Reduced Hamiltonian in ray tracing systems for anisotropic inhomogeneous media

Vlastislav Červený

Department of Geophysics, Faculty of Mathematics and Physics,
Charles University, Ke Karlovu 3, 121 16 Praha 2, Czech Republic.
E-mail vcerveny@seis.karlov.mff.cuni.cz

Summary

The reduced Hamiltonian and its applications in the ray theory of isotropic inhomogeneous media have been well known for a long time. In this article, an analogous reduced Hamiltonian is introduced for anisotropic inhomogeneous media. The reduced Hamiltonian is closely connected with the evolution Hamilton-Jacobi equation, with the factorization of the elastodynamic equation, and with the parabolic equation method. The determination of the reduced Hamiltonian is based on the same 6×6 eigenvalue problem which has been successfully exploited in the 6×6 propagator techniques for 1-D anisotropic inhomogeneous media and in the computation of 6×6 R/T coefficients from anisotropic transition layers. The reduced Hamiltonian ray tracing system, consisting of four ordinary differential equations of the first order, applicable to inhomogeneous anisotropic media, is derived and discussed. It is proved that this system remains valid even for P and S waves propagating in isotropic inhomogeneous media, where it yields the well-known results.

1 Introduction

We shall consider a smooth anisotropic laterally varying elastic medium, and Cartesian coordinates x_i. The eikonal equation for an arbitrarily selected elementary wave propagating in this medium can be expressed in the general Hamiltonian form,

$$\mathcal{H}(x_i, p_i) = 0 \ , \qquad i = 1, 2, 3 \ , \tag{1}$$

where p_i are Cartesian components of slowness vector $\vec{p}(x_i) = \nabla T(x_i)$, and $T(x_i)$ is the travel time. Equation (1) represents a nonlinear partial differential equation of the first order, and is also sometimes called the stationary Hamilton-Jacobi equation. As usually, we shall call $\mathcal{H}(x_i, p_i)$ the Hamiltonian. In the seismic ray theory, the Hamiltonian is usually expressed in terms of $G(x_i, p_i)$, an eigenvalue of the Christoffel matrix $\Gamma_{ik} = a_{ijkl}p_jp_l$, using the relation $\mathcal{H}(x_i, p_i) = \frac{1}{2}[G(x_i, p_i) - 1]$. Here a_{ijkl} are density normalized elastic moduli c_{ijkl}, $a_{ijkl} = \rho^{-1}c_{ijkl}$.

The Hamiltonian ray tracing system reads

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$$\frac{\mathrm{d}x_i}{\mathrm{d}u} = \frac{\partial \mathcal{H}}{\partial p_i} \ , \quad \frac{\mathrm{d}p_i}{\mathrm{d}u} = -\frac{\partial \mathcal{H}}{\partial x_i} \ , \qquad i = 1, 2, 3 \ . \tag{2}$$

Quantity u represents a suitable parameter along the ray trajectory. Hamiltonian $\mathcal{H}(x_i, p_i)$ is invariant along the whole ray. Once $\mathcal{H}(x_i, p_i) = 0$ is valid at an initial point of the ray, it is valid along the whole ray. This is the reason why we speak of the stationary Hamilton-Jacobi equation. Travel time $T(x_i)$ can be calculated along the ray using the relation

$$\frac{\mathrm{d}T}{\mathrm{d}u} = p_i \frac{\partial \mathcal{H}}{\partial p_i} \ . \tag{3}$$

If we use the standard form of Hamiltonian $\mathcal{H} = \frac{1}{2}(G - 1)$, we obtain $\mathrm{d}T/\mathrm{d}u = 1$, as G is a homogeneous function of the second degree in p_i, and $\mathrm{d}T/\mathrm{d}u = \frac{1}{2} p_i \partial G/\partial p_i = 1$. Then ray tracing system (2) reads

$$\frac{\mathrm{d}x_i}{\mathrm{d}T} = \frac{\partial \mathcal{H}}{\partial p_i} = \frac{1}{2}\frac{\partial G}{\partial p_i} \ , \quad \frac{\mathrm{d}p_i}{\mathrm{d}T} = -\frac{\partial \mathcal{H}}{\partial x_i} = -\frac{1}{2}\frac{\partial G}{\partial p_i} \ . \tag{4}$$

System (2) consists of six ordinary differential equations of the first order. The number of equations in each of these systems may be reduced from six to four. One of the equations for p_i can be replaced by the eikonal equation, and one of the equations for x_i can be removed by taking variable u along the ray equal to one of the three coordinates x_i. The general procedure of deriving the reduced ray tracing system is based on the so-called reduced Hamiltonian, see Červený (2001, pp. 107-8). The procedure has been applied to isotropic inhomogeneous media; here we shall apply it to anisotropic inhomogeneous media.

To be more specific, we consider Cartesian coordinate x_3 to be parameter u along the ray. In addition, we solve the eikonal equation (1) for p_3 and denote

$$p_3 = -\mathcal{H}^R(x_i, p_I) \ , \qquad i = 1, 2, 3 \ , \qquad I = 1, 2 \ . \tag{5}$$

Function $\mathcal{H}^R(x_i, p_I)$ is called the *reduced Hamiltonian.* Please note that it depends only on p_1, p_2, not on p_3.

It is well known that Equation (1) represents the slowness surface of the wave under consideration. Similarly, also Equation (5) represents the slowness surface. The difference is that Equation (5) is an explicit, but Equation (1) an implicit equation of the slowness surface. The slowness surface is a closed, centrally symmetric surface. This implies that Equation (5) represents only one half of the slowness surface, when the sign "–" is fixed. Actually, it would be possible to choose also the sign "+" in (5), instead of "–". The sign "–" in (5) is taken for convenience, as it corresponds to the classical form of the Hamilton-Jacobi equation:

$$p_3 + \mathcal{H}^R(x_i, p_I) = 0 \ . \tag{6}$$

As we shall show later, reduced Hamiltonian $\mathcal{H}^R(x_i, p_I)$ is not constant along the ray (it equals $-p_3$). This is the reason why Equation (6) is often called the evolution Hamilton-Jacobi equation in mathematical literature. See, for example, Crandall and Lions (1983). The terms stationary and evolution emphasize the difference between Equations (1) and (6). The stationary Hamilton-Jacobi equation (1) may be used not only for p_3 positive or negative, but also for $p_3 = 0$. The evolution Hamilton-Jacobi equation (6) is, however, only a one-way equation. For the sign of $\mathcal{H}^R(x_i, p_I)$ specified, Equation (6) corresponds either to p_3 positive or to p_3 negative. The case of $p_3 = 0$ is excluded. See the more detailed discussion below.

