Integral superposition of paraxial Gaussian beams in inhomogeneous anisotropic layered structures in Cartesian coordinates

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Summary

Integral superposition of paraxial Gaussian beams in inhomogeneous anisotropic layered structures is studied. It removes certain singularities of the standard ray method, like caustics. Individual quantities in the integral superposition can be calculated by ray tracing and by dynamic ray tracing in Cartesian coordinates. Instead of 3×3 paraxial matrices, it is sufficient to compute only two first columns of these matrices. This simplifies considerably the computations. The wave under consideration may be generated by a point source with an arbitrary radiation function, or by a surface source with the variable initial time along it. For a wave generated by a point-force source, the integral superposition of paraxial Gaussian beams yields the Green function. The receiver point may be situated arbitrarily in the model, including structural interfaces and the Earth's surface. It is customary (but not necessary) to introduce the target surface Σ passing through the receiver (or close to it), along which the data needed in the integral superposition of paraxial Gaussian beams are stored. The same target surface Σ may be used for different elementary waves. The formula for integral superposition may be applied to arbitrary reflected, converted, or multiply reflected waves, propagating in inhomogeneous anisotropic media. It may also be applied to waves propagating in inhomogeneous weakly anisotropic media. For S waves propagating in weakly anisotropic media, the coupling ray theory may be used, in which one coupled, frequency-dependent S wave is considered instead of two separate S1 and S2 waves. The derived integral superposition of paraxial Gaussian beams is valid even for the coupled S wave and removes the unpleasant shear-wave singularities of anisotropic media.

Keywords: integral superposition of paraxial Gaussian beams, inhomogeneous anisotropic media, inhomogeneous weakly anisotropic media, S waves in weakly anisotropic media.

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1 Introduction

The method of integral superposition of paraxial Gaussian beams (also called the method of summation of paraxial Gaussian beams) is a powerful extension of the ray method. The paraxial Gaussian beams are approximate solutions of elastodynamic equation concentrated close to rays, called central, of high-frequency seismic body waves. The amplitudes of paraxial Gaussian beams decrease exponentially with the square of the distance from the central ray along any straight-line profile intersecting the ray. This is the reason why these beams are called paraxial Gaussian beams. The equations for the paraxial Gaussian beams are valid along the whole central ray and have no singularity at caustics.

The paraxial Gaussian beams discussed here are not exact solutions of the elastodynamic equation. Exact Gaussian beams can be computed only exceptionally, e.g., for a point source in a homogeneous medium. Such *exact Gaussian beams* are obtained by moving the point source into the complex space (Felsen, 1976). If we consider Gaussian beams propagating in inhomogeneous media, such an approach cannot be used. We can, however, compute exactly the complex-valued travel time in the vicinity of the central ray. If we determine the travel times in the vicinity of the central ray by exact solution of the eikonal equation, we speak of *strict Gaussian beams* (Červený, Klimeš and Pšenčík, 2007, p.76). In the vicinity of the central ray, called the paraxial vicinity, we can also evaluate the complex-valued travel time of the beam approximately, by its Taylor expansion to quadratic terms at any point of the central ray. To distinguish the beams with approximately evaluated complex-valued travel times from exact and strict Gaussian beams, we call them *paraxial Gaussian beams*. In seismological literature, however, it is common to call them Gaussian beams, without emphasizing their approximate validity in the paraxial vicinity of the central ray. In this paper, we also call them simply "Gaussian beams", without emphasizing the paraxial validity of their equations.

The theory of Gaussian beams in isotropic inhomogeneous layered structures has been described in many papers. For the scalar wave equation, refer to Babich (1968), Babich and Popov (1981), Popov (1982), Červený, Popov and Pšenčík (1982). For the elastodynamic isotropic wave equation, see Červený and Pšenčík (1983a,b), Klimeš (1984), Červený (1985), George, Virieux and Madariaga (1987), White, Norris, Bayliss and Burridge (1987), Popov (2002), Bleistein (2007), Červený, Klimeš and Pšenčík (2007), Kravtsov and Berczynski (2007), Leung, Qian and Burridge (2007). The Gaussian beam summation method has been successfully applied in migration in seismic exploration. A description of the theory of Gaussian beam migration, of its algorithm and excellent results can be found in Hill (1990, 2001), Gray (2005), Vinje, Roberts and Taylor (2008), Gray and Bleistein (2009).

The references to the theory and applications of Gaussian beams propagating in inhomogeneous anisotropic media are not so common. We have to refer to the excellent mathematical treatment by Ralston (1983), devoted to Gaussian beams and propagation of singularities, to Hanyga (1986), to Červený (2000, 2001, sec. 5.8) and to Červený and Pšenčík (2010a). The Gaussian beam summation method was applied to seismic migration in anisotropic media by Alkhalifah (1995) and by Zhu, Gray and Wang (2007).

In most of the above publications, beams were used as building elements in the computation of wavefields based on the method of integral superposition of Gaussian beams. The method removes problems with caustics since Gaussian beams are regular everywhere including caustics. The method of integral superposition of Gaussian beams is not only regular at a caustic point of the central ray, but it yields there approximately correct amplitudes, similarly as at other points of the central ray. The method of integral superposition of Gaussian beams does not require time consuming two-point ray tracing because evaluation of the superposition integral can be performed at any point of the medium sufficiently illuminated by beams in its vicinity. Although reliable two-point ray-tracing procedures are available (see, e.g., Bulant, 1996), which make possible detection of not only first, but also later arrivals, the method of summation of Gaussian beams, combined with the controlled initial-value ray tracing (Bulant, 1996), may be more efficient in retaining later arrivals.

The basic procedure in the computation of Gaussian beams is the dynamic ray tracing (DRT). The dynamic ray tracing system, and, consequently, the expressions for Gaussian beams, can be expressed in various coordinate systems (Cartesian, ray-centred, etc.). Here we concentrate on Cartesian coordinate system, but start from the ray-centred coordinate system, as it yields physically simple and understandable results. For anisotropic media, the DRT system in ray-centred coordinates is, of course, algebraically more complicated than in isotropic media, but the principles remain the same. Similarly, the integral superposition of Gaussian beams remains formally the same for inhomogeneous isotropic and anisotropic media (Klimeš, 1984; Červený et al., 2007).

For practical purposes, it is more comfortable to perform the computations in Cartesian coordinates. In order to make such computations possible, we transform locally the 2×2 matrices $\mathbf{M}^{(q)}$, $\mathbf{Q}^{(q)}$ and $\mathbf{P}^{(q)}$ in ray-centred coordinates to the analogous 3×3 matrices $\hat{\mathbf{M}}^{(x)}$, $\hat{\mathbf{Q}}^{(x)}$ and $\hat{\mathbf{P}}^{(x)}$ in Cartesian coordinates. We could obtain these matrices by using DRT in Cartesian coordinates as, e.g., Červený (1972), Ralston (1983), Leung et al. (2007), Tanushev (2008). In the evaluation of $\hat{\mathbf{Q}}^{(x)}$ and $\hat{\mathbf{P}}^{(x)}$ by dynamic ray tracing along the central ray Ω, it is sufficient to compute only the first two columns of these matrices (Gajewski and Pšenčík, 1990). These two columns of 3×3 matrices $\hat{\mathbf{Q}}^{(x)}$ and $\hat{\mathbf{P}}^{(x)}$ are quite sufficient for the evaluation of the integral superposition of Gaussian beams in Cartesian coordinates.

The derived integral superposition of Gaussian beams can be used also for waves propagating in inhomogeneous weakly anisotropic media, including coupled S waves.

To make the paper more readable and understandable, we try to explain the main procedures based on the ray method as simply as possible, and shift the mathematics to appendices. In the appendices, however, we include all ray-theory prerequisites needed in the computations of Gaussian beams in inhomogeneous anisotropic layered media. In Section 2, we present several basic equations of the ray method for inhomogeneous anisotropic layered media, discuss ray tracing equations and DRT equations, and describe the computation of ray-theory amplitudes. In anisotropic media, both ray tracing and dynamic ray tracing are usually more time-consuming than in isotropic media, particularly for media of lower anisotropic symmetry. We also explain how to simplify the dynamic ray tracing in Cartesian coordinates, which can be reduced to the computation of only two first columns of matrices $\hat{\mathbf{Q}}^{(x)}$ and $\hat{\mathbf{P}}^{(x)}$. Section 3 is devoted to the transformation of the known integral superposition of Gaussian beams in inhomogeneous anisotropic media in ray-centred coordinates to those in Cartesian coordinates. The derived integral superposition in Cartesian coordinates is expressed in terms of only two columns of 3×3 matrices $\hat{\mathbf{Q}}^{(x)}$ and $\hat{\mathbf{P}}^{(x)}$. This considerably simplifies the integral superposition formulae. Section 4 is devoted to integral superposition of Gaussian beams in inhomogeneous weakly anisotropic media. The used weak anisotropy approximation includes automatically the coupling ray theory of S waves. Finally, in section 5 some important concluding remarks are presented. The list of references contains even some references not used in the text. We put them there with the expectation that a reader might find them useful.

To express the equations in the paper in a concise form, we use alternatively the component and matrix notation for vectors and matrices. In the component notation, the upper-case indices (I, J, K,...) take the values 1 or 2, and the lower-case indices (i, j, k,...) the values 1, 2, or 3. The Einstein summation convention is used throughout the paper. The matrices and vectors are denoted by bold upright symbols. The dynamic ray tracing is used here in two coordinate systems, namely in ray-centered coordinates q_i and in Cartesian coordinates x_i. To distinguish the matrices in ray-centred coordinates q_i from the analogous matrices in Cartesian coordinates x_i, we use superscripts (q) and (x) over them. Further, to distinguish between 2×2 and 3×3 matrices, we use the circumflex ($\hat{}$) above the symbol for 3×3 matrices. The vectors are considered as column matrices. In this way, the scalar product of vectors $\mathbf{a}$ and $\mathbf{b}$ reads $\mathbf{a}^T\mathbf{b}$, the dyadic reads $\mathbf{a}\mathbf{b}^T$. Whenever there may be reason for confusion, the dimensions of the matrices are explicitly indicated. The index following the comma in the subscript indicates a partial derivative with respect to the relevant Cartesian coordinate.

2 Ray theory for inhomogeneous anisotropic layered structures

In this section, we discuss basic techniques of computing ray-theory quantities of an arbitrary high-frequency seismic body wave propagating in an inhomogeneous anisotropic layered structure.

2.1 Basic equations of the ray method

The paraxial Gaussian beams represent an extension of the ray concepts. For this reason, it is useful to introduce briefly basics of the ray theory.

Let us consider an inhomogeneous anisotropic perfectly elastic medium. The source-free elastodynamic equation for this medium reads:

$$(c_{ijkl}u_{k,l})_{,j} = \rho\,\ddot{u}_i\ . \qquad (1)$$

Here $u_i(x_n)$ are the Cartesian components of the displacement vector $\mathbf{u}(x_n)$, $c_{ijkl}(x_n)$ are real-valued elastic moduli (components of the stiffness tensor), $\rho(x_n)$ is the density and x_n are the Cartesian coordinates. In the zero-order approximation of the ray method, the time-harmonic solution of (1) for any high-frequency seismic body wave is usually sought in the following form:

$$\mathbf{u}(x_i,t) = \mathbf{U}(x_i)\exp[-\mathrm{i}\omega(t - T(x_j))] \ . \tag{2}$$

Here $T(x_i)$ is the travel time, $\mathbf{U}(x_i)$ the complex-valued vectorial ray-theory amplitude, ω the circular frequency, and t time. Inserting (2) into (1), and setting to zero coefficients of varying powers of ω, we arrive at the basic system of the ray theory equations. Considering the equations corresponding to the highest power of ω (specifically ω^2), we obtain the system of three equations for U_k:

$$(\Gamma_{ik} - \delta_{ik})U_k = 0 \ , \qquad i = 1,2,3 \ . \tag{3}$$

The 3×3 matrix $\hat{\mathbf{\Gamma}}(x_m,p_n)$ is given by the relation

$$\Gamma_{ik}(x_m,p_n) = a_{ijkl}(x_m)p_jp_l \ , \tag{4}$$

and is usually called the generalized Christoffel matrix. Here a_{ijkl} are the density-normalized elastic moduli

$$a_{ijkl}(x_n) = c_{ijkl}(x_n)/\rho(x_n) \ . \tag{5}$$

The quantities $p_i = \partial T/\partial x_i$ are Cartesian components of the slowness vector $\mathbf{p}$.

The Christoffel matrix with elements (4) has three eigenvalues $G_m(x_i,p_j)$ and three corresponding eigenvectors $\mathbf{g}^{(m)}(x_i,p_j)$, $m = 1,2,3$. They correspond to the three elementary waves, propagating in inhomogeneous anisotropic media, specifically P, S1 and S2 waves. Since matrix $\hat{\mathbf{\Gamma}}$ is symmetric and positive definite, all the three eigenvalues G_1, G_2 and G_3 are real-valued and positive. Moreover, they are homogeneous functions of the second degree in p_i. For simplicity, in the following we consider that all three eigenvalues are different.

Let us consider the m-th elementary wave. It follows from (3) that the eigenvalue G_m of this wave satisfies the relation

$$G_m(x_i,p_j) = 1 \ . \tag{6}$$

Equation (6) is a non-linear partial differential equation of the first order for the travel time function $T(x_i)$. It is usually called the eikonal equation for a inhomogeneous anisotropic medium. It can be expressed alternatively in the4 Hamiltonian form

$$\mathcal{H}(x_i,p_j) = \tfrac{1}{2}G_m(x_i,p_j) = \tfrac{1}{2} \ . \tag{7}$$

The Hamiltonian $\mathcal{H}(x_i,p_j)$ is used in ray tracing and dynamic ray tracing (DRT), see Appendices A and B.

The vectorial ray-theory amplitude $\mathbf{U}(x_i)$ of the m-th elementary wave can be expressed in terms of the unit real-valued eigenvector $\mathbf{g}^{(m)}$ of the generalized Christoffel matrix with elements (4) as follows:

$$\mathbf{U}(x_i) = A(x_i)\mathbf{g}^{(m)}(x_i) \ . \tag{8}$$

Here $A(x_i)$ is a complex-valued frequency-independent scalar ray-theory amplitude. See Section 2.4. Equation (8) shows that eigenvector $\mathbf{g}^{(m)}$ specifies the polarisation of the m-th wave. For this reason, we call $\mathbf{g}^{(m)}(x_i)$ the polarisation vector.

2.2 Initial-value ray tracing

Let us consider an arbitrary high-frequency seismic body wave (P, S1, S2; direct, reflected, transmitted, multiply reflected/transmitted, etc.) propagating in a layered medium specified by smooth structural interfaces and by smooth spatial distribution of upto 21 density-normalized elastic moduli inside layers. We can use *ray tracing* resulting from (7), see Appendix A, with proper initial conditions to compute a ray Ω of the two-parametric (orthonomic) system of rays corresponding to a selected wave, and denote its ray parameters γ_1 and γ_2. The ray tracing system consists of a system of generally non-linear ordinary differential equations of the first order. We can introduce a monotonically increasing sampling parameter γ_3 along ray Ω, which uniquely specifies the position of a point on ray Ω. Sampling parameter γ_3 may be chosen in various ways. In inhomogeneous anisotropic media, it is most convenient to take $\gamma_3 = \tau$, where τ is the travel time T along ray Ω of the wave under consideration. The ray parameters γ_1, γ_2, together with the sampling parameter $\gamma_3 = \tau$, may also serve as coordinates, and are therefore called the ray coordinates $\boldsymbol{\gamma} \equiv (\gamma_1, \gamma_2, \gamma_3)$. The ray tracing equations for inhomogeneous anisotropic media and the initial conditions for these equations are given in Appendix A. The transformation equations for a ray reflected/transmitted at a structural interface are also given there.

From ray tracing, we obtain the coordinates $\mathbf{x}(\tau)$ of the points on the ray trajectory Ω and slowness vectors $\mathbf{p}(\tau)$ at these points. As a by-product of ray tracing, we can determine several other useful quantities along the ray Ω, which we shall need in the following: the ray-velocity vector $\boldsymbol{\mathcal{U}}(\tau) = d\mathbf{x}(\tau)/d\tau$, the unit vector $\mathbf{t}(\tau) = \boldsymbol{\mathcal{U}}(\tau)/|\boldsymbol{\mathcal{U}}(\tau)|$ tangent to the ray Ω, the unit vector $\mathbf{N}(\tau) = \mathbf{p}(\tau)/|\mathbf{p}(\tau)|$ perpendicular to the wavefront, the vector $\boldsymbol{\eta}(\tau) = d\mathbf{p}(\tau)/d\tau$, which describes the variation of the slowness vector along the ray, polarization vector $\mathbf{g}(\tau)$, phase velocity $\mathcal{C}(\tau) = 1/|\mathbf{p}(\tau)|$, and ray velocity $\mathcal{U}(\tau) = |\boldsymbol{\mathcal{U}}(\tau)|$. The ray-velocity vector $\boldsymbol{\mathcal{U}}(\tau)$ is also sometimes called the energy-velocity vector or the group-velocity vector. In non-dissipative media, the latter terms have the same meaning. The travel time $T(\tau)$ along a ray is determined automatically as it equals the sampling parameter along the ray, $T(\tau) = \tau$. In the following, we consider the so-called initial-value rays specified by the initial conditions $\tau = \tau_0$, $\mathbf{x}(\tau_0) = \mathbf{x}_0$, $\mathbf{p}(\tau_0) = \mathbf{p}_0$. The specification of $\mathbf{p}(\tau_0)$ in isotropic media is straightforward. In anisotropic media, phase velocity must be found first for a given direction, and only then it is possible to construct $\mathbf{p}(\tau_0)$, see Appendix A.

The ray tracing can be used to compute all the above-mentioned quantities only on the considered ray Ω, not in its vicinity. This is, however, not sufficient in the calculation of the ray-theory amplitudes and/or paraxial Gaussian beams concentrated to ray Ω. This is because the ray-theory amplitudes depend on geometrical spreading, which is a function of the ray field, not of a single ray. In the case of paraxial Gaussian beams, we also need to compute complex-valued paraxial travel times (the complex-valued travel times in the vicinity of the ray Ω). For the computation of the quantities related to the ray field, it is necessary to compute system of rays around Ω or to supplement the ray tracing by an additional procedure called *dynamic ray tracing.*

2.3 Dynamic ray tracing

The dynamic ray tracing (DRT) is a basic procedure for the computation of geometrical spreading and for the computation of second derivatives of the travel time field with respect to spatial coordinates along the ray. Geometrical spreading is a basic quantity in the computation of the ray-theory amplitudes along the ray. Therefore, we speak of dynamic ray tracing in order to distinguish it from the standard kinematic ray tracing. Dynamic ray tracing consists in the solution of a system of linear ordinary differential equations of the first order along the ray Ω. The system may be solved together with ray tracing, or along an already known ray Ω.

The DRT system can be expressed in various coordinate systems (global Cartesian x_i, ray-centred q_i, or local Cartesian wavefront orthonormal y_i, etc.). The DRT system in ray-centred coordinates, with its application to the computation of paraxial Gaussian beams was described in detail in Červený and Pšenčík (2010a). This paper is devoted to three versions of DRT. First we briefly discuss the DRT system in global Cartesian coordinate system x_i, and then in ray-centred coordinates q_i. To distinguish the 2×2 matrices in ray-centred coordinates q_i from the analogous 3×3 matrices in global Cartesian coordinates x_i3, we use superscripts (q) or (x) over relevant symbols. Since the components of vectors are expressed in Cartesian coordinates, we use superscripts (x) and (q) over them only in cases which may lead to misunderstanding. The third version of the DRT is the simplified DRT in global Cartesian coordinates, in which the 3×2 matrices instead of 3×3 matrices are considered. It may represent a more efficient procedure.

