A Self-Consistent Obstacle Scattering Theory for the Diffusion Approximation of the Radiative Transport Equation

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This is to certify that I have examined this copy of a technical report by

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Abstract

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We present a self-consistent theory for scattering by several obstacles contained in a turbid medium. We assume the turbid medium is optically thick so that the diffusion approximation of the radiative transfer equation is valid. This theory is useful for detecting tumors in tissues using near-infrared light.

1 Introduction

Modeling light propagation in biological tissues is important for monitoring and imaging tissue health [1]. For these applications, one seeks to extract useful information from scattered light measurements. Near-infrared light is scattered strongly and absorbed weakly by biological tissues. Hence, the major challenge in this research area is developing accurate models for multiple scattered light measurements.

Light propagation in a multiple scattering medium is governed by the theory of radiative transport [2]. This theory takes into account absorption and scattering due to inhomogeneities in the propagating medium. The radiative transport equation is a partial differential/integral equation. Analytical solutions of the radiative transport equation exist only for relatively simple problems. Even numerical solutions are challenging due to the large number of independent variables in the radiative transport equation. Thus, one must seek approximations to obtain useful results.

The diffusion approximation applies to light propagation in an optically thick medium [1,2]. For that case, the radiance becomes nearly isotropic due to multiple scattering as the penetration depth increases. Then the nearly isotropic radiance is governed by the diffusion equation. The diffusion equation is a partial differential equation. It is significantly easier to solve than the radiative transport equation.

Here, we study light propagation in an optically thick medium containing several absorbing obstacles. To take into account the scattering by multiple obstacles, we derive a self-consistent theory. This theory is similar to the one by Kim and Schotland for the radiative transport equation [3]. We show the results of this theory using numerical calculations. This problem is important for understanding how light interacts with obstacles imbedded in a multiple scattering medium. For biomedical optics applications, this problem is useful for tumor detection problems.

The remainder of this paper is as follows. In Section 2, we give an overview of the theory of radiative transport including a derivation of the radiative transport equation. In Section 3, we give a derivation of the diffusion approximation when the medium is optically thick. In

Section 4, we discuss Green's function for the diffusion equation in the frequency domain. In addition, we discuss the representation formula that plays a crucial role in our scattering theory. In Section 5, we discuss scattering by a single obstacle modeled as an absorbing inhomogeneity. We specialize that formal solution to a "point" obstacle for which we can obtain a closed-form analytical solution. Using that single obstacle solution, we derive a self-consistent scattering theory for several obstacles in Section 6. In Section 7, we show numerical results of our theory. Section 8 is the conclusions.

2 The Theory of Radiative Transport

We discuss the theory of radiative transport. First, we define the physical quantities involved in this theory. Then we give a derivation of the radiative transport equation through a balancing of power considerations.

2.1 Definition of Physical Quantities

Below, we introduce and explain the physical quantities in the theory of radiative transfer.

- **Spectral Radiance** L_υ - is the energy flow per unit normal area per unit solid angle per unit time per unit temporal frequency bandwidth.

- **Radiance** L - is defined as the spectral radiance integrated over a narrow frequency range $[\upsilon, \upsilon + \Delta\upsilon]$

$$L(\vec{r}, \hat{s}, t) = L_\upsilon(\vec{r}, \hat{s}, t)\Delta\upsilon$$

  with r denoting position, $\hat{s}$ denoting the unit direction vector, and t denoting time.

- **Fluence Rate** or **Intensity** Φ - is the energy flow per unit area per unit time:

$$\Phi(\vec{r}, t) = \int_{4\pi} L(\vec{r}, \hat{s}, t) d\Omega \,,$$

  with $d\Omega$ denoting the differential solid angle.

- **Current Density** J - is the net energy flow per unit area per unit time:

$$J(\vec{r},t) = \int_{4\pi} \hat{s} L(\vec{r},\hat{s},t) d\Omega$$

2.2 Derivation of the Radiative Transport Equation

There are four contributions to the radiative transport equation: (1) divergence, (2) extinction, (3) scattering, and (4) source. In what follows, we describe each of these four contributions.