A brief remark to notations. The capital indices $I, J, K, ...$ take the values of 1,2, the lower-case indices $i, j, k, ...$ the values of 1,2,3, and the Greek indices $\alpha, \beta, ...$ the values of 1,2,3,4,5,6. The Einstein summation convention with respect to repetitive indices is used throughout the paper. To distinguish between the 3×3 and 6×6 matrices used in the paper, the 3×3 matrices are denoted by a circumflex above the letter.

2 Reduced Hamiltonian ray tracing system

The basic step in the derivation of the reduced Hamiltonian ray tracing system consists in the definition of Hamiltonian (1) using reduced Hamiltonian $\mathcal{H}^R(x_i, p_I)$ as follows:

$$\mathcal{H}(x_i, p_i) = p_3 + \mathcal{H}^R(x_i, p_I) = 0 \ . \tag{7}$$

For $u = x_3$, the ray tracing system (2) reads:

$$\begin{aligned}
\frac{\mathrm{d}x_1}{\mathrm{d}x_3} &= \frac{\partial \mathcal{H}^R}{\partial p_1} \ , & \frac{\mathrm{d}p_1}{\mathrm{d}x_3} &= -\frac{\partial \mathcal{H}^R}{\partial x_1} \ , \\
\frac{\mathrm{d}x_2}{\mathrm{d}x_3} &= \frac{\partial \mathcal{H}^R}{\partial p_2} \ , & \frac{\mathrm{d}p_2}{\mathrm{d}x_3} &= -\frac{\partial \mathcal{H}^R}{\partial x_2} \ , \\
\frac{\mathrm{d}x_3}{\mathrm{d}x_3} &= 1 \ , & \frac{\mathrm{d}p_3}{\mathrm{d}x_3} &= -\frac{\partial \mathcal{H}^R}{\partial x_3} \ .
\end{aligned}$$

The equation for $\mathrm{d}p_3/\mathrm{d}x_3$, however, may be removed, as it may be replaced by equation $p_3 = -\mathcal{H}^R(x_i, p_I)$. Thus, we obtain

$$\frac{\mathrm{d}x_I}{\mathrm{d}x_3} = \frac{\partial \mathcal{H}^R}{\partial p_I} \ , \qquad \frac{\mathrm{d}p_I}{\mathrm{d}x_3} = -\frac{\partial \mathcal{H}^R}{\partial x_I} \ . \tag{8}$$

This is the final system of four ordinary differential equations of the first order for the ray. We shall call it the *reduced Hamiltonian ray tracing system.*

System (8) should be supplemented by Equation (5) for p_3 and by Equation (3) for the calculation of travel time. Using $u = x_3$ and (7), Equation (3) yields

$$\frac{\mathrm{d}T}{\mathrm{d}x_3} = p_3 + p_I \frac{\partial \mathcal{H}^R}{\partial p_I} = p_I \frac{\partial \mathcal{H}^R}{\partial p_I} - \mathcal{H}^R \ . \tag{9}$$

System (8) with (9) is valid both for isotropic and anisotropic media. In isotropic media, the equations simplify, as the reduced Hamiltonian can be found analytically. See Červený (2001, p. 1078), and Section 5. In anisotropic media, however, analytical expressions for $\mathcal{H}^R(x_i, p_I)$ are not available, and some other approach must be chosen to express the reduced Hamiltonian ray tracing system (8) in a more suitable form.

For anisotropic media, the basic problem in the procedure consists in the solution of the eikonal equation for p_3, with p_1 and p_2 being fixed. This problem has a long tradition in the solution of the R/T problem at an interface between two anisotropic media. It is well known that p_3 can be determined by solving an algebraic equation of the sixth order.

The numerical determination of $p_3 = -\mathcal{H}^R$ is not, however, sufficient to apply ray tracing using system (8); for this we also have to know the derivatives $\partial p_3/\partial p_I (= -\partial\mathcal{H}^R/\partial p_I)$ and $\partial p_3/\partial x_I (= -\partial\mathcal{H}^R/\partial x_I)$.

In Section 3, a straightforward and simple procedure to determine $\partial p_3/\partial p_I$ and $\partial p_3/\partial x_I$ is proposed. It is based on the fact that p_3 are eigenvalues of a 6×6 matrix $\mathbf{A}$. Matrix $\mathbf{A}$ depends just on x_i and p_I, not on p_3. For the definition and properties of the 6×6 matrix $\mathbf{A}$, its eigenvalues and eigenvectors, see Section 4.

The reduced Hamiltonian and the reduced Hamiltonian ray tracing system are closely connected with the evolution Hamilton-Jacobi equation. This equation has found applications in the solution of many important one-way wave propagation problems in isotropic inhomogeneous media. Let us mention the factorization of the acoustic and elastodynamic wave equation, the parabolic wave equation method (ocean acoustics, seismic exploration), finite-difference travel-time computations, etc. Consequently, the generalization of the method for inhomogeneous anisotropic media may be of some interest. As far as the author knows, Thomson (1999) was the first who performed the factorization of the elastodynamic equation for general inhomogeneous anisotropic media. In fact, his Equation (3.7) corresponds strictly to our Equation (8) (with $\mathcal{H}^R = -p_3$).

Reduced Hamiltonian $\mathcal{H}^R(x_i, p_I)$ is not constant along ray (8), only the quantity $p_3 + \mathcal{H}^R(x_i, p_I)$ is constant and equals zero. Thus, $\mathcal{H}^R(x_i, p_I) = -p_3$ along the whole ray.

It should be emphasized once again that the reduced Hamiltonian ray tracing system (8) is applicable only to one-way propagation (with respect to the x_3-coordinate). If reduced Hamiltonian $\mathcal{H}^R(x_i, p_I)$ is specified by (7), ray tracing system (8) corresponds to forward propagation, in the direction of x_3 increasing. For backward propagation, it would be necessary to change the sign of $\mathcal{H}^R(x_i, p_I)$. At the turning point, at which $p_3 = 0$, ray tracing system (8) fails.

