Transformation of spatial and perturbation derivatives of travel time at a curved interface between two arbitrary media

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ABSTRACT

We consider the partial derivatives of travel time with respect to both spatial coordinates and perturbation parameters. These derivatives are very important in studying wave propagation and have already found various applications in smooth media without interfaces. In order to extend the applications to media composed of layers and blocks, we derive the explicit equations for transforming these travel–time derivatives of arbitrary orders at a general smooth curved interface between two arbitrary media. The equations are applicable to both real–valued and complex–valued travel time. The equations are expressed in terms of a general Hamiltonian function and are applicable to the transformation of travel–time derivatives in both isotropic and anisotropic media. The interface is specified by an implicit equation. No local coordinates are needed for the transformation.

Keywords: ray theory, Hamilton–Jacobi equation, eikonal equation, travel time (action), spatial derivatives of travel time, perturbation derivatives of travel time, reflection or refraction at curved interfaces, anisotropy, bianisotropy, heterogeneous media, paraxial approximation, Gaussian beams, wave propagation

1. INTRODUCTION

Travel time, also referred to as action, is a function of spatial coordinates. The spatial coordinates may be arbitrary, including curvilinear coordinates. Travel time satisfies a general partial differential equation of the first order, called the Hamilton–Jacobi equation. For example, various eikonal equations represent important special cases of the Hamilton–Jacobi equation.

Travel time may also depend on one or more perturbation parameters, which parametrize the Hamilton–Jacobi equation. The partial derivatives of travel time with respect to spatial coordinates are referred to as spatial derivatives, whereas the partial derivatives of travel time with respect to perturbation parameters are referred to as perturbation derivatives.

In smooth media, travel time and its first–order spatial derivatives can be calculated by solving the non–linear ordinary differential equations for rays (geodesics) derived by *Hamilton (1837)* and called Hamilton's equations (equations of geodesics, ray–tracing equations). The first–order spatial derivatives of travel time (the components of the slowness vector, called the components of normal slowness by Hamilton) can be transformed at smooth curved interfaces using Snell's law in the form derived by *Hamilton (1837, Eq.* C^7*)*.

In smooth media, the second–order spatial derivatives of travel time can be calculated along the rays by solving the linear ordinary differential equations derived by *Červený (1972)*. The second–order spatial derivatives of travel time can be transformed at smooth curved interfaces using the equation derived by *Hamilton (1837, Eq.* V^7*)*.

In smooth media, the third–order and higher–order spatial derivatives of travel time and all perturbation derivatives of travel time can be calculated along the unperturbed rays by simple numerical quadratures using the equations derived by *Klimeš (2002a)*. These equations have already found various applications (*Duchkov and Goldin, 2001*; *Klimeš, 2002b, 2006, 2013*; *Bulant and Klimeš, 2002, 2008*; *Goldin and Duchkov, 2003*; *Klimeš and Bulant, 2004, 2006, 2012, 2014, 2015, 2016*; *Červený et al., 2008*; *Červený and Pšenčík, 2009*; *Klimeš and Klimeš, 2011*; *Shekar and Tsvankin, 2014*; *Zheng, 2010*), and it is desirable to extend the equations and their applications to media composed of layers and blocks separated by smooth curved interfaces. The perturbation derivatives are especially important for the coupling ray theory and for travel–time inversion. The spatial fourth–order derivatives of travel time are necessary for calculating the first–order term of the ray series in order to estimate the inaccuracy of the zero–order ray theory. The fourth–order and higher–order derivatives of travel time are essential for studying the paraxial Super–Gaussian beams (*Klimeš, 2013*).

In this paper, we thus derive the explicit equations for transforming any spatial and perturbation derivatives of travel time at a general smooth curved interface between two arbitrary media. The equations are applicable to both real–valued and complex–valued travel time. The equations are expressed in terms of a general Hamiltonian function and are applicable to travel–time derivatives of arbitrary orders in smooth heterogeneous media, both isotropic and arbitrarily anisotropic or bianisotropic. The interface represents the surface at which the Hamiltonian function or its partial derivatives may be discontinuous. The interface is specified by an implicit equation. No local coordinates are needed for the transformation of travel–time derivatives.

