Numerical Studies of Inversion Formulas for Diffusion Tomography: Effects of Boundary Conditions

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ABSTRACT

We consider the inverse scattering problem for the diffusion equation with general boundary conditions. Computer simulations are used illustrate our approach in model systems.

Keywords: diffusion tomography, inverse scattering, boundary conditions

The study of the propagation of diffuse light has attracted considerable attention in the context of imaging of highly-scattering systems [1-5]. Such systems are ubiquitous in nature and include biological tissue, the ocean, clouds, and interstellar media. As a result, the inverse scattering problem for the diffusion equation is of fundamental importance. The physical problem under consideration is the reconstruction of the spatial distribution of the optical absorption and diffusion coefficients of an object from a set of measurements taken on its surface. The equations describing the scattering of diffusing photons from fluctuations in the absorption and diffusion coefficients are in general nonlinear [6]. Consequently, numerical reconstruction of these quantities is an extremely complicated and computationally expensive matter. A procedure based on linearization of the forward scattering problem is often employed instead [7,8]. The computational complexity of the resultant image reconstruction algorithm, however, still limits its practical utility.

In this work we present an explicit inversion formula for the linearized inverse scattering problem for the diffusion equation with general boundary conditions. Our results are remarkable in three regards. First, the inversion formula leads directly to an image reconstruction algorithm that is computationally efficient and stable in the presence of added noise. Second, the incorporation of general boundary conditions is of considerable importance for experimental studies [5]. Third, although the main focus of this work is the inverse scattering problem for diffuse light, the results presented are, in fact, very general. Similar equations describe, for example, the propagation of heat in a body with fluctuating thermal conductivity, or the flow of steady current in a body with fluctuating electrical conductivity. In both situations, the proposed solution to the inverse scattering problem can be used to reconstruct the distribution of these conductivities from measurements taken on the boundary of the object.

We begin by considering the propagation of diffusing photons whose energy density $u(\mathbf{r},t)$ obeys the diffusion equation

$$\partial_t u(\mathbf{r},t) = \nabla \cdot (D(\mathbf{r})\nabla u(\mathbf{r},t)) - \alpha(\mathbf{r})u(\mathbf{r},t) + S(\mathbf{r},t) \ , \tag{1}$$

where $D(\mathbf{r})$ and $\alpha(\mathbf{r})$ are the position-dependent diffusion and absorption coefficients, and $S(\mathbf{r},t)$ is the source power density. We consider a slab geometry in which mixed boundary conditions of the form

$$u + \ell \hat{\mathbf{n}} \cdot \nabla u = 0 \ , \tag{2}$$

are specified on the planes $z = 0$ and $z = L$, $\hat{\mathbf{n}}$ is a unit outward normal, and ℓ denotes a parameter with the dimensions of a length. The case of purely absorbing boundaries is obtained when $\ell = 0$, while reflecting boundaries are obtained when $\ell = \infty$.

The average power at the point $\mathbf{r}$ that flows in the direction $\hat{\mathbf{s}}$ is given by $I(\mathbf{r}, \hat{\mathbf{s}}) = \frac{1}{4\pi}\left(cu - 3D\hat{\mathbf{s}} \cdot \nabla u\right)$, where c is the speed of diffusing particles in a non-scattering medium (speed of light for photons) [9,10]. We can now use (2) to obtain the intensity I_S that is measured by detectors located on one of the boundary surfaces which is expressed as $I_S = (c/4\pi)(1 + \ell^*/\ell)u$, where $\ell^* \equiv 3D/c$. The inverse problem can be formulated as the reconstruction of $\alpha(\mathbf{r})$ and $D(\mathbf{r})$ given a set of measurements of $I_S(\boldsymbol{\rho}_s, z_s; \boldsymbol{\rho}_d, z_d)$ produced by sources with coordinates $\mathbf{r}_s = (\boldsymbol{\rho}_s, z_s)$ and measured by detectors with coordinates $\mathbf{r}_d = (\boldsymbol{\rho}_d, z_d)$.