2.3.1 Dynamic ray tracing system in global Cartesian coordinates

Let us consider six paraxial quantities

$$Q_i^{(x)} = \partial x_i/\partial\gamma \ , \qquad P_i^{(x)} = \partial p_i/\partial\gamma \ , \tag{9}$$

where $i = 1, 2, 3$. They describe the changes of the trajectory $\mathbf{x}(\tau)$ and of the relevant slowness vector $\mathbf{p}(\tau)$, caused by the change of a parameter γ. The parameter γ may be any of the initial conditions x_{i0} or p_{i0} for ray tracing, or any ray coordinate. Paraxial quantities (9) can be computed by solving the DRT system in global Cartesian coordinates, see equations (B-1)-(B-2) in Appendix B.

The dynamic ray tracing system in global Cartesian coordinates is often used to seek 3×3 matrices $\hat{\mathbf{Q}}^{(x)}$, $\hat{\mathbf{P}}^{(x)}$, with elements

$$Q_{ij}^{(x)} = \partial x_i/\partial\gamma_j \ , \qquad P_{ij}^{(x)} = \partial p_i/\partial\gamma_j \ . \tag{10}$$

Here γ_i are the ray coordinates or $\gamma_i = x_{i0}$, or $\gamma_i = p_{i0}$. The DRT system in a matrix form is given in (B-5).

The 3×3 matrices $\hat{\mathbf{Q}}^{(x)}$ and $\hat{\mathbf{P}}^{(x)}$ can be used to compute the 3×3 symmetric matrix $\hat{\mathbf{M}}^{(x)}$ of the second-order partial derivatives of the travel time $T(x_m)$ with respect to spatial derivatives x_i:

$$M^{(x)}_{ij} = \partial^2 T(x_m)/\partial x_i \partial x_j \ . \tag{11}$$

It is easy to show that the 3×3 matrix $\hat{\mathbf{M}}^{(x)}$, with nine elements $M^{(x)}_{ij}$, can be simply expressed in terms of 3×3 matrices $\hat{\mathbf{Q}}^{(x)}$ and $\hat{\mathbf{P}}^{(x)}$, obtained from the DRT. As

$$M^{(x)}_{ij} Q^{(x)}_{jk} = \frac{\partial^2 T}{\partial x_i \partial x_j} \frac{\partial x_j}{\partial \gamma_k} = \frac{\partial p_i}{\partial \gamma_k} = P^{(x)}_{ik} \ , \tag{12}$$

we obtain

$$\hat{\mathbf{M}}^{(x)} = \hat{\mathbf{P}}^{(x)} (\hat{\mathbf{Q}}^{(x)})^{-1} \ . \tag{13}$$

Actually, the 3×3 matrix $\hat{\mathbf{M}}^{(x)}$ could be also computed directly without calculation of $\hat{\mathbf{P}}^{(x)}$ and $\hat{\mathbf{Q}}^{(x)}$ from Riccati equation solved along the ray (Ralston, 1983). The Riccati equation is, however, a **non-linear ordinary differential equation**, which is not as suitable for the computation as the system of linear DRT equations.

2.3.2 Dynamic ray tracing in ray-centred coordinates

The basic property of the ray-centred coordinate system is that the selected central ray Ω represents its coordinate axis q_3. The q_1 and q_2 coordinate axes may be introduced in many ways. For an up-to-date review see Klimeš (2006b). Mostly, they are introduced as mutually perpendicular straight lines situated in the plane tangent to the wavefront at its intersection with the central ray Ω. The transformation relation between Cartesian coordinates x_i and ray-centred coordinates q_j then reads

$$x_i(q_j) = x^{\Omega}_i(q_3) + H_{iM}(q_3) q_M \ , \tag{14}$$

where $i, j = 1, 2, 3$ and $M = 1, 2$. Central ray Ω is specified by $q_1 = q_2 = 0$, so that $\mathbf{x}(0, 0, q_3) = \mathbf{x}^{\Omega}(q_3)$, where $\mathbf{x}^{\Omega}$ denotes a point on the ray Ω. Similarly as in kinematic ray tracing, we can take coordinate q_3 equal to the travel time τ along central ray Ω, $q_3 = \tau$. Let us emphasize that the choice $q_3 = \tau$ simplifies the computations considerably, as it leads to the following simple relations, valid at any point of the central ray Ω:

$$\partial T/\partial q_3 = 1 \ , \quad \partial^2 T/\partial q_3 \partial q_i = 0 \ . \tag{15}$$

Note also that $\partial T/\partial q_I = 0$ at any point of Ω. Simple relations (15) are not valid for other choice of the parameter q_3 along Ω, e.g., for the arclength s. It is important to emphasize this, since the arclength along Ω has been commonly used in ray-centred coordinates in inhomogeneous isotropic media. In this respect, our treatment differs from the common treatment in isotropic media.

The elements of the 3×3 transformation matrices $\hat{\mathbf{H}}$ and $\hat{\overline{\mathbf{H}}}$ from ray-centred to Cartesian coordinates and back, are defined as follows:

$$H_{im} = \partial x_i / \partial q_m \ , \quad \overline{H}_{im} = \partial q_i / \partial x_m \ . \tag{16}$$

As the ray-centred coordinate system is curvilinear, we have to distinguish two systems of basis vectors: the contravariant basis vectors $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ (tangential to coordinate axes), and the covariant basis vectors $\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3$ (perpendicular to coordinate surfaces). These basis vectors constitute columns of 3×3 transformation matrices $\hat{\mathbf{H}}$ and $\hat{\overline{\mathbf{H}}}^T$:

$$\hat{\mathbf{H}} = (\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3 = \boldsymbol{\mathcal{U}}) \ , \quad \hat{\overline{\mathbf{H}}}^T = (\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3 = \mathbf{p}) \ . \tag{17}$$

The obvious relation $\overline{H}_{ik} H_{kj} = \delta_{ij}$ can be expressed in terms of $\mathbf{e}_i$ and $\mathbf{f}_i$ as follows:

$$\mathbf{f}_i^T \mathbf{e}_j = \delta_{ij} \ . \tag{18}$$

Equation (18) yields vectorial relations $\mathbf{p}^T \boldsymbol{\mathcal{U}} = 1$, $\mathbf{p}^T \mathbf{e}_I = 0$, $\boldsymbol{\mathcal{U}}^T \mathbf{f}_I = 0$. Thus, vectors $\mathbf{e}_I$ are perpendicular to the slowness vector $\mathbf{p}$, and vectors $\mathbf{f}_I$ are perpendicular to the ray-velocity vector $\boldsymbol{\mathcal{U}}$, i.e. to the ray. Equation (18) also yields:

$$\mathbf{f}_1 = \frac{\mathbf{e}_2 \times \boldsymbol{\mathcal{U}}}{\boldsymbol{\mathcal{U}}^T (\mathbf{e}_1 \times \mathbf{e}_2)} = \mathcal{C}^{-1} (\mathbf{e}_2 \times \boldsymbol{\mathcal{U}}) \ , \quad \mathbf{f}_2 = \frac{\boldsymbol{\mathcal{U}} \times \mathbf{e}_1}{\boldsymbol{\mathcal{U}}^T (\mathbf{e}_1 \times \mathbf{e}_2)} = \mathcal{C}^{-1} (\boldsymbol{\mathcal{U}} \times \mathbf{e}_1) \ . \tag{19}$$

Equations (17) can be also expressed in a more compact way:

$$\hat{\mathbf{H}} = (\boldsymbol{\mathcal{E}}, \boldsymbol{\mathcal{U}}) \ , \quad \hat{\overline{\mathbf{H}}}^T = (\boldsymbol{\mathcal{F}}, \mathbf{p}) \ , \tag{20}$$

where $\boldsymbol{\mathcal{E}}$ and $\boldsymbol{\mathcal{F}}$ are 3×2 matrices

$$\boldsymbol{\mathcal{E}} = \begin{pmatrix} e_{11} & e_{21} \\ e_{12} & e_{22} \\ e_{13} & e_{23} \end{pmatrix} \ , \quad \boldsymbol{\mathcal{F}} = \begin{pmatrix} f_{11} & f_{21} \\ f_{12} & f_{22} \\ f_{13} & f_{23} \end{pmatrix} \ . \tag{21}$$

We also obtain

$$\det \hat{\mathbf{H}} = \det(\boldsymbol{\mathcal{E}}, \boldsymbol{\mathcal{U}}) = C \ , \quad \det \hat{\overline{\mathbf{H}}} = \det(\boldsymbol{\mathcal{F}}, \mathbf{p}) = 1/C \ . \tag{22}$$

The contravariant basis vectors $\mathbf{e}_1$ and $\mathbf{e}_2$ can be determined by solving simple ordinary differential equations of the first order along central ray Ω:

$$\mathrm{d}\mathbf{e}_I / \mathrm{d}\tau = -(\mathbf{e}_I^T \boldsymbol{\eta}) \mathbf{p} / (\mathbf{p}^T \mathbf{p}) \ . \tag{23}$$

Here $\mathbf{p}$ and $\boldsymbol{\eta} = \mathrm{d}\mathbf{p}/\mathrm{d}\tau$ are known from kinematic ray tracing. At a selected point τ_0 of central ray Ω, we take the initial values for $\mathbf{e}_1$ and $\mathbf{e}_2$ such that they form a triplet of mutually perpendicular unit vectors with $\mathbf{N} = \mathcal{C}\mathbf{p}$. It is possible to prove that vectors $\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{N}$ form then right-handed, unit and mutually perpendicular triplet along the whole central ray Ω. Consequently, it is sufficient to calculate only $\mathbf{e}_1(\tau)$ using (23), as $\mathbf{e}_2(\tau) = \mathbf{N}(\tau) \times \mathbf{e}_1(\tau)$. The numerical determination of $\mathbf{e}_1(\tau)$ using (23) is sufficient to determine analytically the 3×2 matrices $\boldsymbol{\mathcal{E}}$ and $\boldsymbol{\mathcal{F}}$. Since $\mathbf{e}_3 = \boldsymbol{\mathcal{U}}$ and $\mathbf{f}_3 = \mathbf{p}$ are known from ray tracing, we can also determine the complete transformation matrices $\hat{\mathbf{H}}$ and $\hat{\overline{\mathbf{H}}}$, see (20). Note that vectors $\mathbf{f}_1$ and $\mathbf{f}_2$ are not necessarily unit and mutually perpendicular, but $\mathbf{e}_1$ and $\mathbf{e}_2$ are.

The DRT system in ray-centred coordinates (Červený and Pšenčík, 2010a) can be used to compute the following partial derivatives along the central ray Ω:

$$Q_I^{(q)} = \partial q_I/\partial\gamma \ , \quad P_I^{(q)} = \partial p_I^{(q)}/\partial\gamma \ . \tag{24}$$

Here γ is any of the ray parameters. Symbol $p_I^{(q)}$ denotes the I-th component of slowness vector $\mathbf{p}$ in the ray-centred coordinate system, $p_I^{(q)} = H_{kI}p_k$. Quantities $Q_I^{(q)}$ and $P_I^{(q)}$ ($I = 1, 2$) specify the off-ray paraxial changes of q_I and $p_I^{(q)}$, caused by the changes of γ. $Q_I^{(q)}$ and $P_I^{(q)}$ may be used to calculate paraxial rays, paraxial travel times, the paraxial slowness vectors, etc. In 3-D models, the DRT system consists of four linear ordinary differential equations of the first order for $Q_I^{(q)}$ and $P_I^{(q)}$. The actual form of the DRT system in ray-centred coordinates and the transformation of this DRT system across a structural interface is described in Červený and Pšenčík (2010a).

In an orthonomic system of rays, in which any ray is specified by two ray parameters γ_1, γ_2, it is useful to express the DRT system in ray-centred coordinates in matrix form. We introduce two 2×2 matrices $\mathbf{Q}^{(q)}$ and $\mathbf{P}^{(q)}$, with elements

$$Q_{IJ}^{(q)} = \partial q_I/\partial\gamma_J \ , \quad P_{IJ}^{(q)} = \partial p_I^{(q)}/\partial\gamma_J \ . \tag{25}$$

To compute the 2×2 matrices $\mathbf{Q}^{(q)}$ and $\mathbf{P}^{(q)}$, we need to solve the dynamic ray tracing system for $Q_I^{(q)}$ and $P_I^{(q)}$, consisting of four equations twice, with different initial conditions corresponding to ray parameters γ_1 and γ_2. The coefficients in both DRT systems, however, remain the same. Both systems can be solved together. As the coefficients in both systems are evaluated only once, the solution for $Q_{IJ}^{(q)}$ and $P_{IJ}^{(q)}$ is not much slower than the solution for $Q_I^{(q)}$ and $P_I^{(q)}$.

From the 2×2 matrices $\mathbf{Q}^{(q)}$ and $\mathbf{P}^{(q)}$, we can obtain the important 2×2 matrix $\mathbf{M}^{(q)}$ of the second derivatives of travel-time field T with respect to ray-centred coordinates q_1 and q_2,

$$M_{IJ}^{(q)} = \partial^2 T/\partial q_I \partial q_J \ . \tag{26}$$

It is easy to show that the symmetric matrix $\mathbf{M}^{(q)}$ with three independent elements $M_{IJ}^{(q)}$ can be expressed in terms of $\mathbf{Q}^{(q)}$ and $\mathbf{P}^{(q)}$. As

$$M_{IJ}^{(q)} Q_{JK}^{(q)} = \frac{\partial^2 T}{\partial q_I \partial q_J} \frac{\partial q_J}{\partial \gamma_K} = \frac{\partial p_I^{(q)}}{\partial q_J} \frac{\partial q_J}{\partial \gamma_K} = \frac{\partial p_I^{(q)}}{\partial \gamma_K} = P_{IK}^{(q)} \ , \tag{27}$$

we obtain

$$\mathbf{M}^{(q)} = \mathbf{P}^{(q)} \mathbf{Q}^{(q)-1} \ . \tag{28}$$

2.3.3 Simplified DRT in global Cartesian coordinates

The disadvantage of the DRT system in the ray-centred coordinates with respect to global Cartesian coordinates is that the DRT system in ray-centred coordinates is more complicated than in global Cartesian coordinates. The reason is that we have to rotate appropriately the whole system at any step of computation. The disadvantage of the DRT system in global Cartesian coordinates is the number of its equations. We can, however, simplify the DRT in global Cartesian coordinates, and compute only the first two columns of 3×3 matrices $\hat{\mathbf{Q}}^{(x)}$ and $\hat{\mathbf{P}}^{(x)}$, namely the elements $Q^{(x)}_{iJ}$ and $P^{(x)}_{iJ}$. These four columns are quite sufficient for the computation of paraxial ray approximations and paraxial Gaussian beams, at any point τ of the central ray. The great advantage of the simplified DRT system is that the DRT system itself remains as simple as in global Cartesian coordinates and, at the same time, the number of equations reduced. The procedure is as follows:

a) At the initial point τ_0 of the ray, we specify the initial conditions $Q^{(x)}_{iN}(\tau_0)$ and $P^{(x)}_{iN}(\tau_0)$. For a point source, see (B-10) and (B-11), and for a surface source, see (B-20) and (B-21).

b) We perform the DRT in global Cartesian coordinates, but only for 3×2 matrices $Q^{(x)}_{iN}(\tau)$ and $P^{(x)}_{iN}(\tau)$, see (B-26).

The simplified DRT system in global Cartesian coordinates is presented in Appendix B, see eq. (B-26). Let us note that the simplified DRT in Cartesian coordinates can be used very efficiently for the Gaussian beam computations with such codes like ANRAY (Gajewski and Pšenčík, 1990). In fact, the simplified Cartesian DRT system with point source initial conditions has been already used in ANRAY, see Pšenčík and Teles (1996). In order to generalize ANRAY for paraxial Gaussian beam computations, it will be sufficient to add solution of the simplified DRT with the plane-wave initial conditions. Let us note that in some cases, the solution with the plane-wave initial conditions is not necessary. For more details see Červený (2001, sec.4.2), Červený and Pšenčík (2009).

2.3.4 Comments on dynamic ray tracing

The applications of the DRT are much broader than discussed in previous sections. As the travel time $T = \tau$ along the ray Ω and its first derivatives $p_i = \partial T/\partial x_i$ are known from ray tracing, and as the second derivatives $M^{(x)}_{ij}$ can be determined using the DRT, we can make a spatial quadratic expansion of the travel time at an arbitrary point of the ray. Consequently, we can determine approximately the travel time $T(x_m)$ even at points x_m situated in the vicinity of the ray Ω. We speak of paraxial travel time and of quadratic (paraxial) vicinity of the ray Ω. We can also construct linear expansion of the slowness vector and compute paraxial rays in the paraxial vicinity of the central ray Ω. Actually, the DRT system itself represents an approximate ray tracing system for paraxial rays in a vicinity of the central ray. For this reason, the dynamic ray tracing is often called paraxial ray tracing. Here, we are not interested in paraxial rays and speak of dynamic ray tracing.

For the evaluation of paraxial travel times, it is useful to transform the 2×2 matrix $\mathbf{M}^{(q)}(\tau)$ in wavefront orthonormal coordinates to 3×3 matrix $\hat{\mathbf{M}}^{(x)}(\tau)$ in global Cartesian coordinates. The appropriate relation was derived by Červený and Klimeš (2010) and reads:

$$\hat{\mathbf{M}}^{(x)} = \boldsymbol{\mathcal{F}}\ \mathbf{M}^{(q)}\ \boldsymbol{\mathcal{F}}^T + \mathbf{p}\boldsymbol{\eta}^T + \boldsymbol{\eta}\mathbf{p}^T - \mathbf{p}\mathbf{p}^T(\boldsymbol{\mathcal{U}}^T\boldsymbol{\eta})\ . \qquad (29)$$

Here $\hat{\mathbf{M}}^{(x)}$ denotes the symmetric 3×3 matrix of the second derivatives of the travel-time field with respect to global Cartesian coordinates, with elements $M_{ij}^{(x)} = \partial^2\tau/\partial x_i \partial x_j$, $\mathbf{M}^{(q)}$ is the 2×2 symmetric matrix of the second derivatives of the travel-time field with respect to ray-centred coordinates, with elements $M_{IJ}^{(q)} = \partial^2\tau/\partial q_I \partial q_J$. The quantities $\mathbf{p}$, $\boldsymbol{\eta}$ and $\boldsymbol{\mathcal{U}}$ are slowness, eta and ray-velocity vectors, which are known from ray tracing. Finally, $\boldsymbol{\mathcal{F}}$ is a 3×2 matrix, $\boldsymbol{\mathcal{F}} = (\mathbf{f}_1, \mathbf{f}_2)$, see (21). The transformation equation (29) can be used for simple computation of the 3×3 matrix $\hat{\mathbf{M}}^{(x)}$ from the 2×2 matrix $\mathbf{M}^{(q)}$ at any point of central ray Ω.

Note that the 3×3 matrix $\hat{\mathbf{M}}^{(x)}$ in global Cartesian coordinates can be also computed directly by dynamic ray tracing in global Cartesian coordinates. Consequently, equation (29) is useful mainly when the DRT system is solved in ray-centred coordinates q_i, or when the simplified DRT in Cartesian coordinates is used.

In the DRT system in Cartesian coordinates, the 3×3 matrices $\hat{\mathbf{Q}}^{(x)}$ and $\hat{\mathbf{P}}^{(x)}$, with elements $Q_{ij}^{(x)}$ and $P_{ij}^{(x)}$, are computed along the ray. Thus the number of solved equations is higher than in ray-centred coordinates. The DRT system in Cartesian coordinates, however, has simpler right-hand sides, especially in anisotropic media. The DRT system in Cartesian coordinates for anisotropic inhomogeneous media was derived by Červený (1972) with the purpose to compute the geometrical spreading and ray amplitudes.

