PHASE SHIFT OF THE GREEN TENSOR DUE TO CAUSTICS IN ANISOTROPIC MEDIA

Luděk Klimeš

Department of Geophysics, Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 121 16 Praha 2, Czech Republic (http://sw3d.cz/staff/klimes.htm)

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ABSTRACT

Equations are presented to determine the phase shift of the amplitude of the elastic Green tensor due to both simple (line) and point caustics in anisotropic media. The phase–shift rules for the Green tensor are expressed in terms of the paraxial–ray matrices calculated by dynamic ray tracing. The phase–shift rules are derived both for 2×2 paraxial–ray matrices in ray–centred coordinates and for 3×3 paraxial–ray matrices in general coordinates. The reciprocity of the phase shift of the Green tensor is demonstrated. Then a simple example is given to illustrate the positive and negative phase shifts in anisotropic media, and also to illustrate the reciprocity of the phase shift of the Green tensor.

Keywords: anisotropy, Green tensor, caustics, KMAH index, paraxial rays

1. INTRODUCTION

Equations for ray tracing and dynamic ray tracing are required to calculate anisotropic ray theory approximations of elastic wavefields or Green tensors. The equations should also be supplemented with rules determining how a ray should be continued through singularities in the ray tracing equations, and which branch of the square root of the determinant of the matrix of geometrical spreading to select when touching a caustic. The correct branch of the square root of the determinant of the matrix of geometrical spreading is determined by the "KMAH index", defined below. The Green tensor also requires the equations of the initial conditions corresponding to a unit force at the point source, including the initial value of the KMAH index. In layered and block models, equations for the reflection/transmission coefficients and for the transformation of the dynamic ray tracing at structural interfaces are also required.

The initial conditions for the Green tensor in an inhomogeneous anisotropic medium are the same as in the anisotropic medium, locally homogeneous in a small

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vicinity of the point source. Refer, e.g., to *Buchwald (1959)* or to *Červený (2001, Sec. 2.5.5)*.

For the reflection/transmission coefficients refer, e.g., to *Fedorov (1968)*.

The dynamic ray tracing equations in Cartesian coordinates, supplementing the ray tracing equations in anisotropic media (*Babich, 1961*), were derived by *Červený (1972)*. For the transformation of the dynamic ray tracing at curved interfaces between anisotropic materials refer, e.g., to *Gajewski and Pšenčík (1990)* and *Červený (2001)*.

The KMAH index determines the phase shift due to caustics. It is named after *Keller (1958)*, *Maslov (1965)*, *Arnold (1967)* and *Hörmander (1971)*. Note that it is referred to as the "path index" by *Maslov (1965)* and *Kravtsov (1968)*. A KMAH index of +1 indicates a phase shift of the complex–valued amplitude by $\frac{\pi}{2}$ in the direction corresponding to increasing *time* (or decreasing *travel time*) of the time–harmonic wave.

The ray–theory wavefield is the limiting case of a Gaussian beam, infinitely narrow at the point source and infinitely broad outside caustics (*Červený, 2001*). The phase shift of a Gaussian beam is included in the the complex–valued amplitude of the Gaussian beam and varies smoothly along the central ray of the beam. We shall thus determine the phase shift of the ray–theory Green tensor as the limiting case of the continuous phase shift of the Gaussian beam.

Hereinafter the time–harmonic wavefield, dependent on time t through the multiplication factor of $\exp(-\mathrm{i}\omega t)$, is chosen for positive circular frequencies ω. The imaginary part of the matrix of the second travel–time derivatives of a Gaussian beam then has to be positive–definite, and the KMAH index of +1 corresponds to the amplitude multiplication factor of $\exp(-\mathrm{i}\frac{\pi}{2})$.

In isotropic media, the increment of the KMAH index is always +2 at a point caustic, and +1 at a simple (line) caustic. However, even in this simple case, an algorithm, robust with respect to finite numerical step along a ray and with respect to rounding errors, is essential for numerical calculations (*Červený et al., 1988*).

Unlike in isotropic media, where the increment of the KMAH index is always positive, the increment of the KMAH index of S waves in anisotropic media may be either positive, or negative, depending on the convexity or non–convexity of the slowness surface. *Lewis (1965)* derived a general phase–shift rule for a point caustic, expressed in terms of the signature of the matrix of second derivatives of travel time. *Garmany (1988a; 1988b)* expressed the phase–shift rule for a 1–D anisotropic medium (a simple caustic) in terms of the second derivatives of the eigenvalue of the Christoffel matrix with respect to the slowness vector. A rule analogous to *Garmany (1988a; 1988b)*, but less explicit, has also been given by *Orlov (1981)* and *Kravtsov and Orlov (1993; 1999)*. *Garmany (2001)* then generalized his phase–shift rule to a simple caustic in a generally heterogeneous and generally anisotropic media. *Bakker (1998)* derived the equations for the phase shift corresponding to a general wavefield, due to both simple and point caustics in 3–D anisotropic media. Bakker's rules are expressed in terms of the second derivatives of the eigenvalue of the Christoffel matrix with respect to the slowness vector, and are closely related to the phase–shift rules derived by *Klimeš (1997)* and presented hereinafter. Note that the criticism of Bakker's approach by *Hanyga and Slawinski (2001)*, based on a different choice of the coordinates for dynamic ray tracing, is inadequate because the differences between their approaches do not affect the phase–shift rules.

For the numerical determination whether a ray touched a caustic, and whether the caustic is a simple caustic or a point caustic, the same algorithm may be used as in the isotropic medium (*Červený et al., 1988, Sec. 5.8.3f; Červený, 2001, Sec. 4.12.1*). The algorithm can identify all caustic points in the isotropic medium. Only in the anisotropic medium and if both the slowness surface and the wavefront are hyperbolic (indefinite curvature matrices), the algorithm may fail to correctly identify a point caustic (or two close simple caustics). Fortunately, in this case, the corresponding increments of the KMAH index are -1 and $+1$, i.e. the caustics do not affect the final value of the KMAH index, see Appendix B. The caustic identification algorithm is thus always reliable with a view of determining the phase shift. The caustic identification algorithm is expressed in terms of the $2{\times}2$ paraxial–ray matrices calculated by dynamic ray tracing in ray–centred coordinates and is briefly recalled in Appendix B. It may be converted into the algorithm expressed in terms of the $3{\times}3$ paraxial–ray matrices calculated in Cartesian coordinates by the substitutions described at the end of Appendix B.

After the caustic is identified, we need to determine the corresponding phase shift. In Sections 2 and 3, we derive the rules determining the sign of the phase shift of the amplitude of the elastic Green tensor due to caustics in anisotropic media. The phase–shift rules are expressed in terms of the paraxial–ray matrices calculated by dynamic ray tracing, similarly as the caustic identification algorithm by *Červený et al. (1988, Sec. 5.8.3f)*. The phase–shift rules are derived both for $2{\times}2$ paraxial–ray matrices in ray–centred coordinates and for $3{\times}3$ paraxial–ray matrices in general coordinates.

The reciprocity of the phase shift of the elastic Green tensor is demonstrated in Section 4.

In Section 5, a simple example is given to simultaneously illustrate the positive and negative phase shifts in anisotropic media, and the reciprocity of the phase shift of the Green tensor.

2. SIMPLE (LINE) CAUSTIC

Assume a simple (line, non–singular, first–order) caustic at the ray bundle originating from a point source. At the simple caustic, the matrix of geometrical spreading has just one zero eigenvalue. We derive the phase–shift rule for the simple caustic in terms of $2{\times}2$ paraxial–ray matrices in ray–centred coordinates in Section 2.1. We then propose conversion of the phase–shift rule into $3{\times}3$ paraxial–ray matrices in general coordinates in Section 2.2.

2.1. Matrices 2×2 in Ray–Centred Coordinates

At the simple caustic, the submatrix $\mathbf{Q}_2$ of the paraxial–ray propagator matrix (*Červený, 2001*)

$$\begin{pmatrix} \mathbf{Q}_1 & \mathbf{Q}_2 \\ \mathbf{P}_1 & \mathbf{P}_2 \end{pmatrix} \tag{1}$$

has just one zero eigenvalue.

In this Section 2.1, paraxial–ray matrices $\mathbf{Q}_1$, $\mathbf{Q}_2$, $\mathbf{P}_1$ and $\mathbf{P}_2$ are 2×2 matrices in the ray–centred coordinates. The phase–shift rules expressed in terms of the 2×2 paraxial–ray matrices in the ray–centred coordinates are independent of the Hamiltonian considered for dynamic ray tracing.

The orthonomic system of rays corresponding to the Green tensor is described by the 2×2 paraxial–ray matrices

$$\mathbf{Q}_{\mathrm{R}} = \mathbf{Q}_2\mathbf{P}_{\mathrm{R0}} \tag{2}$$

and

$$\mathbf{P}_{\mathrm{R}} = \mathbf{P}_2\mathbf{P}_{\mathrm{R0}} \quad . \tag{3}$$

Here matrix $\mathbf{P}_{\mathrm{R0}}$, describing the parametrization of rays, represents the value of matrix $\mathbf{P}_{\mathrm{R}}$ at the point source. Matrices $\mathbf{Q}_{\mathrm{R}}$ and $\mathbf{P}_{\mathrm{R}}$ differ from matrices $\mathbf{Q}_2$ and $\mathbf{P}_2$ by the ray parametrization.