3 Determination of the reduced Hamiltonian and its derivatives

We shall assume that p_3 is an eigenvalue of a 6×6 matrix $\mathbf{A}$. (For the definition of matrix $\mathbf{A}$ see the next section). We wish to determine derivatives $\partial p_3/\partial x_I$ and $\partial p_3/\partial p_I$ in terms of derivatives $\partial \mathbf{A}/\partial x_I$ and $\partial \mathbf{A}/\partial p_I$. The eigenvalue equation reads

$$\mathbf{A}\mathbf{W} = \mathbf{W} p_3 \ , \tag{10}$$

where $\mathbf{W}$ is a 6×1 eigenvector corresponding to the eigenvalue p_3 under consideration.

The actual matrix $\mathbf{A}$ in (10) is not symmetrical, and the eigenvectors $\mathbf{W}_\alpha$ ($\alpha = 1, 2, ..., 6$) are not orthogonal. It will, however, be shown in Section 4 that $\mathbf{A}$ can be symmetrized by multiplying it from the left by the 6×6 matrix $\mathbf{I}_1$,

$$\mathbf{I}_1 = \begin{pmatrix} \hat{\mathbf{0}} & \hat{\mathbf{I}} \\ \hat{\mathbf{I}} & \hat{\mathbf{0}} \end{pmatrix} , \tag{11}$$

where $\hat{\mathbf{0}}$ is a 3×3 null matrix and $\hat{\mathbf{I}}$ a 3×3 identity matrix. Thus, $\mathbf{I}_1\mathbf{A}$ is symmetrical. Matrix $\mathbf{I}_1$ is a 6×6 analogue of the well-known 2×2 Pauli matrix. If we multiply (10) by $\mathbf{W}^T\mathbf{I}_1$ from the left, we obtain

$$\mathbf{W}^T\mathbf{I}_1\mathbf{A}\mathbf{W} = \mathbf{W}^T\mathbf{I}_1\mathbf{W}p_3 \ . \tag{12}$$

This yields

$$p_3 = \frac{\mathbf{W}^T\mathbf{I}_1\mathbf{A}\mathbf{W}}{\mathbf{W}^T\mathbf{I}_1\mathbf{W}} \ . \tag{13}$$

This is the expression for p_3 in terms of matrix $\mathbf{A}$ and of its eigenvectors (corresponding to the selected p_3).

Using (13), we shall find expressions for $\partial p_3/\partial x_I$ and $\partial p_3/\partial p_I$. We denote any of these partial derivatives by $p_3^{'}$. From (13), we obtain

$$\begin{aligned} p_3^{'} &= [(\mathbf{W}^T\mathbf{I}_1\mathbf{A}\mathbf{W})/(\mathbf{W}^T\mathbf{I}_1\mathbf{W})]^{'} \\ &= [(\mathbf{W}^{T\prime}\mathbf{I}_1\mathbf{A}\mathbf{W} + \mathbf{W}^T\mathbf{I}_1\mathbf{A}^{'}\mathbf{W} + \mathbf{W}^T\mathbf{I}_1\mathbf{A}\mathbf{W}^{'})(\mathbf{W}^T\mathbf{I}_1\mathbf{W}) - (\mathbf{W}^T\mathbf{I}_1\mathbf{A}\mathbf{W})(\mathbf{W}^T\mathbf{I}_1\mathbf{W})^{'}] \\ &\quad /(\mathbf{W}^T\mathbf{I}_1\mathbf{W})^2 \ . \end{aligned}$$

We now insert $\mathbf{A}\mathbf{W} = \mathbf{W}p_3$, and the relation $\mathbf{W}^T\mathbf{I}_1\mathbf{A} = \mathbf{W}^T\mathbf{I}_1p_3$, following from (10) and from the fact that $\mathbf{I}_1\mathbf{A}$ is symmetrical. This yields

$$\begin{aligned} p_3^{'} &= (\mathbf{W}^T\mathbf{I}_1\mathbf{A}^{'}\mathbf{W})/(\mathbf{W}^T\mathbf{I}_1\mathbf{W}) \\ &+ [(\mathbf{W}^{T\prime}\mathbf{I}_1\mathbf{W} + \mathbf{W}^T\mathbf{I}_1\mathbf{W}^{'})p_3(\mathbf{W}^T\mathbf{I}_1\mathbf{W}) - (\mathbf{W}^T\mathbf{I}_1\mathbf{W})p_3(\mathbf{W}^T\mathbf{I}_1\mathbf{W})^{'}]/(\mathbf{W}^T\mathbf{I}_1\mathbf{W})^2 \ . \end{aligned}$$

As $\mathbf{W}^{T\prime}\mathbf{I}_1\mathbf{W} + \mathbf{W}^T\mathbf{I}_1\mathbf{W}^{'} = (\mathbf{W}^T\mathbf{I}_1\mathbf{W})^{'}$, the second term vanishes. Thus, the final result is

$$p_3^{'} = \frac{\mathbf{W}^T\mathbf{I}_1\mathbf{A}^{'}\mathbf{W}}{\mathbf{W}^T\mathbf{I}_1\mathbf{W}} \ . \tag{14}$$

This is the result we have been looking for. It expresses the partial derivatives of p_3 in terms of the partial derivatives of $\mathbf{A}$.

The final form of the reduced Hamiltonian ray tracing system (8) is as follows:

$$\frac{\mathrm{d}x_I}{\mathrm{d}x_3} = -\frac{1}{\mathbf{W}^T\mathbf{I}_1\mathbf{W}}\mathbf{W}^T\mathbf{I}_1\frac{\partial\mathbf{A}}{\partial p_I}\mathbf{W} \ , \qquad \frac{\mathrm{d}p_I}{\mathrm{d}x_3} = \frac{1}{\mathbf{W}^T\mathbf{I}_1\mathbf{W}}\mathbf{W}^T\mathbf{I}_1\frac{\partial\mathbf{A}}{\partial x_I}\mathbf{W} \ . \tag{15}$$

This ray tracing system contains the 6×6 matrix $\mathbf{A}$, and its 6×1 eigenvectors. Actually, we can replace these 6×6 and 6×1 matrices by 3×3 and 3×1 matrices. We denote

$$\mathbf{D} = \mathbf{I}_1\mathbf{A} = \begin{pmatrix} \hat{\mathbf{D}}_{11} & \hat{\mathbf{D}}_{12} \\ \hat{\mathbf{D}}_{12}^T & \hat{\mathbf{D}}_{22} \end{pmatrix} \ , \qquad \mathbf{W} = \begin{pmatrix} \hat{\mathbf{G}} \\ -\hat{\mathbf{X}} \end{pmatrix} \ . \tag{16}$$