An alternative version of the simplified DRT in global Cartesian coordinates, called surface-to-surface DRT, is not treated here. For anisotropic inhomogeneous media, the details of surface-to-surface DRT are described in Červený (2001) and Moser and Červený (2007).

2.4 Ray-theory complex-valued amplitudes

Let us again consider a harmonic high-frequency seismic body wave propagating in a laterally varying, anisotropic layered structure and a ray Ω corresponding to this wave. The i-th Cartesian component of the zero-order ray-theory displacement vector $\mathbf{u}(\tau)$ at a point τ on ray Ω is given by the expression resulting from (2) and (8):

$$u_i(\tau) = U_i(\tau)\mathrm{exp}[-\mathrm{i}\omega(t - T(\tau))] = A(\tau)g_i(\tau)\mathrm{exp}[-\mathrm{i}\omega(t - T(\tau))]\ . \qquad (30)$$

Here $U_i(\tau)$ is the i-th Cartesian component of the vectorial ray-theory amplitude $\mathbf{U}(\tau)$ and $A(\tau)$ is the scalar ray-theory amplitude. Both $U_i(\tau)$ and $A(\tau)$ are generally complex-valued. $g_i(\tau)$ is the i-th Cartesian component of the real-valued polarization vector $\mathbf{g}(\tau)$, and $T(\tau) = \tau$ is the travel time along ray Ω. The relation $T(\tau) = \tau$ follows from the homogeneity of the Hamiltonian under consideration. The travel time and the polarization vector are determined during the ray tracing. It remains to discuss the computation of the scalar ray-theory amplitude $A(\tau)$. For this, we need results of the DRT.

For tensorial wave field $u_{ij}(\tau)$ of the Green function generated by a point force situated at τ_0, it is necessary to write (30) as follows:

$$u_{ij}(\tau) = U_{ij}^G(\tau)\exp[-\mathrm{i}\omega(t-T(\tau))] = A^G(\tau)g_i(\tau)g_j(\tau_0)\exp[-\mathrm{i}\omega(t-T(\tau))] \ . \qquad (31)$$

Here $U_{ij}^G(\tau)$ are the Cartesian components of the tensorial ray-theory amplitude of the Green function, and $A^G(\tau)$ the scalar ray-theory amplitude of the Green function. Again, both $U_{ij}^G(\tau)$ and $A^G(\tau)$ are in general complex-valued. The symbols $g_i(\tau)$ and $g_j(\tau_0)$ denote Cartesian components of the polarization vectors $\mathbf{g}$.

In the following, we shall concentrate on computation of scalar ray-theory amplitudes $A(\tau)$ and $A^G(\tau)$. We shall first present the formulae for the amplitudes in ray-centred coordinates, and only later we shall derive the relevant expressions in general Cartesian coordinates from them.

2.4.1 Ray-theory complex-valued amplitudes in ray-centred coordinates

The scalar ray-theory amplitudes can be determined using the continuation relation along ray Ω, which follows from the transport equation. We consider the homogeneous Hamiltonian (7), assume that the DRT in ray-centred coordinates has been performed along the ray specified by proper initial conditions, and that the 2×2 matrix $\mathbf{Q}^{(q)}$ is available along the ray. We further consider two points on the ray specified by τ and τ_0, and assume that $A(\tau_0)$ and $\det\mathbf{Q}^{(q)}(\tau_0)$ are known and $\det\mathbf{Q}^{(q)}(\tau_0)\neq 0$. Then the continuation formula in ray-centred coordinates reads:

$$A(\tau) = \left[\frac{\rho(\tau_0)\mathcal{C}(\tau_0)}{\rho(\tau)\mathcal{C}(\tau)}\right]^{1/2}\left[\frac{\det\mathbf{Q}^{(q)}(\tau_0)}{\det\mathbf{Q}^{(q)}(\tau)}\right]^{1/2}\mathcal{R}^C(\tau,\tau_0)A(\tau_0) \ . \qquad (32)$$

For a detailed derivation, see Červený (2001, equation (5.4.15) with (4.14.39)). In equation (32), ρ is the density, $\mathcal{C}$ the phase velocity (known from ray tracing), $\mathcal{R}^C$ is the complete energy reflection/transmission coefficient along ray Ω from τ_0 to τ, and $\mathbf{Q}^{(q)}$ is the 2×2 matrix, which is a solution of the DRT. Its elements are defined in eq.(25). Matrix $\mathbf{Q}^{(q)}$ is often called the matrix of geometrical spreading, and $|\det\mathbf{Q}^{(q)}|^{1/2}$ the geometrical spreading. In the ray theory, the term $[\det\mathbf{Q}^{(q)}(\tau_0)/\det\mathbf{Q}^{(q)}(\tau)]^{1/2}$ is usually expressed in terms of modulus (related to geometrical spreading) and phase (phase shift due to caustics),

$$A(\tau) = \left[\frac{\rho(\tau_0)C(\tau_0)}{\rho(\tau)C(\tau)}\right]\left[\frac{|\det\mathbf{Q}^{(q)}(\tau_0)|}{|\det\mathbf{Q}^{(q)}(\tau)|}\right]^{1/2}\mathcal{R}^C(\tau,\tau_0)e^{\mathrm{i}T^c}(\tau,\tau_0)A(\tau_0) \ . \qquad (33)$$

The phase shift due to caustics $T^c(\tau,\tau_0)$ can be specified by the so-called KMAH index. Continuation relations (32) and (33) are regular as long as $\det\mathbf{Q}^{(q)}(\tau)$ is non-zero.

The complete energy R/T coefficient $\mathcal{R}^C$ from τ_0 to τ along Ω is a product of the plane-wave energy R/T coefficients determined at all points of incidence of ray Ω on the structural interfaces between τ_0 and τ. Mode conversions at individual interfaces are automatically included in $\mathcal{R}^C$. The algorithms for computing the plane-wave energy R/T coefficients at structural interfaces are well known, see, e.g., Červený (2001), where other references can also be found. For this reason, we do not discuss these algorithms here. Let us emphasize that in the zero-order approximation of the ray method, reflection/transmission of any high-frequency seismic wave at a curved interface separating two inhomogeneous media is described by plane-wave R/T coefficients. They do not depend on the curvatures of the considered interface and of the wavefront of the incident wave at the point of incidence at the interface. They also do not depend on the gradients of the density and the density-normalized elastic moduli at the point of incidence on both sides of the interface. Consequently, the R/T coefficients in the zero-order ray approximation depend only on local values of the density and the density-normalized elastic moduli at the point of incidence (on both sides of the interface) and on the angle of incidence. We further emphasize that $\mathcal{R}^C$ is a product of the energy R/T coefficients, not of the displacement R/T coefficients. With the displacement R/T coefficients, eq.(32) would include a multiplicative factor.

There is an important aspect related to the use of eq.(32) or eq.(33) for the scalar ray-theory amplitude $A(\tau)$, which corresponds to the zero-order approximation of the ray method. The equation is valid along any ray situated in a smoothly varying inhomogeneous medium with smooth structural interfaces. With increasing strength of variations of the medium (with its decreasing smoothness), one must expect decrease of the accuracy of the scalar ray-theory amplitude $A(\tau)$.

We emphasize the important assumption made in the derivation of the continuation relations (32) and (33), namely that $\det \mathbf{Q}^{(q)}(\tau_0) \neq 0$. The case of $\det \mathbf{Q}^{(q)}(\tau_0) = 0$ plays an important role when a point source is situated at τ_0. In this case, it is more useful to use the Green function amplitude $A^G(\tau)$ from (31). It is given by the relation

$$A^G(\tau) = \frac{\mathcal{R}^C \exp[\mathrm{i}T^c(\tau,\tau_0)]}{4\pi[\rho(\tau)\rho(\tau_0)C(\tau)C(\tau_0)]^{1/2}\mathcal{L}(\tau,\tau_0)} \ , \tag{34}$$

see Červený (2001, eq. (5.4.24)) or Červený et al. (2007, eq.78). The function $\mathcal{L}(\tau,\tau_0)$, called the relative geometrical spreading, is given by the relation

$$\mathcal{L}(\tau,\tau_0) = [|\det \mathbf{Q}_2^{(q)}(\tau,\tau_0)|]^{1/2} \ . \tag{35}$$

The 2×2 matrix $\mathbf{Q}_2^{(q)}(\tau,\tau_0)$ is one of 2×2 submatrices of the 4×4 ray propagator matrix $\mathbf{\Pi}(\tau,\tau_0)$ in ray-centred coordinates

$$\mathbf{\Pi}(\tau,\tau_0) = \begin{pmatrix} \mathbf{Q}_1^{(q)}(\tau,\tau_0) & \mathbf{Q}_2^{(q)}(\tau,\tau_0) \\ \mathbf{P}_1^{(q)}(\tau,\tau_0) & \mathbf{P}_2^{(q)}(\tau,\tau_0) \end{pmatrix} \ . \tag{36}$$

The ray propagator matrix $\mathbf{\Pi}(\tau,\tau_0)$ is the solution of dynamic ray tracing in ray-centred coordinates, with initial conditions

$$\mathbf{\Pi}(\tau,\tau_0) = \mathbf{I} \ , \tag{37}$$

where $\mathbf{I}$ is a 4×4 identity matrix. The function $T^c(\tau, \tau_0)$ in (34) is the complete phase shift due to caustics along the ray from the source to the receiver. The possible phase shift directly at the source is included. For details and computation of phase shift due to caustics see Klimeš (2010, 2014c). We do not present here the details, as it is not our intention to use formulae in ray-centred coordinates, but in Cartesian coordinates. The formulae in ray-centred coordinates are used here only as an auxiliary tool.

An alternative expression for the relative geometrical spreading $\mathcal{L}(\tau, \tau_0)$ is obtained from the well-known property of the ray-propagator matrix $\mathbf{\Pi}(\tau, \tau_0)$:

$$\begin{pmatrix} \mathbf{Q}^{(q)}(\tau) \\ \mathbf{P}^{(q)}(\tau) \end{pmatrix} = \mathbf{\Pi}(\tau, \tau_0) \begin{pmatrix} \mathbf{Q}^{(q)}(\tau_0) \\ \mathbf{P}^{(q)}(\tau_0) \end{pmatrix} . \tag{38}$$

See Červený (2001, eq.(4.3.29)). For a point source situated at τ_0 we have $\mathbf{Q}^{(q)}(\tau_0) = \mathbf{0}$, so that

$$\mathbf{Q}^{(q)}(\tau) = \mathbf{Q}_2^{(q)}(\tau, \tau_0)\mathbf{P}^{(q)}(\tau_0) . \tag{39}$$

Then we obtain from (35)

$$\mathcal{L}(\tau, \tau_0) = \left[\frac{|\det \mathbf{Q}^{(q)}(\tau)|}{|\det \mathbf{P}^{(q)}(\tau_0)|} \right]^{1/2} . \tag{40}$$

2.4.2 Ray-theory complex-valued amplitudes in Cartesian coordinates

In this section, we shall present the relations for the ray-theory amplitudes $A(\tau)$ and ray-theory amplitudes of the Green function $A^G(\tau)$ in general Cartesian coordinates.

First we derive the relations for $A(\tau)$. For this, we need a relation between $\hat{\mathbf{Q}}^{(x)}(\tau)$ and $\mathbf{Q}^{(q)}(\tau)$. Let us introduce the matrix $\hat{\mathbf{Q}}^{(q)}(\tau)$ as follows:

$$\hat{\boldsymbol{Q}}^{(q)}(\tau) = \begin{pmatrix} Q_{11}(\tau) & Q_{12}(\tau) & \mathcal{C}(\tau)p_1^{(q)}(\tau) \\ Q_{21}(\tau) & Q_{22}(\tau) & \mathcal{C}(\tau)p_2^{(q)}(\tau) \\ 0 & 0 & 1 \end{pmatrix} . \tag{41}$$

The transformation relation between the 3×3 matrices $\hat{\mathbf{Q}}^{(q)}(\tau)$ and $\hat{\mathbf{Q}}^{(x)}(\tau)$ reads

$$\hat{\mathbf{Q}}^{(x)}(\tau) = \hat{\mathbf{H}}(\tau)\hat{\mathbf{Q}}^{(q)}(\tau) , \tag{42}$$

where $\hat{\mathbf{H}}(\tau)$ is the transformation matrix (17). Equation (42) yields,

$$\hat{\mathbf{Q}}^{(q)}(\tau) = \hat{\mathbf{H}}^{-1}(\tau)\hat{\mathbf{Q}}^{(x)}(\tau) . \tag{43}$$

As $\det \hat{\mathbf{H}}(\tau) = C(\tau)$ and from (41) follows that $\det \hat{\mathbf{Q}}^{(q)}(\tau) = \det \mathbf{Q}^{(q)}(\tau)$, we obtain

$$\det \mathbf{Q}^{(q)}(\tau) = C^{-1}(\tau) \det \hat{\mathbf{Q}}^{(x)}(\tau) . \tag{44}$$

Equation (33) then yields

$$A(\tau) = \left[\frac{\rho(\tau_0)|\det \hat{\mathbf{Q}}^{(x)}(\tau_0)|}{\rho(\tau)|\det \hat{\mathbf{Q}}^{(x)}(\tau)|} \right]^{1/2} \mathcal{R}^C(\tau, \tau_0) e^{\mathrm{i}T^c(\tau,\tau_0)} A(\tau_0) . \tag{45}$$

This is the final relation for $A(\tau)$ expressed in general Cartesian coordinates.

For $|\det \hat{\mathbf{Q}}^{(x)}(\tau)|$ we can also write

$$|\det \hat{\mathbf{Q}}^{(x)}(\tau)| = |\epsilon_{ijk} Q^{(x)}_{i1}\, Q^{(x)}_{j2}\, \mathcal{U}_k| \ . \tag{46}$$

For a homogeneous Hamiltonian, we can write

$$\epsilon_{ijk} Q^{(x)}_{i1} Q^{(x)}_{j2} = \pm |X_1 \times X_2| n_k = \pm |X_1 \times X_2| C p_k \ , \tag{47}$$

where ϵ_{ijk} is the Levi-Civita symbol, and

$$X_{i1} = Q^{(x)}_{i1} \ , \qquad X_{i2} = Q^{(x)}_{i2} \ , . \tag{48}$$

We obtain finally

$$A(\tau) = \left[\frac{\rho(\tau_0)C(\tau_0)}{\rho(\tau)C(\tau)}\right]^{1/2} \left[\frac{|\mathbf{X}_1(\tau_0) \times \mathbf{X}_2(\tau_0)|}{|\mathbf{X}_1(\tau) \times \mathbf{X}_2(\tau)|}\right]^{1/2} \mathcal{R}^C(\tau,\tau_0) e^{\mathrm{i}T^c(\tau,\tau_0)} A(\tau_0) \ . \tag{49}$$

This is an alternative expression for the ray-theory amplitude $A(\tau)$ in Cartesian coordinates. Klimeš (2014b) showed that equation (45), even if we insert (46) into it, is valid even for inhomogeneous Hamiltonians, whereas (49) is valid only for homogeneous Hamiltonians.

For the ray-theory amplitudes of the Green function, expressed in Cartesian coordinates, we have to transform the relative geometrical spreading $\mathcal{L}(\tau,\tau_0)$ given by (40) from ray-centred coordinates to Cartesian coordinates. For the transformation of $|\det \mathbf{Q}^{(q)}(\tau)|$, we can use (44). The transformation between $\det \mathbf{P}^{(q)}(\tau)$ and $\det \mathbf{P}^{(x)}(\tau)$ is, however, more complicated, it contains also $\det \mathbf{Q}^{(q)}(\tau)$. See Klimeš (1994, eq. (30)). We, however, need here only the transformation at $\tau = \tau_0$, where $\mathbf{Q}^{(q)}(\tau_0) = \mathbf{0}$. Then the transformation simplifies:

$$|\det \mathbf{P}^{(q)}(\tau_0)| = |\det \hat{\mathbf{P}}^{(x)}(\tau_0) / \det \hat{\overline{\mathbf{H}}}^T(\tau_0)| = \mathcal{C}(\tau_0) |\det \hat{\mathbf{P}}^{(x)}(\tau_0)| \ , \tag{50}$$

see (22). This yields

$$\mathcal{L}(\tau,\tau_0) = \left\{\frac{|\det \hat{\mathbf{Q}}^{(x)}(\tau)|}{C(\tau_0)C(\tau)|\det \hat{\mathbf{P}}^{(x)}(\tau_0)|}\right\}^{1/2} \ . \tag{51}$$

Equation (51) can be also written in the following form:

$$\mathcal{L}(\tau,\tau_0) = \left\{\frac{|\epsilon_{ijk} Q^{(x)}_{i1}(\tau) Q^{(x)}_{j2}(\tau) \mathcal{U}_k(\tau)|}{C(\tau_0)C(\tau)|\epsilon_{lmn} P^{(x)}_{l1}(\tau_0) P^{(x)}_{m2}(\tau_0) p_n(\tau_0)|}\right\}^{1/2} \ . \tag{52}$$

As the vectors $P^{(x)}_{l1}(\tau_0)$ and $P^{(x)}_{m2}(\tau_0)$ are tangent to the slowness surface, we obtain

$$\epsilon_{lmn} P^{(x)}_{l1}(\tau_0) P^{(x)}_{m2}(\tau_0) = \pm |\mathbf{Y}_1(\tau_0) \times \mathbf{Y}_2(\tau_0)| \, \mathcal{U}_n(\tau_0) / \mathcal{U}(\tau_0) \ , \tag{53}$$

and

$$|\epsilon_{lmn} P^{(x)}_{l1}(\tau_0) P^{(x)}_{m2}(\tau_0) p_n(\tau_0)| = |\mathbf{Y}_1(\tau_0) \times \mathbf{Y}_2(\tau_0)| \mathcal{U}^{-1}(\tau_0) \ . \tag{54}$$

Here we have used the notation

$$Y_{l1}(\tau_0) = P^{(x)}_{l1}(\tau_0) \ , \quad Y_{m2}(\tau_0) = P^{(x)}_{m2}(\tau_0) \ . \tag{55}$$

The final relation for the relative geometrical spreading $\mathcal{L}(\tau, \tau_0)$ reads

$$\mathcal{L}(\tau, \tau_0) = \left\{ \frac{\mathcal{U}(\tau_0) |\mathbf{X}_1(\tau) \times \mathbf{X}_2(\tau)|}{C(\tau_0) |\mathbf{Y}_1(\tau_0) \times \mathbf{Y}_2(\tau_0)|} \right\}^{1/2} \ . \tag{56}$$

We emphasize that equation (56) is valid only for homogeneous Hamiltonians (i.e., for τ corresponding to travel time along the ray). For inhomogeneous Hamiltonians see Klimeš (2014b).