The ray–theory wavefield is the limiting case of the Gaussian beam, infinitely narrow at the point source (*Červený, 2001*). The real part of the matrix of the second travel–time derivatives of the Gaussian beam at the point source is taken to be zero, and the imaginary part is denoted $\mathbf{Y}_0$. The imaginary part $\mathbf{Y}_0$ of the matrix of the second travel–time derivatives of a Gaussian beam is a positive–definite symmetrical matrix. The Gaussian beam approaches the ray–theory wavefield for increasing $\mathbf{Y}_0$, i.e., for the positive–definite symmetrical matrix $\mathbf{Y}_0^{-1}$ limiting to the zero matrix.

The matrix of geometrical spreading of the Gaussian beam is (*Červený, 2001*)

$$\mathbf{Q} = [\mathbf{Q}_1 + \mathrm{i}\mathbf{Q}_2\mathbf{Y}_0]\mathbf{Q}_0 \quad , \tag{4}$$

where $\mathbf{Q}_0$ is the value of the matrix of geometrical spreading of the Gaussian beam at the point source.

The amplitude of the Gaussian beam including the phase shift is proportional to $(\det\mathbf{Q})^{-\frac{1}{2}}$. The increment of the phase of $(\det\mathbf{Q})^{-\frac{1}{2}}$ through the caustic thus converges to the phase shift $\exp(-\mathrm{i}\frac{\pi}{2}KMAH)$ of the anisotropic ray theory.

In the vicinity of the caustic we may approximate $\mathbf{Q}$ by the linear Taylor expansion with respect to the increasing monotonic parameter γ_3 along the ray,

$$\mathbf{Q}(\Delta\gamma_3) \approx [\mathbf{Q}_1 + \mathrm{i}\mathbf{Q}_2\mathbf{Y}_0 + \mathbf{Q}_1'\Delta\gamma_3 + \mathrm{i}\mathbf{Q}_2'\mathbf{Y}_0\Delta\gamma_3]\mathbf{Q}_0 \quad , \tag{5}$$

centred at the caustic where $\Delta\gamma_3 = 0$. Here

$$\mathbf{Q}_1' = \frac{\mathrm{d}\mathbf{Q}_1}{\mathrm{d}\gamma_3} \quad , \qquad \mathbf{Q}_2' = \frac{\mathrm{d}\mathbf{Q}_2}{\mathrm{d}\gamma_3} \quad . \tag{6}$$

For very small $\mathbf{Y}_0^{-1}$ and $\Delta\gamma_3$ we may further approximate Taylor expansion (5) by

$$\mathbf{Q}(\Delta\gamma_3) \approx [\mathbf{Q}_2 - \mathrm{i}\mathbf{Q}_1\mathbf{Y}_0^{-1} + \mathbf{Q}_2'\Delta\gamma_3]\ \mathrm{i}\mathbf{Y}_0\mathbf{Q}_0 \quad . \tag{7}$$

To proceed from the approximation (7) of $\mathbf{Q}(\Delta\gamma_3)$, linear in $\mathbf{Y}_0^{-1}$ and $\Delta\gamma_3$, to the analogous approximation of $\det\mathbf{Q}(\Delta\gamma_3)$, we use identity

$$\partial(\det\mathbf{Q}) = \mathrm{tr}(\mathbf{Q}^{-1}\partial\mathbf{Q})\ \det\mathbf{Q}\ \ , \tag{8}$$

valid for any kind of variations denoted here by ∂. Introducing, at the simple caustic, matrix

$$\mathbf{K} = \mathbf{Q}_2^{-1}\,\det\mathbf{Q}_2 \tag{9}$$

of rank 1 composed of the subdeterminants of $\mathbf{Q}_2$, and considering identity (8), the determinant of matrix (7) may be approximated by expression

$$\det\mathbf{Q}(\Delta\gamma_3) \approx [\mathrm{tr}(\mathbf{K}\mathbf{Q}_2')\Delta\gamma_3 - \mathrm{i}\ \mathrm{tr}(\mathbf{K}\mathbf{Q}_1\mathbf{Y}_0^{-1})]\ \ \det(\mathrm{i}\mathbf{Y}_0\mathbf{Q}_0)\ \ , \tag{10}$$

linear in $\mathbf{Y}_0^{-1}$ and $\Delta\gamma_3$. Note that the range of matrix $\mathbf{K}$ coincides with the null space of matrix $\mathbf{Q}_2$ and vice versa. Matrix $\mathbf{K}$ is always finite, and it is very easy to calculate it numerically from matrix $\mathbf{Q}_2$. For 2×2 matrix $\mathbf{Q}_2$,

$$\mathbf{Q}_2 = \begin{pmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{pmatrix}\ \ , \tag{11}$$

we have

$$\mathbf{K} = \begin{pmatrix} Q_{22} & -Q_{12} \\ -Q_{21} & Q_{11} \end{pmatrix}\ \ . \tag{12}$$

Since matrix $\mathbf{K}$ is of rank 1, it can be expressed as the dyadic product

$$\mathbf{K} = \mathbf{a}\ \mathbf{b}^{\mathrm{T}} \tag{13}$$

of vectors $\mathbf{a}$ and $\mathbf{b}$. Vector $\mathbf{a}$ specifies the singular direction in the ray–parameter domain due to the caustic, $\mathbf{Q}_2\,\mathbf{a} = \mathbf{0}$, whereas vector $\mathbf{b}$ is perpendicular to the caustic surface (spatial singular direction due to the caustic). Matrix $\mathbf{K}$ is thus well suited as the projection matrix to the singular directions at a simple caustic.

If the numbers

$$\widetilde{K}_1 = \mathrm{tr}(\mathbf{K}\mathbf{Q}_1\mathbf{Y}_0^{-1})\ \ , \tag{14}$$

$$K_2 = \mathrm{tr}(\mathbf{K}\mathbf{Q}_2') \tag{15}$$

have equal signs, the determinant (10) passes for increasing $\Delta\gamma_3$ the origin of the complex plane counterclockwise (see Fig. 1), and the increment of the KMAH index is +1. Otherwise, the increment of the KMAH index is −1.

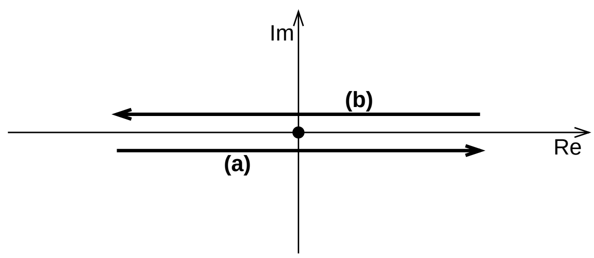

Fig. 1. Values of the function $-\mathrm{i}K_2 + \widetilde{K}_1\Delta\gamma_3$ in the vicinity of the origin of the complex plane: **(a)** for $\widetilde{K}_1 > 0$ and $K_2 > 0$, **(b)** for $\widetilde{K}_1 < 0$ and $K_2 < 0$. The arrows correspond to increasing $\Delta\gamma_3$. The constant multiplication factor of $\det(\mathrm{i}\mathbf{Y}_0\mathbf{Q}_0)$ in expression (10) just rotates the diagram of the functional values around the origin by the corresponding angle.

Multiplying matrix $\mathbf{K}\mathbf{Q}_1\mathbf{Y}_0^{-1}$ in definition (14) by the transposed left–hand side of identity (C.3) of Appendix C, which equals a unit matrix, and considering that $\mathbf{Q}_2\mathbf{K} = \mathbf{0}$, we obtain

$$\widetilde{K}_1 = \mathrm{tr}(\mathbf{K}\mathbf{Q}_1\mathbf{Y}_0^{-1}\mathbf{Q}_1^{\mathrm{T}}\mathbf{P}_2) \quad . \tag{16}$$

Note that $\mathrm{tr}(\mathbf{AB}) = \mathrm{tr}(\mathbf{BA})$ for any two matrices $\mathbf{A}$ and $\mathbf{B}$. Since both $\mathbf{P}_2\mathbf{K}$ and $\mathbf{Q}_1^{\mathrm{T}}\mathbf{P}_2\mathbf{K}\mathbf{Q}_1$ are symmetrical matrices (Appendix C) of rank 1, and $\mathbf{Y}_0^{-1}$ is a positive–definite matrix, the sign of $\widetilde{K}_1$ is the same as the sign of non–zero number

$$K_1 = \mathrm{tr}(\mathbf{K}\mathbf{P}_2) \quad . \tag{17}$$

Since matrix $\mathbf{P}_2$ describes the sensitivity of the slowness vector to the ray parameters, quantity $K_1 = \mathbf{b}^{\mathrm{T}}\mathbf{P}_2\,\mathbf{a}$ is proportional to the derivative of the slowness–vector component, perpendicular to the caustic surface, in the singular direction in the ray–parameter domain. Similarly, since matrix $\mathbf{Q}_2'$ describes the sensitivity of the ray–velocity vector to the ray parameters, quantity $K_2 = \mathbf{b}^{\mathrm{T}}\mathbf{Q}_2'\,\mathbf{a}$ is proportional to the derivative of the the ray–velocity vector component, perpendicular to the caustic surface, in the singular direction in the ray–parameter domain.

