Photon Migration in Turbid Media Using Path Integrals

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We describe the application of path integrals to the problem of light propagation in turbid media. The photon propagation process is separated into an absorption dependent part and a part that depends only on scattering. We determine the nonabsorption photon path and nonabsorption probability distribution function, from which other measurable optical parameters can be obtained. As an example, we calculate the diffuse reflectance for a semi-infinite medium and obtain a new result which reduces to a previously derived expression in the approximate limiting case.

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The propagation of light in a multiply scattering ("turbid") medium has long been studied in astrophysics and atmospheric optics [1], and recently has become important in medical applications [2]. The theory of radiative transfer is widely used to treat this problem by considering the transport of light energy through a random medium and neglecting the wave properties [1,3]. The basic equation in transport theory is the equation of transfer, for which analytic solutions cannot be obtained for most realistic problems. Solutions are often based on the isotropic diffusion approximation, whose primary assumption is that enough scattering events have occurred so that the diffuse radiation is approximately uniformly scattered in all directions. This approach fails near boundaries or sources and when applied to highly anisotropic scattering media for early times. Nonetheless, the diffusion approximation is applied in many instances to obtain approximate solutions [3].

In the present paper we present a new physical picture for treating energy transport in a multiple scattering medium, which we call "the path integral approach to photon migration" (PI). This picture uses the Feynman approach to statistical problems based on his path integral formalism [4], and provides analytic results to the equation of transfer without the need for making the diffusion approximation. It gives new insight into the propagation of light in a turbid medium by making explicit the most probable path taken by photons as they traverse the medium. Below, we compare our results to those of time-dependent diffusion theory [5–7].

Recently, Bonner and co-workers have analyzed multiple scattering transport using an approach called "photon migration" [8,9]. They calculate the probability distribution for the number of steps required by a photon injected into a semi-infinite scattering medium to be emitted at an arbitrary point on the surface. The medium is represented by a three-dimensional cubic lattice and scattering is assumed to be isotropic.

The PI picture also treats light scattering as a probabilistic process, but with a different formalism. The medium is considered to be continuous and scattering need not be isotropic. The evolution of a photon is characterized by two parameters, the *photon weight* [10] and the *no-absorption photon path* [11]. When a photon injected into the medium interacts with a particle, it is considered to have a probability $a=\mu_s/(\mu_s+\mu_a)$ of being scattered and probability $1-a=\mu_a/(\mu_s+\mu_a)$ of being absorbed, with a the albedo and μ_s and μ_a the scattering and absorption coefficients, respectively (i.e., the probabilities per unit length that the photon is scattered and absorbed) [3]. Thus, after each interaction the photon weight is reduced by a factor a, and the photon travels freely in a direction determined by the phase function, which is the probability distribution for the photon to be scattered in a particular direction, until its next interaction with the medium. For a semi-infinite medium all photons are eventually reemitted, but with reduced weights depending upon the photon path. In PI the absorption event is viewed as changing the photon weight according to the albedo, whereas the no-absorption photon path is fully determined by the scattering phase function and the boundary conditions, but independent of the albedo. The experimentally observed diffuse reflectance is equal to the sum of the weights of all the photons which traverse all possible paths. Such separation of albedo from other optical parameters provides good analytic models in turbid media for diffuse reflectance, transmittance, and fluorescence [11].