3 Time-harmonic integral superposition of paraxial Gaussian beams

Consider an arbitrary ray Ω of seismic body wave propagating in an inhomogeneous anisotropic medium, along which ray tracing and dynamic ray tracing in Cartesian coordinates have been performed. Then we can also construct the paraxial Gaussian beam concentrated close to the ray Ω. In the frequency domain, it is given by the relation

$$\begin{aligned} \mathbf{u}^B(x_i, \omega) &= \mathbf{U}^B(x_i, \omega) \exp\{\mathrm{i}\omega[\tau(\tilde{x}_m) + (x_k - \tilde{x}_k) p_k(\tilde{x}_m) \\ &+ \tfrac{1}{2}(x_k - \tilde{x}_k) M^{(x)}_{kl}(\tilde{x}_m)(x_l - \tilde{x}_l)]\} \ . \end{aligned} \tag{57}$$

Here ω is circular frequency, $\tilde{x}_m$ is a point situated on the ray Ω, close to the point x_i situated in the paraxial vicinity of Ω. The quantity $\tau(\tilde{x}_m)$ is a real-valued travel time at $\tilde{x}_m$, calculated from the initial point S of Ω, and $p_k(\tilde{x}_m)$ is the k-th Cartesian component of the real-valued slowness vector at point $\tilde{x}_m$. The 3×3 complex-valued matrix $\hat{\mathbf{M}}^{(x)}(\tilde{x}_m)$ is related to a 2×2 symmetric, positive definite matrix $\mathbf{M}(\tilde{x}_m)$. We call the 2×2 matrix $\mathbf{M}(\tilde{x}_m)$ the matrix of parameters of Gaussian beams. It is because at the initial point S of the ray Ω, it is used to specify the initial conditions for the DRT so that the matrix $\mathbf{M}(\tilde{x}_m)$ satisfies the existence conditions of Gaussian beams at any point of Ω, see eq.(38) and the following discussion in Červený and Pšenčík (2010a). The matrix $\mathbf{M}(\tilde{x}_m)$ controls the shape of Gaussian beam along the ray Ω. For high frequencies ω, the paraxial Gaussian beam (57) is narrow. For lower frequencies ω, the paraxial Gaussian beam is broader.

The relation of the matrix $\hat{\mathbf{M}}^{(x)}(\tilde{x}_m)$ to the matrix of the parameters of Gaussian beams, $\mathbf{M}(\tilde{x}_m)$, has the same form as (29):

$$\hat{\mathbf{M}}^{(x)} = \boldsymbol{\mathcal{F}} \mathbf{M} \boldsymbol{\mathcal{F}}^T + \mathbf{p}\boldsymbol{\eta}^T + \boldsymbol{\eta}\mathbf{p}^T - \mathbf{p}\mathbf{p}^T(\boldsymbol{\mathcal{U}}^T \mathbf{p}) \ . \tag{58}$$

Both matrices in (58) are, however, complex valued and $\mathbf{M}(\tilde{x}_m)$ is positive definite. Throughout this chapter, we understand systematically that $\hat{\mathbf{M}}^{(x)}$ and $\mathbf{M}$ are related by (58).

In equation (57), both for vectorial and tensorial $\mathbf{u}^B(x_i,\omega)$ and $\mathbf{U}^B(x_i,\omega)$ can be used. The exponential in (57) remains the same in both cases.

We do not give here the expression for $\mathbf{U}^B(x_i,\omega)$, as we are not interested in individual paraxial Gaussian beams, but in the integral superposition of paraxial Gaussian beams. The amplitude terms of individual paraxial Gaussian beams in the superposition will be discussed in a great detail in the next section.

The expression for paraxial Gaussian beams in inhomogeneous anisotropic media and for their integral superposition can be used for all the three elementary waves propagating in inhomogeneous anisotropic media, namely the P wave and the two S waves, S1 and S2. The two S waves, however, often interfere and form one coupled S wave. This coupled S wave can be evaluated using the coupling ray theory. We can again construct the paraxial Gaussian beams and integral superposition of paraxial Gaussian beams for coupled S waves.

Integral superposition of Gaussian beams can be also used in inhomogeneous weakly anisotropic media, in which weak anisotropy approximation can be used. This leads to the simplification of ray tracing and dynamic ray tracing. Most importantly, weak anisotropy approach includes automatically the above-mentioned coupling ray theory. As the integral superposition of paraxial Gaussian beams in inhomogeneous weakly anisotropic media is an important topic, we shall discuss the evaluation of quantities, necessary for the integral superposition in weakly anisotropic media in a great detail in Chapter 4.

In the following section, we derive several expressions for time-harmonic integral superposition of paraxial Gaussian beams in Cartesian coordinates, for inhomogeneous anisotropic layered structures. We start with known expressions in ray-centred coordinates, and transform these expressions to Cartesian coordinates. We shall also present expressions for integral superposition along a target surface. This expression may be suitable in many applications.

3.1 Integral superposition of paraxial Gaussian beams in ray-centred coordinates

The expression for integral superposition of paraxial Gaussian beams in 3D isotropic media, was first derived by Klimeš (1984a, equation (77)). See also Červený, Klimeš and Pšenčík (2007, equation (169)). These equations can be used, with a small modification, even for inhomogeneous anisotropic media. The latter equation reads:

$$\begin{aligned}
\mathbf{u}(x_m,\omega) &= (\omega/2\pi)\iint_{\mathcal{D}} \mathrm{d}\gamma_1 \mathrm{d}\gamma_2 \mathbf{U}(x_m)|\det \mathbf{Q}^{(q)}(\tilde{x}_m)| \\
&\times \{-\det[\mathbf{M}^{(q)}(\tilde{x}_m)-\mathbf{M}(\tilde{x}_m)]\}^{1/2} \\
&\times \exp\{\mathrm{i}\omega[\tau(\tilde{x}_m)+(x_k-\tilde{x}_k)p_k(\tilde{x}_m)+\tfrac{1}{2}(x_k-\tilde{x}_k)M^{(x)}_{kl}(\tilde{x}_m)(x_l-\tilde{x}_l)]\}\ .
\end{aligned} \tag{59}$$

Here $\mathbf{Q}^{(q)}(\tilde{x}_m)$, $\mathbf{M}^{(q)}(\tilde{x}_m)$ and $\mathbf{M}(\tilde{x}_m)$ are 2×2 matrices in ray-centred coordinates, and $M^{(x)}_{kl}$ are elements of the 3×3 complex-valued, symmetric matrix $\hat{\mathbf{M}}^{(x)}(\tilde{x}_m)$ specified in Cartesian coordinates. The matrix $\mathbf{M}^{(q)}(\tilde{x}_m)$ is a real-valued matrix of the second derivatives of travel time with respect to ray-centred coordinates q_I. The 3×3 matrix $\hat{\mathbf{M}}^{(x)}(\tilde{x}_m)$ is related to the 2×2 matrix of parameters of paraxial Gaussian beams, $\mathbf{M}(\tilde{x}_m)$, through equation (58).

The integral (59) can be slightly modified. We can write

$$\det \mathbf{Q}^{(q)}(\tilde{x}_m)\{-\det[\mathbf{M}^{(q)}(\tilde{x}_m) - \mathbf{M}(\tilde{x}_m)]\}^{1/2} = [-\det \boldsymbol{\mathcal{N}}(\tilde{x}_m)]^{1/2} \ , \tag{60}$$

where the 2×2 matrix $\boldsymbol{\mathcal{N}}(\tilde{x}_m)$ is given by the relation

$$\boldsymbol{\mathcal{N}}(\tilde{x}_m) = \mathbf{Q}^{(q)T}(\tilde{x}_m)\mathbf{P}^{(q)}(\tilde{x}_m) - \mathbf{Q}^{(q)T}(\tilde{x}_m)\mathbf{M}(\tilde{x}_m)\mathbf{Q}^{(q)}(\tilde{x}_m) \ . \tag{61}$$

The argument of $[-\det \boldsymbol{\mathcal{N}}(\tilde{x}_m)]^{1/2}$ is given by the relation

$$\mathrm{Re}[-\det \boldsymbol{\mathcal{N}}(\tilde{x}_m)]^{1/2} > 0 \qquad \text{for} \ \ \mathrm{Im}\boldsymbol{\mathcal{N}}(\tilde{x}_m) \neq 0 \ . \tag{62}$$

Inserting (60) into (59) we obtain the expression for the integral superposition of Gaussian beams in ray-centred coordinates in the form:

$$\begin{aligned} \mathbf{u}(x_m,\omega) \;&=\; (\omega/2\pi)\iint_{\mathcal{D}} \mathrm{d}\gamma_1 \mathrm{d}\gamma_2 \mathbf{U}(x_m)[-\det \boldsymbol{\mathcal{N}}(\tilde{x}_m)]^{1/2} \\ &\times\; \exp\{\mathrm{i}\omega[\tau(\tilde{x}_m) + (x_k - \tilde{x}_k)p_k(\tilde{x}_m) + \tfrac{1}{2}(x_k - \tilde{x}_k)M^{(x)}_{kl}(\tilde{x}_m)(x_l - \tilde{x}_l)]\} \ . \end{aligned} \tag{63}$$

3.2 Integral superposition of paraxial Gaussian beams in Cartesian coordinates

In this section, we assume that the simplified DRT in Cartesian coordinates has been performed. In such a way, we can determine 3×2 matrices $\mathbf{Q}^{(x)}$ and $\mathbf{P}^{(x)}$ with components

$$Q^{(x)}_{iJ} = \partial x_i/\partial \gamma_J \ , \qquad P^{(x)}_{iJ} = \partial p_i/\partial \gamma_J \ . \tag{64}$$

The simplified DRT for these matrices is given by (B-26). We also introduce the 3×2 matrices $\mathbf{X}$ and $\mathbf{Y}$ by the relations

$$X_{iJ} = \begin{pmatrix} Q^{(x)}_{11} & Q^{(x)}_{12} \\ Q^{(x)}_{21} & Q^{(x)}_{22} \\ Q^{(x)}_{31} & Q^{(x)}_{32} \end{pmatrix} \ , \quad Y_{iJ} = \begin{pmatrix} P^{(x)}_{11} & P^{(x)}_{12} \\ P^{(x)}_{21} & P^{(x)}_{22} \\ P^{(x)}_{31} & P^{(x)}_{32} \end{pmatrix} \ . \tag{65}$$

It is not difficult to transform integral (63) from ray-centred to Cartesian coordinates. For this, we only need to transform $\boldsymbol{\mathcal{N}}$, as the function in the exponent is already given in Cartesian coordinates. We use the transformation relations

$$\mathbf{Q}^{(q)} = \boldsymbol{\mathcal{E}}^T\mathbf{X} \ , \qquad \mathbf{Q}^{(q)T}\mathbf{P}^{(q)} = \mathbf{X}^T\mathbf{Y} \ , \tag{66}$$

see Červený (2000, eq.(6.3)). The 2×2 matrix $\boldsymbol{\mathcal{N}}(\tilde{x}_m)$ is then given by the relation

$$\boldsymbol{\mathcal{N}} = \mathbf{X}^T\mathbf{Y} + \mathbf{X}^T\boldsymbol{\mathcal{E}}\mathbf{M}\boldsymbol{\mathcal{E}}^T\mathbf{X} \ , \tag{67}$$

where all quantities are taken at $\tilde{x}_m$.

Thus, the final integral superposition of paraxial Gaussian beams in Cartesian coordinates is again given by (63), where $\boldsymbol{\mathcal{N}}$ is given by (67) and $M^{(x)}_{kl}$ by (58).

3.3 Integral superposition of paraxial Gaussian beams in Cartesian coordinates along a target surface Σ

It is customary, but not necessary, to introduce the target surface Σ along which the results of ray tracing, dynamic ray tracing and ray-theory amplitudes are stored for further computations. The examples of suitable target surface Σ are the Earth's surface (when the wave fields is evaluated along the Earth's surface), planes perpendicular to the Cartesian coordinate axes x_1, x_2 or x_3, a spherical surface with its center at S, etc. The form of the target surface depends on the application. Receiver R should be also situated on the target surface or in its close vicinity. We denote by R_γ^Σ the point of intersection of ray Ω specified by ray parameters γ_1 and γ_2 with the target surface Σ. Thus, the points R_γ^Σ on the target surface Σ are not specified in advance; they are calculated by initial value ray tracing from the point S to target surface Σ.

Consequently, we can use the notation:

$$\tilde{x}_m = x_m(R_\gamma^\Sigma) \ , \qquad x_k = x_k(R) \ . \tag{68}$$

Inserting (68) into (63), we obtain

$$\begin{aligned}
\mathbf{u}(x_m(R), \omega) \;&=\; (\omega/2\pi) \iint\limits_{\mathcal{D}} \mathrm{d}\gamma_1 \mathrm{d}\gamma_2 \mathbf{U}(x_m(R_\gamma^\Sigma))[-\det \boldsymbol{\mathcal{N}}(x_m(R_\gamma^\Sigma))]^{1/2} \\
&\times\; \exp\{\mathrm{i}\omega[\tau^R(x_m(R_\gamma^\Sigma)) + (x_k(R) - x_k(R_\gamma^\Sigma))p_k(x_m(R_\gamma^\Sigma)) \\
&+\; \tfrac{1}{2}(x_k(R) - x_k(R_\gamma^\Sigma) M_{kl}^{(x)}(x_m(R_\gamma^\Sigma))(x_l(R) - x_l(R_\gamma^\Sigma))]\} \ .
\end{aligned} \tag{69}$$

This is the final formula for the superposition of paraxial Gaussian beams in Cartesian coefficients along the target surface Σ. Again, the 3×3 matrix $\hat{\mathbf{M}}^{(x)}$ is given by (58), where $\mathbf{M}$ is a 2×2 matrix of parameters of Gaussian beams.

We add several short notes to formula (69). We emphasize again that the points R_γ^Σ are situated along the target surface Σ, but the receiver point R may be situated anywhere in its close vicinity. The function $M_{kl}^{(x)}(x_m(R_\gamma^\Sigma))$ is given by relation (58), in which all quantities are taken at point R_γ^Σ, and matrix $\mathbf{M}$ is the 2×2 matrix of parameters of Gaussian beams.

The formula (69) is valid both for vectorial and tensorial $\mathbf{u}$. For vectorial $\mathbf{u}$, we take $\mathbf{U}$ in the integral to equal the vectorial ray-theory amplitude, see (30). For tensorial $\mathbf{u}$, corresponding to the Green function, we take $\mathbf{U}$ in the integral to equal the tensorial ray-theory amplitude of the Green function $\mathbf{U}^G$, see (31). The 2×2 matrix $\boldsymbol{\mathcal{N}}$ is given by (67).

4 Quantities necessary for evaluation of summation integrals in weakly anisotropic media

All the procedures of the previous sections can be also specified for inhomogeneous, weakly anisotropic media. This leads to simplification of ray tracing and dynamic ray tracing equations and also to simpler and explicit expressions for the phase velocity and polarization vectors. S waves, which propagate coupled in weakly anisotropic media and in vicinities of S-wave singularities, represent certain complication. It can be removed if instead of two elementary S waves propagating generally in anisotropic media, we deal with a single coupled S wave. In the following, we consider propagation of P and coupled S waves in inhomogeneous, weakly anisotropic media without interfaces.

For the derivation of weak-anisotropy formulae, the perturbation theory is used, in which deviation of anisotropy from isotropy is considered to be the perturbation. Detailed derivation of the following formulae can be found in Pšenčík and Gajewski (1998), Pšenčík and Farra (2005, 2007) for P waves and Farra and Pšenčík (2008, 2010) for coupled S waves. Many other references can be found in the above papers.

The deviation of anisotropy from isotropy is represented by 21 weak-anisotropy (WA) parameters, which represent an alternative to 21 independent elastic moduli $C_{\alpha\beta}$ or density-normalized elastic moduli $A_{\alpha\beta}$ in the Voigt notation. As $C_{\alpha\beta}$ or $A_{\alpha\beta}$, the WA parameters can be used for the specification of anisotropy of arbitrary symmetry and strength. The WA parameters are a generalization of Thomsen's (1986) parameters introduced to describe a transversely isotropic medium with the vertical axis of symmetry (VTI). Another generalization with respect to Thomsen's (1986) parameters is the use of arbitrarily chosen non-zero constant reference velocities α and β instead of P- and S-wave velocities $\sqrt{A_{33}}$ and $\sqrt{A_{55}}$ along the axis of symmetry used by Thomsen (1986). Important advantage of WA parameters is that they are related to the used coordinate system and not to the symmetry elements (planes of symmetry, axes of symmetry) of the studied medium. This makes their applicability to models with arbitrary anisotropy symmetry and its orientation elementary. The use of constant reference velocities α and β makes the use of WA parameters more flexible. When, for example, a cross-hole experiment is considered, in which waves propagate prevailingly horizontally (and not vertically as in Thomsen's original design), constants α and β can be chosen so that they correspond to the horizontal propagation. It is always desirable to specify α and β so that they make the WA parameters small. Although WA parameters depend on the choice of the reference velocities α and β, the formulae for the P- and S-wave eigenvalues and eigenvectors of the Christoffel matrix, which represent squares of phase velocities and polarization vectors, are *independent* of α and β (Farra and Pšenčík, 2003). For more details on the WA parameters, see Farra et al. (2015).

In contrast to Thomsen's (1986) definition, the WA parameters are related linearly to density-normalized elastic moduli $A_{\alpha\beta}$. Due to this, Thomsen's parameters can be used for the exact specification of phase velocities (Tsvankin, 2001), but WA parameters cannot. This, however, does not matter because WA parameters are designed for weakly anisotropic media, in which, as illustrated by tests in the above-mentioned papers, they work very well. Due to the linear relationship between density-normalized elastic moduli and WA parameters, the transformation between the two types of parameters causes no problems. WA parameters are dimensionless and small (if constants α and β are chosen properly). They are all of comparable size (in contrast to $A_{\alpha\beta}$ parameters, in which the diagonal parameters are much larger than the off-diagonal ones), which is very convenient property when solving various inversion problems, in which WA parameters are the sought quantities, see, for example, Růžek and Pšenčík (2014).

All 21 WA parameters can be expressed in terms of 21 density-normalized elastic parameters $A_{\alpha\beta}$ in Voigt notation and two constant reference velocities α and β in the following way:

$$\epsilon_x = \frac{A_{11}-\alpha^2}{2\alpha^2} \ , \quad \epsilon_y = \frac{A_{22}-\alpha^2}{2\alpha^2} \ , \quad \epsilon_z = \frac{A_{33}-\alpha^2}{2\alpha^2} \ ,$$

$$\delta_x = \frac{A_{23}+2A_{44}-\alpha^2}{\alpha^2} \ , \quad \delta_y = \frac{A_{13}+2A_{55}-\alpha^2}{\alpha^2} \ , \quad \delta_z = \frac{A_{12}+2A_{66}-\alpha^2}{\alpha^2} \ ,$$

$$\chi_x = \frac{A_{14}+2A_{56}}{\alpha^2} \ , \quad \chi_y = \frac{A_{25}+2A_{46}}{\alpha^2} \ , \quad \chi_z = \frac{A_{36}+2A_{45}}{\alpha^2} \ ,$$

$$\epsilon_{15} = \frac{A_{15}}{\alpha^2} \ , \quad \epsilon_{16} = \frac{A_{16}}{\alpha^2} \ , \quad \epsilon_{24} = \frac{A_{24}}{\alpha^2} \ , \quad \epsilon_{26} = \frac{A_{26}}{\alpha^2} \ , \quad \epsilon_{34} = \frac{A_{34}}{\alpha^2} \ , \quad \epsilon_{35} = \frac{A_{35}}{\alpha^2} \ ,$$

$$\epsilon_{46} = \frac{A_{46}}{\alpha^2} \ , \quad \epsilon_{56} = \frac{A_{56}}{\alpha^2} \ , \quad \epsilon_{45} = \frac{A_{45}}{\beta^2} \ ,$$

$$\gamma_x = \frac{A_{44}-\beta^2}{2\beta^2} \ , \quad \gamma_y = \frac{A_{55}-\beta^2}{2\beta^2} \ , \quad \gamma_z = \frac{A_{66}-\beta^2}{2\beta^2} \ . \tag{70}$$

Symbols $A_{\alpha\beta}$ denote the density-normalized elastic parameters in the Voigt notation.

Please, note that the definitions of parameters δ_x and δ_y, and of parameters γ_x and γ_y are interchanged in Pšenčík and Gajewski (1998, eq.(17b)), Farra and Pšenčík (2003, eq.(A3)) and Pšenčík and Farra (2005, eq.(A-1); 2007, eq.(A1)).