Note that both vectors $\mathbf{P}_2\,\mathbf{a}$ and $\mathbf{b}$ are collinear with *Bakker's (1998, Eq. 9)* unit vector $\mathbf{m}_1$. *Bakker's (1998, Eq. 10)* expression $\mathbf{m}_1^{\mathrm{T}}\mathbf{S}_{12}\,\mathbf{m}_1$ is thus identical to K_2/K_1 if the same coordinates and the same Hamiltonian are considered for dynamic ray tracing.

Phase–shift rule for a simple caustic: The increment of the KMAH index is equal to

$$\mathrm{sgn}(K_2/K_1) \quad , \tag{18}$$

where K_1 and K_2 are given by equations (17) and (15) with $\mathbf{K}$ defined by (9).

If the normal curvature of the slowness surface in the direction of vector $\mathbf{b}$ perpendicular to the caustic surface vanishes at a simple spatial caustic,

$$K_2 = 0 \quad , \tag{19}$$

the phase shift depends on the higher–order derivatives of matrix $\mathbf{Q}$ along the ray, see expression (A.4) in Appendix A.

Note that (a) $K_2 = (\det\mathbf{Q}_2)'$ always has the sign of $\det\mathbf{Q}_2$ beyond the caustic, which follows from definition (15) with (9); (b) in an isotropic medium, both K_1 and K_2 have the same sign, and the increment of the KMAH index is thus always positive there, which follows from Eqs. (15), (17), and the dynamic ray tracing equations in ray–centred coordinates; (c) the increment of the KMAH index is negative if the signs of the wavefront curvature in the singular direction ("perpendicular" to the caustic) in front of and beyond the caustic are opposite to the signs the curvature always has in isotropic media; (d) the increment of the KMAH index is negative if the slowness surface is concave in the singular direction ("perpendicular" to the caustic) determined by collinear vectors $\mathbf{b}$ and $\mathbf{P}_2\,\mathbf{a}$, which follows from Eqs. (13), (15), (17), and the dynamic ray tracing equations in ray–centred coordinates, see *Klimeš (1994; 2002)*.

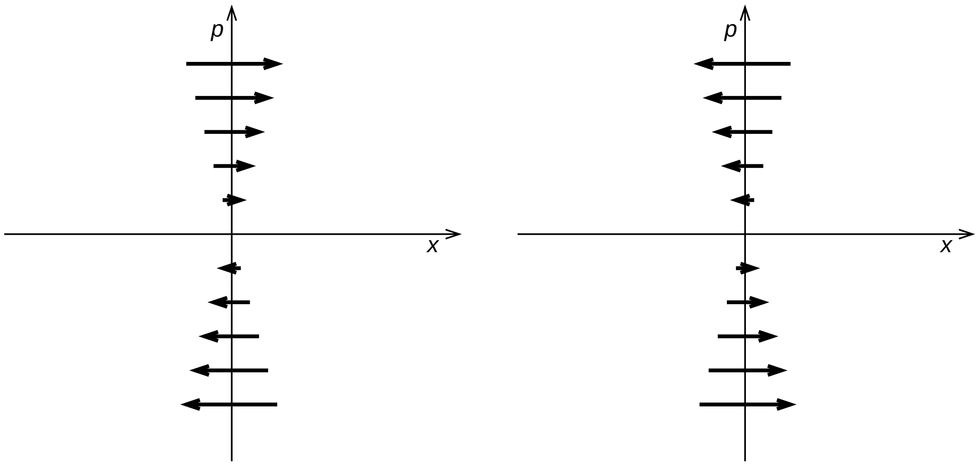

Fig. 2. Phase–space ray tube twisting at a simple caustic for the positive increment of the KMAH index (left), and for the negative increment of the KMAH index (right). The arrows represent short segments of paraxial rays, starting in front of and terminating beyond the caustic.

Note on phase–space twisting at a simple caustic: Let us consider paraxial rays deviating from the axial ray in the singular direction $\mathbf{a}$ in the ray–parameter domain by the value of $\mathbf{a}\,\Delta\gamma$, see matrix (13). Let us project paraxial deviations $\Delta\mathbf{q} = \mathbf{Q}_2(\Delta\gamma_3)\;\mathbf{a}\,\Delta\gamma$ of spatial coordinates in the vicinity of a simple caustic onto the normal to the caustic, given by vector $\mathbf{b}$ in matrix (13), and refer to this projection $x = \mathbf{b}^{\mathrm{T}}\,\Delta\mathbf{q} \approx K_2\,\Delta\gamma_3\,\Delta\gamma$ as the x axis. Let us analogously project paraxial deviations $\Delta\mathbf{p} = \mathbf{P}_2(\Delta\gamma_3)\;\mathbf{a}\,\Delta\gamma$ of slowness vectors in the vicinity of a simple caustic onto the normal to the caustic, and refer to this projection $p = \mathbf{b}^{\mathrm{T}}\,\Delta\mathbf{p} \approx K_1\,\Delta\gamma$ as the p axis. Observed through this xp plane (x horizontal and positive right, p vertical and positive upwards), the phase–space ray tube at a simple caustic is twisted clockwise for the positive increment of the KMAH index, and counterclockwise for the negative increment of the KMAH index, see Fig. 2. The arrows in Fig. 2 represent short segments of paraxial rays corresponding to different values of $\Delta\gamma$. The individual short segments, parametrized by $\Delta\gamma_3$, start in front of and terminate beyond the caustic.

Note on a general orthonomic system of rays: Although the phase–shift rule for a simple caustic has been derived for 2×2 submatrices $\mathbf{Q}_2$ and $\mathbf{P}_2$ of the paraxial–ray propagator matrix, the phase–shift rule (18) also holds if we replace matrices $\mathbf{Q}_2$ and $\mathbf{P}_2$ in Eqs. (9), (15) and (17) by the analogous 2×2 paraxial–ray matrices $\mathbf{Q}_{\mathrm{R}}$ and $\mathbf{P}_{\mathrm{R}}$ defined by Eqs. (2) and (3). If $\mathbf{Q}_2$ in matrix (9) is replaced by $\mathbf{Q}_{\mathrm{R}}$, $\mathbf{a}$ in matrix (13) changes to

$$\mathbf{a}_{\mathrm{R}} = \mathbf{P}_{\mathrm{R0}}^{-1}\,\mathbf{a} \quad , \tag{20}$$

whereas $\mathbf{b}$ remains unchanged. Vector $\mathbf{a}$ specifies the singular direction at the point source in the ray–centred components of the slowness vector, whereas $\mathbf{a}_{\mathrm{R}}$ in ray parameters.

2.2. Matrices 3×3 in General Coordinates

The circumflex is used hereinafter to distinguish the 3×3 matrices in general coordinates from the 2×2 matrices in ray–centred coordinates.

The 6×6 paraxial–ray propagator matrix

$$\begin{pmatrix} \widehat{\mathbf{Q}}_1 & \widehat{\mathbf{Q}}_2 \\ \widehat{\mathbf{P}}_1 & \widehat{\mathbf{P}}_2 \end{pmatrix} \tag{21}$$

in general coordinates depends on the kind of parameter γ_3 along the ray. In Sections 2.2 and 3.2, we assume that rays are parametrized by travel time $\gamma_3 = \tau$. For this parametrization of rays, at a simple caustic, its 3×3 submatrix $\widehat{\mathbf{Q}}_2$ has just one zero eigenvalue, analogously to 2×2 matrix $\mathbf{Q}_2$ (*Klimeš, 1994, Eqs. 59, 64, 65*). The corresponding left and right null eigenvectors of matrices $\mathbf{Q}_2$ and $\widehat{\mathbf{Q}}_2$ differ just by the coordinate transform between the ray–centred and general coordinates at the caustic point and at the point source, respectively.

