# Phase shift of a general wavefield due to caustics in anisotropic media

**Luděk Klimeš**

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

**Summary**

Equations are presented to determine the phase shift of the amplitude of an elastic wavefield due to both simple (line) and point caustics in heterogeneous anisotropic media. The phase–shift rules for a general ray–theory wavefield are expressed in terms of the paraxial matrices calculated by the Hamiltonian equations of geodesic deviation (paraxial ray equations, dynamic ray tracing equations). The phase–shift rules are derived both for 2×2 paraxial matrices in ray–centred coordinates and for 3×3 paraxial matrices in general coordinates.

**Keywords**

Anisotropy, heterogeneity, elastic wavefield, ray theory, caustics, KMAH index, paraxial rays.

## 1. Introduction

Hamilton's equations (equations of rays, ray tracing equations, equations of geodesics) and the Hamiltonian equations of geodesic deviation (paraxial ray equations, dynamic ray tracing equations) are required to calculate anisotropic ray theory approximations of elastic wavefields. The equations should also be supplemented with rules determining how a ray should be continued through singularities in Hamilton's equations of rays, 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. In layered and block models, equations for the reflection/transmission coefficients and for the transformation of the geodesic deviation at structural interfaces are also required. For the reflection/transmission coefficients refer, e.g., to Fedorov (1968).

The Hamiltonian equations of geodesic deviation (paraxial ray equations, dynamic ray tracing equations) in Cartesian coordinates, supplementing Hamilton's equations (equations of rays, ray tracing equations, equations of geodesics) in anisotropic media (Babich, 1961), were derived by Červený (1972). For the transformation of the geodesic deviation at curved interfaces between anisotropic materials refer, e.g., to Farra & Le Bégat (1995, eq. A12) and Klimeš (2010b, eqs. 56–57, 78–80).

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.

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The rules for the phase shift of the Green tensor due to caustics in heterogeneous generally anisotropic elastic media were described by Klimeš (2010a). In this paper, we modify the rules to the phase shift of a wavefield with general initial conditions.

The ray–theory wavefield is the limiting case of a Gaussian beam infinitely broad outside caustics (Červený, 2001). The phase shift of a Gaussian beam is included in 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 wavefield 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 $\omega$. 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, Klimeš, & Pšenčík, 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 Kravtsov & Orlov (1993; 1999). Garmany (2000) 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 hereinafter. Note that the criticism of Bakker's approach by Hanyga & Slawinski (2000), based on a different choice of the coordinates for the Hamiltonian equations of geodesic deviation, 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, Klimeš, & Pšenčík, 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 matrices calculated by the Hamiltonian equations of geodesic deviation in ray–centred coordinates and is briefly recalled in Appendix B. It may be converted into the algorithm expressed in terms of the 3×3 paraxial 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 a general ray–theory wavefield due to caustics in anisotropic media. The phase–shift rules are expressed in terms of the paraxial matrices calculated by the Hamiltonian equations of geodesic deviation, similarly as the caustic identification algorithm by Červený, Klimeš, & Pšenčík (1988, sec. 5.8.3f). The phase–shift rules are derived both for 2×2 paraxial matrices in ray–centred coordinates and for 3×3 paraxial matrices in general coordinates.

In 3–D space, the orthonomic system of rays corresponding to the given initial conditions consists of a two–parametric system of rays which are parametrized by two *ray parameters* $\gamma^1$ and $\gamma^2$. The ray parameters together with the increasing monotonic independent parameter $\gamma^3$ along the rays form *ray coordinates* $\gamma^1$, $\gamma^2$, $\gamma^3$.

The Einstein summation over repetitive lower–case Roman indices, corresponding to the 3 spatial coordinates, is used throughout the paper. Upper–case Roman indices correspond to the first two ray–centred coordinates or to two ray parameters.

## 2. Simple (line) caustic

Assume a simple (line, non–singular, first–order) caustic formed by a general orthonomic system of rays. 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 2×2 paraxial matrices in ray–centred coordinates in Section 2.1. We then propose conversion of the phase–shift rule into 3×3 paraxial matrices in general coordinates in Section 2.2.

### 2.1. Matrices 2×2 in ray–centred coordinates

Gradient

$$p_i = \frac{\partial \tau}{\partial x^i} \tag{1}$$

of travel time is referred to as the *slowness vector*.

