TRANSFORMATION RELATIONS FOR SECOND-ORDER DERIVATIVES OF TRAVEL TIME IN ANISOTROPIC MEDIA

VLASTISLAV ČERVENÝ AND LUDĚK KLIMEŠ

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

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ABSTRACT

In the computation of paraxial travel times and Gaussian beams, the basic role is played by the second-order derivatives of the travel-time field at the reference ray. These derivatives can be determined by dynamic ray tracing (DRT) along the ray. Two basic DRT systems have been broadly used in applications: the DRT system in Cartesian coordinates and the DRT system in ray-centred coordinates. In this paper, the transformation relations between the second-order derivatives of the travel-time field in Cartesian and ray-centred coordinates are derived. These transformation relations can be used both in isotropic and anisotropic media, including computations of complex-valued travel times necessary for the evaluation of Gaussian beams.

Keywords: paraxial travel times, paraxial approximation of the displacement vector, Gaussian beams, dynamic ray tracing, second-order travel-time derivatives

1. INTRODUCTION

In three-dimensional, laterally varying, isotropic or anisotropic media, the ray-theory travel times are computed along rays. If we wish to compute the travel-time field in the vicinity of a reference ray Ω, we have to determine new rays in this vicinity. We can, however, evaluate the travel-time field around Ω approximately. It is sufficient to perform dynamic ray tracing along reference ray Ω and compute the second-order derivatives of the travel time. As the first-order derivatives of travel time are known from ray tracing, we can use the Taylor expansion of the travel-time field $T = T(x_m)$ up to the quadratic terms and determine approximately the travel-time field in the "quadratic" (paraxial) vicinity of the reference ray. The paraxial travel time, although approximate, finds very useful applications in the ray method. The complex-valued paraxial travel times may also be computed and may be applied in the theory of paraxial Gaussian beams connected with the reference ray.

The second-order derivatives of the travel time can be calculated along the ray by the procedure called dynamic ray tracing (DRT). The DRT system is a system of linear, ordinary differential equations for the first-order derivatives of phase-space coordinates (position and slowness vector components) with respect to ray parameters or initial phase-space coordinates. From these partial derivatives of the first order, we can simply determine the second-order derivatives of the travel time, and many other important quantities not discussed here. The DRT system can be solved along a known ray (called the reference or central ray), or together with the ray tracing system.

The DRT system can be formulated in various coordinates. Very common is to use the DRT system in ray-centred coordinates q_1, q_2, q_3, and to determine $\partial^2 T/\partial q_N \partial q_M$, $N = 1, 2$, $M = 1, 2$. Analogously, we can use the DRT system in Cartesian coordinates x_i, $i = 1, 2, 3$, and to determine $\partial^2 T/\partial x_i \partial x_j$.

The DRT system in Cartesian coordinates in generally anisotropic inhomogeneous media was first derived by *Červený (1972)*, see also *Thomson and Chapman (1985)*, *Kendall and Thomson (1989)*, *Červený (2001)* and *Chapman (2004)*. For isotropic inhomogeneous media, a detailed derivation can be found in *Chapman (2004)*.

In isotropic inhomogeneous media, the DRT in ray-centred coordinates was first proposed to compute the geometrical spreading along the ray by *Popov and Pšenčík (1978a,b)*. Later, it was shown how the system can be used to compute the curvatures of the wavefront along the central ray, see *Hubral (1979)*, and *Červený and Hron (1980)*. *Červený and Hron (1980)* proposed that the procedure be called "the dynamic ray tracing" to acknowledge its great importance in the computation of geometrical spreading and ray-theory amplitudes along the central ray. For a detailed treatment of ray-centred coordinates, of DRT in ray-centred coordinates, and of various applications and many references, see *Červený (2001, Sec. 4)*.

For inhomogeneous anisotropic media, the DRT system in ray-centred coordinates was first derived by *Hanyga (1982)*; see also *Kendall et al. (1992)*, *Klimeš (1994, 2006)*, *Bakker (1996)*, and *Červený (2001, 2007)*. At present, the DRT in ray-centred coordinates in both isotropic and anisotropic inhomogeneous layered media, is a well-understood procedure.

The DRT in ray-centred coordinates has found important applications in the theory of paraxial Gaussian beams. In this case, however, the second-order derivatives of the travel time field are complex-valued. Consequently, the paraxial travel time is also complex-valued. It is real-valued only along the central ray, but complex-valued in its paraxial vicinity. The imaginary parts of the second-order derivatives of the travel time cause the Gaussian decrease of amplitudes along any profile intersecting the central ray. The only exception is the profile tangent to the ray.

If we wish to compute the paraxial travel time at a paraxial point approximately, we can use the Taylor expansion of travel time up to the second order at a point on the central ray, either in Cartesian or in ray-centred coordinates. The Cartesian coordinates are more suitable in this case, as they are more flexible.