Matrix

$$\widehat{\mathbf{K}} = \widehat{\mathbf{Q}}_2^{-1} \det\widehat{\mathbf{Q}}_2 \tag{22}$$

of rank 1, analogous to matrix (9), composed of the subdeterminants of $\widehat{\mathbf{Q}}_2$, can again be expressed as the dyadic product

$$\widehat{\mathbf{K}} = \widehat{\mathbf{a}}\, \widehat{\mathbf{b}}^{\mathrm{T}} \tag{23}$$

of vectors $\widehat{\mathbf{a}}$ and $\widehat{\mathbf{b}}$, see matrix (13). Vectors $\widehat{\mathbf{a}}$ and $\widehat{\mathbf{b}}$ specify in general coordinates the same singular directions as vectors $\mathbf{a}$ and $\mathbf{b}$ in ray–centred coordinates, $\widehat{\mathbf{a}}$ at the point source and $\widehat{\mathbf{b}}$ at the caustic point. The phase–shift rule (18) thus also holds if we replace matrices $\mathbf{K}$, $\mathbf{Q}_2'$ and $\mathbf{P}_2$ in Eqs. (15) and (17) by matrices $\widehat{\mathbf{K}}$, $\widehat{\mathbf{Q}}_2'$ and $\widehat{\mathbf{P}}_2$,

$$K_2 = \mathrm{tr}(\widehat{\mathbf{K}}\widehat{\mathbf{Q}}_2') \quad , \tag{24}$$

$$K_1 = \mathrm{tr}(\widehat{\mathbf{K}}\widehat{\mathbf{P}}_2) \quad . \tag{25}$$

Equations (24) and (25) yield the same K_1 and K_2 as Eqs. (15) and (17). The phase–shift rule (18) also holds if we replace matrices $\widehat{\mathbf{Q}}_2$ and $\widehat{\mathbf{P}}_2$ in Eqs. (22), (24) and (25) by the analogous 3×3 paraxial–ray matrices

$$\widehat{\mathbf{Q}}_{\mathrm{R}} = \widehat{\mathbf{Q}}_1\widehat{\mathbf{Q}}_{\mathrm{R0}} + \widehat{\mathbf{Q}}_2\widehat{\mathbf{P}}_{\mathrm{R0}} \tag{26}$$

and

$$\widehat{\mathbf{P}}_{\mathrm{R}} = \widehat{\mathbf{P}}_1\widehat{\mathbf{Q}}_{\mathrm{R0}} + \widehat{\mathbf{P}}_2\widehat{\mathbf{P}}_{\mathrm{R0}} \tag{27}$$

describing the orthonomic system of rays corresponding to the Green tensor. Then vector $\widehat{\mathbf{a}}$ in matrix (23) is replaced by vector $\widehat{\mathbf{a}}_{\mathrm{R}}$, which specifies in general coordinates the same singular direction as vector $\mathbf{a}_{\mathrm{R}}$ in ray parameters,

$$\mathbf{b}^{\mathrm{T}}\mathbf{Q}_{\mathrm{R}}'\,\mathbf{a}_{\mathrm{R}} = \widehat{\mathbf{b}}^{\mathrm{T}}\widehat{\mathbf{Q}}_{\mathrm{R}}'\,\widehat{\mathbf{a}}_{\mathrm{R}} \quad , \tag{28}$$

$$\mathbf{b}^{\mathrm{T}}\mathbf{P}_{\mathrm{R}}\,\mathbf{a}_{\mathrm{R}} = \widehat{\mathbf{b}}^{\mathrm{T}}\widehat{\mathbf{P}}_{\mathrm{R}}\,\widehat{\mathbf{a}}_{\mathrm{R}} \quad . \tag{29}$$

The first two columns of matrix $\widehat{\mathbf{Q}}_{\mathrm{R}0}$ are zero, the third column is tangent to the ray at the point source. The first two columns of matrix $\widehat{\mathbf{P}}_{\mathrm{R}0}$ describe the parametrization of rays at the point source, analogously as matrix $\mathbf{P}_{\mathrm{R}0}$.

In general coordinates, the 3×3 submatrices $\widehat{\mathbf{Q}}_2$ and $\widehat{\mathbf{P}}_2$ of the paraxial–ray propagator matrix are quite different from the 3×3 matrices $\widehat{\mathbf{Q}}_{\mathrm{R}}$ and $\widehat{\mathbf{P}}_{\mathrm{R}}$ describing the orthonomic system of rays corresponding to the Green tensor.

3. POINT CAUSTIC

Assume a point (focus, second–order) caustic at the ray bundle corresponding to a point source. At the caustic, the 2×2 submatrix $\mathbf{Q}_2$ of the paraxial–ray propagator matrix (1) becomes a zero matrix, and the 3×3 submatrix $\widehat{\mathbf{Q}}_2$ of the paraxial–ray propagator matrix (21) has two zero eigenvalues.

3.1. Matrices 2×2 in Ray–Centred Coordinates

For 2×2 matrices expressed in ray–centred coordinates, the determinant of matrix (7) may be approximated by

$$\det\mathbf{Q}(\Delta\gamma_3) \approx \det(-\mathrm{i}\mathbf{B} + \mathbf{Q}_2'\mathbf{P}_2^{-1}\Delta\gamma_3)\ \det(\mathrm{i}\mathbf{P}_2\mathbf{Y}_0\mathbf{Q}_0) \quad . \tag{30}$$

where

$$\mathbf{B} = \mathbf{Q}_1\mathbf{Y}_0^{-1}\mathbf{P}_2^{-1} \quad . \tag{31}$$

Since

$$\mathbf{B} = (\mathbf{P}_2^{\mathrm{T}})^{-1}\mathbf{Y}_0^{-1}\mathbf{P}_2^{-1} \quad , \tag{32}$$

see identity (C.3) of Appendix C, is a small positive–definite symmetrical 2×2 matrix, the phase shift due to caustics depends on the signs of the two eigenvalues of the symmetrical 2×2 matrix $\mathbf{Q}_2'\mathbf{P}_2^{-1}$.

Phase–shift rule for a point caustic:

If

$$\det(\mathbf{Q}_2'\mathbf{P}_2^{-1}) > 0 \quad , \qquad \mathrm{tr}(\mathbf{Q}_2'\mathbf{P}_2^{-1}) > 0 \quad , \tag{33}$$

both the eigenvalues of matrix $-\mathrm{i}\mathbf{B}+\mathbf{Q}_2'\mathbf{P}_2^{-1}\Delta\gamma_3$ pass, for increasing $\Delta\gamma_3$, the origin of the complex plane counterclockwise, and the increment of the KMAH index is +2.

If

$$\det(\mathbf{Q}_2'\mathbf{P}_2^{-1}) > 0 \quad , \qquad \mathrm{tr}(\mathbf{Q}_2'\mathbf{P}_2^{-1}) < 0 \quad , \tag{34}$$

both the eigenvalues of matrix $-\mathrm{i}\mathbf{B}+\mathbf{Q}_2'\mathbf{P}_2^{-1}\Delta\gamma_3$ pass, for increasing $\Delta\gamma_3$, the origin of the complex plane clockwise, and the increment of the KMAH index is −2.

If

$$\det(\mathbf{Q}_2'\mathbf{P}_2^{-1}) < 0 \quad , \tag{35}$$

one eigenvalue of matrix $-\mathrm{i}\mathbf{B} + \mathbf{Q}_2'\mathbf{P}_2^{-1}\Delta\gamma_3$ passes, for increasing $\Delta\gamma_3$, the origin of the complex plane counterclockwise, whereas the other one passes the origin clockwise, and the increment of the KMAH index is 0.

The coincidence of a point spatial caustic with a parabolic line of the slowness surface (*Vavryčuk, 2003*),

$$\det(\mathbf{Q}_2'\mathbf{P}_2^{-1}) = 0 \quad , \tag{36}$$

is not considered in this paper.

Note that, at a point caustic, the 2×2 matrix $\mathbf{Q}_2'\mathbf{P}_2^{-1}$ represents the second derivatives of the Hamiltonian along the plane tangent to the slowness surface. At a point caustic, the 2×2 matrix $\mathbf{Q}_2'\mathbf{P}_2^{-1}$ is identical to *Bakker's (1998)* matrix $\mathbf{S}_{12}$ if the same coordinates and the same Hamiltonian are considered for dynamic ray tracing. The above phase–shift rule is thus identical to the *Bakker's (1998, Eq. 6)* phase–shift rule.