1. Divergence - the energy diverging out of volume element dV

$$dP_{div} = \hat{s}\nabla L(\vec{r},\hat{s},t) d\Omega dV \tag{1}$$

2. Extinction - the energy loss due to absorption and scattering in ds.

$$dP_{ext} = (\mu_t ds)[L(\vec{r},\hat{s},t) dA d\Omega] \tag{2}$$

with $\mu_t ds$ denoting the probability of extinction. Note that light scattering from all directions into solid angle element $d\Omega$ is considered in the next subsection.

3. Scattering - the energy incident on the volume element dV from any direction $\hat{s}'$ and scattered into $d\Omega$ around direction $\hat{s}$ per unit time is given by

$$dP_{sca} = (N_s dV)\left[\int_{4\pi} L(\vec{r},\hat{s}',t) P(\hat{s}',\hat{s}) \sigma_s d\Omega'\right] d\Omega \tag{3}$$

Here, N_s denotes the number density of scatterers and σ_s denotes the scattering cross section of a scatterer. Hence, $N_s dV$ is the number of scatterers in the volume element dV. The phase function $P(\hat{s}',\hat{s})$ is a probability density function, and so $L(\vec{r},\hat{s}',t) P(\hat{s}',\hat{s}) \sigma_s d\Omega'$ is the energy intercepted by a single scatterer within solid angle $d\Omega'$ per unit time.

The product $P(\hat{s}',\hat{s}) d\Omega$ is the probability of light with propagation direction $\hat{s}'$ being scattered into $d\Omega$ around direction $\hat{s}$. Typically, the phase function depends only on the angle between the scattered and incident direction, so $P = P(\hat{s}' \cdot \hat{s})$. For that case, (3) reduces to

$$\mathrm{dP_{sca}} = (\mu_s dV)\left[\int_{4\pi} L(\vec{r},\hat{s}',t)P(\hat{s}'\cdot\hat{s})d\Omega'\right]d\Omega \tag{4}$$

with $\mu_s = N_s \cdot \sigma_s$.

4. Source - the energy produced by a source in the volume element within the solid angle element per unit time:

$$\mathrm{dP_{src}} = Q(\vec{r},\hat{s},t)\ dVd\Omega \tag{5}$$

The change in energy in the volume element dV within solid angle element $d\Omega$ per unit time is given by

$$\mathrm{dP} = \frac{\partial L(\vec{r},\hat{s},t)/c}{\partial t} dVd\Omega \tag{5}$$

Here, L/c is the propagating energy per unit volume per unit solid angle. By the conservation of energy

$$\mathrm{dP} = -\mathrm{dP_{div}} - \mathrm{dP_{ext}} + \mathrm{dP_{sca}} + \mathrm{dP_{src}} \tag{6}$$

Substituting (1), (2), (3), (4), (5), and (6) into (7) we obtain the Radiative Transfer Equation:

$$\frac{1}{c}\frac{\partial L(\vec{r},\hat{s},t)}{\partial t} = -\hat{s}\nabla L(\vec{r},\hat{s},t) - \mu_t L(\vec{r},\hat{s},t) + \mu_s \int_{4\pi} L(\vec{r},\hat{s}',t)P(\hat{s}'\cdot\hat{s})d\Omega' + Q(\vec{r},\hat{s},t) \tag{7}$$

3 The Diffusion Approximation

The diffusion approximation assumes that the radiance in a high-albedo ($\mu_a \ll \mu_s$) scattering medium is nearly isotropic after sufficient scattering. In a high-albedo medium, absorption is much less than scattering. To study the radiance in the diffusion limit, we represent it as an expansion in spherical harmonics:

$$L(\vec{r},\hat{s},t) \approx \sum_{n=0}^{1}\sum_{m=-n}^{n} L_{n,m}(\vec{r},t)Y_{n.m}(\hat{s}) \tag{8}$$