Derivatives of the P-wave and S-wave eigenvalues of the generalized Christoffel matrix play a basic role in ray tracing and dynamic ray tracing equations (A-2) with (7) and (B-1), (B-2) with (7). In the weak-anisotropy approximation, the exact eigenvalues are replaced by their first-order counterparts, expressed in terms of WA parameters. In case of coupled S wave, instead of separate S-wave eigenvalues, their average is used (Bakker, 2002; Bulant and Klimeš, 2002). Thus, when solving the S-waves ray tracing equations, instead of calculating a physical ray, an artificial trajectory, called *common S-wave ray* is calculated, along which the coupled S wave is evaluated.

The explicit expressions for the first-order approximation of the P-wave eigenvalue $G_P(x_m, p_m)$ and of the average of the first-order approximations of S-wave eigenvalues $G_S(x_m, p_m)$ follow from equation

$$G(x_m, p_n) = a_{ijkl}p_j p_l g_i g_k \ , \tag{71}$$

by expanding it with respect to the WA parameters.

The first-order approximation of the P-wave eigenvalue $G_P(x_m, p_m)$ reads (Pšenčík and Farra, 2005, eqs (9), (12)):

$$G_P = \alpha^2\Big(p_k p_k + 2(p_k p_k)^{-1}[(\epsilon_x p_1^4 + \epsilon_y p_2^4 + \epsilon_z p_3^4) + \delta_x p_2^2 p_3^2 + \delta_y p_1^2 p_3^2 + \delta_z p_1^2 p_2^2$$
$$+2(\epsilon_{16} p_2 + \epsilon_{15} p_3) p_1^3 + 2(\epsilon_{24} p_3 + \epsilon_{26} p_1) p_2^3 + 2(\epsilon_{35} p_1 + \epsilon_{34} p_2) p_3^3$$
$$+2(\chi_x p_1 + \chi_y p_2 + \chi_z p_3) p_1 p_2 p_3]\Big). \tag{72}$$

Expression (72) for the P-wave eigenvalue G_P may seem too complicated when compared, for example, with equation (71). But we must realize that the RHS of equation (71) is composed of 81 terms while the RHS of (72) of only 16. Moreover, the exact eigenvalue (71) specified for a P wave depends on all 21 density-normalized elastic parameters $A_{\alpha\beta}$ while (72) depends on only 15 WA parameters. The number of WA parameters further reduces when higher-symmetry anisotropic media are considered. In case of an orthorhombic symmetry with planes of symmetry parallel to coordinate planes, it is 6 WA parameters ϵ_x, ϵ_y, ϵ_z, δ_x, δ_y and δ_z, in a TI symmetry with axis of symmetry parallel to a coordinate axis only 3 parameters, ϵ_x, ϵ_z and δ_x! In an isotropic medium, equation (72) yields exact expression for the P-wave eigenvalue of the Christoffel matrix (4), $V^2(x_m) p_k p_k$, where $V(x_m)$ denotes the P-wave velocity.

Derivatives of $G_P(x_m, p_m)$ with respect to spatial coordinates x_m and components p_m of the slowness vector $\mathbf{p}$, which are necessary for the evaluation of right-hand sides of ray tracing equations (A-2) and dynamic ray tracing equations (B-1) in anisotropic media of arbitrary symmetry, are given in Appendix D. Let us emphasize again that although the constant reference velocity α appears in the expression (72) for $G_P(x_m, p_n)$, and also in its derivatives in Appendix D, $G_P(x_m, p_n)$ and its derivatives are independent of α.

The explicit expression for the first-order approximation of the average of the S-wave eigenvalues, $G_S(x_m, p_m)$, reads (Farra and Pšenčík, 2008, eq. (19)):

$$G_S = \beta^2\Big(p_i p_i + \epsilon_{45} p_1 p_2 + \epsilon_{46} p_1 p_3 + \epsilon_{56} p_2 p_3 + \gamma_y(p_1^2 + p_3^2) + \gamma_x(p_2^2 + p_3^2) + \gamma_z(p_1^2 + p_2^2)\Big)$$
$$-\alpha^2(p_i p_i)^{-1}\Big(\delta_x p_2^2 p_3^2 + \delta_y p_1^2 p_3^2 + \delta_z p_1^2 p_2^2 - \epsilon_x p_1^2(p_2^2 + p_3^2) - \epsilon_y p_2^2(p_1^2 + p_3^2) - \epsilon_z p_3^2(p_1^2 + p_2^2)$$
$$+2(\chi_x p_1 + \chi_y p_2 + \chi_z p_3) p_1 p_2 p_3 - (\epsilon_{16} p_2 + \epsilon_{15} p_3) p_1(p_2^2 + p_3^2 - p_1^2)$$
$$-(\epsilon_{26} p_1 + \epsilon_{24} p_3) p_2(p_1^2 + p_3^2 - p_2^2) - (\epsilon_{34} p_2 + \epsilon_{35} p_1) p_3(p_1^2 + p_2^2 - p_3^2)\Big). \tag{73}$$

Although the expression for $G_S(x_m, p_m)$ is more complicated than that for $G_P(x_m, p_m)$, it still contains less terms than the exact $G_S(x_m, p_m)$ derived from equation (71). Similarly as in the case of $G_P(x_m, p_m)$, the expression (73) simplifies considerably in higher-symmetry anisotropic media. In contrast to $G_P(x_m, p_m)$, the average of S-wave eigenvalues $G_S(x_m, p_m)$ depends on all 21 WA parameters (70) in case of the anisotropy of arbitrary symmetry, on 9 WA parameters ϵ_x, ϵ_y, ϵ_z, δ_x, δ_y, δ_z, γ_x, γ_y and γ_z in orthorhombic media with planes of symmetry parallel with coordinate planes and on 5 WA parameters ϵ_y, ϵ_z, δ_x, γ_x and γ_z in TI media with axis of symmetry parallel to a coordinate axis, see Farra and Pšenčík (2008).

Derivatives of (73) with respect to x_m and p_n have a similar form as derivatives of (72) given in the first part of Appendix D. For the first derivatives necessary for the evaluation of right-hand sides of ray tracing equations (A-2) with (7), see the end of Appendix D.

As in case of $G_P(x_m, p_m)$, the average $G_S(x_m, p_m)$ od S-wave eigenvalues and its derivatives are independent of constant reference velocities α and β. By solving ray tracing equations (A-2) with derivatives of $G_S(x_m, p_m)$, we obtain the first-order common S-wave ray.

Let us note that eqs (72) and (73) can be also used for the evaluation of the first-order approximation of the square of the P-wave phase velocity and of the common S-wave phase velocity since

$$C^2(x_m, N_m) = G(x_m, N_m). \tag{74}$$

It means that for the determination of the corresponding phase velocity it is sufficient to replace the components of the slowness vector p_i in eqs (72) or (73) by the components N_i of a unit vector $\mathbf{N}$ parallel to the slowness vector.

Let us now present expressions for the first-order approximations of polarization vectors.

The first-order P-wave polarization vector $\mathbf{g}_3$ is given by the formula (Pšenčík and Farra, 2007, eq.(10)):

$$\mathbf{g}_3 = \mathbf{N} + \frac{B_{13}(x_m, N_m)\mathbf{e}_1 + B_{23}(x_m, N_m)\mathbf{e}_2}{V_P^2 - V_S^2}. \tag{75}$$

The case of a coupled S wave is similar to the case of an S wave in an isotropic medium. Instead of the determination of specific polarization vectors, we can only determine the coupled S-wave polarization plane. The first-order polarization plane of coupled S wave is specified by two vectors $\mathbf{g}_K$ (Farra and Pšenčík, 2010, eq.(13)):

$$\mathbf{g}_K = \mathbf{e}_K - \frac{B_{K3}(x_m, N_m)}{V_P^2 - V_S^2}\mathbf{e}_3. \tag{76}$$

Symbols V_P and V_S in (75) and (76) denote the P- and S-wave velocities corresponding to a reference isotropic medium closely approximating the studied weakly anisotropic medium along the considered ray. In contrast to constants α and β used in the definition of WA parameters (70), velocities V_P and V_S may vary along the ray. Thus their choice is completely independent from the choice of α and β.

The quantities B_{ij} in (75) and (76) are elements of the matrix $\mathbf{B}(x_m, N_m)$, which plays an important role in the weak-anisotropy approximations. Its elements are defined as:

$$B_{ij}(x_m, N_m) = \Gamma_{kl}(x_m, N_m)e_{ik}e_{jl}. \tag{77}$$

The symbol Γ_{kl} denotes an element of the generalized Christoffel matrix (4) with the slowness vector $\mathbf{p}$ replaced by the unit vector $\mathbf{N}$ in its direction. The symbols e_{jm} denote Cartesian components of three mutually perpendicular unit vectors $\mathbf{e}_1$, $\mathbf{e}_2$ and $\mathbf{e}_3 \equiv \mathbf{N}$ also used in (75) and (76). Vectors $\mathbf{e}_1$ and $\mathbf{e}_2$ can be chosen arbitrarily in the plane perpendicular to $\mathbf{N}$. Matrix $\mathbf{B}(x_m, N_m)$, given in (77), can be obtained by the rotation,

$$\boldsymbol{B} = \boldsymbol{R}^T \bar{\boldsymbol{B}} \boldsymbol{R}, \tag{78}$$

from matrix $\bar{\mathbf{B}}(x_m, N_m)$, specified explicitly in Appendix C, eqs (C-5). Rotation matrix $\boldsymbol{R}$ has the following form:

$$\boldsymbol{R} = \begin{pmatrix} \cos\Phi & -\sin\Phi & 0 \\ \sin\Phi & \cos\Phi & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{79}$$

In (79), the angle Φ is the acute angle between the basis vectors $\mathbf{e}_K$ introduced above and the vectors $\bar{\mathbf{e}}_K$ used in Appendix C, eqs. (C-2) or (C-4). Matrices $\mathbf{B}$ and $\bar{\mathbf{B}}$ are independent of the choice of the constant reference velocities α and β. It can also be shown that the terms B_{33}, $B_{11}+B_{22}$ and $B_{13}^2+B_{23}^2$ are independent of the choice of vectors $\mathbf{e}_1$ and $\mathbf{e}_2$. This property of B_{33} and $B_{11}+B_{22}$ is obvious from equations (72) and (73) if we realize that $G_P(x_m, p_m) = B_{33}(x_m, p_m)$ and $G_S(x_m, p_m) = B_{11}(x_m, p_m) + B_{22}(x_m, p_m)$.

As mentioned above, by solving ray tracing equations (A-2) with the right-hand sides specified in Appendix D, equations (D-1), we obtain first-order P-wave rays and first-order travel times along them. We can easily increase the accuracy of the traveltimes by calculating the second-order P-wave travel time correction $\Delta\tau$ along the first-order ray (Pšenčík and Farra, 2005, eq. (33)):

$$\Delta\tau = -\frac{1}{2}\int c^{-2}(x_m, N_m)\frac{B_{13}^2(x_m, N_m) + B_{23}^2(x_m, N_m)}{V_P^2 - V_S^2}d\tau. \tag{80}$$

The meaning of all quantities appearing in (80) is the same as in the above formulae. We can see that for the evaluation of the correction (80), we can choose vectors $\mathbf{e}_1$ and $\mathbf{e}_2$ arbitrarily because the term $B_{13}^2 + B_{23}^2$ is independent of their choice. Optimum choice of V_P and V_S in (80) is $V^2 = (p_k p_k)^{-1}$ and $V_S^2 = V_P^2/3$, where p_k are components of the first-order slowness vector $\mathbf{p}$ obtained by solving (A-2) with the right-hand sides given in Appendix D. This specification yields the most accurate results.

We have now available all necessary quantities for the evaluation of P-wave elementary ray-theory Green function. It reads

$$G_{ij}^{\mathrm{ray}}(R_\gamma) = \frac{g_{3i}(R_\gamma)g_{3j}(S)}{4\pi[\rho(S)\rho(R_\gamma)C_P(S)C_P(R_\gamma)]^{1/2}}\,\frac{\exp[i\,T^G(R_\gamma, S)]}{\mathcal{L}(R_\gamma, S)}\;. \tag{81}$$

Quantities $\mathbf{g}_3$, C_P and $\mathcal{L}$ in (81) are the first-order counterparts of the exact polarisation vector, phase velocity and relative geometrical spreading.

The evaluation of coupled S-wave elementary ray-theory Green function is slightly more complicated. The i-th Cartesian component of the frequency-dependent vectorial amplitude factor at point R_γ generated by point force at S along the j-th Cartesian axis reads:

$$G_{ij}^{\mathrm{ray}}(R_\gamma) = \frac{\mathcal{A}(R_\gamma)g_{1i}(R_\gamma) + \mathcal{B}(R_\gamma)g_{2i}(R_\gamma)}{[\rho(R_\gamma)C_S(R_\gamma)]^{1/2}\mathcal{L}(R_\gamma, S)}\exp[i\,T^G(R_\gamma, S)]. \tag{82}$$

In (82), $\mathcal{A}$ and $\mathcal{B}$ are the amplitude coefficients, which can be obtained by solving a coupled system of two linear differential equations Farra and Pšenčík, 2010, eq. (21):

$$\begin{pmatrix} d\mathcal{A}/d\tau \\ d\mathcal{B}/d\tau \end{pmatrix} = -\frac{\mathrm{i}\omega}{2}\begin{pmatrix} M_{11}-1 & M_{12} \\ M_{12} & M_{22}-1 \end{pmatrix}\begin{pmatrix} \mathcal{A} \\ \mathcal{B} \end{pmatrix} \tag{83}$$

with the initial conditions

$$\mathcal{A}(S) = \frac{g_{1j}(S)}{4\pi(\rho(S)C_S(S))^{1/2}}, \qquad \mathcal{B}(S) = \frac{g_{2j}(S)}{4\pi(\rho(S)C_S(S))^{1/2}}. \tag{84}$$

The elements of the 2×2 matrix $\boldsymbol{M}$ in (83) read

$$M_{KL}(x_m, p_m) = B_{KL}(x_m, p_m) - C_S^2 \frac{B_{K3}(x_m, p_m) B_{L3}(x_m, p_m)}{V_P^2 - V_S^2}. \tag{85}$$

For the evaluation of elements of matrix $\mathbf{B}(x_m, p_n)$ in equation (85), we need a frame of three orthonormal vectors $\mathbf{e}_i$ continuously varying along the common S-wave ray. For this purpose, we can use the vectorial basis of the wavefront orthonormal coordinate system, see, e.g., Červený (2001). In it, the vector $\mathbf{e}_3$ is obtained as a unit vector parallel to the first-order slowness vector $\mathbf{p}$ and remaining two unit vectors can be determined by solving the following system of ordinary differential equations along the ray:

$$\frac{de_{Ki}}{d\tau} = -C_S^2 (e_{Kk} \frac{dp_k}{d\tau}) p_i, \tag{86}$$

with mutually perpendicular unit vectors $\mathbf{e}_1$ and $\mathbf{e}_2$, chosen arbitrarily in the plane perpendicular to $\mathbf{N}$ at the initial point S. In fact, it is sufficient to calculate only one of the vectors $\mathbf{e}_K$. The other can be found from the condition of orthogonality of all three vectors $\mathbf{e}_i$. In (86), $C_S = C_S(x_m, N_m)$ is the first-order common S-wave phase velocity corresponding to G_S, $C^2 = G_S(x_m, N_m)$.

It is important to note that the travel times obtained by solving the coupled system of differential equations (83) contain automatically the second-order traveltime correction. It is thus not necessary to perform the quadratures along the common S-wave ray as for P waves, see equation (80).

The amplitudes of the first-order elementary ray-theory Green function $G_{ij}^{\text{ray}}(R_\gamma)$ given by (81) for P waves, and by (82) for coupled S wave can be used in the superposition integral (63) or (69) in the same way as the amplitude A^G in (34).

5 Concluding remarks

Here we present several additional remarks and comments to the presented equations for the integral superpositions of paraxial Gaussian beams in Cartesian coordinates. In Chapter 3, we presented two equations for integral superpositions of paraxial Gaussian beams, namely (63) and (69). Equation (63) has a general character, the form of superposition is not specified in it. In equation (69), the superposition along a target surface Σ is performed. For simplicity, we refer here to the integral superposition of paraxial Gaussian beams (69) along a target surface Σ only. Our remarks and comments are, however, in great extent, applicable also to equation (63).

Integral superposition proposed in this paper has the following advantages:

1) All computations, including dynamic ray tracing, are performed in global Cartesian coordinates. Similarly, the position of the initial point S of the ray (e.g., a point source), of the receiver point R and of the points R_γ of the intersection of rays with the target surface Σ are specified in Cartesian coordinates.

2) It is sufficient to use only the simplified version of the dynamic ray tracing described in Section 2.3.3, and compute only 3×2 columns X_1, X_2 and Y_1, Y_2 of the 3×3 matrices $\hat{\mathbf{Q}}^{(x)}$ and $\hat{\mathbf{P}}^{(x)}$. Third columns of paraxial matrices $\hat{\mathbf{Q}}^{(x)}$ and $\hat{\mathbf{P}}^{(x)}$ are not needed at all.

3) Equation (69) is applicable even to other types of wavefields (acoustic waves, electromagnetic waves, radio waves, etc.), not only to seismic wavefields.

4) There is no need for the two point ray tracing. Only an orthonomic system of rays which intersect the target surface Σ should be computed.

5) Equation (69) may be used for both vectorial and tensorial form of the displacement vector $\mathbf{u}$; we must only take vectorial or tensorial ray-theory amplitude $\mathbf{U}$. Thus, we can take the same equation (69) when we compute the wavefield generated at a smooth initial surface and the wavefield generated by a point source (Green function). Only the ray-theory amplitude $\mathbf{U}$ is different in both cases.

6) Equation (69) is applicable to inhomogeneous anisotropic as well as isotropic media and also to pressure waves in liquids. Only the expression for the ray-theory amplitude $\mathbf{U}$ differs in these cases.

7) Equation (69) is also applicable to models with structural interfaces with which the wavefield interacts on a way between the source and the target surface Σ. It is only necessary to take into account the transformation relations for ray tracing and dynamic ray tracing at interfaces and consider the complete energy reflection/transmission coefficients when evaluating amplitudes.

8) Equation (69) may be applied to any of the three waves P, S1, S2 propagating in inhomogeneous anisotropic media. It can be also applied to arbitrary converted, or multiply converted waves. In isotropic inhomogeneous media, it can be applied both to P and S waves, and to converted waves.

9) Evaluation of the superposition integral (69) can simplify considerably in inhomogeneous, weakly anisotropic media when the weak-anisotropy approximation is used, in which deviation of anisotropy from isotropy is considered a perturbation. Weak-anisotropy approximation includes automatically the coupling ray theory (in weakly anisotropic media problems arise not only at singularities, but everywhere where anisotropy differs only little from isotropy). The integral superposition is thus applied to two waves as in isotropic media, to the P wave and to the coupled S wave.

10) Computations of S waves in inhomogeneous anisotropic media often collapse due to the existence of S-wave singularities. The problem of S-wave singularities can be avoided by the use of the coupling ray theory, in which one, coupled S wave, is considered instead of the two separate S waves. Equation (69) can be also used for the integral superposition of such coupled S waves.

11) The target surface Σ used in the computation may be chosen in different ways. It may be taken along the Earth's surface, which is important when we compute the wave field along the surface of the Earth. Another important possibility is to take the target surface along planes perpendicular to the Cartesian coordinate axes.

12) As soon as the required data along the target surface Σ are available, it is possible to compute (69) for receivers R situated arbitrarily at the target surface Σ. Moreover, it is possible to evaluate (69) even for receivers R which are not situated on the target surface Σ, but close to it.

13) A great advantage of equation (69) is that the target surface Σ may be taken the same for different elementary waves. Thus, the complete wave field consisting of several elementary waves, may be computed using the same target surface Σ.

14) The superposition integral (69) may be also used to compute the wavefield generated by various types of point sources, e.g. explosive single force or moment tensor point sources.