Along a particular ray, we may define *ray–centred coordinates* $q^a$ (Klimeš, 2006). We parametrize the points along the ray by an arbitrary monotonic variable $q^3$. At each point $x^i(q^3)$ of the ray, we choose two contravariant basis vectors $h^i_1(q^3)$ and $h^i_2(q^3)$ perpendicular to slowness vector $p_i$,

$$h^i_A(q^3)\, p_i(q^3) = 0 \quad . \tag{2}$$

Contravariant basis vectors $h^i_A$ should vary smoothly along the ray. The transformation from the *ray–centred coordinates* $q^a$ to Cartesian coordinates $x^i$ is defined by relation

$$x^i = x^i(q^3) + h^i_A(q^3)\, q^A \quad . \tag{3}$$

We may then define slowness vector

$$p^{(q)}_i = \frac{\partial \tau}{\partial q^i} \tag{4}$$

in ray–centred coordinates.

There are many points on each ray at which the matrix of geometrical spreading is regular. We thus select one of these points and denote it by $\mathbf{x}_0$.

We consider the propagator matrix

$$\begin{pmatrix} \mathbf{Q}_1 & \mathbf{Q}_2 \\ \mathbf{P}_1 & \mathbf{P}_2 \end{pmatrix} = \begin{pmatrix} \frac{\partial q^I}{\partial q_0^J} & \frac{\partial q^I}{\partial p_{J0}^{(q)}} \\ \frac{\partial p_I^{(q)}}{\partial q_0^J} & \frac{\partial p_I^{(q)}}{\partial p_{J0}^{(q)}} \end{pmatrix} \tag{5}$$

of geodesic deviation (paraxial–ray propagator matrix) from "regular" point $\mathbf{x}_0$ to a caustic. Here $q_0^j$ are the ray–centred coordinates of the initial point $\mathbf{x}_0$ of the ray, and $p_{j0}^{(q)}$ is the initial slowness vector in ray–centred coordinates.

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

We define 2×2 paraxial matrices $\mathbf{Q}_\mathrm{R}$ and $\mathbf{P}_\mathrm{R}$ with elements

$$(Q_\mathrm{R})^I_A = \frac{\partial q^I}{\partial \gamma^A} \tag{6}$$

and

$$(P_\mathrm{R})_{IA} = \frac{\partial p_I^{(q)}}{\partial \gamma^A} \tag{7}$$

in ray–centred coordinates. Matrix $\mathbf{Q}_\mathrm{R}$ represents the matrix of geometrical spreading of the orthonomic system of rays. Matrix $\mathbf{P}_\mathrm{R}$ represents the transformation matrix from ray parameters to the slowness vector.

We denote by $\mathbf{Q}_0$ the matrix of geometrical spreading of the orthonomic system of rays at point $\mathbf{x}_0$. We also denote by $\mathbf{P}_0$ the transformation matrix from ray parameters to the slowness vector at point $\mathbf{x}_0$. The orthonomic system of rays at a caustic is then described by the 2×2 paraxial matrices

$$\mathbf{Q}_\mathrm{R} = \mathbf{Q}_1\mathbf{Q}_0 + \mathbf{Q}_2\mathbf{P}_0 \tag{8}$$

and

$$\mathbf{P}_\mathrm{R} = \mathbf{P}_1\mathbf{Q}_0 + \mathbf{P}_2\mathbf{P}_0 \quad . \tag{9}$$

The ray–theory wavefield is the limiting case of the Gaussian beam infinitely broad at point $\mathbf{x}_0$ (Červený, 2001). The real part of the matrix of the second travel–time derivatives of the Gaussian beam at point $\mathbf{x}_0$ is taken to correspond to the ray–theory wavefield, 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 matrix $\mathbf{Y}_0$ limiting to the zero matrix.

The matrix of geometrical spreading of the Gaussian beam is

$$\mathbf{Q} = \mathbf{Q}_1\mathbf{Q}_0 + \mathbf{Q}_2(\mathbf{P}_0 + \mathrm{i}\mathbf{Y}_0\mathbf{Q}_0) = \mathbf{Q}_\mathrm{R} + \mathrm{i}\mathbf{Q}_2\mathbf{Y}_0\mathbf{Q}_0 \quad . \tag{10}$$

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 $\exp(-\mathrm{i}\frac{\pi}{2}\mathrm{KMAH})$ of the anisotropic ray theory.