Here, $Y_{n,m}$ denote the spherical harmonics and $L_{n,m}$ denote the expansion coefficients. The isotropic component of *L* corresponds to n = 0 and m = 0. When n = 1 and m = -1, 0, 1, we have the anisotropic components. In general, the spherical harmonics are defined as

$$Y_{n,m}(\hat{s}) = Y_{n,m}(\theta,\phi) = (-1)^m \sqrt{\frac{(2n+1)(n-m)!}{4\pi(n+m)!}} P_{n,m}(\cos\theta) e^{im\phi}$$

with $P_{n,m}(x) = \dfrac{(1-x^2)^{m/2}}{2^n n!} \dfrac{d^{m+n}}{dx^{m+n}} (x^2-1)^n$ denoting the associated Legendre polynomials.

For n = 1, the spherical harmonics are as follows.

$$Y_{0,0}(\theta,\phi) = \frac{1}{\sqrt{4\pi}}$$

$$Y_{1,-1}(\theta,\phi) = \sqrt{\frac{3}{8\pi}} \sin\theta e^{-i\phi}$$

$$Y_{1,0}(\theta,\phi) = \sqrt{\frac{3}{4\pi}} \cos\theta$$

$$Y_{1,1}(\theta,\phi) = -\sqrt{\frac{3}{8\pi}} \sin\theta e^{i\phi}$$

Spherical harmonics have the following two properties:

$$Y_{n,-m}(\theta,\phi) = (-1)^m Y^*_{n,m}(\theta,\phi)$$

$$\int_{4\pi} Y_{n,m}(\hat{s}) Y^*_{n',m'}(\hat{s}) d\Omega = \delta_{nn',mm'}$$

Here, the Kronecker delta defined as $\delta_{nn',mm'}$ = 1 when n=n' and m=m' and $\delta_{nn',mm'}$ = 0 otherwise.

Substituting (8) into $\Phi(\vec{r},t) = \int_{4\pi} L(\vec{r},\hat{s},t) d\Omega$ (fluence rate), we obtain

$$\Phi(\vec{r},t) = 4\pi L_{0,0}(\vec{r},t) Y_{0,0}(\hat{s}) \text{ or}$$

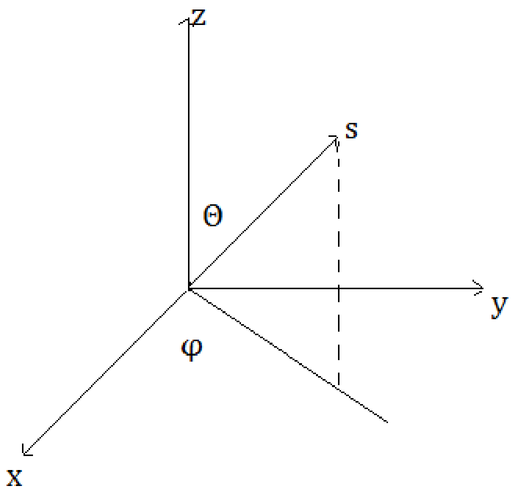
$$L_{0,0}(\vec{r},t) Y_{0,0}(\hat{s}) = \frac{\Phi(\vec{r},t)}{4\pi} \qquad (9)$$

This means that the isotropic term is equal to the fluence rate divided by the entire 4π solid angle.