Here $\hat{\mathbf{D}}_{IJ}$ are 3×3 matrices, $\hat{\mathbf{G}}$ and $\hat{\mathbf{X}}$ 3×1 collumn matrices. Suitable expressions for these matrices will be given in Section 4. Ray tracing system (15) then yields

$$\begin{aligned} \frac{\mathrm{d}x_I}{\mathrm{d}x_3} &= (\hat{\mathbf{G}}^T\frac{\partial\hat{\mathbf{D}}_{11}}{\partial p_I}\hat{\mathbf{G}} - 2\hat{\mathbf{G}}^T\frac{\partial\hat{\mathbf{D}}_{12}}{\partial p_I}\hat{\mathbf{X}} + \hat{\mathbf{X}}^T\frac{\partial\hat{\mathbf{D}}_{22}}{\partial p_I}\hat{\mathbf{X}})/2(\hat{\mathbf{G}}^T\hat{\mathbf{X}}) \ , \\ \frac{\mathrm{d}p_I}{\mathrm{d}x_3} &= -(\hat{\mathbf{G}}^T\frac{\partial\hat{\mathbf{D}}_{11}}{\partial x_I}\hat{\mathbf{G}} - 2\hat{\mathbf{G}}^T\frac{\partial\hat{\mathbf{D}}_{12}}{\partial x_I}\hat{\mathbf{X}} + \hat{\mathbf{X}}^T\frac{\partial\hat{\mathbf{D}}_{22}}{\partial x_I}\hat{\mathbf{X}})/2(\hat{\mathbf{G}}^T\hat{\mathbf{X}}) \ . \end{aligned} \tag{17}$$

4 6×6 matrix $\mathbf{A}$ and its 6×1 eigenvectors $\mathbf{W}$

The 6×6 matrix $\mathbf{A}$ with eigenvalues equal to p_3 has been well known in the seismological literature for a long time. It has been used in the 6×6 propagator technique developed for computing the complete wave field in 1-D isotropic and anisotropic media. As a special case of this, it has also been used in the computation of 6×6 R/T coefficients from transition layers, and in the reflectivity method. For anisotropic media, see, for example, Frazer and Fryer (1989), Chapman (1994), Thomson (1996). For a detailed derivation and discussion, see Červený (2001, Section 5.4.7), where also many other references can be found. Recently, it has also been used in the factorization of the elastodynamic equation, in one-way propagation, in the propagation of surface waves and in the parabolic equation method. See Martin and Thomson (1997), Thomson (1999).

We shall not derive the individual expressions for $\mathbf{A}$, we only refer the reader to Červený (2001, Section 5.4.7). We introduce the 3×3 matrices $\hat{\mathbf{C}}_{jl}$ by the relation

$$\hat{\mathbf{C}}_{jl} = c_{ijkl} \ , \qquad i,j,k,l = 1,2,3 \ . \tag{18}$$

where c_{ijkl} are elastic moduli for anisotropic media. To understand the physical meaning of these matrices more clearly, we shall present them in the Voigt notation:

$$\begin{aligned}
\hat{\mathbf{C}}_{11} &= \begin{pmatrix} C_{11} & C_{16} & C_{15} \\ C_{16} & C_{66} & C_{56} \\ C_{15} & C_{56} & C_{55} \end{pmatrix} , &\qquad \hat{\mathbf{C}}_{22} &= \begin{pmatrix} C_{66} & C_{26} & C_{46} \\ C_{26} & C_{22} & C_{24} \\ C_{46} & C_{24} & C_{44} \end{pmatrix} , \\
\hat{\mathbf{C}}_{33} &= \begin{pmatrix} C_{55} & C_{45} & C_{35} \\ C_{45} & C_{44} & C_{34} \\ C_{35} & C_{34} & C_{33} \end{pmatrix} , &\qquad \hat{\mathbf{C}}_{12} = \hat{\mathbf{C}}_{21}^T &= \begin{pmatrix} C_{16} & C_{12} & C_{14} \\ C_{66} & C_{26} & C_{46} \\ C_{56} & C_{25} & C_{45} \end{pmatrix} , \\
\hat{\mathbf{C}}_{13} = \hat{\mathbf{C}}_{31}^T &= \begin{pmatrix} C_{15} & C_{14} & C_{13} \\ C_{56} & C_{46} & C_{36} \\ C_{55} & C_{45} & C_{35} \end{pmatrix} , &\qquad \hat{\mathbf{C}}_{23} = \hat{\mathbf{C}}_{32}^T &= \begin{pmatrix} C_{56} & C_{46} & C_{36} \\ C_{25} & C_{24} & C_{23} \\ C_{45} & C_{44} & C_{34} \end{pmatrix} ,
\end{aligned} \tag{19}$$

The 6×6 matrix $\mathbf{A}$ is then defined by the relation

$$\mathbf{A} = \begin{pmatrix} \hat{\mathbf{A}}_{11} & \hat{\mathbf{A}}_{12} \\ \hat{\mathbf{A}}_{21} & \hat{\mathbf{A}}_{22} \end{pmatrix} , \tag{20}$$

where the 3×3 matrices $\hat{\mathbf{A}}_{IJ}$ are expressed in terms of $\hat{\mathbf{C}}_{ij}$ and p_I as follows,

$$\begin{aligned}
\hat{\mathbf{A}}_{11} &= -p_L \hat{\mathbf{C}}_{33}^{-1} \hat{\mathbf{C}}_{3L} \ , \\
\hat{\mathbf{A}}_{12} &= -\hat{\mathbf{C}}_{33}^{-1} \ , \\
\hat{\mathbf{A}}_{21} &= -\rho \hat{\mathbf{I}} + p_J p_L (\hat{\mathbf{C}}_{JL} - \hat{\mathbf{C}}_{J3} \hat{\mathbf{C}}_{33}^{-1} \hat{\mathbf{C}}_{3L}) \ , \\
\hat{\mathbf{A}}_{22} &= -p_J \hat{\mathbf{C}}_{J3} \hat{\mathbf{C}}_{33}^{-1} = \hat{\mathbf{A}}_{11}^T \ .
\end{aligned} \tag{21}$$