It is, however, not necessary to perform DRT computations in the coordinate system, in which we wish to determine the second-order travel-time derivatives. The transformation relations derived in this paper allow the computation of the second-order derivatives $\partial^2 T/\partial x_i\, \partial x_j$ from $\partial^2 T/\partial q_N\, \partial q_M$, and vice versa, at an arbitrary point along the ray. Consequently, we can easily determine the second-order derivatives $\partial^2 T/\partial x_i\, \partial x_j$ even when the DRT system is solved in ray-centred coordinates, and vice versa. These transformations simplify the various applications in the paraxial ray theory and in the theory of Gaussian beams considerably, see *Červený and Pšenčík (2009)*.

Briefly to the content of the paper. In Section 2, we review the basic properties of DRT in ray-centred coordinates. The section serves only to show how the complex-valued second-order derivatives $\partial^2 T/\partial q_N \partial q_M$ of the travel time are calculated along the ray using the dynamic ray tracing in ray-centred coordinates. For more detailed explanations and derivations, see *Klimeš (1994, 2006)*. In Section 3, we derive the relations between $\partial^2 T/\partial x_i \partial x_j$ and $\partial^2 T/\partial q_N \partial q_M$. These relations can be used, if we wish to determine $\partial^2 T/\partial x_i\, \partial x_j$ from $\partial^2 T/\partial q_N\, \partial q_M$ at any point of the ray, when the DRT in ray-centred coordinates is used. Finally, in Section 4, we present expressions for the complex-valued paraxial travel times in Cartesian coordinates, using $\partial^2 T/\partial q_N \partial q_M$ calculated by DRT in ray-centred coordinates.

We mostly use the component notation for vectors and matrices, with the upper-case indices (I, J, K...) taking the values of 1 or 2, and the lower-case indices ($i, j, k, ...$) taking the values 1, 2, or 3. The Einstein summation convention is used.

2. DYNAMIC RAY TRACING IN RAY-CENTRED COORDINATES IN HETEROGENEOUS ANISOTROPIC MEDIA

This section has a review character only. For more detailed explanations, derivations and other references, see *Klimeš (1994, 2006)* and *Červený (2001, Sec. 4)*.

We consider the eikonal equation for travel-time field $T(x_i)$ in Hamiltonian form,

$$\mathcal{H}(x_i, p_j) = 0\ . \tag{1}$$

Here $\mathcal{H}$ is the Hamiltonian, x_i are the Cartesian components of position vector $\mathbf{x}$, and $p_i = \partial T/\partial x_i$ are the Cartesian components of slowness vector $\mathbf{p}$, perpendicular to the wavefront. We consider the Hamiltonians, which are homogeneous functions of the second degree in p_i (with a possible additional constant). The kinematic ray tracing equations then read:

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

Here τ is a monotonic variable along the ray, representing the travel time. For a homogeneous Hamiltonian in p_i, vector $\boldsymbol{\mathcal{U}}$, with Cartesian components

$$\mathcal{U}_i = \partial \mathcal{H}/\partial p_i\,, \tag{3}$$

is the ray-velocity vector, tangential to the ray, and vector $\boldsymbol{\eta}$, with Cartesian components

$$\eta_i = -\partial \mathcal{H}/\partial x_i\,, \tag{4}$$

represents the change of slowness vector $\mathbf{p}$ along the ray. Suitable forms of Hamiltonians for heterogeneous anisotropic media are given in *Červený (2001, Sec. 3.6)*. The results presented in this paper are valid for any Hamiltonian; we only require that the Hamiltonian be a homogeneous function of the second degree in p_i.

We now introduce the ray-centred coordinate system q_1, q_2, q_3 connected with the reference ray Ω. The basic property of the ray-centred coordinate system is that ray Ω

represents the q_3 coordinate axis of the system. The remaining coordinates q_1 and q_2 are introduced by the relation, see *Kendall et al. (1992)*, *Klimeš (1994, 2006)*:

$$x_i(q_j) = x_{i0}(q_3) + H_{iM}(q_3)q_M \, , \tag{5}$$

where $i = 1, 2, 3$, $j = 1, 2, 3$, and $M = 1, 2$. Basis vectors H_{i1} and H_{i2} may be introduced in many ways. For an up-to-date review of various possibilities, see *Klimeš (2006)*. The reference ray is specified by $q_1 = q_2 = 0$, for which Eq.(5) yields the relation $x_i(q_3) = x_{i0}(q_3)$. In this paper, we choose $q_3 = \tau$. Coordinates q_1, q_2 are Cartesian coordinates which specify uniquely the position of a point in the plane tangent to the wavefront, intersecting reference ray Ω at the point specified by $q_3 = \tau$.

Equation (5) determines a simple transform from q_1, q_2, q_3 to x_1, x_2, x_3. On the other hand, it is extremely difficult to transform x_1, x_2, x_3 to q_1, q_2, q_3.