$\hat{s}$ can be expressed in spherical harmonics:

$$\hat{s} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$$

$$= \sqrt{\frac{2\pi}{3}}\left(Y_{1,-1}(\hat{s}) - Y_{1,1}(\hat{s}), i[Y_{1,-1}(\hat{s}) + Y_{1,1}(\hat{s})], \sqrt{2}Y_{1,0}(\hat{s})\right)$$



Multiplying (8) by $\hat{s}$ and substituting it into the current density equation $J(\vec{r},t) = \int_{4\pi} \hat{s}L(\vec{r},\hat{s},t)d\Omega$, we get $J(\vec{r},t)\cdot\hat{s} = \frac{4\pi}{3}\sum_{m=-1}^{1} L_{1,m}(\vec{r},t)Y_{1,m}(\hat{s})$ or

$$\sum_{m=-1}^{1} L_{1,m}(\vec{r},t)Y_{1,m}(\hat{s}) = \frac{3}{4\pi}J(\vec{r},t)\cdot\hat{s} \quad (10)$$

Substituting (9) and (10) into (8) we obtain:

$$L(\vec{r},\hat{s},t) = \frac{1}{4\pi}\Phi(\vec{r},t) + \frac{3}{4\pi}J(\vec{r},t)\cdot\hat{s} \quad (11)$$

We assume the source is assumed to be isotropic, i.e. $Q(\vec{r},\hat{s},t)$ is independent of $\hat{s}$;

$$Q(\vec{r},\hat{s},t) = \frac{Q(\vec{r},t)}{4\pi}$$

Substituting equation (11) into equation (7) and integrating over the full 4π solid angle, we obtain the following scalar differential equation:

$$\frac{\partial \Phi(\vec{r},t)}{c\partial t} + \mu_a \Phi(\vec{r},t) + \nabla \cdot J(\vec{r},t) = Q(\vec{r},t) \tag{12}$$

Substituting (11) into the radiative transport equation, multiplying both sides by s, and integrating over the full 4π we obtain,

$$\frac{\partial J(\vec{r},t)}{c\partial t} + (\mu_a + \mu_s^{'})J(\vec{r},t) + \frac{1}{3}\nabla \Phi(\vec{r},t) = 0 \tag{13}$$

where $\mu_s^{'} = \mu_s(1-g)$ is the transport (reduced) scattering coefficient, $g = \int_{4\pi} (\hat{s}' \cdot \hat{s}) P(\hat{s}' \cdot \hat{s}) d\Omega$ is the scattering anisotropy, $\mu_a + \mu_s^{'} = \mu_t^{'}$ denotes the transport (reduced) interaction coefficient, and $\ell_t^{'} = \frac{1}{\mu_t^{'}}$ is the transport mean free path.

To obtain an equation only in $\Phi(\vec{r},t)$, we assume that the fractional change in $J(\vec{r},t)$ within $\ell_t^{'}$ is small, i.e.

$$\left(\frac{\ell_t^{'}}{c}\right)\left(\frac{1}{\left|J(\vec{r},t)\right|}\left|\frac{\partial J(\vec{r},t)}{\partial t}\right|\right) \ll 1 \tag{14}$$

The first parenthesis in (14) is the time duration for photons to transverse $\ell_t^{'}$. The second parenthesis in (14) contains the fractional change in the current density per unit time. Equation (14) can thus be written as

$$\left|\frac{\partial J(\vec{r},t)}{c\partial t}\right| \ll (\mu_a + \mu_s^{'})\left|J(\vec{r},t)\right|$$

Under this assumption, (13) becomes

$$(\mu_a + \mu_s^{'})J(\vec{r},t) = -\frac{1}{3}\nabla \Phi(\vec{r},t)$$

with $D = \frac{1}{3(\mu_a + \mu_s^{'})}$ denoting the diffusion coefficient, so

$$J(\vec{r},t) = -D\nabla \Phi(\vec{r},t) \tag{15}$$

Substituting (15) into (12), we obtain the diffusion equation:

$$\frac{\partial \Phi(\vec{r},t)}{c\partial t} + \mu_a \Phi(\vec{r},t) - \nabla \cdot [D \nabla \Phi(\vec{r},t)] = Q(\vec{r},t) \tag{16}$$

