# Transformation relations <br> for second derivatives of travel time in anisotropic media 

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#### Abstract

Summary In the computation of paraxial travel times and Gaussian beams, the basic role is played by second derivatives of the travel-time field at the reference ray $\Omega$. 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 in ray-centred coordinates. In this paper, the transformation relations between the second derivatives of the travel time field in Cartesian and ray-centred coordinates are derived. These transformation relations can be used in many applications 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 a vicinity of a reference ray $\Omega$, we have to determine new rays in this vicinity. We can, however, evaluate the travel-time field around $\Omega$ approximately. It is sufficient to perform dynamic ray tracing along the reference ray $\Omega$ and compute the second derivatives of the travel time. As the first derivatives are known from ray tracing, we can use quadratic expansion of the travel time field $T=T\left(x_{m}\right)$ 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-

[^0]valued paraxial travel times may be also computed and may be applied in the theory of paraxial Gaussian beams connected with the reference ray.

The DRT used to determine the second order travel-time derivatives can be expressed in various coordinate systems. Most common is to use the DRT in global Cartesian coordinates $x_{i}, i=1,2,3$, and to determine $\partial^{2} T / \partial x_{i} \partial x_{j}$, or to use the DRT in ray-centred coordinates $q_{N}, N=1,2$ and to determine $\partial^{2} T / \partial q_{N} \partial q_{M}$. In ray-centred coordinates, the paraxial travel times are obtained only in the planes tangent to the wavefronts at the reference ray. In Cartesian coordinates, however, they are determined in the whole 3-D vicinity of any point on the reference ray. Consequently, the second derivatives of the travel time field $\partial^{2} T / \partial x_{i} \partial x_{j}$ have much broader applications.

It is, however, not necessary to perform DRT computations in the coordinate system, in which we wish to compute the second travel-time derivatives. The transformation relations derived in this paper allow computation of the second derivatives $\partial^{2} T / \partial x_{i} \partial x_{j}$ from $\partial^{2} T / \partial q_{N} \partial q_{M}$ and vice versa. Consequently, we can simply determine the second 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 considerably various applications in the paraxial ray theory and in the theory of Gaussian beams, see Červený and Pšenčík (2009).

Briefly to the content of the paper. In Sec.2, we introduce basic properties of DRT in ray-centred coordinates. In Sec.3, we derive the relations between $\partial^{2} T / \partial x_{i} \partial x_{j}$ and $\partial^{2} T / \partial q_{N} \partial q_{M}$.

We use here mostly the component notation for vectors and matrices, with the uppercase 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 . Einstein summation convention is used.

## 2 Dynamic ray tracing in ray-centred coordinates in heterogeneous anisotropic media

We consider the eikonal equation for the travel time field $T\left(x_{i}\right)$ in the Hamiltonian form

$$
\begin{equation*}
\mathcal{H}\left(x_{i}, p_{j}\right)=0 . \tag{1}
\end{equation*}
$$

Here $\mathcal{H}$ is the Hamiltonian, $x_{i}$ are the Cartesian components of the position vector $\mathbf{x}$, and $p_{i}=\partial T / \partial x_{i}$ are the Cartesian components of the slowness vector $\mathbf{p}$, vector perpendicular to the wavefront. We consider the Hamiltonians, which are homogeneous functions of second degree in $p_{i}$. The kinematic ray tracing equations then read

$$
\begin{equation*}
\frac{\mathrm{d} x_{i}}{\mathrm{~d} \tau}=\mathcal{U}_{i}=\frac{\partial \mathcal{H}}{\partial p_{i}}, \quad \frac{\mathrm{~d} p_{i}}{\mathrm{~d} \tau}=\eta_{i}=-\frac{\partial \mathcal{H}}{\partial x_{i}} . \tag{2}
\end{equation*}
$$

Here $\tau$ is a monotonic variable along the ray, representing the travel time. The vector $\mathcal{U}$, with Cartesian components $\mathcal{U}_{i}$, is the ray-velocity vector, tangent to the ray, and vector $\boldsymbol{\eta}$, with Cartesian components $\eta_{i}$, 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 is a homogeneous function of second degree in $p_{i}$.