At the simple caustic, matrix $\mathbf{Q}_\mathrm{R}$ has just one zero eigenvalue. In the vicinity of the caustic we may approximate $\mathbf{Q}$ by the linear Taylor expansion with respect to the increasing monotonic parameter $\gamma^3$ along the ray. For very small $\mathbf{Y}_0$ and $\Delta\gamma^3$ we approximate (10) by linear expansion

$$\mathbf{Q}(\Delta\gamma^3) \approx \mathbf{Q}_\mathrm{R} + \mathrm{i}\mathbf{Q}_2\mathbf{Y}_0\mathbf{Q}_0 + \mathbf{Q}'_\mathrm{R}\Delta\gamma^3 \tag{11}$$

centred at the caustic where $\Delta\gamma^3 = 0$. Here

$$\mathbf{Q}'_R = \frac{\mathrm{d}\mathbf{Q}_R}{\mathrm{d}\gamma^3} \quad . \tag{12}$$

To proceed from the approximation (11) 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

$$\partial(\det\mathbf{Q}) = \mathrm{tr}(\mathbf{Q}^{-1}\partial\mathbf{Q})\ \det\mathbf{Q} \quad , \tag{13}$$

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

$$\mathbf{K} = \mathbf{Q}_\mathrm{R}^{-1}\det\mathbf{Q}_\mathrm{R} \tag{14}$$

of rank 1 composed of the subdeterminants of $\mathbf{Q}_\mathrm{R}$, and considering identity (13), the determinant of (11) may be approximated by expression

$$\det\mathbf{Q}(\Delta\gamma^3) \approx \mathrm{tr}(\mathbf{K}\mathbf{Q}'_\mathrm{R})\Delta\gamma^3 + \mathrm{i}\ \mathrm{tr}(\mathbf{K}\mathbf{Q}_2\mathbf{Y}_0\mathbf{Q}_0) \quad , \tag{15}$$

linear in $\mathbf{Y}_0$ and $\Delta\gamma^3$. Note that the range of matrix $\mathbf{K}$ coincides with the null space of matrix $\mathbf{Q}_\mathrm{R}$ and vice versa. Matrix $\mathbf{K}$ is always finite, and it is very easy to calculate it numerically from matrix $\mathbf{Q}_\mathrm{R}$. For $2{\times}2$ matrix $\mathbf{Q}_\mathrm{R}$,

$$\mathbf{Q}_\mathrm{R} = \begin{pmatrix} Q_{\mathrm{R}11} & Q_{\mathrm{R}12} \\ Q_{\mathrm{R}21} & Q_{\mathrm{R}22} \end{pmatrix} \quad , \tag{16}$$

we have

$$\mathbf{K} = \begin{pmatrix} Q_{\mathrm{R}22} & -Q_{\mathrm{R}12} \\ -Q_{\mathrm{R}21} & Q_{\mathrm{R}11} \end{pmatrix} \quad . \tag{17}$$

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

$$\mathbf{K} = \mathbf{a}\ \mathbf{b}^\mathrm{T} \tag{18}$$

of vectors $\mathbf{a}$ and $\mathbf{b}$. Vector $\mathbf{a}$ specifies the singular direction in the ray–parameter domain due to the caustic, $\mathbf{Q}_\mathrm{R}\,\mathbf{a} = \mathbf{0}$, 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

$$\widetilde{K}_1 = -\mathrm{tr}(\mathbf{K}\mathbf{Q}_2\mathbf{Y}_0\mathbf{Q}_0) \quad , \tag{19}$$

$$K_2 = \mathrm{tr}(\mathbf{K}\mathbf{Q}'_\mathrm{R}) \tag{20}$$

have equal signs, the determinant (15) passes for increasing $\Delta\gamma^3$ the origin of the complex plane counterclockwise, and the increment of the KMAH index is +1. Otherwise, the increment of the KMAH index is −1.

Inserting equation (C4) of Appendix C for $\mathbf{Q}_0$ into (19) and considering that $\mathrm{tr}(\mathbf{K}\mathbf{Q}_2\mathbf{Y}_0\mathbf{P}_2^\mathrm{T}\mathbf{Q}_\mathrm{R}) = 0$, we obtain

$$\widetilde{K}_1 = \mathrm{tr}(\mathbf{K}\mathbf{Q}_2\mathbf{Y}_0\mathbf{Q}_2^\mathrm{T}\mathbf{P}_\mathrm{R}) \quad . \tag{21}$$

Since both $\mathbf{P}_{\mathrm{R}}\mathbf{K}$ and $\mathbf{Q}_2^{\mathrm{T}}\mathbf{P}_{\mathrm{R}}\mathbf{K}\mathbf{Q}_2$ are symmetrical matrices of rank 1, and $\mathbf{Y}_0$ is a positive–definite matrix, the sign of $\widetilde{K}_1$ is the same as the sign of

$$K_1 = \mathrm{tr}(\mathbf{K}\mathbf{P}_{\mathrm{R}}) \quad . \tag{22}$$

Since matrix $\mathbf{P}_{\mathrm{R}}$ describes the sensitivity of the slowness vector to the ray parameters, quantity $K_1 = \mathbf{b}^{\mathrm{T}}\mathbf{P}_{\mathrm{R}}\,\mathbf{a}$ 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 $\mathbf{Q}'_{\mathrm{R}}$ describes the sensitivity of the ray–velocity vector to the ray parameters, quantity $K_2 = \mathbf{b}^{\mathrm{T}}\mathbf{Q}'_{\mathrm{R}}\,\mathbf{a}$ 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 $\mathbf{P}_{\mathrm{R}}\,\mathbf{a}$ 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 the Hamiltonian equations of geodesic deviation.