This probabilistic picture, and especially the concept of the "no-absorption photon path," permits the introduction of Feynman path integrals in a very natural way, "due to the ability of path integrals to deal directly with the notion of the probability of a path" [4]. It can be shown that this approach constitutes a rigorous reformulation of the equation of transfer [12,13]. Transport theory is built around a Boltzmann-like kinetic equation for the probability distribution function $f(\mathbf{r},\mathbf{v},t)$ to find single photon at an arbitrary moment of time t at position $\mathbf{r}$ with velocity $\mathbf{v}$. We can also introduce the probability distribution function $P[\mathbf{r}(t)]$ for a photon to travel along a path $\mathbf{r}(t)$ that starts at $[\mathbf{r}_s(0),\mathbf{v}_s(0)]$ at time $t=0$ and finishes at $[\mathbf{r}_f(T),\mathbf{v}_f(T)]$ at $t=T$. Once $P[\mathbf{r}(t)]$ is known, $f(\mathbf{r},\mathbf{v},t)$ can be found using path integrals [4]. The method of deriving $P[\mathbf{r}(t)]$ directly from the scatter-

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ing phase function is discussed below. Because time appears so naturally in this formation, it is very easy to connect these results with the work on time-dependent optical spectroscopy being carried out by Chance and coworkers [6,7].

To illustrate the method we calculate the diffuse reflectance, R, in the semi-infinite geometry for index-matched boundary conditions. In the PI picture R is the sum of all the photons, appropriately weighted, exiting the medium [11]

$$R(\mu_s,\mu_a,g)=\sum_1^\infty a^n f_n(g)=\int_0^\infty a^n f_n(g)dn\,, \qquad (1)$$

where $f_n(g)$ is the nonabsorption probability distribution function for a photon being reemitted after n interactions with the medium, and g is the mean cosine of the scattering angle. Since in the semi-infinite geometry all photons eventually escape from the medium surface and are detected, the normalizing condition

$$\sum_1^\infty f_n(g)=\int_0^\infty f_n(g)dn=1$$

is required. The problem thus reduces to determining $f_n(g)$. In an earlier paper $f_n(g)$ was approximated by fitting Monte Carlo generated curves [11]. Here we derive $f_n(g)$ from first principles.

In photon migration the photon's path is formed as a result of the very large number of interactions with the medium. Every interaction randomly changes the direction of the photon's motion mostly by a small angle. For convenience we chose a two-dimensional normal distribution as the phase function [14]:

$$p(\Delta)=(2\pi\sigma^2)^{-1}\exp(-\Delta^2/2\sigma^2)\,, \qquad (2)$$

where $\Delta\cong\sqrt{\Delta_{x'z'}^2+\Delta_{y'z'}^2}$ and $\Delta_{x'z'},\Delta_{y'z'}\ll 1$ are the projections of the deflection angle on the local coordinate system (x',y',z') with the z' axis chosen along the photon's propagation direction before the scattering event. Here

$$g=\int\int d\Delta_{x'z'}d\Delta_{y'z'}\,p\left(\sqrt{\Delta_{x'z'}^2+\Delta_{y'z'}^2}\right)\cos\Delta\,,$$

and $g\approx 1-\sigma^2$ for small σ.

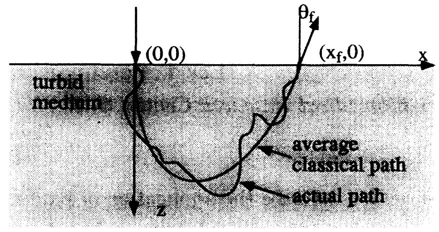

FIG. 1. Path integral picture of photon migration: actual and average classical paths. The actual path as well as classical path need not lie in the plane.

We calculate $f_n(g)$ by considering the propagation of photons in the medium with $\mu_a=0$. The number of scattering events in time interval dt is $\mu_s dt$. (The speed of light in the medium is taken to be unity.) We choose the entry point as the origin of the laboratory coordinate system, define the normal to the surface at this point as the z axis, and choose the line from the origin passing through the exit point as the x axis (Fig. 1). To simplify, we assume that the photon travels in the x-z plane and calculate the photon's resulting *average classical path* which closely approximates the *classical paths* of all photons that enter the medium at the origin at normal incidence and terminate at the given exit point. (A *classical path* is that path which minimizes the classical action [4].) The motion in any other plane can be treated similarly.