We now introduce the ray-centred coordinate system $q_{1}, q_{2}, q_{3}$ connected with the reference ray $\Omega$. The basic property of the ray-centred coordinate system is that the ray $\Omega$ represents the $q_{3}$ coordinate axis of the system. The remaining coordinates $q_{1}$ and $q_{2}$ are introduced by the relation, see Klimeš (1994, 2006):

$$
\begin{equation*}
x_{i}\left(q_{j}\right)=x_{i 0}\left(q_{3}\right)+H_{i M}\left(q_{3}\right) q_{M} \tag{3}
\end{equation*}
$$

where $i=1,2,3$, and $M=1,2$. Basis vectors $H_{i 1}$ and $H_{i 2}$ 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. (3) yields the relation $x_{i}\left(q_{3}\right)=x_{i 0}\left(q_{3}\right)$, with $q_{3}=\tau$. Coordinates $q_{1}, q_{2}$ are Cartesian coordinates which specify uniquely the position of a point in the plane tangent to the wavefront, intersecting the reference ray $\Omega$ at the point specified by $q_{3}=\tau$.

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

$$
\begin{equation*}
H_{i m}=\frac{\partial x_{i}}{\partial q_{m}}, \quad \bar{H}_{i m}=\frac{\partial q_{i}}{\partial x_{m}} \tag{4}
\end{equation*}
$$

The elements satisfy the relation

$$
\begin{equation*}
\bar{H}_{m i} H_{i n}=\delta_{m n} \tag{5}
\end{equation*}
$$

Six elements of the transformation matrices are known from kinematic ray tracing:

$$
\begin{equation*}
H_{i 3}=\frac{\partial x_{i}}{\partial q_{3}}=\mathcal{U}_{i}, \quad \bar{H}_{3 i}=\frac{\partial q_{3}}{\partial x_{i}}=p_{i} \tag{6}
\end{equation*}
$$

From eqs (5) and (6), we obtain $p_{i} \mathcal{U}_{i}=1, p_{i} H_{i I}=0, \mathcal{U}_{i} \bar{H}_{I i}=0$. Thus, the vectors $H_{i I}$ are perpendicular to the slowness vector and the vectors $\bar{H}_{I i}$ are perpendicular to the ray-velocity vector.

In this paper, we shall specify the contravariant basis vectors $H_{i 1}(\tau)$ and $H_{i 2}(\tau)$ along the ray by a simple ordinary differential equation of the first order:

$$
\begin{equation*}
\mathrm{d} H_{i I} / \mathrm{d} \tau=-\left(H_{j I} \eta_{j}\right) p_{i} /\left(p_{k} p_{k}\right) \tag{7}
\end{equation*}
$$

In eq. (7), we used the relation $d p_{i} / d \tau=\eta_{i}$. Consequently, the vectors $H_{i I}(\tau)$ can be obtained by solving eq. (7) numerically along the ray $\Omega$. In this paper, we assume that the vectors $H_{i I}$ and $\mathcal{C} p_{i}$, where $\mathcal{C}$ denotes the phase velocity, have been chosen at a point $\tau_{0}$ of the ray $\Omega$ in such a way that they form a right-handed triplet of mutually perpendicular unit vectors. It can be proved that the vectors are then unit, mutually perpendicular and right handed along the whole ray. Thus, it is sufficient to compute only one of the vectors $H_{i I}$, say $H_{i 1}$, by solving numerically eq. (7). The vector $H_{i 2}$ can be calculated from known $H_{i 1}$ and $\mathcal{C} p_{i}$ at any point of the ray. Using relation $H_{i 3}=\mathcal{U}_{i}$ from eq. (6), we have the complete $3 \times 3$ matrix $\mathbf{H}$. The $3 \times 3$ matrix $\overline{\mathbf{H}}$ can be then determined by inversion of $\mathbf{H}$, see eq. (5).