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

$$\mathrm{sgn}(K_2/K_1) \quad , \tag{23}$$

where $K_1$ and $K_2$ are given by equations (22) and (20) with $\mathbf{K}$ defined by (14).

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,

$$K_2 = 0 \quad , \tag{24}$$

the phase shift depends on the higher–order derivatives of matrix $\mathbf{Q}$ along the ray, see equation (A4) in Appendix A.

Note that (a) $K_2$ always has the sign of $\det\mathbf{Q}_{\mathrm{R}}$ beyond the caustic, which follows from equation (15) with $\mathbf{Y}_0 = \mathbf{0}$; (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 (20), (22), and the Hamiltonian equations of geodesic deviation 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 $\mathbf{P}_{\mathrm{R}}\,\mathbf{a}$, which follows from (18), (20), (22), and the Hamiltonian equations of geodesic deviation in ray–centred coordinates.

## 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.

We consider paraxial rays with initial coordinates $x_0^j$ and initial slowness vector $p_{j0}$. The 6×6 propagator matrix

$$\begin{pmatrix} \widehat{\mathbf{Q}}_1 & \widehat{\mathbf{Q}}_2 \\ \widehat{\mathbf{P}}_1 & \widehat{\mathbf{P}}_2 \end{pmatrix} = \begin{pmatrix} \frac{\partial x^i}{\partial x_0^j} & \frac{\partial x^i}{\partial p_{j0}} \\ \frac{\partial p_i}{\partial x_0^j} & \frac{\partial p_i}{\partial p_{j0}} \end{pmatrix} \tag{25}$$

of geodesic deviation in general coordinates depends on the kind of parameter $\gamma^3$ along the ray.

We define 3×3 paraxial matrices $\widehat{\mathbf{Q}}_\mathrm{R}$ and $\widehat{\mathbf{P}}_\mathrm{R}$ with elements

$$(\widehat{Q}_\mathrm{R})^i_a = \frac{\partial x^i}{\partial \gamma^a} \tag{26}$$

and

$$(\widehat{P}_\mathrm{R})_{ia} = \frac{\partial p_i}{\partial \gamma^a} \quad . \tag{27}$$

We denote the initial values of 3×3 paraxial matrices $\widehat{\mathbf{Q}}_\mathrm{R}$ and $\widehat{\mathbf{P}}_\mathrm{R}$ as $\widehat{\mathbf{Q}}_0$ and $\widehat{\mathbf{P}}_0$. The orthonomic system of rays at a caustic is then described by 3×3 paraxial matrices

$$\widehat{\mathbf{Q}}_\mathrm{R} = \widehat{\mathbf{Q}}_1\widehat{\mathbf{Q}}_0 + \widehat{\mathbf{Q}}_2\widehat{\mathbf{P}}_0 \tag{28}$$

and

$$\widehat{\mathbf{P}}_\mathrm{R} = \widehat{\mathbf{P}}_1\widehat{\mathbf{Q}}_0 + \widehat{\mathbf{P}}_2\widehat{\mathbf{P}}_0 \quad . \tag{29}$$

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, 3×3 matrix $\widehat{\mathbf{Q}}_\mathrm{R}$ has just one zero eigenvalue, analogously to 2×2 matrix $\mathbf{Q}_\mathrm{R}$ (Klimeš, 1994, eqs. 59, 64, 65). The corresponding left and right null eigenvectors of matrices $\mathbf{Q}_\mathrm{R}$ and $\widehat{\mathbf{Q}}_\mathrm{R}$ differ just by the coordinate transform between the ray–centred and general coordinates at the caustic point and at the point source, respectively.