15) The superposition integral (69) can also be used for other than point source, for example, voluminal, surficial or line sources. The ray-theory expressions for line sources required in (69) can be found in Červený and Moser (2007).

16) The computation of all quantities included in the integral superposition of paraxial Gaussian beams is described in the paper in detail. The exception is the computation of phase shift due to caustics, which is also needed in our equations. The computation of the phase shift due to caustics is described in the paper Klimeš (2014c).

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Appendix A

Ray-tracing in inhomogeneous anisotropic media with interfaces

We consider the eikonal equation for inhomogeneous anisotropic media with Hamiltonian defined by the relation

$$\mathcal{H}(x_i, p_j) = \tfrac{1}{2} G_m(x_i, p_j) \ , \qquad (A-1)$$

where $G_m(x_i, p_j)$ is one of the three eigenvalues of the generalized Christoffel matrix $\Gamma_{ik} = a_{ijkl} p_j p_l$. We assume that the eigenvalue G_m differs from the other two eigenvalues.

A1) **Ray tracing system**

The ray tracing system is given by the system of six nonlinear ordinary differential equations of the first order,

$$\frac{\mathrm{d}x_i}{\mathrm{d}\tau} = \frac{\partial\mathcal{H}}{\partial p_i}\ , \quad \frac{\mathrm{d}p_i}{\mathrm{d}\tau} = -\frac{\partial\mathcal{H}}{\partial x_i}\ . \tag{A-2}$$

Here the parameter τ along the ray represents the travel time. The right-hand sides of the ray tracing system (A-2) represent components $\mathcal{U}_i = \partial\mathcal{H}/\partial p_i$ of the ray velocity vector $\boldsymbol{\mathcal{U}}$, and $\eta_i = -\partial\mathcal{H}/\partial x_i$ of vector $\boldsymbol{\eta}$. They can be determined from the equations

$$\frac{\partial\mathcal{H}}{\partial p_i} = \mathcal{U}_i = a_{ijkl}p_l g_j^{(m)} g_k^{(m)}\ , \quad -\frac{\partial\mathcal{H}}{\partial x_i} = \eta_i = -\frac{1}{2}\frac{\partial a_{jkln}}{\partial x_i}p_k p_n g_j^{(m)} g_l^{(m)} \tag{A-3}$$

(no summation over m). Vector $\mathbf{g}^{(m)}$ denotes the eigenvector of the Christoffel matrix corresponding to the eigenvalue G_m of the wave under consideration (P, S1, S2).

In equations (A-2), we can use alternative expressions for $\partial\mathcal{H}/\partial p_i$ and $-\partial\mathcal{H}/\partial x_i$, which do not contain eigenvector $\mathbf{g}^{(m)}$ explicitly. These expressions are, however, algebraically more complicated. They read (Červený, 1972):

$$\frac{\partial\mathcal{H}}{\partial p_i} = \mathcal{U}_i = a_{ijkl}p_l D_{jk}/D_{ss}\ , \quad -\frac{\partial\mathcal{H}}{\partial x_i} = \eta_i = -\frac{1}{2}\frac{\partial a_{jkln}}{\partial x_i}p_k p_n D_{jl}/D_{ss}\ . \tag{A-4}$$

Here

$$D_{ij} = \tfrac{1}{2}\epsilon_{ikl}\epsilon_{jrs}(\Gamma_{kr} - \delta_{kr})(\Gamma_{ls} - \delta_{ls})\ . \tag{A-5}$$

Symbol ϵ_{ijk} represents the Levi-Civita symbol ($\epsilon_{123} = \epsilon_{312} = \epsilon_{231} = 1$, $\epsilon_{132} = \epsilon_{213} = \epsilon_{321} = -1$, $\epsilon_{ijk} = 0$ otherwise).

Another alternative expression for $\partial\mathcal{H}/\partial x_i$ in ray tracing equations (A-2) is as follows. Taking into account that $G_m(x_i, p_j)$ in (A-1) is a homogeneous function of the second degree in p_j, we have $G_m(x_i, p_j) = p_k p_k G_m(x_i, N_j)$ and $G_m(x_i, N_j) = \mathcal{C}^2(x_i, N_j)$, where $\mathbf{N} = \mathbf{p}/|\mathbf{p}|$ and $p_k p_k = \mathcal{C}^{-2}(x_i, N_j)$, $\mathcal{C}(x_i, N_j)$ being the phase velocity in the direction of the vector $\mathbf{N}$. Then we can write

$$-\frac{\partial\mathcal{H}(x_n, p_j)}{\partial x_i} = -\frac{1}{2}\frac{\partial G_m(x_n, p_j)}{\partial x_i} = -\frac{1}{2}\mathcal{C}^{-2}(x_n, N_j)\frac{\partial\mathcal{C}^2(x_n, N_j)}{\partial x_i}\ . \tag{A-6}$$

For $\partial\mathcal{H}/\partial p_i$ and $-\partial\mathcal{H}/\partial x_i$ we can thus write:

$$\frac{\partial\mathcal{H}}{\partial p_i} = \mathcal{U}_i(x_n, p_j)\ , \quad -\frac{\partial\mathcal{H}}{\partial x_i} = -\mathcal{C}^{-1}(x_n, N_j)\frac{\partial\mathcal{C}(x_n, N_j)}{\partial x_i}\ . \tag{A-7}$$

The ray tracing system (A-2) with (A-7) was proposed by Zhu, Gray and Wang (2005). The phase velocity $\mathcal{C}$ and the ray-velocity vector $\boldsymbol{\mathcal{U}}$ can be expressed exactly or approximately in terms of Thomsen's (1986) or weak-anisotropy (WA) parameters. In the case of approximate expressions and WA parameters, the ray tracing system (A-2) with (A-7) corresponds to the system proposed by Pšenčík and Farra (2005) for P-wave ray tracing.

A2) **Initial conditions for rays**

The initial conditions for the ray tracing system (A-2) differ from the initial conditions for ray tracing in isotropic media. For a given direction $\mathbf{N}$ specifying the direction of the slowness vector at the initial point of the ray, we can determine phase velocities of all three waves, $\mathcal{C}$. The phase velocities are obtained as a solution of a cubic equation resulting from the condition of solvability of the Christoffel equation

$$\det(a_{ijkl}N_jN_l - \mathcal{C}\delta_{ik}) = 0 \ . \qquad (A-8)$$

Selecting the value of $\mathcal{C}$ corresponding to the studied wave, we can construct the slowness vector of the studied wave at the initial point of the ray, $\mathbf{p} = \mathbf{N}/\mathcal{C}$. The initial conditions for the ray-velocity vector $\boldsymbol{\mathcal{U}}$ need not be specified among initial conditions for (A-2).

Anisotropic ray tracing system (A-2), with (A-3) or (A-4) or (A-7), can be used quite universally for P waves, including P waves in inhomogeneous isotropic and weakly anisotropic media. For S waves, however, the situation is more complicated. Ray tracing fails in the vicinity of S-wave singularities, where the two eigenvalues corresponding to S waves are equal or close to each other. Ray tracing for S waves may fail globally in very weakly anisotropic media, and fails fully in isotropic media. Remember that two eigenvalues of S waves are equal in isotropic media. These problems can be removed if the coupling ray theory for shear waves or its various modifications are used (Kravtsov, 1968; Coates and Chapman, 1990; Bulant and Klimeš, 2008; Farra and Pšenčík, 2010).

To use the ray-tracing system (A-2) for computations, we have to know initial conditions $\mathbf{x}(\tau_0)$, $\mathbf{p}(\tau_0)$ at the initial point $\tau = \tau_0$ of the ray. We denote here the initial point of the ray by S. We first present here the initial conditions $\mathbf{x}(\tau_0)$, $\mathbf{p}(\tau_0)$ for a point source situated at S, and after this the initial conditions $\mathbf{x}(\tau_0)$, $\mathbf{p}(\tau_0)$ for the point S situated at an initial surface Σ.

a) At a **point source** S, the initial conditions $x_i(\tau_0)$, $p_i(\tau_0)$ are simple. It is most common to express them in terms of the called ray parameters γ_1, γ_2. At a point source S, the ray parameters γ_1, γ_2 are mostly taken to be the take-off angles φ_0, δ_0. The initial conditions for $x_i(\tau_0)$, $p_i(\tau_0)$ for a non-moving source situated at point S are then as follows:

$$x_i(\tau_0) = x_i(S) \ , \qquad p_i(\tau_0) = \mathcal{C}^{-1}(\varphi_0, \delta_0)N_i(S) \ . \qquad (A-9)$$

Here $\mathbf{N}(S)$ is the unit vector specified by take-off angles φ_0, δ_0 as follows

$$N_i(S) = (\cos\varphi_0\cos\delta_0,\ \sin\varphi_0\cos\delta_0,\ \sin\delta_0) \ , \qquad (A-10)$$

and $\mathcal{C}(\varphi_0, \delta_0)$ is the phase velocity corresponding to the relevant direction $\mathbf{N}(S)$,

$$\mathcal{C}(\varphi_0, \delta_0) = [G_m(x_i(S), N_j(S))]^{1/2} \ . \qquad (A-11)$$

We have to emphasize that the take-off angles φ_0, δ_0 do not specify the initial direction of the ray, but the initial direction of the slowness vector $\mathbf{p}(S)$. The initial direction of the ray is given by the ray-velocity vector $\boldsymbol{\mathcal{U}}(S)$. $\boldsymbol{\mathcal{U}}(S)$, however, may be simply calculated from $\mathbf{p}(S)$ using the first equation in (A-3). The opposite calculation of $\mathbf{p}(S)$ from $\boldsymbol{\mathcal{U}}(S)$ is, however, very complicated.

b) At a **point** S **situated on the initial surface** Σ the initial conditions $x_i(\tau_0)$, $p_i(\tau_0)$ of a ray are more complicated. Consider a smooth initial surface Σ, given by the parameteric equation

$$\mathbf{x} = \mathbf{g}^{\Sigma}(u_1, u_2) \ , \qquad (A-12)$$

where u_1 and u_2 are the initial surface coordinates, which may represent, e.g., the Gaussian coordinates of the surface Σ. Alternatively, we can use a local Cartesian coordinate system u_1, u_2 in the plane tangent to Σ with its origin at the point S. The initial travel time T^0 along Σ may be constant, or may vary with surface coordinates u_1, u_2,

$$T^0 = T^0(u_1, u_2) \ . \qquad (A-13)$$

We denote

$$\mathbf{g}_I^\Sigma = \partial \mathbf{g}^\Sigma / \partial u_I \ , \qquad \mathbf{g}_{IJ}^\Sigma = \partial^2 \mathbf{g}^\Sigma / \partial u_I \partial u_J \ ,$$
$$T_I^0 = \partial T^0 / \partial u_I \ , \qquad T_{IJ}^0 = \partial^2 T^0 / \partial u_I \partial u_J \ . \qquad (A-14)$$

The unit vector $\mathbf{n}^\Sigma$ perpendicular to Σ is given by the relation

$$\mathbf{n}^\Sigma(u_1, u_2) = (\mathbf{g}_1^\Sigma \times \mathbf{g}_2^\Sigma)/|\mathbf{g}_1^\Sigma \times \mathbf{g}_2^\Sigma| \ . \qquad (A-15)$$

The initial conditions $x_i(\tau_0)$, $p_i(\tau_0)$ at a point S situated on the initial surface Σ are then given by the relations

$$x_i(\tau_0) = x_i(S) \ , \qquad p_i(\tau_0) = \sigma n_i^\Sigma + p_i^\Sigma \ , \qquad (A-16)$$

where $\mathbf{n}^\Sigma$ is given by (A-15), $\mathbf{p}^\Sigma$ by the relation

$$\mathbf{p}^\Sigma = A_{IJ} T_I^0 g_J \ , \qquad (A-17)$$

and $\mathbf{A}$ is the 2×2 matrix defined by the formula

$$\mathbf{A}^{-1} = \begin{pmatrix} \mathbf{g}_1^{\Sigma T} \mathbf{g}_1^\Sigma & \mathbf{g}_1^{\Sigma T} \mathbf{g}_2^\Sigma \\ \mathbf{g}_1^{\Sigma T} \mathbf{g}_2^\Sigma & \mathbf{g}_2^{\Sigma T} \mathbf{g}_2^\Sigma \end{pmatrix} \ . \qquad (A-18)$$

The scalar σ can be determined from the eikonal equation $\mathcal{H}(x_i, p_j) = \frac{1}{2}$, for the choice of the wave mode (P,S1,S2). For general anisotropy and for $\mathbf{p}^\Sigma \neq 0$, the following algebraic equation of the sixth degree for σ is obtained:

$$\det[a_{ijkl}(\sigma n_j^\Sigma + p_j^\Sigma)(\sigma n_i^\Sigma + p_i^\Sigma) - \delta_{ik}] = 0 \ . \qquad (A-19)$$

As in the case of reflection/transmission, see the next section, three roots corresponding to three generated waves, P, S1, S2, must be selected from the six roots of (A-19).

A3) **Rays across structural interfaces**

Let us now assume that a ray hits a curved structural interface. In the framework of the zero-order ray method, the reflection/transmission problem at the point of incidence of an arbitrary wave at a curved interface Σ separating two inhomogeneous media reduces to the problem of incidence of a plane wave at a plane interface separating two homogeneous media. Three reflected and three transmitted waves (P, S1, S2) are generated at the point of incidence; some of them may be inhomogeneous. The slowness vector of any of reflected or transmitted waves at the point of reflection/transmission is given by the relation

$$\tilde{\mathbf{p}} = \sigma \mathbf{n} + \mathbf{p}^\Sigma \ . \qquad (A-20)$$

Tilde indicates that the quantity corresponds to a generated wave. In (A-20), $\mathbf{n}$ is the unit normal to the interface Σ at the point of incidence. Symbol $\mathbf{p}^\Sigma$ denotes the tangential component to the interface of the slowness vector of the incident wave. Component $\mathbf{p}^\Sigma$ is the same for the incident and all generated waves. This equality is just another expression of the Snell law. The projection σ of slowness vector $\tilde{\mathbf{p}}$ to normal $\mathbf{n}$ is a root of the algebraic equation of the sixth degree:

$$\det[a_{ijkl}(\sigma n_k + p_k^\Sigma)(\sigma n_l + p_l^\Sigma) - \delta_{ij}] = 0 \ . \qquad (A-21)$$

For reflected waves, we use the same elastic moduli a_{ijkl} as for incident waves. For transmitted waves, we use a_{ijkl} corresponding to the halfspace on the other side of the interface.

Equation (A-21) has six roots for each halfspace. The roots corresponding to the three reflected and three transmitted waves are selected from them according to the direction of the relevant ray-velocity vector $\tilde{\boldsymbol{\mathcal{U}}}$ (for real-valued roots) and according to the radiation conditions (for complex-valued roots). For more details, see Gajewski and Pšenčík (1987), Červený (2001, section 2.3.3).

A4) **Concluding note**

The ray method was first proposed for the computation of high-frequency seismic wave fields in inhomogeneous anisotropic media by Babich (1961). Ray-tracing equations, namely (A-2) with (A-4), were first derived by Červený (1972). For more details on ray tracing in inhomogeneous anisotropic media, see Červený (2001, Chap.3.6). The computer program for ray tracing in inhomogeneous anisotropic layered structures based on the above-mentioned formulae is the computer package ANRAY (Gajewski and Pšenčík, 1987,1990). The package ANRAY is freely available on the web pages of the SW3D Consortium Seismic Waves in Complex 3D Structures (http://sw3d.cz).

Appendix B
Dynamic ray tracing in inhomogeneous anisotropic media

Dynamic ray tracing consists in the solution of a system of linear ordinary differential equations of the first order along the ray Ω. The dynamic ray tracing system in various forms of Cartesian coordinates (general, local) was studied by several authors. For a detailed derivations and for references see Červený (2001). We shall present here only formulae for the DRT system based on global Cartesian coordinates x_1, x_2, x_3 and for the simplified DRT system in global Cartesian coordinates x_1, x_2, x_3.

B1) **DRT system in global Cartesian coordinates** x_i.

The DRT in global Cartesian coordinates consists of six equations for $Q_i^{(x)} = \partial x_i/\partial\gamma$ and $P_i^{(x)} = \partial p_i/\partial\gamma$, where γ is any of initial values x_{i0}, p_{i0}, or any ray parameter or a variable along the ray. The DRT system reads

$$\mathrm{d}Q_i^{(x)}/\mathrm{d}\tau = A_{ij}^{(x)}Q_j^{(x)} + B_{ij}^{(x)}P_j^{(x)} \ , \quad \mathrm{d}P_i^{(x)}/\mathrm{d}\tau = -C_{ij}^{(x)}Q_j^{(x)} - D_{ij}^{(x)}P_j^{(x)} \ , \qquad (B-1)$$

where

$$A_{ij}^{(x)} = \partial^2\mathcal{H}/\partial p_i \partial x_j \ , \quad B_{ij}^{(x)} = \partial^2\mathcal{H}/\partial p_i \partial p_j \ ,$$
$$C_{ij}^{(x)} = \partial^2\mathcal{H}/\partial x_i \partial x_j \ , \quad D_{ij}^{(x)} = \partial^2\mathcal{H}/\partial x_i \partial p_j \ , \qquad (B-2)$$

and where the Hamiltonian $\mathcal{H}(x_i, p_j)$ is given by (7). The elements of 3×3 matrices $A_{ij}^{(x)}$, $B_{ij}^{(x)}$, $C_{ij}^{(x)}$ and $D_{ij}^{(x)}$ satisfy three symmetry relations:

$$B_{ij}^{(x)} = B_{ji}^{(x)} \ , \quad C_{ij}^{(x)} = C_{ji}^{(x)} \ , \quad D_{ij}^{(x)} = A_{ji}^{(x)} \ . \qquad (B-3)$$

The 3×1 vectors $\mathbf{Q}^{(x)}$ and $\mathbf{P}^{(x)}$ in (B-1) satisfy the following constrain relation:

$$\mathcal{U}_k Q_k^{(x)} - \eta_k P_k^{(x)} = 0 \qquad (B-4)$$

along the ray Ω. It is common to write the dynamic ray tracing system (B-1) in a matrix form:

$$\mathrm{d}\hat{\mathbf{Q}}^{(x)}/\mathrm{d}\tau = \hat{\mathbf{A}}^{(x)}\hat{\mathbf{Q}}^{(x)} + \hat{\mathbf{B}}^{(x)}\hat{\mathbf{P}}^{(x)} \ , \quad \mathrm{d}\hat{\mathbf{P}}^{(x)}/\mathrm{d}\tau = -\hat{\mathbf{C}}^{(x)}\hat{\mathbf{Q}}^{(x)} - \hat{\mathbf{D}}^{(x)}\hat{\mathbf{P}}^{(x)} \ , \qquad (B-5)$$

where elements of the 3×3 matrices $\hat{\mathbf{Q}}^{(x)}$ and $\hat{\mathbf{P}}^{(x)}$ have the following form:

$$Q_{ij}^{(x)} = \partial x_i/\partial\gamma_j \ , \qquad P_{ij}^{(x)} = \partial p_i/\partial\gamma_j \ . \qquad (B-6)$$

Here we consider γ_j (j=1,2,3) to be the ray coordinates, with γ_1 and γ_2 the ray parameters and $\gamma_3 = \tau$ the travel time along the ray.

a) **Initial conditions for DRT at a point source**. The initial conditions for $\hat{\mathbf{Q}}^{(x)}$ are simple:

$$Q_{iJ}^{(x)}(S) = 0 \ , \qquad Q_{i3}^{(x)}(S) = \mathcal{U}_i(S) \ . \qquad (B-7)$$

The initial conditions for $P_{ij}^{(x)}$ are more involved. If we consider the ray parameters γ_1 and γ_2 to be the take-off angles $\gamma_1 = \varphi_0$ and $\gamma_2 = \delta_0$, for which the unit vector $N(S)$, perpendicular to the wavefront at S is given by the relation (A-10), we get

$$\begin{aligned} P_{iJ}^{(x)}(S) &= (Z_{iJ}(S) - p_i(S)\mathcal{U}_k(S)Z_{kJ}(S))/\mathcal{C}(\varphi_0,\delta_0) \ , \\ P_{i3}^{(x)}(S) &= \eta_i(S) \ , \end{aligned} \qquad (B-8)$$

where

$$\begin{aligned} Z_{11}(S) &= -\sin\varphi_0\cos\delta_0 \ , \quad Z_{21}(S) = \cos\varphi_0\cos\delta_0 \ , \quad Z_{31}(S) = 0 \ , \\ Z_{12}(S) &= -\cos\varphi_0\sin\delta_0 \ , \quad Z_{22}(S) = -\sin\varphi_0\sin\delta_0 \ , \quad Z_{32}(S) = \cos\delta_0 \ . \end{aligned} \qquad (B-9)$$

See Pšenčík and Teles (1996, eq. A-4), Červený and Moser (2009, eq. 42), for the derivation and more details.