If the diffusion coefficient is space-invariant we have

$$\frac{\partial \Phi(\vec{r},t)}{c\partial t} + \mu_a \Phi(\vec{r},t) - D \nabla^2 \Phi(\vec{r},t) = Q(\vec{r},t) \tag{17}$$

4 Green's Function

We study Green's function for the diffusion equation in the frequency domain. By Fourier transforming (17) with respect to time we obtain,

$$\frac{-i\omega}{c} u + \mu_a u - D \nabla^2 u = Q \tag{18}$$

where $u = \frac{1}{2\pi} \int_{-\infty}^{\infty} \Phi(\vec{r},t) e^{i\omega t} dt$. By rearranging terms in (18), we obtain

$$-D \Delta u + k^2 u = Q \tag{19}$$

with $k^2 = (\mu_a - i\omega / c)$.

Green's function, denoted by $G(r - r')$, is the solution of (19) when $Q = \delta(r - r')$. Because the laplacian is invariant under translation, we consider the coordinate system in which r' is the origin, i.e.

$$-D \Delta G + k^2 G = \delta(r) \tag{20}$$

Changing equation (20) to spherical coordinates gives us:

$$-D \frac{1}{\rho^2} \frac{d}{d\rho} \left(\rho^2 \frac{dG}{d\rho} \right) + k^2 G = \delta(\rho) \tag{21}$$

where $G = G(\rho)$ and $r = (\rho, \varphi, \theta)$.

We now consider the situation in which $\rho \neq 0$. For that case, $\delta(\rho) = 0$. By the change of variables $G = \rho^{-1} \upsilon$ we obtain:

$$-D \frac{d^2 \upsilon}{d\rho^2} + k^2 \upsilon = 0 \tag{22}$$

The general solution to (22) is:

$$\upsilon(\rho) = c_1 e^{-k\rho/\sqrt{D}} + c_2 e^{k\rho/\sqrt{D}} \tag{23}$$

To ensure that this solution is bounded for all ρ, we must set $c_2 = 0$. Hence, we obtain:

$$G(\rho) = p^{-1}\upsilon(\rho) = \frac{c_1 e^{-k\rho/\sqrt{D}}}{\rho} \tag{24}$$

To determine our coefficient c_1, we integrate equation (20) over the volume V defined as a ball of radius ρo and obtain:

$$\int_{V(\rho o)} (-D\Delta G + k^2 G)dV = \int_{V(\rho o)} \delta(\rho)dV = 1 \tag{25}$$

Applying the divergence theorem to the first term of the left-hand side of (25):

$$-D\int_{v(\rho o)} \Delta G dV = -D\int_{S(\rho o)} \frac{dG}{d\rho} dS \tag{26}$$

Substituting (24) into (26),

$$-D\int_{S(\rho o)} \frac{dG}{d\rho} dS = c_1 D\left[\frac{k}{\sqrt{D}}\frac{e^{-k\rho o/\sqrt{D}}}{\rho o} + \frac{e^{-k\rho o/\sqrt{D}}}{\rho o^2}\right]\int_{S(\rho o)} dS$$

$$= c_1 D\left[\frac{k}{\sqrt{D}}\frac{e^{-k\rho o/\sqrt{D}}}{\rho o} + \frac{e^{-k\rho o/\sqrt{D}}}{\rho o^2}\right]4\pi\rho o^2$$

$$= c_1 4\pi D\left[\frac{k}{\sqrt{D}}\rho o e^{-k\rho o/\sqrt{D}} + e^{-k\rho o/\sqrt{D}}\right] \tag{27}$$

In the limit as $\rho o \to 0$, the result in (27) reduces and we obtain $c_1 = \frac{1}{4\pi D}$ and therefore,

$$G(\rho) = \frac{e^{-k\rho o/\sqrt{D}}}{4\pi D\rho} \tag{28}$$

Generalizing this result we obtain our Green's Function:

$$G(r - r') = \frac{e^{-k|r-r'|/\sqrt{D}}}{4\pi D|r - r'|} \tag{29}$$

Green's second identity for the volume V with boundary S is given by [4]

$$\int_V (w\Delta v - v\Delta w)dV = \int_S \left(w\frac{\partial v}{\partial n} - v\frac{\partial w}{\partial n} \right) dS$$