Several partial derivatives of travel time T with respect to ray-centred coordinates are constant along the central ray. It is not difficult to see that

$$\frac{\partial T}{\partial q_I} = 0 \tag{6}$$

at any point of the central ray. This relation is valid generally, for any choice of q_3. The choice $q_3 = \tau$ leads further to the following simple relations valid at any point of ray Ω:

$$\frac{\partial T}{\partial q_3} = 1 \, , \qquad \frac{\partial^2 T}{\partial q_3 \partial q_i} = 0 \, . \tag{7}$$

Relations (7) are not valid for any other monotonic parameter (e.g., the arclength) along the ray. It is important to emphasize this, since the arclength along the ray has most commonly been used in ray-centred coordinates in heterogeneous isotropic media. In this respect, our treatment differs from the usual treatment in isotropic media.

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

$$H_{im} = \frac{\partial x_i}{\partial q_m} \, , \qquad \overline{H}_{im} = \frac{\partial q_i}{\partial x_m} \, . \tag{8}$$

The elements satisfy the relation

$$\overline{H}_{mi} H_{in} = \delta_{mn} \, . \tag{9}$$

Six elements of the transformation matrices are known from kinematic ray tracing. For $q_3 = \tau$, the third column of matrix $\mathbf{H}$ reads:

$$H_{i3} = \frac{\partial x_i}{\partial q_3} = \frac{\partial x_i}{\partial \tau} = \mathcal{U}_i \, , \tag{10}$$

where $\boldsymbol{\mathcal{U}}$ is the ray velocity vector. We now determine the third line of $\overline{\mathbf{H}}$. Taking into account that $\partial T / \partial q_K = 0$, $q_3 = \tau$, and $\partial T / \partial \tau = 1$ along the ray, we obtain

$$p_i = \frac{\partial T}{\partial x_i} = \frac{\partial T}{\partial q_m} \frac{\partial q_m}{\partial x_i} = \frac{\partial T}{\partial q_3} \frac{\partial q_3}{\partial x_i} = \frac{\partial T}{\partial \tau} \overline{H}_{3i} = \overline{H}_{3i} \, . \tag{11}$$

From Eqs.(9) – (11), we then obtain $p_i H_{iI} = 0$, $\mathcal{U}_i \overline{H}_{Ii} = 0$. Thus, vectors H_{i1} and H_{i2} are perpendicular to the slowness vector and vectors $\overline{H}_{1i}$ and $\overline{H}_{2i}$ are perpendicular to the ray-velocity vector.

Let us now consider an orthonomic (two-parametric) system of rays, in which each ray is specified by two ray parameters γ_1, γ_2. They may represent the take-off angles at a point source, curvilinear Gaussian coordinates of initial points of rays at a curved initial surface, etc. We introduce two 2×2 matrices $\mathbf{Q}^{(q)}$ and $\mathbf{P}^{(q)}$, with elements $Q_{IJ}^{(q)}$ and $P_{IJ}^{(q)}$ ($I = 1, 2$; $J = 1, 2$) along central ray Ω by the relation

$$Q_{IJ}^{(q)} = \partial q_I / \partial \gamma_J \ , \quad P_{IJ}^{(q)} = \partial p_I^{(q)} / \partial \gamma_J \ . \tag{12}$$

Here $p_I^{(q)} = \partial T / \partial q_I$. The expressions for $Q_{IJ}^{(q)}$ and $P_{IJ}^{(q)}$ show, how q_I and $p_I^{(q)}$ vary when parameters γ_1, γ_2 change (i.e. when we pass from one ray to another). Matrices $Q_{IJ}^{(q)}$ and $P_{IJ}^{(q)}$ can be computed by solving a system of ordinary differential equations of the first order along ray Ω, called the *dynamic ray tracing* (DRT) *system*. The DRT system in ray-centred coordinates consists of four matrix equations, see *Klimeš (2006)*,

$$\frac{\mathrm{d}Q_{NI}^{(q)}}{\mathrm{d}\tau} = A_{NM}^{(q)} Q_{MI}^{(q)} + B_{NM}^{(q)} P_{MI}^{(q)} \ , \qquad \frac{\mathrm{d}P_{NI}^{(q)}}{\mathrm{d}\tau} = -C_{NM}^{(q)} Q_{MI}^{(q)} - D_{NM} P_{MI}^{(q)} \ , \tag{13}$$

where

$$A_{NM}^{(q)} = \overline{H}_{Ni} H_{jM} A_{ij} - d_{NM} \ , \quad B_{NM}^{(q)} = \overline{H}_{Ni} \overline{H}_{Mj} B_{ij} \ ,$$
$$C_{NM}^{(q)} = H_{iN} H_{jM} (C_{ij} - \eta_i \eta_j) \ , \quad D_{NM}^{(q)} = H_{iN} \overline{H}_{Mj} D_{ij} - d_{MN} \ . \tag{14}$$