Let us emphasize that the choice of $q_{3}=\tau$ simplifies considerably the computations as it leads to the following simple relations valid at any point of the ray $\Omega$ :

$$
\begin{equation*}
\frac{\partial T}{\partial q_{3}}=1, \quad \frac{\partial T}{\partial q_{I}}=0, \quad \frac{\partial^{2} T}{\partial q_{3} \partial q_{i}}=0 \tag{8}
\end{equation*}
$$

These simple relations are not valid for any other monotonic parameter (e.g., the arclength) along the ray. This is important to emphasize since the arclength along the ray has been mostly used in ray-centred coordinates in heterogeneous isotropic media. In this respect, our treatment differs from common treatment in isotropic media.

We now introduce six quantities $Q_{n}^{(q)}$ and $P_{n}^{(q)}(n=1,2,3)$ on the ray by the relations

$$
\begin{equation*}
Q_{n}^{(q)}=\partial q_{n} / \partial \gamma, \quad P_{n}^{(q)}=\partial p_{n}^{(q)} / \partial \gamma, \tag{9}
\end{equation*}
$$

where $\gamma$ is a chosen ray parameter and $p_{n}^{(q)}=\partial T / \partial q_{n}$. The expressions for $Q_{n}^{(q)}$ and $P_{n}^{(q)}$ show how $q_{n}$ and $p_{n}^{(q)}$ change when the ray parameter $\gamma$ changes. The quantities $Q_{3}^{(q)}$ and $P_{3}^{(q)}$ are available from the ray tracing, but $Q_{N}^{(q)}$ and $P_{N}^{(q)}$ must be computed by solving a system of ordinary differential equations of the first order along the ray $\Omega$, called dynamic ray tracing (DRT) system. The DRT system in ray-centred coordinates consists of four equations:

$$
\begin{align*}
\frac{\mathrm{d} Q_{N}^{(q)}}{\mathrm{d} \tau} & =A_{N M}^{(q)} Q_{M}^{(q)}+B_{N M}^{(q)} P_{M}^{(q)} \\
\frac{\mathrm{d} P_{N}^{(q)}}{\mathrm{d} \tau} & =-C_{N M}^{(q)} Q_{M}^{(q)}-D_{N M} P_{M}^{(q)} \tag{10}
\end{align*}
$$

where

$$
\begin{align*}
& A_{N M}^{(q)}=\bar{H}_{N i} H_{j M} A_{i j}-d_{N M}, \quad B_{N M}^{(q)}=\bar{H}_{N i} \bar{H}_{M j} B_{i j} \\
& C_{N M}^{(q)}=H_{i N} H_{j M}\left(C_{i j}-\eta_{i} \eta_{j}\right), \quad D_{N M}^{(q)}=H_{i N} \bar{H}_{M j} D_{i j}-d_{M N} \tag{11}
\end{align*}
$$

The $3 \times 3$ matrices $\mathbf{A}, \mathbf{B}, \mathbf{C}$ and $\mathbf{D}$ with elements $A_{i j}, B_{i j}, C_{i j}$ and $D_{i j}$ represent the second derivatives of the Hamiltionians:

$$
\begin{align*}
A_{i j} & =\frac{\partial^{2} \mathcal{H}}{\partial p_{i} \partial x_{j}}, \quad B_{i j}=\frac{\partial^{2} \mathcal{H}}{\partial p_{i} \partial p_{j}} \\
C_{i j} & =\frac{\partial^{2} \mathcal{H}}{\partial x_{i} \partial p_{j}}, \quad D_{i j}=\frac{\partial^{2} \mathcal{H}}{\partial x_{i} \partial p_{j}} \tag{12}
\end{align*}
$$

Note that $D_{i j}=A_{j i}$. The symbol $d_{N M}$ in (11) denotes

$$
\begin{equation*}
d_{N M}=\bar{H}_{N i} \mathrm{~d} H_{i M} / \mathrm{d} \tau=-\left(\bar{H}_{N i} p_{i}\right)\left(H_{j M} \eta_{j}\right) /\left(p_{k} p_{k}\right) . \tag{13}
\end{equation*}
$$