We shall also present here the symmetrical 6×6 matrix $\mathbf{D} = \mathbf{I}_1 \mathbf{A}$:

$$\mathbf{D} = \mathbf{I}_1 \mathbf{A} = \begin{pmatrix} \hat{\mathbf{D}}_{11} & \hat{\mathbf{D}}_{12} \\ \hat{\mathbf{D}}_{21} & \hat{\mathbf{D}}_{22} \end{pmatrix} = \begin{pmatrix} \hat{\mathbf{A}}_{21} & \hat{\mathbf{A}}_{22} \\ \hat{\mathbf{A}}_{11} & \hat{\mathbf{A}}_{12} \end{pmatrix} , \tag{22}$$

where

$$\begin{aligned}
\hat{\mathbf{D}}_{11} &= -\rho \hat{\mathbf{I}} + p_J p_L (\hat{\mathbf{C}}_{JL} - \hat{\mathbf{C}}_{J3} \hat{\mathbf{C}}_{33}^{-1} \hat{\mathbf{C}}_{3L}) \ , \\
\hat{\mathbf{D}}_{12} &= \hat{\mathbf{D}}_{21}^T = -p_L \hat{\mathbf{C}}_{L3} \hat{\mathbf{C}}_{33}^{-1} \ , \\
\hat{\mathbf{D}}_{22} &= -\hat{\mathbf{C}}_{33}^{-1} \ .
\end{aligned} \tag{23}$$

It is easy to see that the 6×6 matrix $\mathbf{D}$ is symmetrical.

It may also be useful to introduce the 3×3 matrices $\hat{\mathbf{A}}_L$ and $\hat{\mathbf{B}}_{JL}$:

$$\hat{\mathbf{A}}_L = \hat{\mathbf{C}}_{33}^{-1}\hat{\mathbf{C}}_{3L} \ , \quad \hat{\mathbf{B}}_{JL} = \hat{\mathbf{C}}_{JL} - \hat{\mathbf{C}}_{J3}\hat{\mathbf{C}}_{33}^{-1}\hat{\mathbf{C}}_{3L} \ . \tag{24}$$

The 3×3 matrices $\hat{\mathbf{D}}_{IJ}$ then read, see (23) and (24)

$$\begin{aligned}
\hat{\mathbf{D}}_{11} &= -\rho\hat{\mathbf{I}} + p_J p_L \hat{\mathbf{B}}_{JL} \ , \\
\hat{\mathbf{D}}_{12} &= \hat{\mathbf{D}}_{21}^T = -p_L \hat{\mathbf{A}}_L^T \ , \\
\hat{\mathbf{D}}_{22} &= -\hat{\mathbf{C}}_{33}^{-1} \ .
\end{aligned} \tag{25}$$

Note that $\hat{\mathbf{A}}_L$ and $\hat{\mathbf{B}}_{JL}$ do not depend on p_I.

Now we shall discuss the determination of eigenvectors $\mathbf{W}_\alpha$, $\alpha = 1, 2, ..., 6$. As soon as eigenvalue p_3 is known, the relevant eigenvectors $\mathbf{W}$ can be determined from (10). Actually, it is possible to determine it in a simpler way, proposed in Červený (2001, Section 5.4.7). We determine the 3×3 Christoffel matrix $\Gamma_{ik} = c_{ijkl}p_j p_l$ and its eigenvector $\vec{g}$ corresponding to the wave under consideration. We can then express $\mathbf{W}$ analytically:

$$\mathbf{W} = (g_1, g_2, g_3, -X_1, -X_2, -X_3)^T \ , \tag{26}$$

where

$$X_i = c_{i3kl} g_k p_l \ . \tag{27}$$

Thus,

$$\mathbf{W} = \begin{pmatrix} \hat{\mathbf{G}} \\ -\hat{\mathbf{X}} \end{pmatrix} , \tag{28}$$

where

$$\hat{\mathbf{G}} = (g_1, g_2, g_3)^T \ , \qquad \hat{\mathbf{X}} = (X_1, X_2, X_3)^T \ . \tag{29}$$

Note that eigenvectors $\mathbf{W}_\alpha$, $\alpha = 1, 2, ..., 6$, are not orthogonal, but matrix $\mathbf{W}_\alpha^T \mathbf{I}_1 \mathbf{W}_\beta$, is diagonal in the following sense

$$\begin{aligned}
\mathbf{W}_\alpha^T \mathbf{I}_1 \mathbf{W}_\beta &= 0 \qquad\qquad \text{for } \alpha \neq \beta \ , \\
\mathbf{W}_\alpha^T \mathbf{I}_1 \mathbf{W}_\beta &= -2\rho\mathcal{U}_3 \qquad \text{for } \alpha = \beta \ .
\end{aligned} \tag{30}$$

We then speak of the I_1-orthogonality of eigenvectors $\mathbf{W}_\alpha$, $i = 1, 2, ..., 6$, see Frazer and Fryer (1989). The validity of (30) for $\alpha = \beta$ can be proved simply:

$$\mathbf{W}_\alpha^T \mathbf{I}_1 \mathbf{W}_\alpha = (\hat{\mathbf{G}}^T, -\hat{\mathbf{X}}^T) \begin{pmatrix} \hat{\mathbf{0}} & \hat{\mathbf{I}} \\ \hat{\mathbf{I}} & \hat{\mathbf{0}} \end{pmatrix} \begin{pmatrix} \hat{\mathbf{G}} \\ -\hat{\mathbf{X}} \end{pmatrix} = -2\hat{\mathbf{G}}^T\hat{\mathbf{X}} = -2\rho\mathcal{U}_3 \ . \tag{31}$$

Here $\mathcal{U}_3$ is the Cartesian component of the group velocity vector.