The 3×3 matrices $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$ and $\mathbf{D}$ with elements A_{ij}, B_{ij}, C_{ij} and D_{ij} represent the second-order derivatives of the Hamiltonian:

$$A_{ij} = \frac{\partial^2 \mathcal{H}}{\partial p_i \partial x_j} \ , \quad B_{ij} = \frac{\partial^2 \mathcal{H}}{\partial p_i \partial p_j} \ ,$$
$$C_{ij} = \frac{\partial^2 \mathcal{H}}{\partial x_i \partial p_j} \ , \quad D_{ij} = \frac{\partial^2 \mathcal{H}}{\partial x_i \partial p_j} \ . \tag{15}$$

Note that $D_{ij} = A_{ji}$. Symbol d_{NM} in Eq.(14) denotes

$$d_{NM} = \overline{H}_{Ni} \mathrm{d}H_{iM} / \mathrm{d}\tau \ . \tag{16}$$

From the known 2×2 matrices $\mathbf{Q}^{(q)}$ and $\mathbf{P}^{(q)}$, we can also determine the matrix of the second-order derivatives of travel-time field $\mathbf{M}^{(q)}$, with elements

$$M_{IJ}^{(q)} = \partial^2 T / \partial q_I \partial q_J \ . \tag{17}$$

We use

$$M_{IJ}^{(q)} Q_{JK}^{(q)} = \frac{\partial^2 T}{\partial q_I \partial q_J} \frac{\partial q_J}{\partial \gamma_K} = \frac{\partial p_I^{(q)}}{\partial \gamma_J} \frac{\partial q_I}{\partial \gamma_K} = \frac{\partial p_I^{(q)}}{\partial \gamma_K} = P_{IK}^{(q)} \ . \tag{18}$$

This yields

$$\mathbf{M}^{(q)} = \mathbf{P}^{(q)}(\mathbf{Q}^{(q)})^{-1} . \tag{19}$$

Once the DRT system (13) for $Q_{IJ}^{(q)}(\tau)$ and $P_{IJ}^{(q)}(\tau)$ is solved along ray Ω, and $M_{IJ}^{(q)}(\tau)$ is determined using Eq.(19), we can write the Taylor series expansion of the paraxial travel time field $T(q_1, q_2, q_3)$, up to the quadratic terms of q_1, q_2, at any fixed point of ray Ω, specified by $q_3 = \tau$:

$$T(q_1, q_2, q_3) = T(q_3) + \tfrac{1}{2}\mathbf{q}^T\mathbf{M}^{(q)}(q_3)\mathbf{q} , \tag{20}$$

where $\mathbf{q} = (q_1, q_2)^T$ and $T(q_3) = T(0, 0, q_3)$. Equation (20) plays an important role in the paraxial ray method, in the computation of the paraxial approximation of the displacement vector and in the theory of Gaussian beams, etc. For fixed q_3, it yields the paraxial travel time (possibly complex valued) in plane $q_3 = constant$, which is tangential to the wavefront at the given point of ray Ω.

Equation (20) could be used if the complex-valued paraxial travel time $T(q_1, q_2, q_3)$ were computed at point $R(q_1, q_2, q_3)$, specified in ray-centred coordinates q_1, q_2, q_3. In this case, the plane passing through point R would be tangential to the wavefront at point $R_\Omega(0, 0, q_3 = \tau)$. Consequently, if we specify point R_Ω situated on ray Ω, we can calculate the complex-valued paraxial travel times (20) parametrized by q_1, q_2 in the whole plane tangential to the wavefront at R_Ω. Varying the position of R_Ω along the ray, we can determine the complex-valued paraxial travel times (20) parametrized by q_1, q_2, q_3 in the vicinity of the central ray Ω.

A considerably more complicated problem appears, however, if we wish to compute the complex-valued paraxial travel time $T(x_1, x_2, x_3)$ in general Cartesian coordinates. We can proceed in two ways: a) Transform x_1, x_2, x_3 to q_1, q_2, q_3. This is, however, usually a very cumbersome procedure, even in isotropic inhomogeneous media. b) We transform the 2×2 matrix $\mathbf{M}^{(q)}$ in (20) to the 3×3 matrix $\mathbf{M}^{(x)}$ of the second-order derivatives of the travel time with respect to Cartesian coordinates. It would then be possible to compute simply the paraxial travel-time field in the whole vicinity of point q_3 of ray Ω, not only in the plane tangential to the wavefront. The computation of $\partial^2 T/\partial x_i \partial x_j$ from known $\partial^2 T/\partial q_N \partial q_M$ is discussed in Section 3, and the computation of $T(x_1, x_2, x_3)$ in Cartesian coordinates in Section 4.