Matrix

$$\widehat{\mathbf{K}} = \widehat{\mathbf{Q}}_\mathrm{R}^{-1}\,\det\widehat{\mathbf{Q}}_\mathrm{R} \tag{30}$$

of rank 1, analogous to matrix (14), composed of the subdeterminants of $\widehat{\mathbf{Q}}_\mathrm{R}$, can again be expressed as the dyadic product

$$\widehat{\mathbf{K}} = \widehat{\mathbf{a}}\,\widehat{\mathbf{b}}^\mathrm{T} \tag{31}$$

of vectors $\widehat{\mathbf{a}}$ and $\widehat{\mathbf{b}}$, see (18). 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 (23) thus also holds if we replace matrices $\mathbf{K}$, $\mathbf{Q}'_\mathrm{R}$ and $\mathbf{P}_\mathrm{R}$ in (20) and (22) by matrices $\widehat{\mathbf{K}}$, $\widehat{\mathbf{Q}}'_\mathrm{R}$ and $\widehat{\mathbf{P}}_\mathrm{R}$,

$$K_2 = \mathrm{tr}(\widehat{\mathbf{K}}\widehat{\mathbf{Q}}'_\mathrm{R}) \quad , \tag{32}$$

$$K_1 = \mathrm{tr}(\widehat{\mathbf{K}}\widehat{\mathbf{P}}_\mathrm{R}) \quad . \tag{33}$$

Equations (32) and (33) yield the same $K_1$ and $K_2$ as equations (20) and (22).

## 3. Point caustic

Assume a point (focus, second–order) caustic at an orthonomic system of rays. At the caustic, 2×2 matrix (8) in ray–centred coordinates becomes a zero matrix, and 3×3 matrix (28) 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 (11) may be approximated by

$$\det\mathbf{Q}(\Delta\gamma^3) \approx \det(-\mathrm{i}\mathbf{B} + \mathbf{Q}'_{\mathrm{R}}\mathbf{P}_{\mathrm{R}}^{-1}\Delta\gamma^3)\ \det(\mathbf{P}_{\mathrm{R}}) \quad , \tag{34}$$

where

$$\mathbf{B} = -\mathbf{Q}_2\mathbf{Y}_0\mathbf{Q}_0\mathbf{P}_{\mathrm{R}}^{-1} \quad . \tag{35}$$

Since

$$\mathbf{B} = \mathbf{Q}_2\mathbf{Y}_0\mathbf{Q}_2^{\mathrm{T}} \quad , \tag{36}$$

see equation (C4) 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 $\mathbf{Q}'_{\mathrm{R}}\mathbf{P}_{\mathrm{R}}^{-1}$.

*Phase–shift rule for a point caustic:*

If

$$\det(\mathbf{Q}'_{\mathrm{R}}\mathbf{P}_{\mathrm{R}}^{-1}) > 0 \quad , \qquad \mathrm{tr}(\mathbf{Q}'_{\mathrm{R}}\mathbf{P}_{\mathrm{R}}^{-1}) > 0 \quad , \tag{37}$$

both the eigenvalues of matrix $-\mathrm{i}\mathbf{B} + \mathbf{Q}'_{\mathrm{R}}\mathbf{P}_{\mathrm{R}}^{-1}\Delta\gamma^3$ pass, for increasing $\Delta\gamma^3$, the origin of the complex plane counterclockwise, and the increment of the KMAH index is +2.

If

$$\det(\mathbf{Q}'_{\mathrm{R}}\mathbf{P}_{\mathrm{R}}^{-1}) > 0 \quad , \qquad \mathrm{tr}(\mathbf{Q}'_{\mathrm{R}}\mathbf{P}_{\mathrm{R}}^{-1}) < 0 \quad , \tag{38}$$

both the eigenvalues of matrix $-\mathrm{i}\mathbf{B} + \mathbf{Q}'_{\mathrm{R}}\mathbf{P}_{\mathrm{R}}^{-1}\Delta\gamma^3$ pass, for increasing $\Delta\gamma^3$, the origin of the complex plane clockwise, and the increment of the KMAH index is −2.

If

$$\det(\mathbf{Q}'_{\mathrm{R}}\mathbf{P}_{\mathrm{R}}^{-1}) < 0 \quad , \tag{39}$$

one eigenvalue of matrix $-\mathrm{i}\mathbf{B} + \mathbf{Q}'_{\mathrm{R}}\mathbf{P}_{\mathrm{R}}^{-1}\Delta\gamma^3$ 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),

$$\det(\mathbf{Q}'_{\mathrm{R}}\mathbf{P}_{\mathrm{R}}^{-1}) = 0 \quad , \tag{40}$$

is not considered in this paper.

