PHYSICAL REVIEW E, VOLUME 64, 035601(R)

Inverse scattering for the diffusion equation with general boundary conditions

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(Received 26 July 2000; published 28 August 2001)

We consider the inverse scattering problem for the diffusion equation. A solution to this problem in the form of an explicit inversion formula is derived. Computer simulations are used illustrate our approach in model systems.

DOI: 10.1103/PhysRevE.64.035601 PACS number(s): 42.30.Wb, 41.20.Jb, 42.62.Be

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 Rapid Communication 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 particles (photons in the case of light) whose energy density $u(\mathbf{r},t)$ obeys the diffusion equation

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

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

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

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 $I(\mathbf{r},\hat{\mathbf{s}}) = (1/4\pi)(cu - 3D\hat{\mathbf{s}}\cdot\nabla u)$, where c is the speed of diffusing particles in a nonscattering medium (speed of light for photons) [9,10]. We can now use Eq. (2) to obtain the intensity I_S that is measured by detectors located on one of the boundary surfaces that 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 $\mathbf{r}_d = (\boldsymbol{\rho}_d, z_d)$.

We now present the derivation of the inversion formula. We rewrite Eq. (1) in Dirac notation as

$$\partial_t|u(t)\rangle + H|u(t)\rangle = |S(t)\rangle, \quad (3)$$

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

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

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, $G(\omega) = 1/(H - i\omega)$, and the resulting solution is given by $|u(\omega)\rangle = G(\omega)|S(\omega)\rangle$.

It is conventient 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

$$H = H_0 + V, \quad (5)$$

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$$H_0 = -D_0\nabla^2 + \alpha_0, \tag{6}$$

$$V = -\nabla\cdot\delta D(\mathbf{r})\nabla + \delta\alpha(\mathbf{r}). \tag{7}$$

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 $G=G_0-G_0VG$.

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:

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

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

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:

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

where

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

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

Note that in order to obtain Eq. (12), an integration by parts was performed to evaluate the action of the operator $-\nabla\cdot\delta D\nabla$. Also, the expression (11) for g is valid as long as at least one of the variables in the pairs (z_s,z) or (z,z_d) is on the boundary surface, which is evidently the case in Eqs. (13) and (14).

We now change variables according to $\mathbf{q}_s=\mathbf{p}+\mathbf{q}/2$, $\mathbf{q}_d=\mathbf{p}-\mathbf{q}/2$, where $\mathbf{q}$ and $\mathbf{p}$ are two independent two-dimensional vectors and rewrite Eq. (12) as

$$\phi(\mathbf{p}+\mathbf{q}/2,\mathbf{p}-\mathbf{q}/2)=\int d^3r\,\exp(-i\mathbf{q}\cdot\boldsymbol{\rho})[\kappa_A(\mathbf{p},\mathbf{q};z)\,\delta\alpha(\mathbf{r})+\kappa_D(\mathbf{p},\mathbf{q};z)\,\delta D(\mathbf{r})], \tag{15}$$

with the dependence on z_s and z_d of all quantities under the integral implied. Now we notice that the transverse part of Eq. (15) is a Fourier transform that can be inverted separately from the longitudinal part. To this end we put $a(\mathbf{q},z)=\int e^{-i\mathbf{q}\cdot\boldsymbol{\rho}}\delta\alpha(\boldsymbol{\rho},z)d^2\rho$, $b(\mathbf{q},z)=\int e^{-i\mathbf{q}\cdot\boldsymbol{\rho}}\delta D(\boldsymbol{\rho},z)d^2\rho$ and arrive at the equation

$$\phi(\mathbf{p}+\mathbf{q}/2,\mathbf{p}-\mathbf{q}/2)=\int_0^L[\kappa_A(\mathbf{p},\mathbf{q};z)a(\mathbf{q},z)+\kappa_D(\mathbf{p},\mathbf{q};z)b(\mathbf{q},z)]dz. \tag{16}$$