3. RELATION BETWEEN $\partial^2 T/\partial x_i \partial x_j$ AND $\partial^2 T/\partial q_N q_M$

In this section, we derive the relation between the 3×3 matrix $\mathbf{M}^{(x)}$ of the second-order derivatives of the travel-time field in Cartesian coordinates x_i $(i = 1, 2, 3)$ and the 2×2 matrix $\mathbf{M}^{(q)}$ of the second-order derivatives of the travel-time field in ray-centred coordinates $q_I (I = 1, 2)$. The nine components of $\mathbf{M}^{(x)}$ are denoted $\partial^2 T/\partial x_i \partial x_j$, and the four components of $\mathbf{M}^{(q)}$ are denoted $\partial^2 T/\partial q_I \partial q_J$. Both matrices are symmetric. The relation we derive is valid at any point of central ray Ω, and for any choice of basis vectors (8) of the ray-centred coordinate system. We assume that vectors $\mathbf{p}$, $\boldsymbol{\eta}$ and $\boldsymbol{\mathcal{U}}$ are known from ray tracing. We can express $\partial^2 T/\partial x_i \partial x_j$as

$$\frac{\partial^2 T}{\partial x_i \partial x_j} = \frac{\partial}{\partial x_i}\left(\frac{\partial T}{\partial x_j}\right) = \frac{\partial}{\partial x_i}\left(\frac{\partial T}{\partial q_n}\frac{\partial q_n}{\partial x_j}\right). \tag{21}$$

This equation yields

$$\frac{\partial^2 T}{\partial x_i \partial x_j} = \frac{\partial}{\partial x_i}\left(\frac{\partial T}{\partial q_n}\right)\frac{\partial q_n}{\partial x_j} + \frac{\partial T}{\partial q_n}\frac{\partial^2 q_n}{\partial x_i \partial x_j}\,. \tag{22}$$

Along the central ray, $\partial T/\partial q_n = \delta_{n3}$, see Eqs.(6) and (7). On performing the differentiation in the first term in Eq.(22), we obtain

$$\frac{\partial^2 T}{\partial x_i \partial x_j} = \frac{\partial q_m}{\partial x_i}\frac{\partial^2 T}{\partial q_n \partial q_m}\frac{\partial q_n}{\partial x_j} + \frac{\partial^2 q_3}{\partial x_i \partial x_j}\,. \tag{23}$$

Now we split the summation over $n = 1, 2, 3$ in Eq.(23) into the summation over $n = N$ and $n = 3$, and analogously the summation over m. We obtain

$$\frac{\partial^2 T}{\partial x_i \partial x_j} = \frac{\partial q_M}{\partial x_i}\frac{\partial^2 T}{\partial q_M \partial q_N}\frac{\partial q_N}{\partial x_j} + \frac{\partial q_m}{\partial x_i}\frac{\partial^2 T}{\partial q_m \partial q_3}\frac{\partial q_3}{\partial x_j} +$$

$$+ \frac{\partial q_3}{\partial x_i}\frac{\partial^2 T}{\partial q_3 \partial q_n}\frac{\partial q_n}{\partial x_j} - \frac{\partial q_3}{\partial x_i}\frac{\partial^2 T}{\partial q_3 \partial q_3}\frac{\partial q_3}{\partial x_j} + \frac{\partial^2 q_3}{\partial x_i \partial x_j}\,. \tag{24}$$

Taking into account Eq.(7) we obtain

$$\frac{\partial^2 T}{\partial x_i \partial x_j} = \frac{\partial q_M}{\partial x_i}\frac{\partial^2 T}{\partial q_M \partial q_N}\frac{\partial q_N}{\partial x_j} + \frac{\partial^2 q_3}{\partial x_i \partial x_j} \tag{25}$$

The result (25) is, indeed, surprisingly simple. The first term can be fully computed by dynamic ray tracing in ray-centred coordinates. Alternatively, it can be calculated by dynamic ray tracing in orthonormal wavefront coordinates, or by incomplete dynamic ray tracing in Cartesian coordinates. What remains to be determined is $\partial^2 q_3/\partial x_i \partial x_j$.

We use the obvious relation

$$\frac{\partial}{\partial x_i}\left(\frac{\partial q_3}{\partial x_k}\frac{\partial x_k}{\partial q_m}\right) = 0\,. \tag{26}$$

This relation yields

$$\frac{\partial^2 q_3}{\partial x_i \partial x_k}\frac{\partial x_k}{\partial q_m} + \frac{\partial q_3}{\partial x_k}\frac{\partial}{\partial x_i}\left(\frac{\partial x_k}{\partial q_m}\right) = 0\,. \tag{27}$$

Multiplying (27) by $\partial q_m/\partial x_j$, we obtain

$$\frac{\partial^2 q_3}{\partial x_i \partial x_j} = -\frac{\partial q_m}{\partial x_j}\frac{\partial q_3}{\partial x_k}\frac{\partial q_n}{\partial x_i}\frac{\partial^2 x_k}{\partial q_m \partial q_n}\,. \tag{28}$$