The same DRT system (10) can be used if we consider two ray parameters $\gamma_{1}, \gamma_{2}$ (orthonomic system of rays). In this case, we compute the $2 \times 2$ matrices $\mathbf{Q}^{(q)}$ and $\mathbf{P}^{(q)}$, with elements $Q_{I J}^{(q)}=\partial q_{I} / \partial \gamma_{J}, P_{I J}^{(q)}=\partial p_{I}^{(q)} / \partial \gamma_{J}$, with $I=1,2, J=1,2$. The DRT system (10) must be then solved twice (eight equations must be solved).

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

$$
\begin{equation*}
M_{I J}^{(q)}=\partial^{2} T / \partial q_{I} \partial q_{J} \tag{14}
\end{equation*}
$$

The $2 \times 2$ matrix $\mathbf{M}^{(q)}$ can be easily expressed in terms of $2 \times 2$ matrices $\mathbf{Q}^{(q)}$ and $\mathbf{P}^{(q)}$ as follows:

$$
\begin{equation*}
\mathbf{M}^{(q)}=\mathbf{P}^{(q)}\left(\mathbf{Q}^{(q)}\right)^{-1} \tag{15}
\end{equation*}
$$

Once the DRT system $(10)$ for $Q_{I J}^{(q)}(\tau)$ and $P_{I J}^{(q)}(\tau)$ is solved along the ray $\Omega$ and $M_{I J}^{(q)}(\tau)$ is determined using (15), we can write the quadratic expansion for paraxial travel time $T\left(q_{i}\right)$ in the vicinity of the ray $\Omega$ :

$$
\begin{equation*}
T\left(q_{1}, q_{2}, q_{3}\right)=T\left(q_{3}\right)+\frac{1}{2} \mathbf{q} \mathbf{M}^{(q)}\left(q_{3}\right) \mathbf{q}^{T} \tag{16}
\end{equation*}
$$

where $\mathbf{q}=\left(q_{1}, q_{2}\right)$ and $T\left(q_{3}\right)=T\left(\mathbf{q}=0, q_{3}\right)$. Equation (16) plays a basic role in the paraxial ray method, in the computation of paraxial approximation of the displacement vector and in the theory of Gaussian beams, etc. It gives the paraxial travel time (possibly complex valued) in the plane tangent to the wavefront at the point of its intersection with the ray $\Omega$.

The disadvantage of the expression (16) is that it can be used only in planes tangent to the wavefronts at $\Omega$. Thus, if we wish to determine the paraxial travel time at a point $R\left(q_{1}, q_{2}, \tau\right)$ situated in a vicinity of the ray $\Omega$, we must first find the relevant plane tangent to the wavefront at the point $\tau$ on the ray $\Omega$. The relevant value of $\tau$ is, however, not known. Its determination might be a cumbersome procedure.

The procedure could be considerably simplified if the $3 \times 3$ matrix $\mathbf{M}^{(x)}$ of the second derivatives of travel time with respect to Cartesian coordinates is known instead of the $2 \times 2$ matrix $\mathbf{M}^{(q)}$. Then it would be possible to compute simply the paraxial travel time field in the whole vicinity of the point $\tau$ on the ray $\Omega$, not only in the plane tangent 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.

## 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 $3 \times 3$ matrix $\mathbf{M}^{(x)}$ of second derivatives of the travel time field in Cartesian coordinates $x_{i}(i=1,2,3)$ and the $2 \times 2$ matrix $\mathbf{M}^{(q)}$ of second 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 the central ray $\Omega$. We assume that the vectors $\mathbf{p}, \boldsymbol{\eta}$ and $\boldsymbol{U}$ are known from ray tracing. For $\partial^{2} T / \partial x_{i} \partial x_{j}$, we can write

$$
\begin{equation*}
\frac{\partial^{2} T}{\partial x_{i} \partial x_{j}}=\frac{\partial}{\partial x_{i}}\left(\frac{\partial T}{\partial x_{j}}\right)=\frac{\partial}{\partial x_{i}}\left(\frac{\partial T}{\partial q_{n}} \frac{\partial q_{n}}{\partial x_{j}}\right) . \tag{17}
\end{equation*}
$$