A note on the elastic moduli c_{ijkl}. Instead of c_{ijkl}, density normalized elastic moduli $a_{ijkl} = c_{ijkl}/\rho$ have often been used. They have the dimension of (velocity)^2. Indeed, all the expressions given in this contribution remain valid if a_{ijkl} are used instead of c_{ijkl} in (18) and (27), and if the density ρ is replaced by unity in (21), (23), (25), (30) and (31). Using (24), ray tracing system (17) can then be expressed in the following form:

$$\begin{aligned}
\frac{\mathrm{d}x_I}{\mathrm{d}x_3} &= [p_K \hat{\mathbf{G}}^T(\hat{\mathbf{B}}_{IK} + \hat{\mathbf{B}}_{KI})\hat{\mathbf{G}} + 2\hat{\mathbf{G}}^T\mathbf{A}_I^T\hat{\mathbf{X}}]/2(\hat{\mathbf{G}}^T\hat{\mathbf{X}}) \ , \\
\frac{\mathrm{d}p_I}{\mathrm{d}x_3} &= -[p_K p_L \hat{\mathbf{G}}^T \frac{\partial\hat{\mathbf{B}}_{KL}}{\partial x_I}\hat{\mathbf{G}} + 2p_K\hat{\mathbf{G}}^T\frac{\partial\hat{\mathbf{A}}_K^T}{\partial x_I}\hat{\mathbf{X}} - \hat{\mathbf{X}}^T\frac{\partial\hat{\mathbf{C}}_{33}^{-1}}{\partial x_I}\hat{\mathbf{X}}]/2(\hat{\mathbf{G}}^T\hat{\mathbf{X}}) \ ,
\end{aligned} \tag{32}$$

where $\hat{\mathbf{G}}^T\hat{\mathbf{X}} = \mathcal{U}_3$.

5 Isotropic media

The reduced Hamiltonian ray tracing systems (15), (17) and (32), derived for general anisotropic inhomogeneous media, must remain valid even for isotropic media. For isotropic media, however, the reduced Hamiltonian ray tracing systems may also be simply derived analytically. We shall first present these analytical solutions, as they are very transparent. Only then, shall we show that general ray tracing system (32) yields the same results for isotropic media.

The stationary Hamilton-Jacobi equation (1), representing the eikonal equation, reads

$$\mathcal{H}(x_i, p_i) = \tfrac{1}{2}(V^2 p_i p_i - 1) = 0 \ . \tag{33}$$

Here $V = \alpha$ for P waves, and $V = \beta$ for S waves. The solution for p_3 is

$$p_3 + \mathcal{H}^R(x_i, p_I) = 0 \ , \tag{34}$$

where

$$\mathcal{H}^R(x_i, p_I) = -[V^{-2}(x_i) - p_1^2 - p_2^2]^{1/2} \ . \tag{35}$$

The sign "–" in (35) corresponds to the one-way propagation in the direction of increasing x_3. For the opposite direction of propagation, it would be necessary to take "+" in (35). Reduced Hamiltonian ray tracing system (7) then reads

$$\begin{aligned} \frac{\mathrm{d}x_I}{\mathrm{d}x_3} &= \frac{V p_I}{[1 - V^2(p_1^2 + p_2^2)]^{1/2}} \ , \\ \frac{\mathrm{d}p_I}{\mathrm{d}x_3} &= \frac{1}{[1 - V^2(p_1^2 + p_2^2)]^{1/2}} \frac{\partial}{\partial x_I}\left(\frac{1}{V}\right) \ . \end{aligned} \tag{36}$$

For travel time T, we can use (9):

$$\frac{\mathrm{d}T}{\mathrm{d}x_3} = [V^{-2} - p_1^2 - p_2^2]^{1/2} + p_i p_i [V^{-2} - p_1^2 - p_2^2]^{-1/2} = V^{-2}[V^{-2} - p_1^2 - p_2^2]^{-1/2} \ . \tag{37}$$

Equations (33)–(37) yield the complete solution for isotropic inhomogeneous media.

Now we would like to check whether the general equations derived in Sections 2–4 for anisotropic media would yield the same equations (34)–(37), if they were specified for isotropic media. Instead of elastic moduli c_{ijkl}, we shall consider the density normalized elastic moduli. Consequently, we can start from (32).

We shall first specify the 3×3 matrices $\hat{\mathbf{C}}_{jl}$, given by (19). In the Voigt notation, for isotropic media,

$$\begin{aligned} &C_{11} = C_{22} = C_{33} = \alpha^2 \ , \qquad C_{44} = C_{55} = C_{66} = \beta^2 \ , \\ &C_{12} = C_{21} = C_{13} = C_{31} = C_{23} = C_{32} = \alpha^2 - 2\beta^2 \ . \end{aligned} \tag{38}$$

All other C_{ij} vanish. The 3×3 matrices $\hat{\mathbf{C}}_{kl}$, given by (19), then read,

$$
\hat{\mathbf{C}}_{11} = \begin{pmatrix} \alpha^2 & 0 & 0 \\ 0 & \beta^2 & 0 \\ 0 & 0 & \beta^2 \end{pmatrix} , \qquad \hat{\mathbf{C}}_{22} = \begin{pmatrix} \beta^2 & 0 & 0 \\ 0 & \alpha^2 & 0 \\ 0 & 0 & \beta^2 \end{pmatrix} ,
$$

$$
\hat{\mathbf{C}}_{33} = \begin{pmatrix} \beta^2 & 0 & 0 \\ 0 & \beta^2 & 0 \\ 0 & 0 & \alpha^2 \end{pmatrix} , \qquad \hat{\mathbf{C}}_{12} = \hat{\mathbf{C}}_{21}^T = \begin{pmatrix} 0 & \alpha^2 - 2\beta^2 & 0 \\ \beta^2 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} , \tag{39}
$$

$$
\hat{\mathbf{C}}_{13} = \hat{\mathbf{C}}_{31}^T = \begin{pmatrix} 0 & 0 & \alpha^2 - 2\beta^2 \\ 0 & 0 & 0 \\ \beta^2 & 0 & 0 \end{pmatrix} , \qquad \hat{\mathbf{C}}_{23} = \hat{\mathbf{C}}_{32}^T = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \alpha^2 - 2\beta^2 \\ 0 & \beta^2 & 0 \end{pmatrix} .
$$