Note that, at a point caustic, the 2×2 matrix $\mathbf{Q}'_{\mathrm{R}}\mathbf{P}_{\mathrm{R}}^{-1}$ represents the second derivatives of the Hamiltonian along the plane tangent to the slowness surface. At a point caustic, the 2×2 matrix $\mathbf{Q}'_{\mathrm{R}}\mathbf{P}_{\mathrm{R}}^{-1}$ is identical to Bakker's (1998) matrix $\mathbf{S}_{12}$ if the same coordinates and the same Hamiltonian are considered for the Hamiltonian equations of geodesic deviation. 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 $\mathbf{Q}'_{\mathrm{R}}$ is known, matrix $\mathbf{Q}'_{\mathrm{R}}\mathbf{P}_{\mathrm{R}}^{-1}$ in conditions (37) to (40) may also be replaced by matrix $\mathbf{P}_{\mathrm{R}}^{\mathrm{T}}\mathbf{Q}'_{\mathrm{R}}$,

$$\mathbf{Q}'_{\mathrm{R}}\mathbf{P}_{\mathrm{R}}^{-1} \quad \longrightarrow \quad \mathbf{P}_{\mathrm{R}}^{\mathrm{T}}\mathbf{Q}'_{\mathrm{R}} \quad . \tag{41}$$

### 3.2. Matrices 3×3 in general coordinates

We consider here the 3×3 paraxial matrices $\widehat{\mathbf{Q}}_{\mathrm{R}}$ and $\widehat{\mathbf{P}}_{\mathrm{R}}$ given by (28) and (29), which describe the orthonomic system of rays. The propagator matrix (25) of geodesic deviation depends on the kind of parameter $\gamma^3$ 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)

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

where $\mathrm{sub}(\widehat{\mathbf{A}})$ stands for the upper left 2×2 submatrix of 3×3 matrix $\widehat{\mathbf{A}}$.

Conditions (37) to (40) may thus be converted by substitution

$$\mathbf{Q}'_{\mathrm{R}}\mathbf{P}_{\mathrm{R}}^{-1} \quad \longrightarrow \quad \mathrm{sub}(\widehat{\mathbf{P}}_{\mathrm{R}}^{\mathrm{T}}\widehat{\mathbf{Q}}'_{\mathrm{R}}) \quad . \tag{43}$$

Other conversions of conditions (37) to (40) may be derived using transformation equations by Klimeš (1994; 2002).

## 4. Conclusions

The phase–shift rule for a general ray–theory wavefield at a simple (line) caustic is given by equation (23), with equations (20) and (22) for 2×2 paraxial matrices in ray–centred coordinates, or with equations (32) and (33) for 3×3 paraxial matrices in general coordinates. The phase–shift rules for a general ray–theory wavefield at a point caustic, expressed in terms of 2×2 paraxial matrices in ray–centred coordinates, are given by equations (37), (38) and (39). These phase–shift rules for a general ray–theory wavefield at a point caustic can be expressed in terms of 3×3 paraxial matrices in general coordinates using substitution (43).

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 $\gamma^1$, $\gamma^2$, $\gamma^3$ may be decomposed into subdomains of equal sign of function

$$D = \det(\mathbf{Q}_\mathrm{R}) \quad , \tag{A1}$$

separated by the zero isosurface of function $D = D(\gamma^k)$, determined by equation (Kravtsov & Orlov, 1993, eq. 2.3.2)

$$D = 0 \quad . \tag{A2}$$

Matrix $\mathbf{Q}_\mathrm{R}$ in (A1) represents the 2×2 matrix of geometrical spreading in ray–centred coordinates, see (8).

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 $\gamma^K$ =*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

$$D' = \mathrm{tr}(\mathbf{Q}'_\mathrm{R}\mathbf{Q}_\mathrm{R}^{-1})\det(\mathbf{Q}_\mathrm{R}) = \mathrm{tr}(\mathbf{K}\mathbf{Q}'_\mathrm{R}) = K_2 \quad . \tag{A3}$$

For the given sign of $K_1$, the phase shift depends on the third component (A3) of the gradient of $D$, see (23). 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, (A3) has opposite signs at the bottom and at the top of the fold. If a ray–coordinate line $\gamma^K$ =*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 $\gamma^3$ 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 (39).

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 $\gamma^3$ is of the odd order. The corresponding increment of the KMAH index is

$$\mathrm{sgn}(D^{(n)}/K_1) \quad , \tag{A4}$$

where $K_1$ is given by equation (22). This should be the case if a simple caustic is identified. If the first derivative $D'$ of $D$ with respect to $\gamma^3$ is non–zero at a simple caustic, (A4) is identical to (23). If equality (24) holds at a simple caustic, the first non–zero derivative $D^{(n)}$ of $D$ with respect to $\gamma^3$ should be of the odd order. Equality (24) implies that the slowness surface at the simple caustic is hyperbolic or, by coincidence, parabolic.