For fixed $\mathbf{q}$, Eq. (16) defines an integral equation for $a(\mathbf{q},z)$ and $b(\mathbf{q},z)$. Recall that when f and g belong to *different* Hilbert spaces, a solution to the equation $Af=g$ is defined to be a minimizer of $\|Af-g\|$. Among all such solutions it is conventional to choose the one with minimum norm. This so-called generalized solution is unique and may be shown to be given by $f=A^*(AA^*)^{-1}g$ where A^* denotes the adjoint of the operator A [12]. Then it is readily seen that the minimum L^2 norm solution to Eq. (16) has the form

$$a(\mathbf{q},z)=\int d^2p\,d^2p'\,\kappa_A^*(\mathbf{p},\mathbf{q};z)\langle\mathbf{p}|T^{-1}(\mathbf{q})|\mathbf{p}'\rangle\times\phi(\mathbf{p}'+\mathbf{q}/2,\mathbf{p}'-\mathbf{q}/2), \tag{17}$$

$$b(\mathbf{q},z)=\int d^2p\,d^2p'\,\kappa_D^*(\mathbf{p},\mathbf{q};z)\langle\mathbf{p}|T^{-1}(\mathbf{q})|\mathbf{p}'\rangle\times\phi(\mathbf{p}'+\mathbf{q}/2,\mathbf{p}'-\mathbf{q}/2), \tag{18}$$

where the matrix elements of $T(\mathbf{q})$ are given by the overlap integral

$$\langle\mathbf{p}|T(\mathbf{q})|\mathbf{p}'\rangle=\int_0^L[\kappa_A(\mathbf{p},\mathbf{q};z)\kappa_A^*(\mathbf{p}',\mathbf{q};z)+\kappa_D(\mathbf{p},\mathbf{q};z)\kappa_D^*(\mathbf{p}',\mathbf{q};z)]dz. \tag{19}$$

It may be verified by direct substitution that Eqs. (17) and (18) satisfy Eq. (16). Note that the inversion formulas (17) and (18) can be easily generalized to the case of multiple modulation frequencies by inserting additional integrations over frequencies and taking into account the implicit dependence of all quantities in the integrals on ω.

Finally, we apply the inverse Fourier transform in the transverse direction to arrive at our main result:

$$\delta\alpha(\mathbf{r}) = \int \frac{d^2q}{(2\pi)^2} e^{i\mathbf{q}\cdot\boldsymbol{\rho}} \int d^2p\, d^2p'\, \kappa_A^*(\mathbf{p},\mathbf{q};z) \times \langle \mathbf{p}|T^{-1}(\mathbf{q})|\mathbf{p}'\rangle \phi(\mathbf{p}'+\mathbf{q}/2,\mathbf{p}'-\mathbf{q}/2), \quad (20)$$

$$\delta D(\mathbf{r}) = \int \frac{d^2q}{(2\pi)^2} e^{i\mathbf{q}\cdot\boldsymbol{\rho}} \int d^2p\, d^2p'\, \kappa_D^*(\mathbf{p},\mathbf{q};z) \times \langle \mathbf{p}|T^{-1}(\mathbf{q})|\mathbf{p}'\rangle \phi(\mathbf{p}'+\mathbf{q}/2,\mathbf{p}'-\mathbf{q}/2), \quad (21)$$

which are the required inversion formulas.

Several comments on Eqs. (20) and (21) are necessary. First, the solution we have constructed to the inverse problem is the minimum L^2 norm solution to Eq. (12) given the data function $\phi(\mathbf{q}_s,\mathbf{q}_d)$. This solution always exists and is unique [12]. Note that the uniqueness of solutions to the *nonlinear* inverse problem is a different matter [5]. Existence and uniqueness of solutions to the *linear* inverse problem is guaranteed by the results of [13]. Second, the inversion formulas (20) and (21) employ four-dimensional data to reconstruct two unknown three-dimensional functions. If only one modulation frequency is employed the problem is underdetermined and simultaneous reconstruction of $\delta\alpha$ and δD can result in a loss of image quality. A single frequency is sufficient for reconstructing either $\delta\alpha$ or δD alone, while at least two frequencies are necessary for simultaneous reconstruction. Third, in practice one must deal with discrete data. The discretized problem is, obviously, underdetermined and in principle allows multiple solutions. Although these solutions will satisfy Eq. (12) and will minimize the discrepancy norm, the inversion formulas we have constructed will pick from among these minimizers the unique solution which has the smallest L^2 norm. To obtain this solution, the integrations in Eqs. (20) and (21) must be replaced by summations over the discrete values of $\mathbf{p}$ and $\mathbf{q}$. In addition the operator T becomes a finite matrix that can be diagonalized by the usual methods of linear algebra. Note that numerical inversion of $T(\mathbf{q})$, whose determinant is extremely small, requires regularization. This may be achieved by setting

$$T^{-1}(\mathbf{q}) = \sum_{\mathbf{q}'} \Theta(\sigma(\mathbf{q}')-\epsilon) \frac{|c(\mathbf{q},\mathbf{q}')\rangle\langle c(\mathbf{q},\mathbf{q}')|}{\sigma^2(\mathbf{q},\mathbf{q}')}, \quad (22)$$