This equation yields

$$
\begin{equation*}
\frac{\partial^{2} T}{\partial x_{i} \partial x_{j}}=\frac{\partial}{\partial x_{i}}\left(\frac{\partial T}{\partial q_{n}}\right) \frac{\partial q_{n}}{\partial x_{j}}+\frac{\partial T}{\partial q_{n}} \frac{\partial^{2} q_{n}}{\partial x_{i} \partial x_{j}} . \tag{18}
\end{equation*}
$$

Along the central ray, $\partial T / \partial q_{n}=\delta_{n 3}$, see (8). Performing the differentiation in the first term in (18), we obtain

$$
\begin{equation*}
\frac{\partial^{2} T}{\partial x_{i} \partial x_{j}}=\frac{\partial q_{m}}{\partial x_{i}} \frac{\partial^{2} T}{\partial q_{n} \partial q_{m}} \frac{\partial q_{n}}{\partial x_{j}}+\frac{\partial^{2} q_{3}}{\partial x_{i} \partial x_{j}} . \tag{19}
\end{equation*}
$$

Now we split the summation over $n=1,2,3$ in (19) in the summation over $n=N$ and $n=3$, and analogously the summation over $m$. We obtain

$$
\begin{gather*}
\frac{\partial^{2} T}{\partial x_{i} \partial x_{j}}=\frac{\partial q_{M}}{\partial x_{i}} \frac{\partial^{2} T}{\partial q_{M} \partial q_{N}} \frac{\partial q_{N}}{\partial x_{j}}+\frac{\partial q_{m}}{\partial x_{i}} \frac{\partial^{2} T}{\partial q_{m} \partial q_{3}} \frac{\partial q_{3}}{\partial x_{j}} \\
+\frac{\partial q_{3}}{\partial x_{i}} \frac{\partial^{2} T}{\partial q_{3} \partial q_{n}} \frac{\partial q_{n}}{\partial x_{j}}-\frac{\partial q_{3}}{\partial x_{i}} \frac{\partial^{2} T}{\partial q_{3} \partial q_{3}} \frac{\partial q_{3}}{\partial x_{j}}+\frac{\partial^{2} q_{3}}{\partial x_{i} \partial x_{j}} . \tag{20}
\end{gather*}
$$

Taking into account eq.(8) we obtain

$$
\begin{equation*}
\frac{\partial^{2} T}{\partial x_{i} \partial x_{j}}=\frac{\partial q_{M}}{\partial x_{i}} \frac{\partial^{2} T}{\partial q_{M} \partial q_{N}} \frac{\partial q_{N}}{\partial x_{j}}+\frac{\partial^{2} q_{3}}{\partial x_{i} \partial x_{j}} . \tag{21}
\end{equation*}
$$

The result (21) is surprisingly simple, indeed. 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

$$
\begin{equation*}
\frac{\partial}{\partial x_{i}}\left(\frac{\partial q_{3}}{\partial x_{k}} \frac{\partial x_{k}}{\partial q_{m}}\right)=0 . \tag{22}
\end{equation*}
$$

This relation yields

$$
\begin{equation*}
\frac{\partial^{2} q_{3}}{\partial x_{i} \partial x_{k}} \frac{\partial x_{k}}{\partial q_{m}}+\frac{\partial q_{3}}{\partial x_{k}} \frac{\partial}{\partial x_{i}}\left(\frac{\partial x_{k}}{\partial q_{m}}\right)=0 . \tag{23}
\end{equation*}
$$