Along the photon's path,

$$\ddot{x}(t)^2+\ddot{z}(t)^2=\dot{\theta}_{xz}(t)^2\,, \qquad (3)$$

with θ_{xz} the angle the photon makes with the z axis and $d\theta=\dot{\theta}_{xz}dt$ the variation in the photon's angle in the x-z plane during time interval dt. Because $\dot{\theta}_{xz}(t)$ is a random function with a normal distribution, we can write for the probability to observe this function [4]

$$P(\dot{\theta}_{xz}(t))=\exp\left[-(2\mu_s\sigma^2)^{-1}\int\dot{\theta}_{xz}(t)^2dt\right]. \qquad (4)$$

This means that the photon escape probability through the surface point $(x_f,0)$, with angle $\theta_{xz}\equiv\theta_f$ can be written as a path integral:

$$f[x_f,\theta_f,T]=\int\int\exp\left[-(2\mu_s\sigma^2)^{-1}\int_0^T[\ddot{x}(t)^2+\ddot{z}(t)^2]dt\right]\mathcal{D}x(t)\mathcal{D}z(t)\,, \qquad (5)$$

where $\mathcal{D}x(t)\mathcal{D}z(t)$ means integration along the different paths that satisfy initial and final conditions. The term in the exponent of Eq. (5) is an "effective classical action" for a photon in a highly scattering medium; it must be supplemented by the additional condition $\dot{x}^2+\dot{z}^2=c^2=1$. The effective Lagrangian of the photon in such a medium is

$$L(\dot{\mathbf{r}},\ddot{\mathbf{r}},t)=\ddot{x}(t)^2+\ddot{z}(t)^2+\xi(t)[\dot{x}(t)^2+\dot{z}(t)^2-1]\,, \qquad (6)$$

where $\xi(t)$ is a Lagrange multiplier. The analytical solution of the Euler's equation for such a Lagrangian is not trivial. An approximate solution can be obtained by employing the initial conditions that the velocity is equal to unity along the z axis at the origin, the final conditions that $x(T)=x_f$, $z(T)=0$, $\dot{x}(T)=v_x$, $\dot{z}(T)=v_z$, and setting the average square of the velocity over the path equal to unity. Treating the motion in the x and z directions as independent, we obtain the following approximate equations of motions: $\dddot{x}=0$ and $\dddot{z}=0$. These equations, along

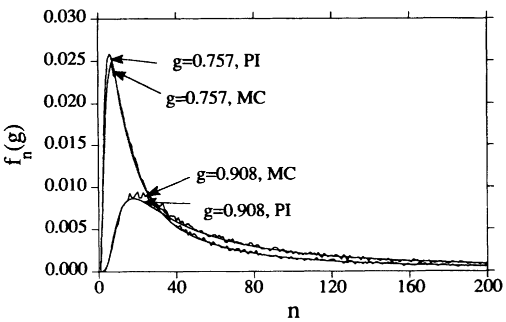

FIG. 2. Comparison of PI and MC simulation of the nonabsorption probability distribution function, $f_n(g)$, as a function of the number of scattering events, n, for $\sigma^2=0.3$ ($g=0.757$) and $\sigma^2=0.1$ ($g=0.908$).

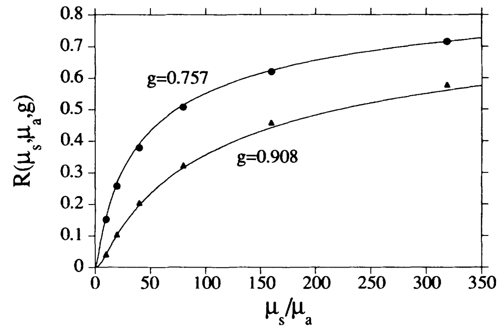

FIG. 3. Diffuse reflectance, R, calculated from PI (solid lines) and MC simulation (points) as a function of the ratio of the scattering coefficient to the absorption coefficient, for $\sigma^2=0.3$ ($g=0.757$) and $\sigma^2=0.1$ ($g=0.908$).