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. Fourth, it is important to note that an image reconstruction algorithm based on Eqs. (20) and (21) has, with the use of the fast Fourier transform to compute $\phi(\mathbf{q}_s,\mathbf{q}_d)$, computational complexity $O(M\log M)$, where M is the number of source-detector pairs. This should be compared with the $O(M^3)$ complexity

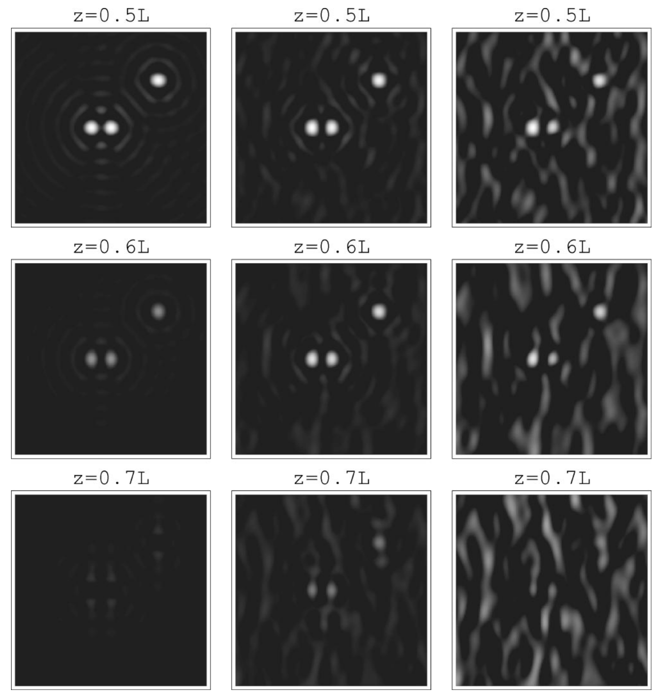

FIG. 2. Tomographic images of three point absorbers located in the $z=0.5L$ plane for different levels of noise n and different depths z. (a) $n=0$ and $\epsilon=10^{-17}$; (b) $n=1\%$ and $\epsilon=10^{-8}$; (c) $n=5\%$ and $\epsilon=10^{-8}$. The field of view is $2L\times 2L$. A linear color scale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

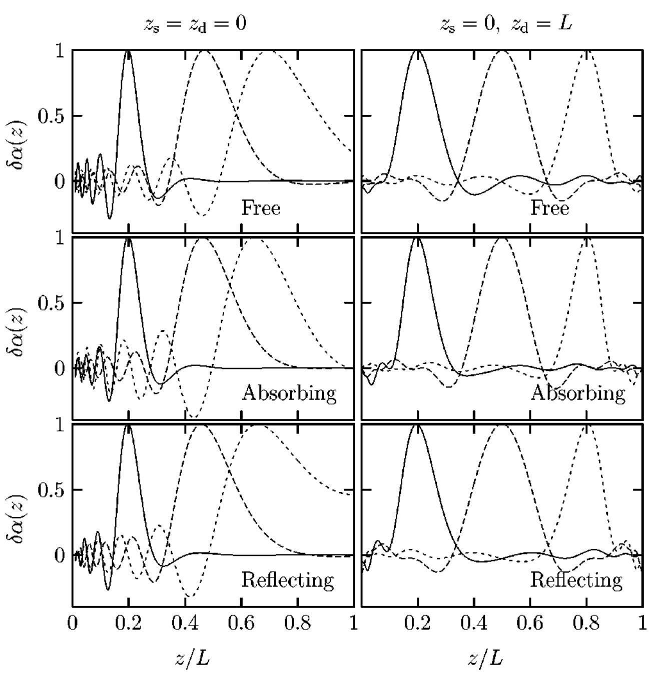

FIG. 1. Reconstruction of a point absorber that is located at $z/L=0.2$ (solid line), $z/L=0.5$ (long dash), and $z/L=0.8$ (short dash). The reconstructed value of $\delta\alpha$ is normalized by its maximum value.

of a direct numerical inversion of the integral equation (15). Finally, the inversion formulas presented here may be used as the basis for an alternative nonlinear reconstruction algorithm via a simplified Newton's method [5,14] in which the generalized inverse of the functional derivative of the nonlinear forward scattering operator is computed from Eqs. (20) and (21).

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 Eq. (15) by one or more delta functions. The numerical integrations in Eqs. (20) and (21) 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 wave vectors $\mathbf{p}$ which were chosen on a line ranging in length from 0 to $M\Delta q$.

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 as indicated.

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.

We wish to thank Dr. P. Scott Carney for valuable discussions. This research was supported in part by a grant from the NIH.

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