We now again split the summation over $n = 1, 2, 3$ into the summation over $n = N$ and $n = 3$, and similarly for m:

$$\frac{\partial^2 q_3}{\partial x_i \partial x_j} = -\frac{\partial q_M}{\partial x_j}\frac{\partial q_3}{\partial x_k}\frac{\partial q_N}{\partial x_i}\frac{\partial^2 x_k}{\partial q_M \partial q_N} - \frac{\partial q_3}{\partial x_j}\frac{\partial q_3}{\partial x_k}\frac{\partial q_n}{\partial x_i}\frac{\partial^2 x_k}{\partial q_3 \partial q_n} - \\ - \frac{\partial q_m}{\partial x_j}\frac{\partial q_3}{\partial x_k}\frac{\partial q_3}{\partial x_i}\frac{\partial^2 x_k}{\partial q_m \partial q_3} + \frac{\partial q_3}{\partial x_j}\frac{\partial q_3}{\partial x_k}\frac{\partial q_3}{\partial x_i}\frac{\partial^2 x_k}{\partial q_3 \partial q_3} \, . \tag{29}$$

Equation (29) can be simplified further if we use the obvious identity

$$\frac{\partial}{\partial q_3}\left(\frac{\partial q_3}{\partial x_k}\frac{\partial x_k}{\partial q_m}\right) = 0 \, . \tag{30}$$

As from Eq.(26), we similarly obtain

$$\frac{\partial}{\partial q_3}\left(\frac{\partial q_3}{\partial x_k}\right)\frac{\partial x_k}{\partial q_m} + \frac{\partial q_3}{\partial x_k}\frac{\partial^2 x_k}{\partial q_3 \partial q_m} = 0 \, . \tag{31}$$

This yields

$$\frac{\partial q_3}{\partial x_k}\frac{\partial^2 x_k}{\partial q_3 \partial q_m} = -\eta_k \frac{\partial x_k}{\partial q_m} \, , \tag{32}$$

as $\partial(\partial q_3/\partial x_k)/\partial q_3 = \partial p_k/\partial q_3 = \eta_k$. Inserting Eq.(32) into Eq.(29), and taking into account that the first term in Eq.(29) is zero ($\partial^2 x_k/\partial q_M \partial q_N$ vanishes since q_N and q_M are Cartesian coordinates in the plane tangent to the wavefront), we obtain

$$\frac{\partial^2 q_3}{\partial x_i \partial x_j} = \frac{\partial q_3}{\partial x_j}\frac{\partial q_n}{\partial x_i}\frac{\partial x_k}{\partial q_n}\eta_k + \frac{\partial q_m}{\partial x_j}\frac{\partial q_3}{\partial x_i}\frac{\partial x_k}{\partial q_m}\eta_k - \frac{\partial q_3}{\partial x_j}\frac{\partial q_3}{\partial x_i}\frac{\partial x_k}{\partial q_3}\eta_k \, . \tag{33}$$

We now take into account that

$$\frac{\partial q_3}{\partial x_j} = p_j \, , \qquad \frac{\partial x_k}{\partial q_3} = \mathcal{U}_k \, , \qquad \frac{\partial x_k}{\partial q_n}\frac{\partial q_n}{\partial x_i} = \delta_{ki} \, , \tag{34}$$

see Eqs.(9) and (10), and obtain from Eq.(33):

$$\frac{\partial^2 q_3}{\partial x_i \partial x_j} = p_i \eta_j + p_j \eta_i - p_i p_j (\mathcal{U}_k \eta_k) \, . \tag{35}$$

Equations (23) and (35) yield the final equation for $\partial^2 T/\partial x_i \partial x_j$:

$$\frac{\partial^2 T}{\partial x_i \partial x_j} = \frac{\partial q_M}{\partial x_i}\frac{\partial^2 T}{\partial q_M \partial q_N}\frac{\partial q_N}{\partial x_j} + p_i \eta_j + p_j \eta_i - p_i p_j \mathcal{U}_k \eta_k \, . \tag{36}$$

Equation (36) can also be used to express $\partial^2 T/\partial q_M \partial q_N$ in terms of $\partial^2 T/\partial x_i \partial x_j$. Multiplying (36) by $\partial x_i/\partial q_N \; \partial x_j/\partial q_M$ yields:

$$\frac{\partial x_i}{\partial q_N}\frac{\partial^2 T}{\partial x_i \partial x_j}\frac{\partial x_j}{\partial q_M} = \frac{\partial^2 T}{\partial q_M \partial q_N} + \frac{\partial x_i}{\partial q_N}\left(p_i \eta_j + p_j \eta_i - p_i p_j \mathcal{U}_k \eta_k\right)\frac{\partial x_j}{\partial q_M} \, . \tag{37}$$

We now take into account that $\partial x_i/\partial q_N$ is situated in the plane tangential to the wavefront at central ray Ω. Consequently, it is perpendicular to slowness vector $\mathbf{p}$, and $p_i \partial x_i/\partial q_N = 0$. Eq.(37) then yields a simple relation

$$\frac{\partial^2 T}{\partial q_N \partial q_M} = \frac{\partial x_i}{\partial q_N} \frac{\partial^2 T}{\partial x_i \partial x_j} \frac{\partial x_j}{\partial q_M} \, . \tag{38}$$

Equations (36) and (38) present the main result of this paper.