It is useful to rewrite (1) in Dirac notation as

$$\partial_t |u(t)\rangle + H|u(t)\rangle = |S(t)\rangle \ , \tag{3}$$

where the energy density is given by $u(\mathbf{r}, t) = \langle \mathbf{r}|u(t)\rangle$, $S(\mathbf{r}, t) = \langle \mathbf{r}|S(t)\rangle$, and $H = -\nabla \cdot D(\mathbf{r})\nabla + \alpha(\mathbf{r})$. Equation (3) is the Schrödinger equation in imaginary time where $\alpha(\mathbf{r})$ can be interpreted as the interaction potential and $D(\mathbf{r})$ as a position-dependent mass. The time evolution of $|u(t)\rangle$ can be described by the Green's function $G(t) = \Theta(t)\exp(-Ht)$, $\Theta(t)$ being the unit step function, according to

$$|u(t)\rangle = \int_{-\infty}^{\infty} G(t - t')|S(t')\rangle dt' \tag{4}$$

The Green's function $G(t)$ describes the results of a time-resolved experiment. Alternatively, we can perform measurements with a source that is harmonically modulated at the frequency ω. In this case, the intensity I_S is obtained from the Fourier-transformed Green's function, $G(\omega) = 1/\left(H - i\omega\right)$, and the resulting solution is given by $|u(\omega)\rangle = G(\omega)|S(\omega)\rangle$.

It is convenient to decompose $\alpha(\mathbf{r})$ and $D(\mathbf{r})$ as $\alpha(\mathbf{r}) = \alpha_0 + \delta\alpha(\mathbf{r})$ and $D(\mathbf{r}) = D_0 + \delta D(\mathbf{r})$, where α_0 and D_0 are the background values of the respective coefficients, and represent the Hamiltonian in the form

$$H = H_0 + V \ , \tag{5}$$
$$H_0 = -D_0 \nabla^2 + \alpha_0 \ , \tag{6}$$
$$V = -\nabla \cdot \delta D(\mathbf{r})\nabla + \delta\alpha(\mathbf{r}) \ . \tag{7}$$

The unperturbed Green's function $G_0(\omega) = 1/(H_0 - i\omega)$ can be calculated analytically given the boundary conditions (2), and the complete Green's function satisfies the Dyson equation $G = G_0 - G_0 V G$.

The change in the measured intensity due to the presence of fluctuations in α and D, $\Delta I_S(\mathbf{r}_s, \mathbf{r}_d)$, is given by

$$\Delta I_S(\mathbf{r}_s,\mathbf{r}_d) = \frac{cS_0(\omega)}{4\pi}\left(1+\frac{\ell^*}{\ell}\right)^2 \langle \mathbf{r}_s|G_0 - G|\mathbf{r}_d\rangle \ , \tag{8}$$

The extra factor of $(1+\ell^*/\ell)$ can be explained by the general reciprocity of sources and detectors [11]. Next, we use perturbation theory to express G to leading order in V as $G = G_0 - G_0VG_0$. We define the *data function* $\phi(\mathbf{r}_s,\mathbf{r}_d)$, which is proportional to the experimentally measurable quantity $\Delta I_S(\mathbf{r}_s,\mathbf{r}_d)$, as

$$\phi(\mathbf{r}_s,\mathbf{r}_d) = \left(1+\frac{\ell^*}{\ell}\right)^2 \langle \mathbf{r}_s|G_0VG_0|\mathbf{r}_d\rangle \ , \tag{9}$$