with the conditions at $t=0$ and $t=T$, give the following average classical photon path:

$$x(t)=(Tv_x-2x_f)(t/T)^3+(3x_f-Tv_x)(t/T)^2,\quad z(t)=T(1+v_z)(t/T)^3-T(2+v_z)(t/T)^2+t. \tag{7}$$

Integrating Eq. (5) first along the above path and then x_f, and taking into account the velocity condition, we obtain

$$f(\theta_f,T)=C\left(\frac{6}{\pi\mu_s\sigma^2T^3}\right)^{1/2}\left(\frac{1}{2\pi\mu_s\sigma^2T}\right)^{1/2}\exp\left[-\frac{1}{\mu_s\sigma^2T}[\beta+9/5(v_z+7/12)^2]\right], \tag{8}$$

with C a normalization constant and $\beta=2.68$. Integrating over v_z, we obtain an expression for the probability for the photon to return to the surface at time T:

$$f(T)=\left(\frac{\beta}{\mu_s^3\pi\sigma^2}\right)^{1/2}T^{-3/2}\exp\left(-\frac{\beta}{\mu_s\sigma^2T}\right). \tag{9}$$

Equivalently, we may write $f_n(g)=f(T)$, with $T=n/\mu_s$ and $\beta_{\rm eff}(g)\equiv\beta(1-g)/\sigma^2$. This function, which is actually the time-dependent diffuse reflectance for $\mu_a=0$, varies with time in the same way as that calculated from the time-dependent diffusion approximation in Ref. [7]. [In Ref. [7] the numerical coefficient corresponding to $\beta_{\rm eff}$ is 0.75. Using a more appropriate boundary condition from Ref. [3] in the time dependent diffusion approximation gives $\beta_{\rm eff}=0.75(1.71)^2=2.19$.] For the highly forward scattering case, $g=0.908$, where the diffusion approximation is poor, PI gives $\beta_{\rm eff}=2.47$. For the more isotropic case, $g=0.757$, PI gives $\beta_{\rm eff}=2.17$.

In order to test the validity of Eq. (9), we used a Monte Carlo (MC) program with a Gaussian phase function. Comparison of the numerical simulation with the analytical results, shown in Fig. 2, shows excellent agreement between the two methods, indicating the validity of our approximation within PI.

The steady-state diffuse reflectance can be obtained from Eq. (1) using Eq. (9). This gives

$$R(\mu_s,\mu_a,g)=\exp\left[-2\left(\beta_{\rm eff}\frac{-\ln a}{1-g}\right)^{1/2}\right]. \tag{10}$$

Again, this expression agrees with MC simulations (Fig. 3). We note that in the derivation the escape probability can be explicitly obtained as a function of the coordinates (x,y) on the surface of the sample and the escape angle, θ_f, as well as the number of scattering events, n. Consequently, the diffuse reflectance can be calculated as a function of these variables. Note that this result can be readily inverted.

These results are very encouraging and indicate the potential of PI. Work is in progress to extend the calculations to other geometries and boundary conditions. We are examining the feasibility of removing the approximations made in deriving the classical path, and will report this work in the future. Of greatest significance, particularly in medical applications, is the ability to solve the inverse problem, i.e., given external optical measurements, to be able to infer the distribution and composition of embedded inhomogeneities, such as diseased tissue embedded in normal. In addition, the explicit picture of the most probable photon path given by PI provides beautiful physical insights into the light scattering problem.

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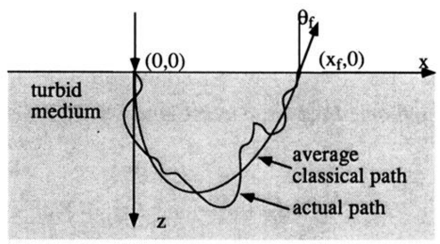

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