With initial conditions (B-8)-(B-9), the elements of matrices $\hat{\mathbf{Q}}^{(x)}$ and $\hat{\mathbf{P}}^{(x)}$ along ray Ω have the meaning shown in equations (B-6) with $\gamma_1 = \varphi_0$, $\gamma_2 = \delta_0$ and $\gamma_3 = \tau$. Let us note that the quantities Q_{i3} and P_{i3} can be obtained from ray tracing equations (A-2). Thus, it is not necessary to seek them as the solution of (B-5), see Sec. B2. For the computation of relative geometrical spreading $\mathcal{L}(R_\gamma, S)$, which will be needed in the following, slightly modified initial conditions are required. They should correspond to the point-source initial conditions of the ray propagator matrix. They read (Pšenčík and Teles, 1996, eq.(A5); Červený, 2001, eq.(4.2.51)):

$$Q^{(x)}_{nK}(S) = 0, \qquad P^{(x)}_{iJ}(S) = R_{iJ} - p_i(S)\mathcal{U}_k(S)\, R_{kJ} \ , \qquad (B-10)$$

where

$$\begin{array}{lll} R_{11} = -\sin\varphi_0 \ , & R_{21} = \cos\varphi_0 \ , & R_{31} = 0 \ , \\ R_{12} = -\cos\varphi_0\sin\delta_0 \ , & R_{22} = -\sin\varphi_0\sin\delta_0 \ , & R_{32} = \cos\delta_0 \ . \end{array} \qquad (B-11)$$

Due to the linearity of the DRT system (B-5), its solution with initial conditions (B-7)-(B-8) can be obtained from solutions of dynamic ray tracing with initial conditions (B-10) and (B-11) simply by multiplication of $Q^{(x)}_{i1}(R_\gamma)$ and $P^{(x)}_{i1}(R_\gamma)$ by the constant factor $C^{-1}(\varphi_0,\delta_0)\cos\delta_0$ and of $Q^{(x)}_{i2}(R_\gamma)$ and $P^{(x)}_{i2}(R_\gamma)$ by $C^{-1}(\varphi_0,\delta_0)$. Thus as basic initial conditions for dynamic ray tracing we consider equations (B-10) and (B-11).

Dynamic ray tracing (B-5) with the initial conditions (B-10) and (B-11) is used for the determination of a quantity important for the evaluation of Gaussian beams and paraxial ray approximations, the relative geometrical spreading $\mathcal{L}(R_\gamma, S)$. We can use equation (56), but for specific initial conditions (B-10) equation (56) can be simplified. The vectorial product in the denominator of (56) can be expressed as

$$\epsilon_{ijk}Y_{1j}(S)Y_{2k}(S) = \epsilon_{ijk}[R_{j1}R_{k2} - R_{j1}p_k(\mathcal{U}_mR_{ml}) - p_jR_{k2}(\mathcal{U}_nR_{n1})] \ . \qquad (B-12)$$

As R_{j1} and R_{k2} are mutually perpendicular unit vectors tangent to the wavefront, we obtain

$$\epsilon_{ijk}R_{j1}R_{k2} = N_i \ , \quad \epsilon_{ijk}R_{j1}p_k = -C^{-1}R_{i2} \ , \quad \epsilon_{ijk}p_jR_{k2} = -C^{-1}R_{i2} \ . \qquad (B-13)$$

Inserting (B-13) into (B-12), we obtain

$$\begin{aligned} \epsilon_{ijk}Y_{1j}(S)Y_{2k}(S) &= N_i + C^{-1}R_{22}(\mathcal{U}_mR_{m2}) + C^{-1}R_{j1}(\mathcal{U}_nR_{n1}) \\ &= N_i + C^{-1}(R_{i2}R_{n2} + R_{i1}R_{n1})\mathcal{U}_n \\ &= N_i + C^{-1}(\delta_{in} + N_iN_n)\mathcal{U}_n = N_i + C^{-1}(\mathcal{U}_j + N_j(N_n\mathcal{U}_n)) \ . \end{aligned} \qquad (B-14)$$

As $N_n\mathcal{U}_n = C^{-1}(p_n\mathcal{U}_n) = C^{-1}$, we obtain finally

$$|\mathbf{Y}_1(S) \times \mathbf{Y}_2(S)| = |\epsilon_{ijk}Y_{1j}(S)Y_{2k}(S)| = \mathcal{U}/\mathcal{C} \ . \qquad (B-15)$$

Inserting (B-15) into (56), we obtain finally

$$\mathcal{L}(R_\gamma, S) = |\mathbf{X}_1(\tau) \times \mathbf{X}_2(\tau)| = |\mathbf{Q}^{(x)}_1(R_\gamma) \times \mathbf{Q}^{(x)}_2(R_\gamma)|^{1/2} \ . \qquad (B-16)$$

Here the 3×1 matrices $\mathbf{Q}^{(x)}_1$ and $\mathbf{Q}^{(x)}_2$ are the first and second columns of the 3×3 matrix $\hat{\mathbf{Q}}^{(x)}$.

If we choose the ray parameters γ_1 and γ_2 by relations $\gamma_1 = p_1(S)$, $\gamma_2 = p_2(S)$, the initial conditions for $P^{(x)}_{iJ}$ are simpler,

$$P^{(x)}_{iJ}(S) = (\delta_{1J},\, \delta_{2J},\, -\mathcal{U}_i(S)/\mathcal{U}_3(S)) \ . \qquad (B-17)$$

If $\gamma_3 = \tau$, then the elements $P^{(x)}_{i3}(S)$ remain the same as in (B-8), $P^{(x)}_{i3}(S) = \eta_i(S)$. These simple expressions, however, fail for initial directions of the ray specified in the (x_1, x_2) plane, as $\mathcal{U}_3(S) = 0$ in this case. It is then necessary to rotate the Cartesian coordinate system suitably.

b) **Initial conditions for DRT at the point S situated at a smooth initial surface Σ.** We introduce initial surface Σ and the relevant notations in the same way as in Appendix A2/b. We further introduce the vectors $\mathbf{h}_1, \mathbf{h}_2$ and $\mathbf{h}_3$ at the point S as follows:

$$\mathbf{h}_1 = (\mathbf{g}^{\Sigma}_2 \times \boldsymbol{\mathcal{U}})/\det\mathbf{X} \ , \quad \mathbf{h}_2 = (\boldsymbol{\mathcal{U}} \times \mathbf{g}^{\Sigma}_1)/\det\mathbf{X} \ , \quad \mathbf{h}_3 = (\mathbf{g}^{\Sigma}_1 \times \mathbf{g}^{\Sigma}_2)/\det\mathbf{X} \ , \qquad (B-18)$$

where

$$\mathbf{X}^{-T} = (\mathbf{h}_1, \mathbf{h}_2, \mathbf{h}_3) \ . \qquad (B-19)$$

The vectors $\mathbf{h}_1$ and $\mathbf{h}_2$ are perpendicular to the ray at S, the vector $\mathbf{h}_3$ is perpendicular to the wavefront at S. Then we obtain the initial conditions for $Q^{(x)}_{ij}(S)$ in the following form:

$$Q^{(x)}_{iJ}(S) = g^{\Sigma}_{Ji}(S) - T^0_J(S)\mathcal{U}_i(S) \ , \qquad Q^{(x)}_{i3}(S) = \mathcal{U}_i(S) \ , \qquad (B-20)$$

and the initial conditions for $P^{(x)}_{ij}(S)$:

$$\begin{aligned} &P^{(x)}_{iJ}(S) = h_{Ki}(S)[T^0_{JK}(S) - ((\mathbf{g}^{\Sigma}_{JK}(S))^T\mathbf{p}(S))] + h_{3i}(S)((\mathbf{g}^{\Sigma}_J(S))^T\boldsymbol{\eta}(S)) - T^0_J(S)\eta_i(S) \ , \\ &P^{(x)}_{i3}(S) = \eta_i(S) \ . \end{aligned} \qquad (B-21)$$

where T^0_J is defined in (A-14). Again, $Q^{(x)}_{i3}(R_\gamma)$ and $P^{(x)}_{i3}(R_\gamma)$ can be obtained by solving the ray tracing equations.

c) **Transformation of DRT in Cartesian coordinates across an interface**. We consider a smooth structural interface $\Sigma(x_i)$ described in Appendix A3. We keep the symbols $Q^{(x)}_{kJ}$ and $P^{(x)}_{kJ}$ for the incident paraxial matrices, and denote $Q^{(x)G}_{kJ}$ and $P^{(x)G}_{kJ}$ the paraxial matrices of any generated wave (reflected, transmitted). The relation between the generated paraxial matrices and incident paraxial matrices is given by the following relations

$$Q^{(x)G}_{iJ} = W_{ik}Q^{(x)}_{kJ} \ , \qquad P^{(x)G}_{iJ} = R_{ik}Q^{(x)}_{kJ} + S_{ik}P^{(x)}_{kJ} \ . \qquad (B-22)$$

Here the 3×3 matrices $\hat{\mathbf{W}}, \hat{\mathbf{R}}, \hat{\mathbf{S}}$ are given by relations,

$$\begin{aligned} &W_{ij} = \delta_{ij} + \eta^{-1}(Q^{(x)G}_{j3} - Q^{(x)}_{i3})n_j \ , \\ &S_{ij} = \delta_{ij} - (\eta^G)^{-1}(Q^{(x)G}_{j3} - Q^{(x)}_{j3})n_i \ , \\ &R_{ij} = \eta^{-1}(P^{(x)G}_{i3} - P^{(x)}_{i3})n_j + (\eta^G)^{-1}(P^{(x)G}_{j3} - P^{(x)}_{j3})n_i \\ &+(\eta\eta^G)^{-1}(Q^{(x)G}_{k3}P^{(x)}_{k3} - Q_{k3}P^{(x)G}_{k3})n_in_j \\ &+(\Sigma_{,m}\Sigma_{,m})^{-1/2}(\zeta^G - \zeta)\Sigma_{,lk}[\delta_{il} - (\eta^G)^{-1}Q^{(x)G}_{l3}n_i][\delta_{kj} - \eta^{-1}Q^{(x)}_{k3}n_j] \ . \end{aligned} \qquad (B-23)$$

Here $\mathbf{n}$ is the unit normal to the interface at the point of incidence, and

$$\begin{aligned} &\zeta^G = p^G_m n_m \ , \qquad \zeta = p_m n_m \ , \\ &\eta^G = Q^{(x)G}_{m3} n_m \ , \quad \eta = Q^{(x)}_{m3} n_m \ . \end{aligned} \qquad (B-24)$$

For the derivation and more details see Farra and LeBégat (1995), Pšenčík and Farra (2014).

It should be emphasized that the transformation relations (B-20) must be used even at interfaces of the second order (where gradients of parameters of the medium or of density vary discontinuously, but parameters and density themselves are continuous). Ignoring this may lead to inaccuracies and cause instability of the solution of the DRT system. Let us mention that interfaces of the second order are often introduced to the model artificially, during the approximation of the model, for example, when bi- or trilinear interpolation in a rectangular grid is used or if a piece-wise polynomial approximation using triangles (2D) or tetrahedrons (3D) is used. From these reasons, it is recommended to use splines or other approximations, which do not generate interfaces of the second order. The mentioned approximations may, on the other hand, generate false oscillations of the distribution of density-normalized elastic moduli. To avoid these effects, techniques developed for isotropic media and based on Sobolev scalar products and Lyapunov exponents (see Klimeš, 2000 for theory and Bulant, 2002 and Žáček, 2002 for numerical examples; see also Červený et al., 2007, Sec.6.2.1) should be extended to anisotropic media.

B2) **Simplified DRT system in global Cartesian coordinates x_i**

As shown in the previous text, it is sufficient to solve the DRT system (B-5) for only six elements of matrix $\mathbf{Q}^{(x)}$ and six elements of matrix $\mathbf{P}^{(x)}$:

$$Q^{(x)}_{iN} = \partial x_i/\partial\gamma_N \ , \qquad P^{(x)}_{iN} = \partial p_i/\partial\gamma_N \ , \qquad (B-25)$$

where γ_1 and γ_2 are ray parameters. The elements $Q^{(x)}_{i3}$ and $P^{(x)}_{i3}$, $i = 1, 2, 3$, are not necessary to compute, they can be obtained from ray tracing. The simplified DRT system in global Cartesian coordinates x_i reads:

$$\mathrm{d}Q^{(x)}_{iN}/\mathrm{d}\tau = A^{(x)}_{ij}Q^{(x)}_{jN} + B^{(x)}_{ij}P^{(x)}_{jN} \ , \qquad \mathrm{d}P^{(x)}_{iN}/\mathrm{d}\tau = -C^{(x)}_{ij}Q^{(x)}_{jN} - D^{(x)}_{ij}P^{(x)}_{jN} \ . \qquad (B-26)$$

Here the 3×3 matrices $A^{(x)}_{ij}$, $B^{(x)}_{ij}$, $C^{(x)}_{ij}$ and $D^{(x)}_{ij}$ are again given by (B-2). The system (B-26) consists of twelve equations, not eighteen like (B-1).

Appendix C

Explicit expressions for matrix $\bar{\mathbf{B}}$

The elements $\bar{B}_{ij}$ of matrix $\bar{\mathbf{B}}$ used for the determination of matrix $\mathbf{B}$, see equation (7), are given by the formula

$$\bar{B}_{mn}(\mathbf{x}, \mathbf{N}) = a_{ijkl}(\mathbf{x})N_jN_l\bar{e}_{mi}\bar{e}_{nk}. \qquad (C-1)$$

Here a_{ijkl} are density-normalized elastic moduli (elements of the stiffness tensor). Symbols N_i denote components of unit vector $\mathbf{N}$ parallel to the slowness vector. Explicit expressions for elements of matrix $\bar{\mathbf{B}}$, given below, correspond to a special choice of vectors $\mathbf{e}_i$:

$$\bar{\mathbf{e}}_1 \equiv D^{-1}(N_1N_3, N_2N_3, N_3^2-1), \quad \bar{\mathbf{e}}_2 \equiv D^{-1}(-N_2, N_1, 0), \quad \bar{\mathbf{e}}_3 = \mathbf{N} \equiv (N_1, N_2, N_3), \qquad (C-2)$$

where

$$D = (N_1^2 + N_2^2)^{1/2}, \quad N_1^2 + N_2^2 + N_3^2 = 1. \qquad (C-3)$$

For the sake of brevity, we use components of vector $\mathbf{N}$ for the definition of vectors $\mathbf{e}_i$ and elements of matrix $\bar{\mathbf{B}}$. This introduces the term D in the denominators of formulae (C-2) and also in expressions for elements of $\bar{\mathbf{B}}$. The artificial term D disappears if (C-2) is rewritten as:

$$\bar{\mathbf{e}}_1 \equiv (\cos\varphi\cos\theta, \sin\varphi\cos\theta, -\sin\theta),$$
$$\mathbf{e}_2 \equiv (-\sin\varphi, \cos\varphi, 0),$$
$$\mathbf{e}_3 \equiv (\cos\varphi\sin\theta, \sin\varphi\sin\theta, \cos\theta). \qquad (C-4)$$

Here φ denotes an azimuthal angle, θ a polar angle, $(0 \le \varphi \le 2\pi,\ 0 \le \theta \le \pi)$.

Explicit expressions for elements of matrix $\bar{\mathbf{B}}$ for a weakly anisotropic medium of arbitrary symmetry in terms of 21 WA parameters were introduced by Farra and Pšenčík (2003). Note interchanges of parameters δ_x and δ_y, and parameters γ_x and γ_y in the mentioned paper and here. We can see that in case of P waves, it is sufficient to deal with only 3 elements of matrix $\bar{\mathbf{B}}$, namely with $\bar{B}_{13}$, $\bar{B}_{23}$ and $\bar{B}_{33}$. In case of S waves, it is necessary to deal with elements $\bar{B}_{11}$, $\bar{B}_{22}$, $\bar{B}_{12}$, $\bar{B}_{13}$ and $\bar{B}_{23}$. Elements $\bar{B}_{11}(\mathbf{N})$, $\bar{B}_{22}(\mathbf{N})$ and $\bar{B}_{33}(\mathbf{N})$ represent the first-order approximations of the squares of S1-, S2- and P-wave phase velocities, $C^2_{S1}(\mathbf{x},\mathbf{N}) = \bar{B}_{11}(\mathbf{x},\mathbf{N})$, $C^2_{S2}(\mathbf{x},\mathbf{N}) = \bar{B}_{22}(\mathbf{x},\mathbf{N})$ and $C^2_P(\mathbf{x},\mathbf{N}) = \bar{B}_{33}(\mathbf{x},\mathbf{N})$, respectively. It is also good to note that $G_P(\mathbf{x},\mathbf{p}) = \bar{B}_{33}(\mathbf{x},\mathbf{p})$ and $G_S(\mathbf{x},\mathbf{p}) = \bar{B}_{11}(\mathbf{x},\mathbf{p}) + \bar{B}_{22}(\mathbf{x},\mathbf{p})$.