The 3×3 matrices $\hat{\mathbf{A}}_L$ and $\hat{\mathbf{B}}_{JL}$, given by (24), then become:

$$
\hat{\mathbf{A}}_1 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 - 2\beta^2/\alpha^2 & 0 & 0 \end{pmatrix} , \qquad \hat{\mathbf{A}}_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 - 2\beta^2/\alpha^2 & 0 \end{pmatrix} ,
$$

$$
\hat{\mathbf{B}}_{11} = \begin{pmatrix} 4\beta^2(1 - \beta^2/\alpha^2) & 0 & 0 \\ 0 & \beta^2 & 0 \\ 0 & 0 & 0 \end{pmatrix} , \qquad \hat{\mathbf{B}}_{12} = \begin{pmatrix} 0 & 2\beta^2(1 - 2\beta^2/\alpha^2) & 0 \\ \beta^2 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} , \tag{40}
$$

$$
\hat{\mathbf{B}}_{21} = \begin{pmatrix} 0 & \beta^2 & 0 \\ 2\beta^2(1 - 2\beta^2/\alpha^2) & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} , \qquad \hat{\mathbf{B}}_{22} = \begin{pmatrix} \beta^2 & 0 & 0 \\ 0 & 4\beta^2(1 - \beta^2/\alpha^2) & 0 \\ 0 & 0 & 0 \end{pmatrix} .
$$

Now it is simple to construct the 6×6 system matrix $\mathbf{A}$, see (20), (21), (24) and (40),

$$
\mathbf{A} = \begin{pmatrix} 0 & 0 & -p_1 & -1/\beta^2 & 0 & 0 \\ 0 & 0 & -p_2 & 0 & -1/\beta^2 & 0 \\ -\Delta_2 p_1 & -p_2\Delta_2 & 0 & 0 & 0 & -1/\alpha^2 \\ U_1 + p_1^2\beta^2\Delta_1 & p_1 p_2 \beta^2 \Delta_1 & 0 & 0 & 0 & -p_1\Delta_2 \\ p_1 p_2 \beta^2 \Delta_1 & U_1 + p_2^2\beta^2\Delta_1 & 0 & 0 & 0 & -p_2\Delta_2 \\ 0 & 0 & -1 & -p_1 & -p_2 & 0 \end{pmatrix} . \tag{41}
$$

Here

$$
U_1 = -1 + \beta^2(p_1^2 + p_2^2) , \qquad \Delta_1 = 3 - 4\beta^2/\alpha^2 , \qquad \Delta_2 = 1 - 2\beta^2/\alpha^2 . \tag{42}
$$

We wish to calculate the eigenvalues p_3 of the 6×6 matrix $\mathbf{A}$. They are solutions of the secular equation

$$
\det(\mathbf{A} - p_3\mathbf{I}) = 0 , \tag{43}
$$

where $\mathbf{I}$ is the 6×6 identity matrix. It is simple to see that (43) represents an algebraic equation of the sixth order, so that six eigenvalues must be obtained. After some cumbersome algebra, we can express equation (43) in the following form:

$$
\begin{aligned}
p_3^6 &- p_3^4\Big[\Big(\frac{1}{\alpha^2} - p_1^2 - p_2^2\Big) + 2\Big(\frac{1}{\beta^2} - p_1^2 - p_2^2\Big)\Big] \\
&+ p_3^2\Big[\Big(\frac{1}{\beta^2} - p_1^2 - p_2^2\Big)\Big]\Big[\Big(\frac{1}{\beta^2} - p_1^2 - p_2^2\Big) + 2\Big(\frac{1}{\alpha^2} - p_1^2 - p_2^2\Big)\Big] \\
&- \Big(\frac{1}{\alpha^2} - p_1^2 - p_2^2\Big)\Big(\frac{1}{\beta^2} - p_1^2 - p_2^2\Big)^2 = 0 .
\end{aligned} \tag{44}
$$

The simplest derivation of (44) from (43) and (41) is probably based on the Laplace expansion of determinant (43) with respect to the first two columns. This expansion yields a sum of products of the 2×2 minors with their 4×4 cofactors. All relevant 2×2 and 4×4 determinants are very simple.

Equation (44) can be expressed in the final form:

$$\left[p_3^2 - \left(\frac{1}{\alpha^2} - p_1^2 - p_2^2\right)\right]\left[p_3^2 - \left(\frac{1}{\beta^2} - p_1^2 - p_2^2\right)\right]^2 = 0 \; . \tag{45}$$

Equation (45) shows that the six eigenvalues of the 6×6 matrix $\mathbf{A}$ are as follows:

a) Two eigenvalues corresponding to P waves:

$$p_3 = \pm\left[\frac{1}{\alpha^2} - p_1^2 - p_2^2\right]^{1/2} \; . \tag{46}$$

b) Four eigenvalues corresponding to S waves:

$$p_3 = \pm\left[\frac{1}{\beta^2} - p_1^2 - p_2^2\right]^{1/2} \; .$$

The eigenvalues of S waves correspond to the double roots of (45). As $p_3 = -\mathcal{H}^R$, we have confirmed the result (35), using the general 6×6 system matrix $\mathbf{A}$.

We now wish to prove that the general anisotropic system (32) yields (36) for isotropic media. For this, we have to calculate the eigenvectors $\mathbf{W}$, expressed in terms of $\hat{\mathbf{G}}$ and $\hat{\mathbf{X}}$, see (24)–(27). This must be done independently for P and S waves.

1. **P waves**

We remind the reader that $p_3 = [1/\alpha^2 - p_1^2 - p_2^2]^{1/2}$ for forward P-wave propagation in isotropic media. To determine $\hat{\mathbf{G}}$ and $\hat{\mathbf{X}}$, we shall use (24)–(27), and take into account that the normalized eigenvectors of the Christoffel matrix are given by relations $g_i = \alpha p_i$. Then

$$\hat{\mathbf{G}} = \alpha\begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix} \; , \qquad \hat{\mathbf{X}} = \alpha\begin{pmatrix} 2\beta^2 p_1 p_3 \\ 2\beta^2 p_2 p_3 \\ (1 - 2\beta^2/\alpha^2) + 2\beta^2 p_3^2 \end{pmatrix} \; . \tag{47}$$

We also take into account that $\hat{\mathbf{G}}^T\hat{\mathbf{X}} = \mathcal{U}_3 = \alpha^2 p_3$, see (31) for $\rho = 1$. This can be easily verified from (47),

$$\hat{\mathbf{G}}^T\hat{\mathbf{X}} = 2\alpha^2 p_3 \beta^2 p_i p_i + \alpha^2\left(1 - 2\frac{\beta^2}{\alpha^2}\right)p_3 = 2\beta^2 p_3 + \alpha^2 p_3 - 2\beta^2 p_3 = \alpha^2 p_3 \; . \tag{48}$$