Using Green's second identity, we derive the representation formula for the diffusion approximation:

$$u(r) = \int_V GQdr + \int_S \left(G\frac{\partial u}{\partial n} - u\frac{\partial G}{\partial n} \right) \tag{30}$$

Evaluating (30) in the limit as $V \to \mathbb{R}^3$, we get

$$u(r) = u_{inc}(r) + \int_V GQdr \tag{31}$$

with u_{inc} denoting the incident field. We will make use of (31) to study the direct obstacle scattering problem.

5 The Direct Obstacle Scattering Problem

We now consider light propagating in a multiple scattering medium containing an obstacle. We model this obstacle as an absorbing inhomogeneity. Consider (19) with the absorption coefficient equal an absorption constant plus a spatially varying function:

$$\mu_a = \overline{\mu}_a + V(r)$$

Substituting this absorption coefficient into the homogeneous diffusion equation

$$-D\Delta u + k^2 u = 0$$

We find that

$$\begin{aligned} k^2 &= -iw/c + \mu_a \\ &= -iw/c + \overline{\mu}_a + V \\ &= K^2 + V \end{aligned} \tag{32}$$

Plugging (32) into the homogeneous equation, we derive the direct obstacle scattering problem:

$$-D\Delta u + K^2 u + Vu = 0$$
$$-D\Delta u + K^2 u = -Vu$$
(33)

We apply the representation formula given by (31) to (33) and obtain the following representation of the solution:

$$u(r) = u_{inc}(r) - K^2 \int GVudr \qquad (34)$$

Equation (34) is called the Lippmann-Schwinger equation which is a Fredholm integral equation of the second kind. The formal solution of (34) is given by the Born series:

$$u(r) = u_{inc}(r) + \sum_{n=1}^{\infty} u_n(r) \qquad (35)$$

where each of the u_n are obtained by a recursion relation and satisfy

$u_n = -K^2 \int GVu_{n-1}dr$ and where $u_1 = -K^2 \int GVu_{inc}dr$

Thus, our first Born approximation is obtained by looking only at the first term of the recursive relation

$$u = u_{inc} - K^2 \int GVu_{inc}dr$$

5.1 Point Obstacle Solution

We now consider the special case in which the size of the obstacle is very small. For that case, we approximate the absorbing inhomogeneity by

$$V(r) \approx \sigma_a \delta(r - r_0)$$

with σ_a denoting the absorption cross-section for the obstacle. Taking the case when n = 1:

$$u(r) = u_{inc}(r) - K^2 \int G(r,r')V(r')u_{inc}(r')dr' \qquad (36)$$

Thus, $u \approx u_{inc} - K^2 \int G\sigma_a \delta(r - r_0)u_{inc}dr$ which implies our first Born approximation:

$$u \approx u_{inc} - K^2 G\sigma_a u_{inc} \qquad (37)$$

5.2 Several Point Obstacles

Now consider *N* point scatters, at locations $r_1, r_2, ..., r_n$ with corresponding absorption cross sections sigma… For that case, we represent the solution as the sum of the incident field and all of the "scattered" fields from each of the obstacles:

$$u = u_{inc} - \sum_{n=1}^{N} K^2 G(r, r_n)\sigma_{an} u_n^E \tag{39}$$

Here, u_n^E denotes the exciting field on obstacle *n*. To derive these exciting fields, we use a self-consistent argument: the exciting field for each obstacle is the sum of incident field on the obstacle and the fields scattered by all of the other obstacles. According to this argument,

$$u_n^E = u_{inc} - \sum_{m \neq n} K^2 G(r_{n,} r_m)\sigma_{am} u_n^E \tag{40}$$

for *n* = 1, 2, 3, …, *N*. Equation (40) defines a linear system of equations since Green's function is known explicitly. Upon solution of (40), we obtain the exciting fields u_n^E that we substitute into (39) to obtain the total field.