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

## Appendix B: Caustic identification algorithm

We first repeat the caustic identification algorithm by Červený, Klimeš, & Pšenčík (1988, sec. 5.8.3f) and Červený (2001, sec. 4.12.1), expressed in terms of the 2×2 paraxial matrices calculated by the Hamiltonian equations of geodesic deviation 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 matrices calculated by the Hamiltonian equations of geodesic deviation in Cartesian coordinates.

Let us denote by $\mathbf{Q}_{\rm A}$ and $\mathbf{Q}_{\rm B}$ the values of the 2×2 matrix of geometrical spreading at the endpoints A and B of a sufficiently short segment of a ray. The 2×2 matrix of geometrical spreading in ray–centred coordinates is given by (8). We also define the 2×2 matrix

$$\mathbf{K}_{\rm A} = \mathbf{Q}_{\rm A}^{-1} \det(\mathbf{Q}_{\rm A}) \quad , \tag{B1}$$

see (17). Quantity

$$\mathrm{tr}(\mathbf{K}_{\rm A}\mathbf{Q}_{\rm B}) = Q_{\rm A11}Q_{\rm B22} + Q_{\rm A22}Q_{\rm B11} - Q_{\rm A12}Q_{\rm B21} - Q_{\rm A21}Q_{\rm B12} \tag{B2}$$

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

*Caustic identification algorithm:*

If

$$\det(\mathbf{Q}_{\rm A})\,\det(\mathbf{Q}_{\rm B}) < 0 \quad , \tag{B3}$$

there is a simple caustic between points A and B.

If

$$\det(\mathbf{Q}_{\rm A})\,\det(\mathbf{Q}_{\rm B}) > 0 \quad , \tag{B4}$$

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

$$\mathrm{tr}(\mathbf{K}_{\rm A}\mathbf{Q}_{\rm B})\,\det(\mathbf{Q}_{\rm A}) < 0 \quad . \tag{B5}$$

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

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

$$\mathrm{tr}(\mathbf{K}_{\rm A}\mathbf{Q}_{\rm B})\,\det(\mathbf{Q}_{\rm B}) < 0 \quad . \tag{B6}$$

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

$$\mathrm{tr}(\mathbf{K}_{\rm A}\mathbf{Q}_{\rm B})\,\det(\mathbf{Q}_{\rm A}) < 0 \quad . \tag{B7}$$

In the case (39) of hyperbolic slowness surface, condition (B5) 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 (39) and (B4) 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 (B5) for two intersecting smooth parts of the zero isosurface of $D$ is

$$\mathrm{tr}(\mathbf{K}_\mathrm{A}\mathbf{Q}_\mathrm{B})\ \mathrm{sgn}[\det(\mathbf{Q}_\mathrm{A})] \le -2\sqrt{\det(\mathbf{Q}_\mathrm{A})\det(\mathbf{Q}_\mathrm{B})} \quad , \tag{B8}$$

but this condition is only approximate. In deriving condition (B8), we approximated the matrix of geometrical spreading between points A and B by linear interpolation and studied analytically its determinant. The equal sign in (B8) 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 (B8), 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 (B4) and the slowness surface is not hyperbolic, $\det(\mathbf{Q}'_\mathrm{R}\mathbf{P}_\mathrm{R}^{-1}) \ge 0$, see (37) and (38), then approximately

$$|\mathrm{tr}(\mathbf{K}_\mathrm{A}\mathbf{Q}_\mathrm{B})| \ge 2\sqrt{\det(\mathbf{Q}_\mathrm{A})\det(\mathbf{Q}_\mathrm{B})} \quad , \tag{B9}$$

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 $\mathbf{P}_\mathrm{R}$ represent matrices (8) and (9). In this case $\det(\mathbf{Q}'_\mathrm{R}\mathbf{P}_\mathrm{R}^{-1}) \ge 0$, the approximations and numerical errors should not affect the sign of the left–hand side of (B5), and condition (B5) reliably detects a point caustic (or two close simple caustics), whereas application of approximate condition (B8) would be hazardous.