To avoid matrix inversion if the derivative $\mathbf{Q}_2'$ is known, matrix $\mathbf{Q}_2'\mathbf{P}_2^{-1}$ in conditions (33) to (36) may also be replaced by matrix $\mathbf{P}_2^{\mathrm{T}}\mathbf{Q}_2'$,

$$\mathbf{Q}_2'\mathbf{P}_2^{-1} \quad \longrightarrow \quad \mathbf{P}_2^{\mathrm{T}}\mathbf{Q}_2' \quad . \tag{37}$$

Note on a general orthonomic system of rays: Although the phase–shift rule for a point caustic is expressed in terms of the 2×2 submatrices $\mathbf{Q}_2$ and $\mathbf{P}_2$ of the paraxial–ray propagator matrix, the phase–shift rule also holds if we replace matrices $\mathbf{Q}_2$ and $\mathbf{P}_2$ by the analogous paraxial–ray matrices (2) and (3) describing the orthonomic system of rays corresponding to the Green tensor,

$$\mathbf{Q}_2'\mathbf{P}_2^{-1} = \mathbf{Q}_{\mathrm{R}}'\mathbf{P}_{\mathrm{R}}^{-1} \quad . \tag{38}$$

To avoid matrix inversion if the derivative $\mathbf{Q}_{\mathrm{R}}'$ is known, matrix $\mathbf{Q}_2'\mathbf{P}_2^{-1} = \mathbf{Q}_{\mathrm{R}}'\mathbf{P}_{\mathrm{R}}^{-1}$ in conditions (33) to (36) may also be replaced by matrix $\mathbf{P}_{\mathrm{R}}^{\mathrm{T}}\mathbf{Q}_{\mathrm{R}}'$,

$$\mathbf{Q}_2'\mathbf{P}_2^{-1} \quad \longrightarrow \quad \mathbf{P}_{\mathrm{R}}^{\mathrm{T}}\mathbf{Q}_{\mathrm{R}}' \quad . \tag{39}$$

3.2. Matrices 3×3 in General Coordinates

We may consider the 3×3 submatrices $\widehat{\mathbf{Q}}_2$ and $\widehat{\mathbf{P}}_2$ of the paraxial–ray propagator matrix, or the 3×3 paraxial–ray matrices $\widehat{\mathbf{Q}}_{\mathrm{R}}$ and $\widehat{\mathbf{P}}_{\mathrm{R}}$ describing the orthonomic system of rays corresponding to the Green tensor. The paraxial–ray propagator matrix (21) depends on the kind of parameter γ_3 along the ray. In Sections 2.2 and 3.2, we assume that rays are parametrized by travel time $\gamma_3 = \tau$. For this parametrization of rays, at a point caustic, we may derive equality (*Klimeš, 1994, Eqs. 37a, 39a, 53*)

$$\mathbf{P}_{\mathrm{R}}^{\mathrm{T}}\mathbf{Q}_{\mathrm{R}}' = \mathrm{sub}(\widehat{\mathbf{P}}_{\mathrm{R}}^{\mathrm{T}}\widehat{\mathbf{Q}}_{\mathrm{R}}') \quad , \tag{40}$$

where $\mathrm{sub}(\widehat{\mathbf{A}})$ stands for the upper left 2×2 submatrix of 3×3 matrix $\widehat{\mathbf{A}}$. Inserting matrices (26) and (27) into (40) and considering that the first two columns of matrix $\widehat{\mathbf{Q}}_{\mathrm{R0}}$ are zero, we arrive at

$$\mathbf{P}_{\mathrm{R}}^{\mathrm{T}}\mathbf{Q}_{\mathrm{R}}' = \mathrm{sub}(\widehat{\mathbf{P}}_{\mathrm{R0}}^{\mathrm{T}}\widehat{\mathbf{P}}_2^{\mathrm{T}}\widehat{\mathbf{Q}}_2'\widehat{\mathbf{P}}_{\mathrm{R0}}) \quad . \tag{41}$$

We denote by $\widehat{\mathbf{h}}_0$ the matrix which columns are formed by the covariant basis vectors of the ray–centred coordinate system at the point source (*Klimeš, 2002, Eq. 16*).

Then the first two columns of matrix $\widehat{\mathbf{P}}_{\mathrm{R}0}$ equal the first two columns of matrix $\widehat{\mathbf{h}}_0$ multiplied by $\mathbf{P}_{\mathrm{R}0}$ from the right, and thus

$$\mathbf{P}_{\mathrm{R}}^{\mathrm{T}}\mathbf{Q}'_{\mathrm{R}} = \mathbf{P}_{\mathrm{R}0}^{\mathrm{T}}\,\mathrm{sub}(\widehat{\mathbf{h}}_0^{\mathrm{T}}\widehat{\mathbf{P}}_2^{\mathrm{T}}\widehat{\mathbf{Q}}'_2\widehat{\mathbf{h}}_0)\,\mathbf{P}_{\mathrm{R}0} \quad . \tag{42}$$

Conditions (33) to (36) may thus be converted by substitution

$$\mathbf{Q}'_2\mathbf{P}_2^{-1} \quad \longrightarrow \quad \mathrm{sub}(\widehat{\mathbf{h}}_0^{\mathrm{T}}\widehat{\mathbf{P}}_2^{\mathrm{T}}\widehat{\mathbf{Q}}'_2\widehat{\mathbf{h}}_0) \quad , \tag{43}$$

or by substitution

$$\mathbf{Q}'_2\mathbf{P}_2^{-1} \quad \longrightarrow \quad \mathrm{sub}(\widehat{\mathbf{P}}_{\mathrm{R}}^{\mathrm{T}}\widehat{\mathbf{Q}}'_{\mathrm{R}}) \quad . \tag{44}$$

The first two columns of matrix $\widehat{\mathbf{h}}_0$ in substitution (43) may be selected arbitrarily in the plane perpendicular to the ray. Other conversions of conditions (33) to (36) may be derived using transformation equations by *Klimeš (1994; 2002)*.

4. RECIPROCITY OF THE PHASE SHIFT

Kendall et al. (1992) show the reciprocity of the anisotropic–ray–theory Green tensor except for the discussion of the reciprocity of the phase shift of the Green tensor due to caustics. The phase–shift reciprocity is thus demonstrated in this section.

The anisotropic–ray–theory Green tensor is infinite along the rays corresponding to the parabolic lines of the slowness surface at the source. For other rays, the phase shift of the Green tensor due to caustics is obviously reciprocal for two very close points A and B because there can be no Green–tensor caustic between sufficiently close points and because the initial phase shifts are equal. Now let us fix point A and move point B along a ray away from point A.

Assuming that we have hereinbefore considered initial conditions $\mathbf{Y}_0$, $\mathbf{Q}_0$ at point A and have studied the determinant of matrix $\mathbf{Q}$ at point B, we shall now consider initial conditions $\mathbf{Y}_0$, $\mathbf{Q}_0$ at point B and study the determinant of matrix $\mathbf{Q}$ at point A.

The inverse matrix of the paraxial–ray propagator matrix (1) from point A to point B is

$$\begin{pmatrix} \mathbf{P}_2^{\mathrm{T}} & -\mathbf{Q}_2^{\mathrm{T}} \\ -\mathbf{P}_1^{\mathrm{T}} & \mathbf{Q}_1^{\mathrm{T}} \end{pmatrix} \quad , \tag{45}$$

which follows from the symplectic property of the paraxial–ray propagator matrix (*Thomson and Chapman, 1985*). Matrix (45) is the paraxial–ray propagator matrix from point B to point A, but still corresponds to the wave propagation from point A to point B. The opposite wave propagation implies the opposite orientation of the slowness vectors. Keeping the same spatial coordinates and changing the signs of all slowness vector components in matrix (45), including the initial conditions, we thus arrive at the paraxial–ray propagator matrix

$$\begin{pmatrix} \mathbf{P}_2^{\mathrm{T}} & \mathbf{Q}_2^{\mathrm{T}} \\ \mathbf{P}_1^{\mathrm{T}} & \mathbf{Q}_1^{\mathrm{T}} \end{pmatrix} \tag{46}$$

from point B to point A, consistent with the direction of propagation.

Equations (1) to (36) may thus be modified for the propagation from point B to point A by the substitution

$$\mathbf{Q}_1 \longrightarrow \mathbf{P}_2^{\mathrm{T}} \ , \qquad \mathbf{P}_1 \longrightarrow \mathbf{P}_1^{\mathrm{T}} \ , \qquad \mathbf{Q}_2 \longrightarrow \mathbf{Q}_2^{\mathrm{T}} \ , \qquad \mathbf{P}_2 \longrightarrow \mathbf{Q}_1^{\mathrm{T}} \ , \tag{47}$$

including the derivatives of these matrices. Since matrices $\mathbf{Q}_2$ and $\mathbf{Q}_2^{\mathrm{T}}$ have the same rank, the caustics arise for the same distances between points A and B for both the directions of propagation.

With a simple (line) caustic, substitution (47) implies the substitution

$$K_2 \longrightarrow K_2 \ , \qquad K_1 \longrightarrow \widetilde{\widetilde{K}}_1 \ , \tag{48}$$

where

$$\widetilde{\widetilde{K}}_1 = \mathrm{tr}(\mathbf{K}\mathbf{Q}_1) \ . \tag{49}$$

Since $\mathbf{K}\mathbf{Q}_1$ is a symmetrical matrix (Appendix C) of rank 1, and $\mathbf{Y}_0^{-1}$ is a positive–definite matrix, the sign of $\widetilde{\widetilde{K}}_1$ is the same as the sign of $\widetilde{K}_1$ given by definition (14), which is in turn the same as the sign of K_1. Conditions (33), (34) and (35) determine the same phase shift for both the directions of propagation. Increment (18) of the KMAH index due to a simple caustic is thus equal for both the directions of propagation.