Now we can calculate the RHS's of (32). After some cumbersome, but straightforward algebra, we obtain

$$\begin{aligned} 2p_1\hat{\mathbf{G}}^T\hat{\mathbf{B}}_{11}\hat{\mathbf{G}} + p_2\mathbf{G}^T(\hat{\mathbf{B}}_{12} + \hat{\mathbf{B}}_{21})\hat{\mathbf{G}} + 2\hat{\mathbf{G}}^T\hat{\mathbf{A}}_1^T\hat{\mathbf{X}} &= 2\alpha^2 p_1 \; , \\ p_1\hat{\mathbf{G}}^T(\hat{\mathbf{B}}_{12} + \hat{\mathbf{B}}_{21})\hat{\mathbf{G}} + 2p_2\hat{\mathbf{G}}^T\hat{\mathbf{B}}_{22}\hat{\mathbf{G}} + 2\hat{\mathbf{G}}^T\hat{\mathbf{A}}_2^T\hat{\mathbf{X}} &= 2\alpha^2 p_2 \\ p_K p_L\hat{\mathbf{G}}^T\frac{\partial\hat{\mathbf{B}}_{KL}}{\partial x_I}\hat{\mathbf{G}} + 2p_K\hat{\mathbf{G}}^T\frac{\partial\hat{\mathbf{A}}_K^T}{\partial x_I}\hat{\mathbf{X}} - \hat{\mathbf{X}}^T\frac{\partial\hat{\mathbf{C}}_{33}^{-1}}{\partial x_I}\hat{\mathbf{X}} &= -2\alpha\frac{\partial(1/\alpha)}{\partial x_I} \; . \end{aligned} \tag{49}$$

Inserting (48) and (49) into (32) yields the reduced Hamiltonian ray tracing system of P waves in isotropic inhomogeneous media:

$$\frac{\mathrm{d}x_I}{\mathrm{d}x_3} = \frac{\alpha p_I}{[1-\alpha^2(p_1^2+p_2^2)]^{1/2}} , \qquad \frac{\mathrm{d}p_I}{\mathrm{d}x_3} = \frac{1}{[1-\alpha^2(p_1^2+p_2^2)]^{1/2}} \frac{\partial}{\partial x_I}\Big(\frac{1}{\alpha}\Big) . \tag{50}$$

This is exactly the same as (36). Thus, we have confirmed that the general ray tracing system (32), valid for anisotropic media, reduces to ray tracing system (50) for P waves in isotropic media.

2. **S waves**

We remind the reader that $p_3 = [1/\beta^2 - p_1^2 - p_2^2]^{1/2}$ for forward S waves propagation in isotropic media. To determine $\hat{\mathbf{G}}$ and $\hat{\mathbf{X}}$, we shall use (24)–(27) and take into account that the normalized eigenvector of the Christoffel matrix is $\vec{e}$, perpendicular to the slowness vector $\vec{p}$. Thus, $p_i e_i = 0$. Then

$$\hat{\mathbf{G}} = \begin{pmatrix} e_1 \\ e_2 \\ e_3 \end{pmatrix} , \qquad \hat{\mathbf{X}} = \beta^2 \begin{pmatrix} e_1 p_3 + e_3 p_1 \\ e_2 p_3 + e_3 p_2 \\ 2 e_3 p_3 \end{pmatrix} . \tag{51}$$

We also take into account that $\hat{\mathbf{G}}^T\hat{\mathbf{X}} = \mathcal{U}_3 = \beta^2 p_3$, see (31) for $\rho = 1$. This also follows simply from (51):

$$\hat{\mathbf{G}}^T\hat{\mathbf{X}} = \beta^2 e_i e_i p_3 + \beta^2 e_i p_i e_3 = \beta^2 p_3 . \tag{52}$$

The computation of the RHS's of (32) is again cumbersome, but straightforward. We obtain

$$\begin{aligned} 2p_1\hat{\mathbf{G}}^T\hat{\mathbf{B}}_{11}\hat{\mathbf{G}} + p_2\hat{\mathbf{G}}^T(\hat{\mathbf{B}}_{12}+\hat{\mathbf{B}}_{21})\hat{\mathbf{G}} + 2\hat{\mathbf{G}}^T\hat{\mathbf{A}}_1^T\hat{\mathbf{X}} &= 2p_1\beta^2 , \\ p_1\hat{\mathbf{G}}^T(\hat{\mathbf{B}}_{12}+\hat{\mathbf{B}}_{21})\hat{\mathbf{G}} + 2p_2\hat{\mathbf{G}}^T\hat{\mathbf{B}}_{22}\hat{\mathbf{G}} + 2\hat{\mathbf{G}}^T\hat{\mathbf{A}}_2^T\hat{\mathbf{X}} &= 2p_2\beta^2 , \\ p_K p_L \hat{\mathbf{G}}^T\frac{\partial\hat{\mathbf{B}}_{KL}}{\partial x_I}\hat{\mathbf{G}} + 2p_K\hat{\mathbf{G}}^T\frac{\partial\hat{\mathbf{A}}_K^T}{\partial x_I}\hat{\mathbf{X}} - \hat{\mathbf{X}}^T\frac{\partial\hat{\mathbf{C}}_{33}^{-1}}{\partial x_I}\hat{\mathbf{X}} &= -2\beta\frac{\partial\beta^{-1}}{\partial x_I} . \end{aligned} \tag{53}$$

Inserting (52) and (53) into (32) yields the reduced Hamiltonian ray tracing system of S waves, in isotropic inhomogeneous media:

$$\frac{\mathrm{d}x_I}{\mathrm{d}x_3} = \frac{\beta p_I}{[1-\beta^2(p_1^2+p_2^2)]^{1/2}} , \qquad \frac{\mathrm{d}p_I}{\mathrm{d}x_3} = \frac{1}{[1-\beta^2(p_1^2+p_2^2)]^{1/2}} \frac{\partial}{\partial x_I}\Big(\frac{1}{\beta}\Big) . \tag{54}$$

This is exactly the same as (36). Thus, we have confirmed also for S waves, that the general ray tracing system (32), valid for anisotropic media, reduces to ray tracing system (54) in isotropic media. Equations (52)–(54) remain valid for arbitrarily oriented unit vector $\vec{e}$ in a plane perpendicular to $\vec{p}$.

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