Multiplying (23) by $\partial q_{m} / \partial x_{j}$, we obtain

$$
\begin{equation*}
\frac{\partial^{2} q_{3}}{\partial x_{i} \partial x_{j}}=-\frac{\partial q_{m}}{\partial x_{j}} \frac{\partial q_{3}}{\partial x_{k}} \frac{\partial q_{n}}{\partial x_{i}} \frac{\partial^{2} x_{k}}{\partial q_{m} \partial q_{n}} . \tag{24}
\end{equation*}
$$

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

$$
\begin{align*}
\frac{\partial^{2} q_{3}}{\partial x_{i} \partial x_{j}} & =-\frac{\partial q_{M}}{\partial x_{j}} \frac{\partial q_{3}}{\partial x_{k}} \frac{\partial q_{N}}{\partial x_{i}} \frac{\partial^{2} x_{k}}{\partial q_{M} \partial q_{N}}-\frac{\partial q_{3}}{\partial x_{j}} \frac{\partial q_{3}}{\partial x_{k}} \frac{\partial q_{n}}{\partial x_{i}} \frac{\partial^{2} x_{k}}{\partial q_{3} \partial q_{n}} \\
& -\frac{\partial q_{m}}{\partial x_{j}} \frac{\partial q_{3}}{\partial x_{k}} \frac{\partial q_{3}}{\partial x_{i}} \frac{\partial^{2} x_{k}}{\partial q_{m} \partial q_{3}}+\frac{\partial q_{3}}{\partial x_{j}} \frac{\partial q_{3}}{\partial x_{k}} \frac{\partial q_{3}}{\partial x_{i}} \frac{\partial^{2} x_{k}}{\partial q_{3} \partial q_{3}} . \tag{25}
\end{align*}
$$

Equation (25) can be further simplified if we use the obvious identity

$$
\begin{equation*}
\frac{\partial}{\partial q_{3}}\left(\frac{\partial q_{3}}{\partial x_{k}} \frac{\partial x_{k}}{\partial q_{m}}\right)=0 . \tag{26}
\end{equation*}
$$

Similarly as from (22), we obtain

$$
\begin{equation*}
\frac{\partial}{\partial q_{3}}\left(\frac{\partial q_{3}}{\partial x_{k}}\right) \frac{\partial x_{k}}{\partial q_{m}}+\frac{\partial q_{3}}{\partial x_{k}} \frac{\partial^{2} x_{k}}{\partial q_{3} \partial q_{m}}=0 . \tag{27}
\end{equation*}
$$

This yields

$$
\begin{equation*}
\frac{\partial q_{3}}{\partial x_{k}} \frac{\partial^{2} x_{k}}{\partial q_{3} \partial q_{m}}=-\eta_{k} \frac{\partial x_{k}}{\partial q_{m}} \tag{28}
\end{equation*}
$$

as $\partial\left(\partial q_{3} / \partial x_{k}\right) / \partial q_{3}=\partial p_{k} / \partial q_{3}=\eta_{k}$. Inserting (28) into (25), and taking into account that the first term in (25) 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

$$
\begin{equation*}
\frac{\partial^{2} q_{3}}{\partial x_{i} \partial x_{j}}=\frac{\partial q_{3}}{\partial x_{j}} \frac{\partial q_{n}}{\partial x_{i}} \frac{\partial x_{k}}{\partial q_{n}} \eta_{k}+\frac{\partial q_{m}}{\partial x_{j}} \frac{\partial q_{3}}{\partial x_{i}} \frac{\partial x_{k}}{\partial q_{m}} \eta_{k}-\frac{\partial q_{3}}{\partial x_{j}} \frac{\partial q_{3}}{\partial x_{i}} \frac{\partial x_{k}}{\partial q_{3}} \eta_{k} . \tag{29}
\end{equation*}
$$

We now take into account that

$$
\begin{equation*}
\frac{\partial q_{3}}{\partial x_{j}}=p_{j}, \quad \frac{\partial x_{k}}{\partial q_{3}}=\mathcal{U}_{k}, \quad \frac{\partial x_{k}}{\partial q_{n}} \frac{\partial q_{n}}{\partial x_{i}}=\delta_{k i}, \tag{30}
\end{equation*}
$$

see (5) and (6), and obtain from (29):

$$
\begin{equation*}
\frac{\partial^{2} q_{3}}{\partial x_{i} \partial x_{j}}=p_{i} \eta_{j}+p_{j} \eta_{i}-p_{i} p_{j}\left(\mathcal{U}_{k} \eta_{k}\right) \tag{31}
\end{equation*}
$$