With a point caustic, substitution (47) implies the substitution

$$\mathbf{Q}_2'\,\mathbf{P}_2^{-1} \longrightarrow [\mathbf{Q}_2^{\mathrm{T}}]'\,[\mathbf{Q}_1^{\mathrm{T}}]^{-1} \tag{50}$$

in conditions (33), (34) and (35). Since, at a point caustic,

$$[\mathbf{Q}_2^{\mathrm{T}}]'\,[\mathbf{Q}_1^{\mathrm{T}}]^{-1} = [\mathbf{Q}_2^{\mathrm{T}}]'\,\mathbf{P}_2 = \mathbf{P}_2^{\mathrm{T}}\,[\mathbf{Q}_2'\mathbf{P}_2^{-1}]^{\mathrm{T}}\,\mathbf{P}_2 \ , \tag{51}$$

see identity (C.3) of Appendix C, eigenvalues of matrices $\mathbf{Q}_2'\,\mathbf{P}_2^{-1}$ and $[\mathbf{Q}_2^{\mathrm{T}}]'\,[\mathbf{Q}_1^{\mathrm{T}}]^{-1}$ have equal signs, and conditions (33), (34) and (35) determine the same phase shift for both the directions of propagation.

5. EXAMPLE

Assume a 2–D homogeneous anisotropic medium with a triplication on the S–wave ray–velocity surface. Select a ray corresponding to the reverse branch of the ray–velocity surface as the axial ray. Assume that the homogeneous anisotropic medium is separated from the homogeneous isotropic medium by a planar interface perpendicular to the axial ray. For the sake of simplicity, we may assume that the slowness vector at the axial ray is parallel with the ray–velocity vector, and that the (phase and ray) velocities in the direction of the axial ray are almost equal in both media. Note that this configuration for demonstrating the anomalous phase shift has been proposed by *Kravtsov and Orlov (1993; 1999, Fig. 10.3)*.

The slowness vectors of the paraxial rays, propagating in the anisotropic medium to one side of the axial ray, point to the other side of the axial ray, see Fig. 3. On entering the isotropic medium, the paraxial rays are refracted to the direction of the slowness vector and cross the axial ray at the caustic.

Consider 3 points on the axial ray: Point A in the anisotropic medium, point B situated in the isotropic medium between the interface and the caustic corresponding to the point source at A, and point C situated in the isotropic medium beyond the caustic corresponding to the point source at A. The paraxial rays from all 3 points are depicted in Fig. 3. The paraxial rays corresponding to the same paraxial slowness vector are parallel in each of the halfspaces.

Accumulation of the phase shift along the four rays between points A, B and C is shown in Figures 4, 5, 6 and 7.

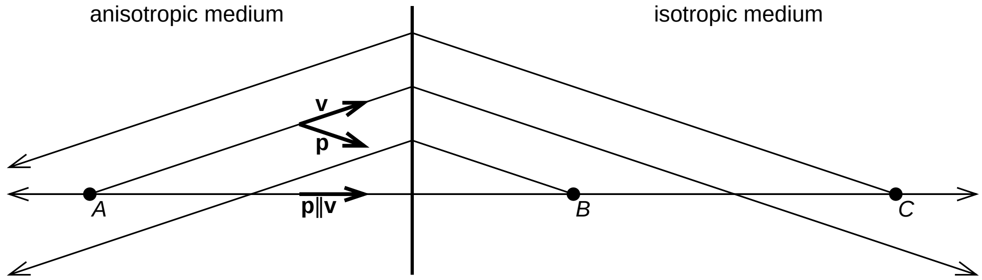

Fig. 3. The axial ray and paraxial rays from points A, B, C in the discussed example. In the anisotropic halfspace, paraxial ray–velocity vector **v** and slowness vector **p** are deflected in opposite directions.

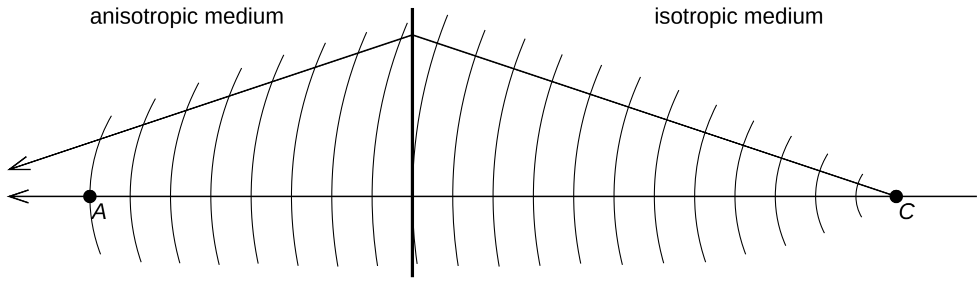

Fig. 4. $C \rightarrow A$: There is no caustic along the ray from point C to point A. If the KMAH index is defined zero at the point source in the isotropic medium, the resulting KMAH index at point A is 0.

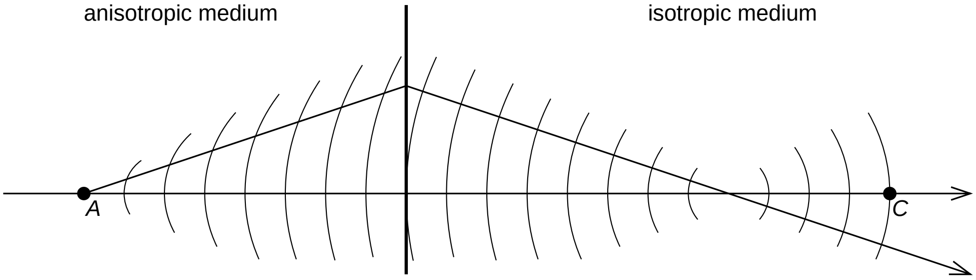

Fig. 5. $A{\rightarrow}C$: The initial KMAH index at point A on the reverse wavefront branch must be smaller by 1 than on the forward branch (*Pšenčík and Teles, 1996; Hanyga and Slawinski, 2001*), i.e. -1 in our 2–D case with the zero initial value of the KMAH index in the isotropic medium. There is a single caustic along the ray from point A to point C, located in the isotropic medium, causing the KMAH index to increase by 1. The resulting KMAH index at point C is then 0.

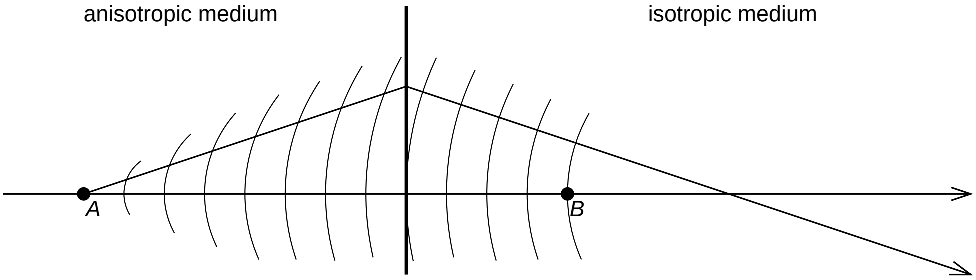

Fig. 6. $A{\rightarrow}B$: The initial KMAH index at point A is again -1, but there is no caustic along the ray from point A to point B. The resulting KMAH index at point B is now -1.

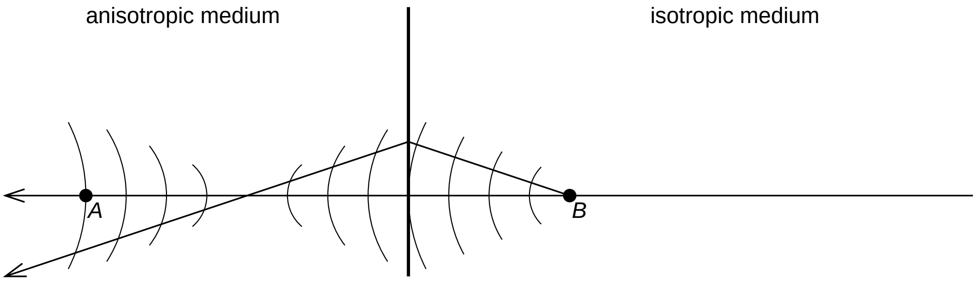

Fig. 7. $B{\rightarrow}A$: The initial KMAH index at point B is 0, as for $C{\rightarrow}A$. There is a single caustic along the ray from point B to point A, located in the anisotropic medium on the reverse branch of the ray–velocity surface, causing the KMAH index to decrease by 1. The resulting KMAH index at point A is then -1.

6. CONCLUSIONS

The phase–shift rules for the Green tensor at a simple (line) caustic, expressed in terms of 2×2 paraxial–ray matrices in ray–centred coordinates or 3×3 paraxial–ray matrices in general coordinates, are given by equations (15), (17) and (18). The phase–shift rules for the Green tensor at a point caustic, expressed in terms of 2×2 paraxial–ray matrices in ray–centred coordinates or 3×3 paraxial–ray matrices in general coordinates, are given by conditions (33), (34) and (35). The phase–shift rules for the Green tensor at a point caustic can be expressed in terms of 3×3 paraxial–ray matrices in general coordinates using substitutions (43) or (44).

The reciprocity of the phase shift of the Green tensor is demonstrated in Section 4. In Section 5, a simple example is given to illustrate the positive and negative phase shifts in anisotropic media, and also to illustrate the reciprocity of the phase shift of the Green tensor.