An equivalent, and more convenient description can be obtained in the two-dimensional basis of the form $|\mathbf{q}_a z_a\rangle$ $(a = s, d)$, where $\langle \mathbf{r}|\mathbf{q}_a z_a\rangle = \delta(z - z_a)\exp(i\mathbf{q}_a \cdot \boldsymbol{\rho})$ and $\mathbf{q}_a$ is a two-dimensional vector parallel to the plane $z = 0$. Note that this description leads to Fourier transforming the data function with respect to $\boldsymbol{\rho}_s$ and $\boldsymbol{\rho}_d$. The matrix elements of the unperturbed Green's function in this basis can be readily obtained:

$$\langle \mathbf{q}_s z_s|G_0(\omega)|\mathbf{q}_d z_d\rangle = \frac{(2\pi)^2\ell}{D_0}\delta(\mathbf{q}_s - \mathbf{q}_d) g\left(\mathbf{q}_s; z_s, z_d\right) \ , \tag{10}$$

$$g\left(\mathbf{q}; z_s, z_d\right) = \frac{\sinh\left[Q\left(L - |z_s - z_d|\right)\right] + Q\ell\cosh\left[Q\left(L - |z_s - z_d|\right)\right]}{\sinh\left(QL\right) + 2Q\ell\cosh\left(QL\right) + \left(Q\ell\right)^2\sinh\left(QL\right)} \ . \tag{11}$$

where $Q \equiv Q(\mathbf{q}) = (\mathbf{q}^2 + k_0^2)^{1/2}$ and the wave number is given by $k_0^2 = (\alpha_0 - i\omega)/D_0$. Combining (9), (10), and (7), we obtain the following integral equation that relates the unknown functions $\delta\alpha$, δD to the data function ϕ in the $|\mathbf{q}_a, z_a\rangle$ basis:

$$\phi(\mathbf{q}_s,\mathbf{q}_d) = \int d^3r \exp\left[i(\mathbf{q}_d - \mathbf{q}_s)\cdot\boldsymbol{\rho}\right]\left[\kappa_A(\mathbf{q}_s,\mathbf{q_d},z_s,z_d;z)\delta\alpha(\mathbf{r}) + \kappa_D(\mathbf{q}_s,\mathbf{q}_d,z_s,z_d;z)\delta D(\mathbf{r})\right] \tag{12}$$

where

$$\kappa_A(\mathbf{q}_s,\mathbf{q}_s,z_s,z_d;z) = \left(\frac{\ell+\ell^*}{D_0}\right)^2 g(\mathbf{q}_s;z_s,z)g(\mathbf{q}_d;z,z_d) \ , \tag{13}$$

$$\kappa_D(\mathbf{q}_s,\mathbf{q}_d,z_s,z_d;z) = \left(\frac{\ell+\ell^*}{D_0}\right)^2 \left[\frac{\partial g(\mathbf{q}_s;z_s,z)}{\partial z}\frac{\partial g(\mathbf{q}_d;z,z_d)}{\partial z} + \mathbf{q}_s\cdot\mathbf{q}_d g(\mathbf{q}_s;z_s,z)g(\mathbf{q}_d;z,z_d)\right] \tag{14}$$

It can be shown that the solution to the integral equation (12) is given by

$$\delta\alpha(\mathbf{r}) = \int \frac{d^2q}{(2\pi)^2} e^{i\mathbf{q}\cdot\boldsymbol{\rho}} \int d^2p d^2p' \kappa_A^*\left(\mathbf{p}+\frac{\mathbf{q}}{2},\mathbf{p}-\frac{\mathbf{q}}{2};z\right)\langle \mathbf{p}|T^{-1}(\mathbf{q})|\mathbf{p}'\rangle\phi(\mathbf{p}'+\mathbf{q}/2,\mathbf{p}'-\mathbf{q}/2) \ , \tag{15}$$