Equations (19) and (31) yield the final equation for $\partial^{2} T / \partial x_{i} \partial x_{j}$ :

$$
\begin{equation*}
\frac{\partial^{2} T}{\partial x_{i} \partial x_{j}}=\frac{\partial q_{M}}{\partial x_{i}} \frac{\partial^{2} T}{\partial q_{M} \partial q_{N}} \frac{\partial q_{N}}{\partial x_{j}}+p_{i} \eta_{j}+p_{j} \eta_{i}-p_{i} p_{j} \mathcal{U}_{k} \eta_{k} \tag{32}
\end{equation*}
$$

It may be useful to express the important equation (32) in the matrix form. Let us consider the matrices $\mathbf{H}$ and $\overline{\mathbf{H}}$, see eq. (4) defined along the ray $\Omega$. We denote the columns of the matrix $\mathbf{H}$, which represent contravariant basis vectors of the ray-centred coordinate system, by $\mathbf{e}_{i}$, and the lines of the matrix $\overline{\mathbf{H}}$, which represent covariant basis vectors, by $\mathbf{f}_{i}$ :

$$
\begin{equation*}
\mathbf{H}=\left(\mathbf{e}_{1}, \mathbf{e}_{2}, \mathbf{e}_{3}=\mathcal{U}\right), \quad \overline{\mathbf{H}}^{T}=\left(\mathbf{f}_{1}, \mathbf{f}_{2}, \mathbf{f}_{3}=\mathbf{p}\right) . \tag{33}
\end{equation*}
$$

The basis vectors $\mathbf{e}_{i}$ are tangential to the coordinate lines, and the basis vectors $\mathbf{f}_{i}$ are perpendicular to the coordinate surfaces. The vectors $\mathbf{e}_{i}$ and $\mathbf{f}_{j}$ satisfy the relation (5):

$$
\begin{equation*}
\mathbf{e}_{i}^{T} \mathbf{f}_{j}=\delta_{i j} \tag{34}
\end{equation*}
$$

Then the matrix form of eq. (32) reads

$$
\begin{equation*}
\mathbf{M}^{(x)}=\mathbf{f} \mathbf{M}^{(q)} \mathbf{f}^{T}+\mathbf{p} \boldsymbol{\eta}^{T}+\boldsymbol{\eta} \mathbf{p}^{T}-\mathbf{p}\left(\boldsymbol{\mathcal { U }}^{T} \boldsymbol{\eta}\right) \mathbf{p}^{T} \tag{35}
\end{equation*}
$$

Here $\mathbf{f}=\left(\mathbf{f}_{1}, \mathbf{f}_{2}\right)$ is the $3 \times 2$ matrix with column vectors $\mathbf{f}_{1}$ and $\mathbf{f}_{2}$. The vectors $\mathbf{f}_{I}$ are perpendicular to the ray $\Omega$.

## 4 Concluding remarks

Equations (32) or (35) play a very important role in the paraxial ray methods, particularly in the computation of paraxial travel time, paraxial approximation of the displacement vector and Gaussian beams. See more details in Cervený and Pšenčík (2009).

For dynamic ray tracing in ray-centred coordinates, eqs (32) or (35) are very useful when we wish to find the paraxial travel time at an arbitrary point, specified in Cartesian coordinates, in the vicinity of the reference ray.

For dynamic ray tracing in Cartesian coordinates, eqs (32) or (35) are useful for the specification of the initial conditions. The specification of the initial conditions for $\mathbf{M}^{(x)}$ is very simple if we express $\mathbf{M}^{(x)}$ in terms of $\mathbf{M}^{(q)}$, for which it has a very simple physical meaning.

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