This self-consistent argument makes the assumption that there are no self-interacting fields. In other words, the field that excites an individual object is not affected by itself. This assumption is reasonable when the distribution of obstacles is sufficiently dilute so that one needs to take into account "far-field" interactions only.

6 Numerical Results

For our numerical results, we consider only two point absorbers so that we can study carefully their interactions. In particular, we study light propagation in the whole space composed of a uniform absorbing and scattering medium except for two point absorbers. The diffusion coefficient is set to D = 0.5168 and the absorption coefficient is set to 0.034. Both of the point absorbers have absorption cross-sections 0.03. These are known values for cervical tissue [3]. A diffusing plane wave of the form

u(z) = exp(-k z)

is incident on the two absorbing obstacles contained in the halfspace {z > 0}. We evaluate the solution given by (40) on the plane {z = 0} which we call the detector plane. We plot in the figures below the intensity on the detector plane u(x,y,z=0).

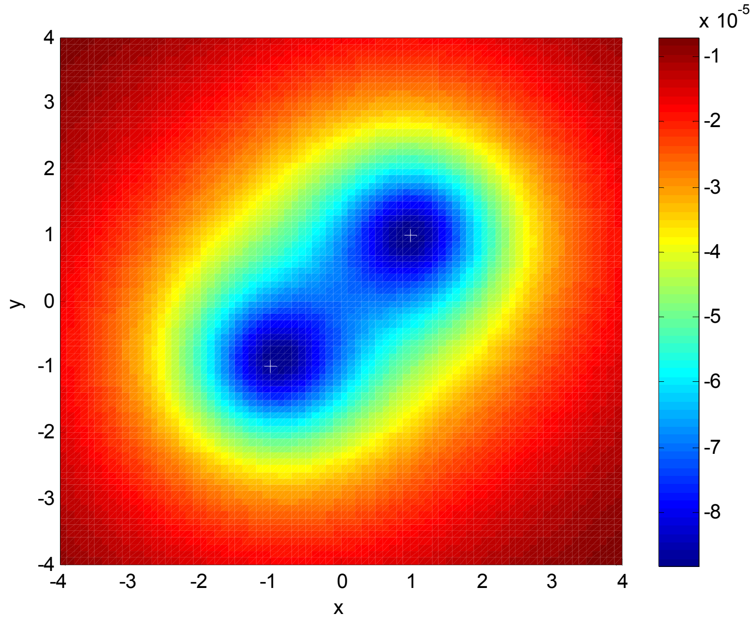


Figure (1)

Figure (1) shows the intensity of the two point absorbers on the plane z=0 when point absorber r_1 is at location (1.0, 1.0, 1.0) and point absorber r_2 is at location (-1.0, -1.0, 1.0).