$$\delta D(\mathbf{r}) = \int \frac{d^2q}{(2\pi)^2} e^{i\mathbf{q}\cdot\boldsymbol{\rho}} \int d^2p d^2p' \kappa_D^*\left(\mathbf{p}+\frac{\mathbf{q}}{2},\mathbf{p}-\frac{\mathbf{q}}{2};z\right)\langle \mathbf{p}|T^{-1}(\mathbf{q})|\mathbf{p}'\rangle\phi(\mathbf{p}'+\mathbf{q}/2,\mathbf{p}'-\mathbf{q}/2) \ , \tag{16}$$

where

$$\langle \mathbf{p}|T(\mathbf{q})|\mathbf{p}'\rangle = \int_0^L \left[\kappa_A\left(\mathbf{p}+\frac{\mathbf{q}}{2},\mathbf{p}-\frac{\mathbf{q}}{2};z\right)\kappa_A^*\left(\mathbf{p}'+\frac{\mathbf{q}}{2},\mathbf{p}'-\frac{\mathbf{q}}{2};z\right)\right.$$
$$\left.+\kappa_D\left(\mathbf{p}+\frac{\mathbf{q}}{2},\mathbf{p}-\frac{\mathbf{q}}{2};z\right)\kappa_D^*\left(\mathbf{p}'+\frac{\mathbf{q}}{2},\mathbf{p}'-\frac{\mathbf{q}}{2};z\right)\right]dz \qquad (17)$$

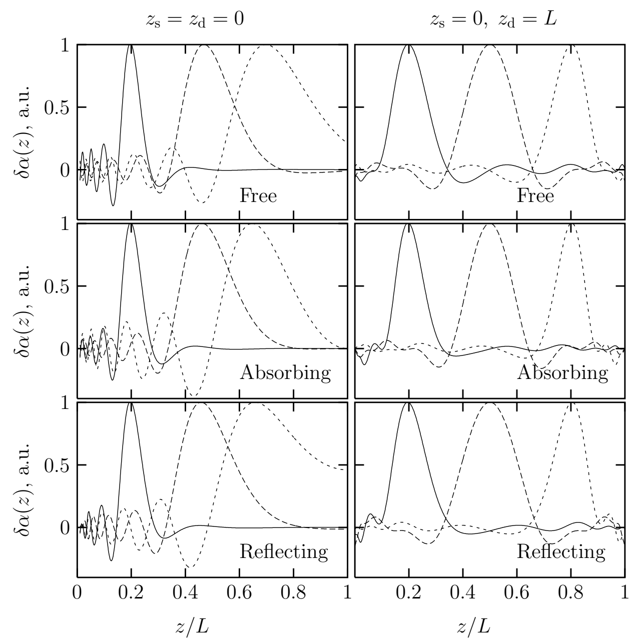
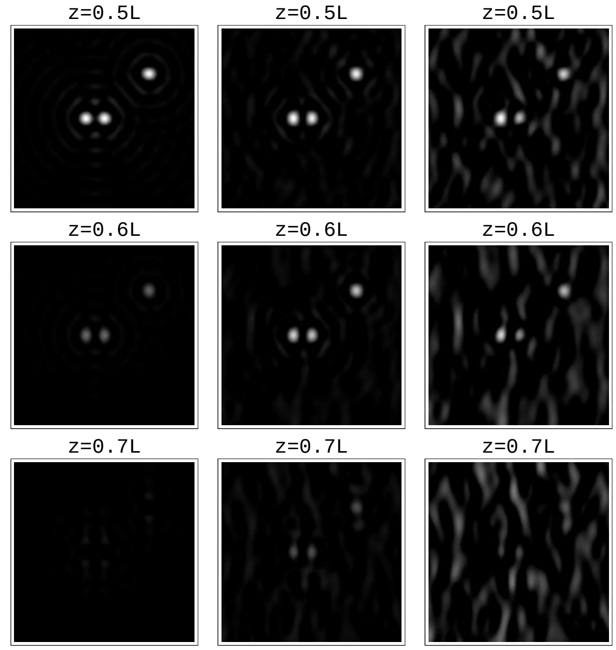


Fig. 1. Reconstruction of a point absorber which is located at $z/L = 0.2$ (solid line), $z/L = 0.5$ (long dash) and $z/L = 0.8$ (short dash). The reconstructed value of $\delta\alpha$ is normalized by its maximum value.