The elements of matrix $\bar{\mathbf{B}}$ are specified here in the form used by Farra and Pšenčík (2003, (A4)), which is convenient fro retrieval of WA parameters from elements of matrix $\bar{\mathbf{B}}$. Detailed analysis of the dependence of matrix $\bar{\mathbf{B}}$ on WA parameters can be found in Farra and Pšenčík (2003). The elements of matrix $\bar{\mathbf{B}}(\mathbf{x},\mathbf{N})$ have the following form:

$$\bar{B}_{11} = \beta^2 + 2\alpha^2 D^{-2}\Big(N_3^3[(\epsilon_{15}-\epsilon_{35})N_1^3 + (\epsilon_{24}-\epsilon_{34})N_2^3 + (\chi_x-\epsilon_{34})N_1^2N_2 + (\chi_y-\epsilon_{35})N_1N_2^2]$$
$$+N_3^2[(\epsilon_x-\delta_y+\epsilon_z)N_1^4 + (\epsilon_y-\delta_x+\epsilon_z)N_2^4 + (\delta_z-\delta_x-\delta_y+2\epsilon_z)N_1^2N_2^2$$
$$+2(\epsilon_{16}-\chi_z)N_1^3N_2 + 2(\epsilon_{26}-\chi_z)N_1N_2^3]$$
$$+N_3[(\epsilon_{35}-\epsilon_{15})N_1^5 + (\epsilon_{34}-\epsilon_{24})N_2^5 + (\epsilon_{34}-\chi_x)N_1^4N_2 + (\epsilon_{35}-\chi_y)N_1N_2^4$$
$$+(2\epsilon_{35}-\chi_y-\epsilon_{15})N_1^3N_2^2 + (2\epsilon_{34}-\chi_x-\epsilon_{24})N_1^2N_2^3]\Big)$$
$$+2\beta^2D^{-2}(\gamma_yN_1^2 + \gamma_xN_2^2 + \epsilon_{45}N_1N_2),$$

$$\bar{B}_{12} = \alpha^2D^{-2}\Big(N_3^2[(\chi_x-\epsilon_{34})N_1^3 - (\chi_y-\epsilon_{35})N_2^3 + (\epsilon_{35}+\chi_y-2\epsilon_{15})N_1^2N_2$$
$$+(2\epsilon_{24}-\chi_x-\epsilon_{34})N_1N_2^2] + N_3[(\epsilon_{16}-\chi_z)N_1^4 - (\epsilon_{26}-\chi_z)N_2^4 + (\delta_y-\delta_x-2\epsilon_x+\delta_z)N_1^3N_2$$
$$+(\delta_y-\delta_x+2\epsilon_y-\delta_z)N_1N_2^3 + 3(\epsilon_{26}-\epsilon_{16})N_1^2N_2^2] + [(\epsilon_{15}-\chi_y)N_1^4N_2$$
$$+(\chi_x-\epsilon_{24})N_1N_2^4 + (\epsilon_{15}-\chi_y)N_1^2N_2^3 + (\chi_x-\epsilon_{24})N_1^3N_2^2$$
$$+\epsilon_{46}N_2^3 - \epsilon_{56}N_1^3 + \epsilon_{46}N_1^2N_2 - \epsilon_{56}N_1N_2^2]\Big) + \beta^2D^{-2}N_3[2(\gamma_x-\gamma_y)N_1N_2 + \epsilon_{45}N_1^2 - \epsilon_{45}N_2^2],$$

$$\bar{B}_{22} = \beta^2 + 2\beta^2 D^{-2} N_3^2 (\gamma_y N_2^2 + \gamma_x N_1^2 - \epsilon_{45} N_1 N_2)$$
$$+2\alpha^2 D^{-2} \Big(N_3 [\epsilon_{46} N_1^3 + \epsilon_{56} N_2^3) + (\epsilon_{56} - \chi_x + \epsilon_{24}) N_1^2 N_2 + (\epsilon_{46} - \chi_y + \epsilon_{15}) N_1 N_2^2]$$
$$+(\epsilon_x + \epsilon_y - \delta_z) N_1^2 N_2^2 + (\epsilon_{26} - \epsilon_{16}) N_1^3 N_2 - (\epsilon_{26} - \epsilon_{16}) N_1 N_2^3] \Big) + 2\beta^2 \gamma_z (N_1^2 + N_2^2),$$

$$\bar{B}_{13} = \alpha^2 D^{-1} \{ N_3^4 (\epsilon_{34} N_2 + \epsilon_{35} N_1) + N_3^3 [(\delta_y - \epsilon_x - \epsilon_z) N_1^2 + (\delta_x - \epsilon_y - \epsilon_z) N_2^2 + 2\chi_z N_1 N_2]$$
$$+N_3^2 [(4\chi_x - 3\epsilon_{34}) N_1^2 N_2 + (4\chi_y - 3\epsilon_{35}) N_1 N_2^2 + (4\epsilon_{15} - 3\epsilon_{35}) N_1^3 + (4\epsilon_{24} - 3\epsilon_{34}) N_2^3]$$
$$+N_3 [(2\delta_z - \delta_x - \delta_y - \epsilon_x - \epsilon_y + 2\epsilon_z) N_1^2 N_2^2 + 2(2\epsilon_{16} - \chi_z) N_1^3 N_2 + 2(2\epsilon_{26} - \chi_z) N_1 N_2^3$$
$$+(\epsilon_x + \epsilon_z - \delta_y) N_1^4 + (\epsilon_y + \epsilon_z - \delta_x) N_2^4 + (\epsilon_x - \epsilon_z) N_1^2 + (\epsilon_y - \epsilon_z) N_2^2]$$
$$-\chi_x N_1^2 N_2 - \chi_y N_1 N_2^2 - \epsilon_{15} N_1^3 - \epsilon_{24} N_2^3 \},$$

$$\bar{B}_{23} = \alpha^2 D^{-1} \{ N_3^3 (\epsilon_{34} N_1 - \epsilon_{35} N_2) + N_3^2 [(\delta_x - \delta_y - \epsilon_y + \epsilon_x) N_1 N_2 + \chi_z N_1^2 - \chi_z N_2^2]$$
$$+N_3 [(2\chi_y - 3\epsilon_{15}) N_1^2 N_2 - (2\chi_x - 3\epsilon_{24}) N_1 N_2^2 + \chi_x N_1^3 - \chi_y N_2^3]$$
$$+(\delta_z - \epsilon_x - \epsilon_y) N_1^3 N_2 - (\delta_z - \epsilon_x - \epsilon_y) N_1 N_2^3 + 3(\epsilon_{26} - \epsilon_{16}) N_1^2 N_2^2 + \epsilon_{16} N_1^4 - \epsilon_{26} N_2^4 + (\epsilon_y - \epsilon_x) N_1 N_2 \},$$

$$\bar{B}_{33} = \alpha^2 + 2\alpha^2 [2 N_3^3 (\epsilon_{34} N_2 + \epsilon_{35} N_1) + N_3^2 ((\delta_y - \epsilon_x - \epsilon_z) N_1^2 + (\delta_x - \epsilon_y - \epsilon_z) N_2^2$$
$$+2\chi_z N_1 N_2 + \epsilon_z) + 2 N_3 (\chi_x N_1^2 N_2 + \chi_y N_1 N_2^2 + \epsilon_{15} N_1^3 + \epsilon_{24} N_2^3) + \epsilon_x N_1^2 + \epsilon_y N_2^2$$
$$+(\delta_z - \epsilon_x - \epsilon_y) N_1^2 N_2^2 + 2\epsilon_{16} N_1^3 N_2 + 2\epsilon_{26} N_1 N_2^3]. \qquad (C-5)$$

The symbols α and β in (C-5) denotes the constant reference P- and S-wave velocities. Although the WA parameters depend on velocities α and β, and these velocities also appear in the expressions for the elements $\bar{B}_{mn}$ of matrix $\bar{\mathbf{B}}$, the matrix $\bar{\mathbf{B}}$ is *independent* of α and β.

Appendix D

a) First and second derivatives of the first-order P-wave eigenvalue $G_P(x_m, p_m)$ for a weakly anisotropic medium of an arbitrary symmetry

The first derivatives of the first-order P-wave eigenvalue in eq.(73) appearing on the RHS of ray tracing equations (A-2) depend on x_m and p_m. They have the following explicit form:

$$\frac{\partial G}{\partial p_1} = 2\alpha^2 \Big(p_1 + 2\epsilon_x p_1 + 2c^4 [A p_{23} p_1 + B(p_{23} - p_1^2) + C(3p_{23} + p_1^2) p_1^2 - D p_1 p_2 p_3] \Big),$$

$$\frac{\partial G}{\partial p_2} = 2\alpha^2\Big(p_2 + 2\epsilon_y p_2 + 2c^4[Ep_{13}p_2 + F(p_{13} - p_2^2) + G(3p_{13} + p_2^2)p_2^2 - Hp_1p_2p_3]\Big),$$

$$\frac{\partial G}{\partial p_3} = 2\alpha^2\Big(p_3 + 2\epsilon_z p_3 + 2c^4[Pp_{12}p_3 + Q(p_{12} - p_3^2) + R(3p_{12} + p_3^2)p_3^2 - Sp_1p_2p_3]\Big),$$

$$\frac{\partial G}{\partial x_i} = 2\alpha^2\Big(T_{,i} + c^2[2R_{,i}p_3^3 + P_{,i}p_3^2 + 2Q_{,i}p_3 + S_{,i}p_1p_2]\Big). \qquad (D-1)$$

The second derivatives of the first-order P-wave eigenvalue in eq.(73) appearing on the RHS of dynamic ray tracing equations (B-11) depend on x_m and p_m too. They have the following explicit form:

$$\frac{\partial^2 G}{\partial p_1^2} = 2\alpha^2\Big(1 + 2\epsilon_x + 2c^6[(Ap_{23} - Dp_2p_3)(p_{23} - 3p_1^2) + 2p_1(Cp_{23} - B)(3p_{23} - p_1^2)]\Big),$$

$$\begin{aligned}\frac{\partial^2 G}{\partial p_1 \partial p_2} &= 4\alpha^2\Big(c^4[2(\chi_x p_3 + \eta_z p_2)p_1p_{23} + (\chi_z p_3^2 + 2\chi_y p_2p_3 + 3\epsilon_{26}p_2^2)(p_{23} - p_1^2)\\ &+\epsilon_{16}(p_1^2 + 3p_{23})p_1^2 - (\eta_x p_3 + 4\epsilon_{24}p_2)p_1p_2p_3] - c^6[2A(p_{23} - p_1^2)p_1p_2 + 2B(p_{23} - 3p_1^2)p_2\\ &+2C(3p_{23} - p_1^2)p_1^2p_2 + D(p_{13} - 3p_2^2)p_1p_3]\Big),\end{aligned}$$

$$\begin{aligned}\frac{\partial^2 G}{\partial p_1 \partial p_3} &= 4\alpha^2\Big(c^4[2(\chi_x p_2 + \eta_y p_3)p_1p_{23} + (\chi_y p_2^2 + 2\chi_z p_2p_3 + 3\epsilon_{35}p_3^2)(p_{23} - p_1^2)\\ &+\epsilon_{15}(p_1^2 + 3p_{23})p_1^2 - (\eta_x p_2 + 4\epsilon_{34}p_3)p_1p_2p_3] - c^6[2A(p_{23} - p_1^2)p_1p_3 + 2B(p_{23} - 3p_1^2)p_3\\ &+2C(3p_{23} - p_1^2)p_1^2p_3 + D(p_{12} - 3p_3^2)p_1p_2]\Big),\end{aligned}$$

$$\frac{\partial^2 G}{\partial p_2^2} = 2\alpha^2\Big(1 + 2\epsilon_y + 2c^6[(Ep_{13} - Hp_1p_3)(p_{13} - 3p_2^2) + 2p_2(Gp_{13} - F)(3p_{13} - p_2^2)]\Big),$$

$$\begin{aligned}\frac{\partial^2 G}{\partial p_2 \partial p_3} &= 4\alpha^2\Big(c^4[2(\chi_y p_1 + \eta_x p_3)p_2p_{13} + (\chi_x p_1^2 + 2\chi_z p_1p_3 + 3\epsilon_{34}p_3^2)(p_{13} - p_2^2)\\ &+\epsilon_{24}(p_2^2 + 3p_{13})p_2^2 - (\eta_y p_1 + 4\epsilon_{35}p_3)p_1p_2p_3] - c^6[2E(p_{13} - p_2^2)p_2p_3 + 2F(p_{13} - 3p_2^2)p_3\\ &+2G(3p_{13} - p_2^2)p_2^2p_3 + H(p_{12} - 3p_3^2)p_1p_2]\Big),\end{aligned}$$

$$\frac{\partial^2 G}{\partial p_3^2} = 2\alpha^2\Big(1 + 2\epsilon_z + 2c^6[(Pp_{12} - Sp_1p_2)(p_{12} - 3p_3^2) + 2p_3(Rp_{12} - Q)(3p_{12} - p_3^2)]\Big),$$

$$\frac{\partial^2 G}{\partial x_i \partial p_1} = 4\alpha^2\Big(\epsilon_{x,i}p_1 + c^4[(A_{,i}p_{23}p_1 + B_{,i}(p_{23} - p_1^2) + C_{,i}(3p_{23} + p_1^2)p_1^2 - D_{,i}p_1p_2p_3]\Big),$$

$$\frac{\partial^2 G}{\partial x_i \partial p_2} = 4\alpha^2\Big(\epsilon_{y,i}p_2 + c^4[(E_{,i}p_{13}p_2 + F_{,i}(p_{13} - p_2^2) + G_{,i}(3p_{13} + p_2^2)p_2^2 - H_{,i}p_1p_2p_3]\Big),$$

$$\frac{\partial^2 G}{\partial x_i \partial p_3} = 4\alpha^2\Big(\epsilon_{z,i}p_3 + c^4[(P_{,i}p_{12}p_3 + Q_{,i}(p_{12} - p_3^2) + R_{,i}(3p_{12} + p_3^2)p_3^2 - S_{,i}p_1p_2p_3]\Big),$$

$$\frac{\partial^2 G}{\partial x_i \partial x_j} = 2\alpha^2\Big(T_{,ij} + c^2[2R_{,ij}p_3^3 + P_{,ij}p_3^2 + 2Q_{,ij}p_3 + S_{,ij}p_1p_2]\Big). \qquad (D-2)$$

In eqs (D-1) and (D-2),

$$c^2 = (p_k p_k)^{-1}, \qquad (D-3)$$

and the following notation is used:

$$p_{13} = p_1^2 + p_3^2, \quad p_{23} = p_2^2 + p_3^2, \quad p_{12} = p_1^2 + p_2^2,$$

$$A = \eta_y p_3^2 + 2\chi_x p_2 p_3 + \eta_z p_2^2, \quad B = \epsilon_{35} p_3^3 + \chi_z p_2 p_3^2 + \chi_y p_2^2 p_3 + \epsilon_{26} p_2^3,$$

$$C = \epsilon_{15} p_3 + \epsilon_{16} p_2, \quad D = 2\epsilon_{34} p_3^2 + \eta_x p_2 p_3 + 2\epsilon_{24} p_2^2,$$

$$E = \eta_x p_3^2 + 2\chi_y p_1 p_3 + \eta_z p_1^2, \quad F = \epsilon_{34} p_3^3 + \chi_z p_1 p_3^2 + \chi_x p_1^2 p_3 + \epsilon_{16} p_1^3,$$

$$G = \epsilon_{24} p_3 + \epsilon_{26} p_1, \quad H = 2\epsilon_{35} p_3^2 + \eta_y p_1 p_3 + 2\epsilon_{15} p_1^2,$$

$$P = \eta_y p_1^2 + 2\chi_z p_1 p_2 + \eta_x p_2^2, \quad Q = \epsilon_{15} p_1^3 + \chi_x p_1^2 p_2 + \chi_y p_1 p_2^2 + \epsilon_{24} p_2^3,$$

$$R = \epsilon_{34} p_2 + \epsilon_{35} p_1, \quad S = 2\epsilon_{16} p_1^2 + \eta_z p_1 p_2 + 2\epsilon_{26} p_2^2,$$

$$T = \epsilon_x p_1^2 + \epsilon_y p_2^2 + \epsilon_z p_3^2,$$

$$\eta_x = \delta_x - \epsilon_y - \epsilon_z, \quad \eta_y = \delta_y - \epsilon_x - \epsilon_z, \quad \eta_z = \delta_z - \epsilon_x - \epsilon_y. \qquad (D-4)$$

b) First derivatives of the first-order common S-wave eigenvalue $G_S(x_m, p_m)$ for a weakly anisotropic medium of an arbitrary symmetry

The first derivatives of the first-order common S-wave eigenvalue in eq.(74) appearing on the RHS of ray tracing equations (A-2) depend on x_m and p_m. They have the following explicit form:

$$\frac{\partial G_S}{\partial p_1} = \beta^2[2p_1(1+\gamma_y+\gamma_z) + \epsilon_{45}p_2 + \epsilon_{46}p_3]$$
$$+\alpha^2 c^4 \Big(2p_1 p_{23}(\epsilon_x p_{23} - \delta_y p_3^2 - \delta_z p_2^2) + 2p_1(\epsilon_y p_2^4 + \epsilon_z p_3^4 + \delta_x p_2^2 p_3^2)$$
$$-2(2\chi_x p_1 + \chi_y p_2 + \chi_z p_3)p_2 p_3(p_{23} - p_1^2) + (\epsilon_{16}p_2 + \epsilon_{15}p_3)[(p_{23}-p_1^2)^2 - 2p_1^2 c^{-2}]$$
$$+[\epsilon_{26}p_2(p_{13}-p_2^2) + \epsilon_{35}p_3(p_{12}-p_3^2)]c^{-2} + 4p_1[(\epsilon_{26}p_1 + \epsilon_{24}p_3)p_2^3 + (\epsilon_{34}p_2 + \epsilon_{35}p_1)p_3^3]\Big),$$

$$\frac{\partial G_S}{\partial p_2} = \beta^2[2p_2(1+\gamma_x+\gamma_z) + \epsilon_{45}p_1 + \epsilon_{56}p_3]$$
$$+\alpha^2 c^4 \Big(2p_2 p_{13}(\epsilon_y p_{13} - \delta_x p_3^2 - \delta_z p_1^2) + 2p_2(\epsilon_x p_1^4 + \epsilon_z p_3^4 + \delta_y p_1^2 p_3^2)$$
$$-2(\chi_x p_1 + 2\chi_y p_2 + \chi_z p_3)p_1 p_3(p_{13} - p_2^2) + (\epsilon_{26}p_2 + \epsilon_{24}p_3)[(p_{13}-p_2^2)^2 - 2p_2^2 c^{-2}]$$
$$+[\epsilon_{16}p_1(p_{23}-p_1^2) + \epsilon_{34}p_3(p_{12}-p_3^2)]c^{-2} + 4p_2[(\epsilon_{16}p_2 + \epsilon_{15}p_3)p_1^3 + (\epsilon_{34}p_2 + \epsilon_{35}p_1)p_3^3]\Big),$$

$$\frac{\partial G_S}{\partial p_3} = \beta^2[2p_3(1+\gamma_x+\gamma_y) + \epsilon_{46}p_1 + \epsilon_{56}p_2]$$
$$+\alpha^2 c^4 \Big(2p_3 p_{12}(\epsilon_z p_{12} - \delta_x p_2^2 - \delta_y p_1^2) + 2p_3(\epsilon_x p_1^4 + \epsilon_y p_2^4 + \delta_z p_1^2 p_2^2)$$
$$-2(\chi_x p_1 + \chi_y p_2 + 2\chi_z p_3)p_1 p_2(p_{12} - p_3^2) + (\epsilon_{34}p_2 + \epsilon_{35}p_1)[(p_{12}-p_3^2)^2 - 2p_3^2 c^{-2}]$$

$$+[\epsilon_{15}p_1(p_{23}-p_1^2)+\epsilon_{24}p_2(p_{13}-p_2^2)]c^{-2}+4p_3[(\epsilon_{16}p_2+\epsilon_{15}p_3)p_1^3+(\epsilon_{26}p_1+\epsilon_{24}p_3)p_2^3]\Big),$$

$$\frac{\partial G_S}{\partial x_i}=\beta^2\Big(\epsilon_{45,i}p_1p_2+\epsilon_{46,i}p_1p_3+\epsilon_{56,i}p_2p_3+\gamma_{y,i}p_{13}+\gamma_{x,i}p_{23}+\gamma_{z,i}p_{12}\Big)$$
$$-\alpha^2(p_ip_i)^{-1}\Big(\delta_{x,i}p_2^2p_3^2+\delta_{y,i}p_1^2p_3^2+\delta_{z,i}p_1^2p_2^2-\epsilon_{x,i}p_1^2p_{23}-\epsilon_{y,i}p_2^2p_{13}-\epsilon_{z,i}p_3^2p_{12}$$
$$+2(\chi_{x,i}p_1+\chi_{y,i}p_2+\chi_{z,i}p_3)p_1p_2p_3-(\epsilon_{16,i}p_2+\epsilon_{15,i}p_3)p_1(p_{23}-p_1^2)$$
$$-(\epsilon_{26,i}p_1+\epsilon_{24,i}p_3)p_2(p_{13}-p_2^2)-(\epsilon_{34,i}p_2+\epsilon_{35,i}p_1)p_3(p_{12}-p_3^2)\Big). \qquad (D-5)$$

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