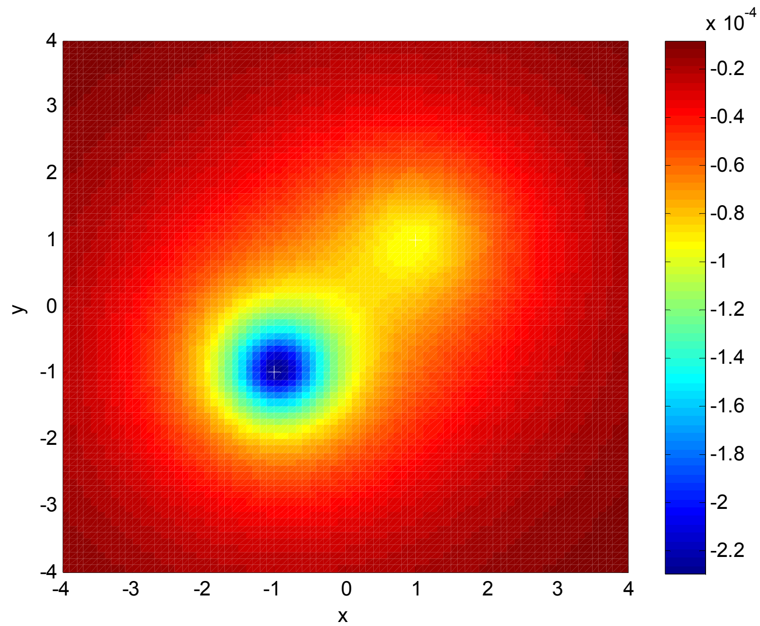


Figure (2)

For Figure (2), the locations for point absorbers r_1 and r_2 are (1.0, 1.0, 1.0) and (-1.0, -1.0, 0.5), respectively.

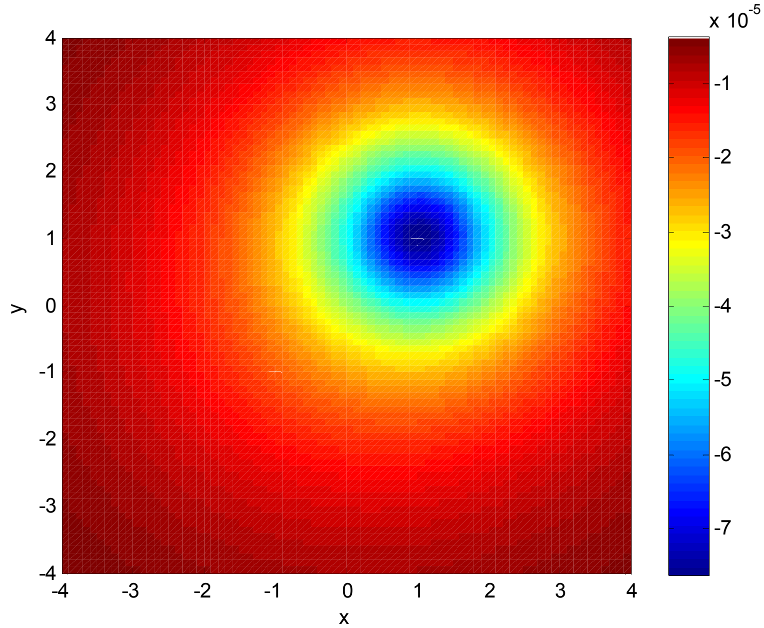


Figure (3)

For Figure (3), the locations for point absorbers r_1 and r_2 are (1.0, 1.0, 1.0) and (-1.0, -1.0, 3.0), respectively.

We can see in Figure (1) that the point absorbers have the same intensity when they are the same distance away from the detector (z=0) plane. But as the point absorber gets farther away from the detector plane, the intensity of the absorber is less. In Figure (2), point absorber r_2 is closer to the detector plane and thus its intensity is stronger than point absorber r_1. In Figure (3) point absorber r_2 is farther from the detector plane and so its intensity is much less than r_1. In fact, in figure (3), it is difficult to see r_2.

7 Conclusions

We have presented a self-consistent theory to study the diffusion of light in a multiple scattering medium containing several absorbing obstacles. This theory gives valuable insight into the interactions of light between obstacles and a surrounding turbid medium. This insight is needed for obtaining quantitative resolution estimates for imaging in tissues, for example. Moreover, this theory provides a means to quantify how well one can distinguish different obstacles from scattered light measurements.

To extend this theory further to take into account problems of practical interest, we can consider different geometries, *e.g.* halfspace, slab, etc, which would require the corresponding Green's function and proper boundary conditions. An interesting extension would be to consider the inverse problem, namely *can one determine the number and* *locations of absorbing obstacles from scattered light measurements?* Certainly developing this self-consistent theory provides an important first-step toward solving that inverse problem.

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