(a) (b) (c)

Fig. 2. Tomographic images of three point absorbers located in the $z = 0.5L$ plane for different levels of noise n and different depths z. (a) n=0 and $\epsilon = 10^{-17}$; (b) n=1% and $\epsilon = 10^{-8}$; (c) n=5% and $\epsilon = 10^{-8}$. The field of view is $2L \times 2L$. A linear color scale is employed.

To illustrate the use of the inversion formulas, we have numerically simulated the reconstruction of $\delta\alpha$ for one or more point absorbers of the form $\delta\alpha(\mathbf{r}) = \alpha_0\delta(\mathbf{r}-\mathbf{r}_0)$ under the assumption that $\delta D = 0$. The simulations were performed with the single modulation frequency $\omega = 0$ for three types of boundary conditions: purely absorbing, purely reflecting, and free. The forward data $\phi(\mathbf{q}_s, \mathbf{q}_d)$ was calculated analytically, by replacing $\delta\alpha$ in (12) by one or more delta functions. The numerical integrations in (15) and (16) were carried out by choosing $\mathbf{q}$ to lie on a rectangular grid with spacing Δq and inside the circle $|\mathbf{q}| < M\Delta q$. The values of the parameters were $\Delta q = L^{-1} = 2\pi/k_0$ and $M = 40$. We also used M discrete wavevectors $\mathbf{p}$ which were chosen on a line ranging in length from 0 to $M\Delta q$. Note that in this case the operator T is a finite-dimensional matrix which can be diagonalized using standard methods of linear algebra (Jacobi diagonalization was used in numerical examples shown here). It is also important to note that the inversion of T must be *regularized* because T has very small eigenvalues. We have used the regularization formula

$$T^{-1}(\mathbf{q}) = \sum_{q'} \Theta\left(\sigma(\mathbf{q}') - \epsilon\right) \frac{|c(\mathbf{q},\mathbf{q}')\rangle\langle c(\mathbf{q},\mathbf{q}')|}{\sigma^2(\mathbf{q},\mathbf{q}')}, \tag{18}$$

where $|c(\mathbf{q},\mathbf{q}')\rangle$ are eigenvectors of $T(\mathbf{q})$ and ϵ is a small regularization parameter. The optimum value of ϵ is determined by several factors including the level of noise in the data. The regularization parameter also serves to set the spatial resolution of the reconstruction.

In Fig. 1 we illustrate the depth resolution for the three types of the boundary conditions and two possible arrangements of sources and detectors (on the same or different planes). The plots in Fig. 1 represent the reconstructed value of $\delta\alpha$ along the line perpendicular to the $z = 0$ plane and intersecting a single absorbing inhomogeneity. Evidently, the best resolution is obtained here with absorbing boundary conditions when the sources and detectors are located on different planes.

To demonstrate the robustness of the inversion procedure in the presence of noise we present three tomographic slices drawn at $z = 0.5L$, $z = 0.6L$ and $z = 0.7L$ with the forward data calculated for three point absorbers located in the plane $z = 0.5L$ as shown in Fig. 2 and absorbing boundary conditions. Gaussian noise of zero mean was added to the data function $\phi(\mathbf{q}_s, \mathbf{q}_d)$ at various levels of the noise-to-signal ratio (n) as indicated; different values of the regularization parameter were also used (see figure caption). It can be seen from the figure that when the regularization parameter is increased, the reconstructions become more stable in the presence of noise, but the depth resolution decreases.

In conclusion, we have described an inverse scattering method for the diffusion equation with general boundary conditions. We emphasize that our results are of general physical interest since they are applicable to inverse scattering with any multiply-scattered wave in the diffusion regime.

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