It may be useful to express the important Eqs.(36) and (38) in matrix form. Let us consider matrices $\mathbf{H}$ and $\overline{\mathbf{H}}$, see Eq.(8), defined along ray Ω. We denote the columns of matrix $\mathbf{H}$, which represent the contravariant basis vectors of the ray-centred coordinate system, by $\mathbf{e}_i$, and the rows of matrix $\overline{\mathbf{H}}$, which represent covariant basis vectors, by $\mathbf{f}_i$:

$$\mathbf{H} = (\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3 = \boldsymbol{\mathcal{U}}) \, , \qquad \overline{\mathbf{H}}^T = (\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3 = \mathbf{p}) \, . \tag{39}$$

Basis vectors $\mathbf{e}_I$ are perpendicular to slowness vector $\mathbf{p}$, and basis vectors $\mathbf{f}_I$ are perpendicular to ray-velocity vector $\boldsymbol{\mathcal{U}}$, i.e. to central ray Ω. Vectors $\mathbf{e}_i$ and $\mathbf{f}_i$ are used in dynamic ray tracing in ray-centred coordinates, so that they are known at any point of ray Ω. They satisfy relation (9):

$$\mathbf{e}_i^T \mathbf{f}_j = \delta_{ij} \, . \tag{40}$$

Consequently, $\mathbf{f}_1$ and $\mathbf{f}_2$ can be expressed in terms of $\mathbf{e}_1$ and $\mathbf{e}_2$ as follows:

$$\mathbf{f}_1 = \frac{\mathbf{e}_2 \times \boldsymbol{\mathcal{U}}}{\boldsymbol{\mathcal{U}}^T(\mathbf{e}_1 \times \mathbf{e}_2)} = \mathcal{C}^{-1}(\mathbf{e}_2 \times \boldsymbol{\mathcal{U}}) \, , \quad \mathbf{f}_2 = \frac{\boldsymbol{\mathcal{U}} \times \mathbf{e}_1}{\boldsymbol{\mathcal{U}}^T(\mathbf{e}_1 \times \mathbf{e}_2)} = \mathcal{C}^{-1}(\boldsymbol{\mathcal{U}} \times \mathbf{e}_1) \, . \tag{41}$$

The matrix form of Eq.(36) then reads

$$\mathbf{M}^{(x)} = \mathbf{f} \; \mathbf{M}^{(q)} \; \mathbf{f}^T + \mathbf{p}\boldsymbol{\eta}^T + \boldsymbol{\eta}\mathbf{p}^T - \mathbf{p}(\boldsymbol{\mathcal{U}}^T \boldsymbol{\eta})\mathbf{p}^T \, . \tag{42}$$

Here $\mathbf{f} = (\mathbf{f}_1, \mathbf{f}_2)$ is the 3×2 matrix with column vectors $\mathbf{f}_1$ and $\mathbf{f}_2$. Vectors $\mathbf{f}_I$ are perpendicular to ray Ω. Similarly, the matrix form of Eq.(38) reads

$$\mathbf{M}^{(q)} = \mathbf{e}^T \mathbf{M}^{(x)} \mathbf{e} \, . \tag{43}$$

Here $\mathbf{e} = (\mathbf{e}_1, \mathbf{e}_2)$ is the 3×2 matrix with column vectors $\mathbf{e}_1$ and $\mathbf{e}_2$.

Let us now consider paraxial Gaussian beams. If we use the 2×2 matrix $\mathbf{M}^{(q)}(\tau_0)$ complex-valued, finite and symmetric at the initial point $\tau = \tau_0$ of the ray, with $\mathrm{Im}\mathbf{M}(\tau_0)$ positive definite, the 2×2 matrix $\mathbf{M}^{(q)}(\tau)$ is complex-valued, finite and symmetric, and $\mathrm{Im}\mathbf{M}^{(q)}$ is positive definite at any point of ray Ω. Vectors $\mathbf{p}$, $\boldsymbol{\eta}$, $\boldsymbol{\mathcal{U}}$, $\mathbf{f}_1$, $\mathbf{f}_2$, $\mathbf{e}_1$ and $\mathbf{e}_2$ are real-valued. Consequently, only the 2×2 matrix $\mathbf{M}^{(q)}$ is complex-valued in the expression (42) for the relevant 3×3 matrix $\mathbf{M}^{(x)}$.