Using condition (B5) instead of (B8) 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 (B5) 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 $\gamma^3$ 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

$$\widehat{\mathbf{Q}}_\mathrm{A} = \widehat{\mathbf{h}}_\mathrm{A} \begin{pmatrix} \multicolumn{2}{c}{\mathbf{Q}} & \begin{matrix}0\\0\end{matrix} \\ \frac{\mathrm{d}q^3}{\mathrm{d}\gamma^1} & \frac{\mathrm{d}q^3}{\mathrm{d}\gamma^2} & \frac{\mathrm{d}q^3}{\mathrm{d}\gamma^3} \end{pmatrix}_\mathrm{A} \quad , \tag{B10}$$

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

$$\det(\widehat{\mathbf{Q}}_\mathrm{A}) = \det(\mathbf{Q}_\mathrm{A})\det(\widehat{\mathbf{h}}_\mathrm{A})\ \frac{\mathrm{d}q^3}{\mathrm{d}\gamma^3}\bigg|_\mathrm{A} \tag{B11}$$

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

$$\widehat{\mathbf{K}}_\mathrm{A} = \widehat{\mathbf{Q}}_\mathrm{A}^{-1}\det(\widehat{\mathbf{Q}}_\mathrm{A}) \quad , \tag{B12}$$

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

$$\mathrm{tr}[\mathrm{sub}(\widehat{\mathbf{K}}_\mathrm{A}\widehat{\mathbf{Q}}_\mathrm{B})] \approx \mathrm{tr}(\mathbf{K}_\mathrm{A}\mathbf{Q}_\mathrm{B})\,\det(\widehat{\mathbf{h}}_\mathrm{A})\,\left.\frac{\mathrm{d}q^3}{\mathrm{d}\gamma^3}\right|_\mathrm{A} \quad . \tag{B13}$$

Approximation

$$\widehat{\mathbf{h}}_\mathrm{A} \approx \widehat{\mathbf{h}}_\mathrm{B} \tag{B14}$$

is used in deriving (B13).

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

$$\det(\mathbf{Q}_\mathrm{A}) \quad\longrightarrow\quad \det(\widehat{\mathbf{Q}}_\mathrm{A}) \quad , \tag{B15}$$

$$\det(\mathbf{Q}_\mathrm{B}) \quad\longrightarrow\quad \det(\widehat{\mathbf{Q}}_\mathrm{B}) \quad , \tag{B16}$$

$$\mathrm{tr}(\mathbf{K}_\mathrm{A}\mathbf{Q}_\mathrm{B}) \quad\longrightarrow\quad \mathrm{tr}[\mathrm{sub}(\widehat{\mathbf{K}}_\mathrm{A}\widehat{\mathbf{Q}}_\mathrm{B})] \quad , \tag{B17}$$

$$\mathbf{Q}_\mathrm{A} = \mathbf{0} \quad\longrightarrow\quad \widehat{\mathbf{K}}_\mathrm{A} = \widehat{\mathbf{0}} \quad , \tag{B18}$$

$$\mathbf{Q}_\mathrm{B} = \mathbf{0} \quad\longrightarrow\quad \widehat{\mathbf{K}}_\mathrm{B} = \widehat{\mathbf{0}} \tag{B19}$$

to the caustic identification algorithm expressed in terms of the 3×3 paraxial matrices calculated by the Hamiltonian equations of geodesic deviation in Cartesian coordinates.

## Appendix C: Symplecticity

The symplectic property of of the propagator matrix (5) of geodesic deviation may be expressed in the form of

$$\begin{pmatrix} \mathbf{Q}_1^\mathrm{T} & \mathbf{P}_1^\mathrm{T} \\ \mathbf{Q}_2^\mathrm{T} & \mathbf{P}_2^\mathrm{T} \end{pmatrix} \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ -\mathbf{1} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{Q}_1 & \mathbf{Q}_2 \\ \mathbf{P}_1 & \mathbf{P}_2 \end{pmatrix} = \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ -\mathbf{1} & \mathbf{0} \end{pmatrix} \quad , \tag{C1}$$

or of

$$\begin{pmatrix} \mathbf{Q}_1 & \mathbf{Q}_2 \\ \mathbf{P}_1 & \mathbf{P}_2 \end{pmatrix} \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ -\mathbf{1} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{Q}_1^\mathrm{T} & \mathbf{P}_1^\mathrm{T} \\ \mathbf{Q}_2^\mathrm{T} & \mathbf{P}_2^\mathrm{T} \end{pmatrix} = \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ -\mathbf{1} & \mathbf{0} \end{pmatrix} \quad . \tag{C2}$$

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

$$\mathbf{P}_2^\mathrm{T}\mathbf{Q}_1 - \mathbf{Q}_2^\mathrm{T}\mathbf{P}_1 = \mathbf{1} \quad . \tag{C3}$$

Symmetry of matrix $\mathbf{Q}_2^\mathrm{T}\mathbf{P}_2$ and identity (C3) imply the identity

$$\mathbf{P}_2^\mathrm{T}\mathbf{Q}_\mathrm{R} - \mathbf{Q}_2^\mathrm{T}\mathbf{P}_\mathrm{R} = \mathbf{Q}_0 \tag{C4}$$

for matrices (8) and (9).

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