For additional information, including electronic reprints, computer codes and data, refer to the consortium research project "Seismic Waves in Complex 3–D Structures" ("http://sw3d.cz").

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APPENDIX A
KMAH INDEX DISPLAYED IN RAY COORDINATES

The domain of ray coordinates γ_1, γ_2, γ_3 may be decomposed into subdomains of equal sign of function

$$D = \det(\mathbf{Q}_\mathrm{R}) \quad , \tag{A.1}$$

separated by the zero isosurface of function $D = D(\gamma_k)$, determined by equation (*Kravtsov and Orlov, 1993, Eq. 2.3.2*)

$$D = 0 \quad . \tag{A.2}$$

Matrix $\mathbf{Q}_\mathrm{R}$ in function (A.1) represents 2×2 matrix (2) of geometrical spreading in ray–centred coordinates. It may coincide with 2×2 submatrix $\mathbf{Q}_2$ of paraxial–ray propagator matrix (1).

The KMAH index is constant in the subdomains but changes at the zero isosurface, which represent the caustic surfaces. Smooth parts of the zero isosurface represent simple (line) caustics, intersections of different parts of the zero isosurface represent point caustics. Ray–coordinate lines γ_K = constant, $K = 1, 2$ represent rays. The points of intersection of these lines with the zero isosurface represent the points where the rays touch the caustics.

The normal to the zero isosurface is given by the gradient $\frac{\partial D}{\partial \gamma_i}$ of function $D = D(\gamma_k)$. The third component $\frac{\partial D}{\partial \gamma_3}$ of the gradient is

$$D' = \mathrm{tr}(\mathbf{Q}'_{\mathrm{R}}\mathbf{Q}_{\mathrm{R}}^{-1})\det(\mathbf{Q}_{\mathrm{R}}) = \mathrm{tr}(\mathbf{K}\mathbf{Q}'_{\mathrm{R}}) = K_2 \quad . \tag{A.3}$$

For the given sign of K_1, the phase shift depends on the third component (A.3) of the gradient of D, see expression (18). Note that the sign of K_1 is constant in the vicinity of each smooth part of the zero isosurface of D, but both K_1 and K_2 change their signs at the intersection with another smooth part of the zero isosurface.

In a case of a local return fold of the zero isosurface, derivative (A.3) has opposite signs at the bottom and at the top of the fold. If a ray–coordinate line γ_K = constant, $K = 1, 2$, intersects a small local return fold of the zero isosurface, the both corresponding phase shifts cancel, yielding effectively no phase shift. Similarly, no phase shift occurs if a ray–coordinate line closely bypass a local return fold of the zero isosurface. We thus define no phase shift also if a ray–coordinate line touches a local return fold of the zero isosurface of D. This occurs if $D' = 0$ and if the first non–zero derivative $D^{(n)}$ of D with respect to γ_3 is of the even order. The paraxial rays corresponding to the singular direction then mutually touch but do not cross. If a short segment of a ray crosses a small local return fold of the zero isosurface, having both its endpoints situated outside the fold, the crossing can hardly be identified.

A local return fold of the zero isosurface should not occur if a simple caustic is indicated. A local return fold of the zero isosurface may occur only if both the slowness surface and the wavefront are hyperbolic, see condition (35).

On the other hand, a respective phase shift is generated if a ray–coordinate line crosses the zero isosurface of D. This happens if the first non–zero derivative $D^{(n)}$ of D with respect to γ_3 is of the odd order. The corresponding increment of the KMAH index is

$$\mathrm{sgn}(D^{(n)}/K_1) \quad , \tag{A.4}$$

where K_1 is given by Eq. (17). This should be the case if a simple caustic is identified. If the first derivative D' of D with respect to γ_3 is non–zero at a simple caustic, expression (A.4) is identical to expression (18). If equality (19) holds at a simple caustic, the first non–zero derivative $D^{(n)}$ of D with respect to γ_3 should be of the odd order. Equality (19) implies that the slowness surface at the simple caustic is hyperbolic or, by coincidence, parabolic.

Unfortunately, the n^{th}–order derivative of D depends on the n^{th}–order derivative of $\mathbf{Q}_{\mathrm{R}}$, which in turn depends on the $(n+2)^{\mathrm{nd}}$–order spatial derivatives of the density–normalized elastic moduli.

APPENDIX B
CAUSTIC IDENTIFICATION ALGORITHM

We first repeat the caustic identification algorithm by *Červený et al. (1988, Sec. 5.8.3f)* and *Červený (2001, Sec. 4.12.1)*, expressed in terms of the 2×2 paraxial–ray matrices calculated by dynamic ray tracing in ray–centred coordinates. The algorithm may fail to correctly identify a point caustic (or two close simple caustics) if both the slowness surface and the wavefront are hyperbolic, but is always reliable with a view of determining the phase shift. We then express the caustic identification algorithm also in terms of the 3×3 paraxial–ray matrices calculated by dynamic ray tracing in Cartesian coordinates.

Let us denote by $\mathbf{Q}_{\mathrm{A}}$ and $\mathbf{Q}_{\mathrm{B}}$ the values of 2×2 matrix $\mathbf{Q}_{\mathrm{R}}$ of geometrical spreading in ray–centred coordinates at the endpoints A and B of a sufficiently short segment of a ray. It may coincide with 2×2 submatrix $\mathbf{Q}_2$ of paraxial–ray propagator matrix (1) in ray–centred coordinates. We also define the 2×2 matrix

$$\mathbf{K}_{\mathrm{A}} = \mathbf{Q}_{\mathrm{A}}^{-1} \det(\mathbf{Q}_{\mathrm{A}}) \quad , \tag{B.1}$$

see matrix (12). Quantity

$$\mathrm{tr}(\mathbf{K}_{\mathrm{A}}\mathbf{Q}_{\mathrm{B}}) = Q_{\mathrm{A}11}Q_{\mathrm{B}22} + Q_{\mathrm{A}22}Q_{\mathrm{B}11} - Q_{\mathrm{A}12}Q_{\mathrm{B}21} - Q_{\mathrm{A}21}Q_{\mathrm{B}12} \tag{B.2}$$

is then symmetric with respect to the endpoints A and B of the segment of the ray.

Caustic identification algorithm:

If

$$\det(\mathbf{Q}_{\mathrm{A}})\,\det(\mathbf{Q}_{\mathrm{B}}) < 0 \quad , \tag{B.3}$$

there is a simple caustic between points A and B.

If

$$\det(\mathbf{Q}_{\mathrm{A}})\,\det(\mathbf{Q}_{\mathrm{B}}) > 0 \quad , \tag{B.4}$$

there is a point caustic (or two close simple caustics) between points A and B if

$$\mathrm{tr}(\mathbf{K}_{\mathrm{A}}\mathbf{Q}_{\mathrm{B}})\,\det(\mathbf{Q}_{\mathrm{A}}) < 0 \quad . \tag{B.5}$$

If $\mathbf{Q}_{\mathrm{A}} = \mathbf{0}$ or $\mathbf{Q}_{\mathrm{B}} = \mathbf{0}$, there is a point caustic at point A or B, respectively.

Otherwise, if $\det(\mathbf{Q}_{\mathrm{A}}) = 0$ or $\det(\mathbf{Q}_{\mathrm{B}}) = 0$, there is a simple caustic at point A or B, respectively. If $\det(\mathbf{Q}_{\mathrm{A}}) = 0$ and $\det(\mathbf{Q}_{\mathrm{B}}) \neq 0$, there is an additional simple caustic between points A and B if

$$\mathrm{tr}(\mathbf{K}_{\mathrm{A}}\mathbf{Q}_{\mathrm{B}})\,\det(\mathbf{Q}_{\mathrm{B}}) < 0 \quad . \tag{B.6}$$

If $\det(\mathbf{Q}_{\mathrm{A}}) \neq 0$ and $\det(\mathbf{Q}_{\mathrm{B}}) = 0$, there is an additional simple caustic between points A and B if

$$\mathrm{tr}(\mathbf{K}_{\mathrm{A}}\mathbf{Q}_{\mathrm{B}})\,\det(\mathbf{Q}_{\mathrm{A}}) < 0 \quad . \tag{B.7}$$

In the case (35) of hyperbolic slowness surface, condition (B.5) is not correct, but it does not affect the final value of the KMAH index because the increment of the KMAH index is zero. A caustic occurring under conditions (35) and (B.4) means that both the slowness surface and the wavefront are hyperbolic, which may happen only in the anisotropic medium.

Note that the correct version of condition (B.5) for two intersecting smooth parts of the zero isosurface of D is

$$\mathrm{tr}(\mathbf{K}_\mathrm{A}\mathbf{Q}_\mathrm{B})\ \mathrm{sgn}[\det(\mathbf{Q}_\mathrm{A})] \leq -2\sqrt{\det(\mathbf{Q}_\mathrm{A})\det(\mathbf{Q}_\mathrm{B})}\ \ , \tag{B.8}$$

but this condition is only approximate. In deriving condition (B.8), we approximated the matrix of geometrical spreading between points A and B by linear interpolation and studied analytically its determinant. The equal sign in condition (B.8) corresponds to a point caustic at the intersection of two smooth parts of the zero isosurface of D. In cases close to the equality in condition (B.8), we may miss a point caustic (or two close simple caustics) or we may consider no caustic to be a point caustic (or two close simple caustics).