Equations (36), (38), (42) and (43) are valid for an arbitrary choice of basis vectors $\mathbf{e}_I$ of the ray-centred coordinate system, defined by Eqs.(8) and (39). Several possibilities of computing $\mathbf{e}_I$ are discussed in *Klimeš (2006).*

4. PARAXIAL REAL-VALUED OR COMPLEX-VALUED TRAVEL TIMES

Equations (36) and (42) play a very important role in paraxial ray methods, particularly in the computation of the paraxial travel time, paraxial approximation of the displacement vector and Gaussian beams. For more details we refer the reader to *Červený and Pšenčík (2009)*.

For dynamic ray tracing in ray-centred coordinates, Eqs.(36) or (42) are very useful if we wish to find the paraxial travel time at an arbitrary point, specified in Cartesian coordinates, in the vicinity of the reference ray.

We shall consider point R, situated arbitrarily in the paraxial vicinity of ray Ω, and point R_Ω, situated arbitrarily on ray Ω. We introduce vector $\Delta\mathbf{x}$ with components Δx_i as follows:

$$\Delta x_i = x_i(R) - x_i(R_\Omega)\,. \tag{44}$$

For small $|\Delta\mathbf{x}|$, we can then write the Taylor series expansion upto quadratic terms for the paraxial travel-time field at R,

$$T(R) = T(R_\Omega) + \mathbf{p}^T(R_\Omega)\Delta\mathbf{x} + \frac{1}{2}\,(\Delta\mathbf{x})^T\mathbf{M}^{(x)}(R_\Omega)\Delta\mathbf{x}\,. \tag{45}$$

Here $\mathbf{M}^{(x)}(R_\Omega)$ is given by Eq.(42). Expression (45) for $T(R)$ is, of course, only approximate. Roughly speaking, its accuracy becomes higher as the distance between R and R_Ω, i.e. $|\Delta\mathbf{x}|$, grows smaller.

More explicitly, the quadratic expansion for the paraxial travel-time $T(R)$ reads:

$$T(R) = T(R_\Omega) + \mathbf{p}^T\Delta\mathbf{x} + (\mathbf{p}^T\Delta\mathbf{x})(\boldsymbol{\eta}^T\Delta\mathbf{x}) - \frac{1}{2}\,(\mathbf{p}^T\Delta\mathbf{x})^2(\boldsymbol{\mathcal{U}}^T\boldsymbol{\eta}) + \\ + \frac{1}{2}\,(\mathbf{f}_1^T\Delta\mathbf{x}, \mathbf{f}_2^T\Delta\mathbf{x})\mathbf{M}^{(q)}\begin{pmatrix} \mathbf{f}_1^T\Delta\mathbf{x} \\ \mathbf{f}_2^T\Delta\mathbf{x} \end{pmatrix}. \tag{46}$$

Here $\mathbf{p}$, $\boldsymbol{\mathcal{U}}$, $\boldsymbol{\eta}$, $\mathbf{f}_1$, $\mathbf{f}_2$ and $\mathbf{M}^{(q)}$ do not depend on the position of point R, but only on the position of point R_Ω on ray Ω. Vectors $\mathbf{p}$, $\boldsymbol{\mathcal{U}}$ and $\boldsymbol{\eta}$ are known from kinematic ray tracing, vectors $\mathbf{f}_1$, $\mathbf{f}_2$ and the 2×2 matrix $\mathbf{M}^{(q)}$ from dynamic ray tracing. See the relevant discussion above Eq.(42).

Equation (46) for the paraxial travel time $T(R)$ expressed in the Cartesian coordinates of points R and R_Ω is considerably more flexible than Eq.(20), expressed in ray-centred coordinates q_1, q_2, q_3. The determination of the ray-centred coordinates $q_1(R)$, $q_2(R)$, $q_3(R)$ of the observation point R, whose position is known in Cartesian coordinates only, is very difficult. It requires finding the appropriate point R_Ω on ray Ω and the relevant plane tangent to the wavefront at R_Ω, which passes through the known observation point R. This may be a cumbersome numerical procedure.

Equation (46) is valid both for the paraxial travel-time approximation, when the 2×2 matrix $\mathbf{M}^{(q)}$ is real-valued, and for the paraxial Gaussian beams, when $\mathbf{M}^{(q)}$ is complex-valued. For paraxial Gaussian beams,

$$\mathrm{Im}T(R) = \frac{1}{2}\,(\mathbf{f}_1^T\Delta\mathbf{x}, \mathbf{f}_2^T\Delta\mathbf{x})\mathrm{Im}\mathbf{M}^{(q)}(R_\Omega)\begin{pmatrix}\mathbf{f}_1^T\Delta\mathbf{x}\\ \mathbf{f}_2^T\Delta\mathbf{x}\end{pmatrix}. \tag{47}$$

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