to $z_{max}/2$.

V. DISCUSSION

Our analysis has been developed for cw measurements. More detailed information is potentially available from the ratio $\langle z_{av}/z_{max}\rangle$ as a function of space and time for the time-gated measurement. However, a physical argument suggests that if the distance is large the trajectory should flatten out and remain close to the absorbing interface. Our present results indicate that in the cw measurement $\langle z_{av}/z_{max}\rangle$ is approximately equal to 1/2 except at the very smallest values of the absorption coefficient, suggesting that there is a volume of tissue that is uniformly probed by photons.

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