If (B.4) and the slowness surface is not hyperbolic, $\det(\mathbf{Q}'_\mathrm{R}\mathbf{P}_\mathrm{R}^{-1}) \geq 0$, see conditions (33) and (34), then approximately

$$|\mathrm{tr}(\mathbf{K}_\mathrm{A}\mathbf{Q}_\mathrm{B})| \geq 2\sqrt{\det(\mathbf{Q}_\mathrm{A})\det(\mathbf{Q}_\mathrm{B})}\ \ , \tag{B.9}$$

because matrix $\mathbf{P}_\mathrm{R}\mathbf{Q}_\mathrm{R}^{-1}$ is symmetric and matrix $\mathbf{Q}'_\mathrm{R}\mathbf{P}_\mathrm{R}^{-1}$ is approximately symmetric in the vicinity of a point caustic. Here $\mathbf{Q}_\mathrm{R}$ and $\mathbf{P}_\mathrm{R}$ may coincide with submatrices $\mathbf{Q}_2$ and $\mathbf{P}_2$ of paraxial–ray propagator matrix (1) in ray–centred coordinates. In case of $\det(\mathbf{Q}'_\mathrm{R}\mathbf{P}_\mathrm{R}^{-1}) \geq 0$, the approximations and numerical errors should not affect the sign of the left–hand side of condition (B.5), and condition (B.5) reliably detects a point caustic (or two close simple caustics), whereas application of approximate condition (B.8) would be hazardous.

Using condition (B.5) instead of condition (B.8) thus results in false indication of a point caustic (or two close simple caustics) with no phase shift at regions where there is no caustic, but condition (B.5) is superior with respect to the correct phase shift.

If a short segment of a ray crosses a small local return fold of the zero isosurface of D, having both its endpoints A and B situated outside the fold, the corresponding two simple caustics are missed by our caustic identification algorithm, but this does not affect the correct phase shift.

Let us denote by $\widehat{\mathbf{Q}}_\mathrm{A}$ and $\widehat{\mathbf{Q}}_\mathrm{B}$ the 3×3 matrices in Cartesian coordinates, analogous to the 2×2 matrices $\mathbf{Q}_\mathrm{A}$ and $\mathbf{Q}_\mathrm{B}$ in ray–centred coordinates. Let us denote by $\widehat{\mathbf{h}}_\mathrm{A}$ and $\widehat{\mathbf{h}}_\mathrm{B}$ the 3×3 transformation matrices from ray–centred coordinates q_1, q_2, q_3 to Cartesian coordinates. Lets us also denote by γ_3 the ray coordinate along the ray, and by q_3 the ray–centred coordinate along the ray. The matrices in Cartesian and ray–centred coordinates are related by equation

$$\widehat{\mathbf{Q}}_\mathrm{A} = \widehat{\mathbf{h}}_\mathrm{A} \begin{pmatrix} \multicolumn{2}{c}{\mathbf{Q}} & 0 \\ & & 0 \\ \frac{\mathrm{d}q_3}{\mathrm{d}\gamma_1} & \frac{\mathrm{d}q_3}{\mathrm{d}\gamma_2} & \frac{\mathrm{d}q_3}{\mathrm{d}\gamma_3} \end{pmatrix}_\mathrm{A}\ \ , \tag{B.10}$$

and by the analogous equation for $\widehat{\mathbf{Q}}_\mathrm{B}$. Then

$$\det(\widehat{\mathbf{Q}}_\mathrm{A}) = \det(\mathbf{Q}_\mathrm{A})\det(\widehat{\mathbf{h}}_\mathrm{A})\left.\frac{\mathrm{d}q_3}{\mathrm{d}\gamma_3}\right|_\mathrm{A} \tag{B.11}$$

and analogously for $\det(\widehat{\mathbf{Q}}_\mathrm{B})$. The 3×3 analogue of $\mathbf{K}_\mathrm{A}$ is

$$\widehat{\mathbf{K}}_\mathrm{A} = \widehat{\mathbf{Q}}_\mathrm{A}^{-1} \det(\widehat{\mathbf{Q}}_\mathrm{A}) \quad , \tag{B.12}$$

and similarly for $\mathbf{K}_\mathrm{B}$. Denote by $\mathrm{sub}(\widehat{\mathbf{K}}_\mathrm{A}\widehat{\mathbf{Q}}_\mathrm{B})$ the upper left 2×2 submatrix of 3×3 matrix $\widehat{\mathbf{K}}_\mathrm{A}\widehat{\mathbf{Q}}_\mathrm{B}$ (not of $\widehat{\mathbf{Q}}_\mathrm{B}\widehat{\mathbf{K}}_\mathrm{A}$). Then

$$\mathrm{tr}[\mathrm{sub}(\widehat{\mathbf{K}}_\mathrm{A}\widehat{\mathbf{Q}}_\mathrm{B})] \approx \mathrm{tr}(\mathbf{K}_\mathrm{A}\mathbf{Q}_\mathrm{B}) \det(\widehat{\mathbf{h}}_\mathrm{A}) \left.\frac{\mathrm{d}q_3}{\mathrm{d}\gamma_3}\right|_\mathrm{A} \quad . \tag{B.13}$$

Approximation

$$\widehat{\mathbf{h}}_\mathrm{A} \approx \widehat{\mathbf{h}}_\mathrm{B} \tag{B.14}$$

is used in deriving approximation (B.13).

The caustic identification algorithm expressed in terms of the 2×2 paraxial–ray matrices calculated by dynamic ray tracing in ray–centred coordinates may thus be converted by substitutions

$$\det(\mathbf{Q}_\mathrm{A}) \quad \longrightarrow \quad \det(\widehat{\mathbf{Q}}_\mathrm{A}) \quad , \tag{B.15}$$

$$\det(\mathbf{Q}_\mathrm{B}) \quad \longrightarrow \quad \det(\widehat{\mathbf{Q}}_\mathrm{B}) \quad , \tag{B.16}$$

$$\mathrm{tr}(\mathbf{K}_\mathrm{A}\mathbf{Q}_\mathrm{B}) \quad \longrightarrow \quad \mathrm{tr}[\mathrm{sub}(\widehat{\mathbf{K}}_\mathrm{A}\widehat{\mathbf{Q}}_\mathrm{B})] \quad , \tag{B.17}$$

$$\mathbf{Q}_\mathrm{A} = \mathbf{0} \quad \longrightarrow \quad \widehat{\mathbf{K}}_\mathrm{A} = \widehat{\mathbf{0}} \quad , \tag{B.18}$$

$$\mathbf{Q}_\mathrm{B} = \mathbf{0} \quad \longrightarrow \quad \widehat{\mathbf{K}}_\mathrm{B} = \widehat{\mathbf{0}} \tag{B.19}$$

to the caustic identification algorithm expressed in terms of the 3×3 paraxial–ray matrices calculated by dynamic ray tracing in Cartesian coordinates.

APPENDIX C
SYMPLECTICITY

The symplectic property of the paraxial–ray propagator matrix (1) may be expressed in the form of

$$\begin{pmatrix} \mathbf{Q}_1^\mathrm{T} & \mathbf{P}_1^\mathrm{T} \\ \mathbf{Q}_2^\mathrm{T} & \mathbf{P}_2^\mathrm{T} \end{pmatrix} \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ -\mathbf{1} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{Q}_1 & \mathbf{Q}_2 \\ \mathbf{P}_1 & \mathbf{P}_2 \end{pmatrix} = \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ -\mathbf{1} & \mathbf{0} \end{pmatrix} \quad , \tag{C.1}$$

or of

$$\begin{pmatrix} \mathbf{Q}_1 & \mathbf{Q}_2 \\ \mathbf{P}_1 & \mathbf{P}_2 \end{pmatrix} \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ -\mathbf{1} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{Q}_1^\mathrm{T} & \mathbf{P}_1^\mathrm{T} \\ \mathbf{Q}_2^\mathrm{T} & \mathbf{P}_2^\mathrm{T} \end{pmatrix} = \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ -\mathbf{1} & \mathbf{0} \end{pmatrix} \quad . \tag{C.2}$$

It implies, inter alia, the symmetry of matrices $\mathbf{Q}_1\mathbf{Q}_2^\mathrm{T}$ and $\mathbf{Q}_2^\mathrm{T}\mathbf{P}_2$, and consequently of matrices $\mathbf{K}\mathbf{Q}_1$ and $\mathbf{P}_2\mathbf{K}$, and the identity

$$\mathbf{P}_2^\mathrm{T}\mathbf{Q}_1 - \mathbf{Q}_2^\mathrm{T}\mathbf{P}_1 = \mathbf{1} \quad . \tag{C.3}$$

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