We follow the approach of *Hamilton (1837)*. Section 2 is devoted to the specification of the problem and to the description of the notation used hereinafter for partial derivatives. The derivation of equations for transforming the first–order and second–order derivatives of travel time in Sections 3 and 4 follows the corresponding derivation by *Hamilton (1837)*, but it is generalized towards perturbation derivatives and mixed spatial–perturbation derivatives.

The derivation is then extended to the transformation of the third–order and fourth–order derivatives of travel time in Sections 5 and 6. The equations for transforming any higher–order spatial and perturbation derivatives of travel time at a curved interface between two arbitrary media are given in Section 7.

We present three examples of application of the proposed transformation relations in Section 8 in order to illustrate the notation used and the equations derived.

We use the componental notation for vectors and matrices. For example, p_i stands for the covariant vector with components p_i. The Einstein summation over repetitive indices is used throughout the paper.

2. TRAVEL TIME AT A SMOOTH INTERFACE

Travel time $\tau(x^i, f^\alpha)$ is a function of spatial coordinates x^i, and may also depend on one or several perturbation parameters f^α. We consider a smooth interface implicitly described by equation (*Hamilton, 1837, Eq.* B[7])

$$F(x^i, f^\alpha) = 0 \ . \tag{1}$$

The interface represents the surface at which the Hamiltonian function or its partial derivatives of an arbitrary order may be discontinuous. Note that perturbation derivatives $F_{,\alpha}$ describe perturbations of the interface.

We denote the incident travel time by $\widetilde{\tau}(x^i, f^\alpha)$. It satisfies the Hamilton–Jacobi equation (*Hamilton, 1837, Eq.* C)

$$\widetilde{H}\big(x^i, \widetilde{\tau}_{,j}(x^m, f^\mu), f^\alpha\big) = \widetilde{C} \ , \tag{2}$$

where Hamiltonian function $\widetilde{H} = \widetilde{H}(x^i, p_j, f^\alpha)$ and constant $\widetilde{C}$ are given, but we do not need this equation, because the incident travel time and its spatial and perturbation derivatives are assumed to be known along the interface.

The transformed travel time $\tau(x^i, f^\alpha)$ satisfies the Hamilton–Jacobi equation (*Hamilton, 1837, Eq.* F[7])

$$H\big(x^i, \tau_{,j}(x^m, f^\mu), f^\alpha\big) = C \ , \tag{3}$$

where Hamiltonian function $H = H(x^i, p_j, f^\alpha)$ and constant C are given. The domains for solving Hamilton–Jacobi equations (2) and (3) are situated on the same side of the interface if travel time $\tau(x^i, f^\alpha)$ corresponds to a reflected wave, and on the opposite sides if travel time $\tau(x^i, f^\alpha)$ corresponds to a refracted wave. The positions of the domain for solving Hamilton–Jacobi equation (3) should be prescribed uniquely by the ray code (*Červený et al., 1988, Sec. 4*; *Červený, 2001, Sec. 3.2.2*).

The transformed travel time must be equal to the incident travel time along the interface (*Hamilton, 1837, Eq.* A[7]),

$$\tau(x^i, f^\alpha) = \widetilde{\tau}(x^i, f^\alpha) \tag{4}$$

for x^i satisfying constraint (1). Condition (4) thus represents the initial conditions for Hamilton–Jacobi equation (3). We have to seek expressions for the spatial and perturbation derivatives of the transformed travel time τ in terms of the spatial and perturbation derivatives of the incident travel time $\widetilde{\tau}$.

Hamiltonian function $H = H(x^i, p_j, f^\alpha)$ is a function of spatial coordinates x^i, of slowness–vector components p_i, and may also depend on one or several perturbation parameters f^α. We use notation

$$H^{,a\ldots f}_{,i\ldots n\alpha\ldots\nu} = \frac{\partial}{\partial p_a}\cdots\frac{\partial}{\partial p_f}\frac{\partial}{\partial x^i}\cdots\frac{\partial}{\partial x^n}\frac{\partial}{\partial f^\alpha}\cdots\frac{\partial}{\partial f^\nu}H \tag{5}$$

for the partial derivatives of the Hamiltonian function, and the analogous notation for the partial derivatives of other functions such as $F(x^i, f^\alpha)$, $\widetilde{\tau}(x^i, f^\alpha)$, $\tau(x^i, f^\alpha)$.

The equations for the transformation of perturbation derivatives of travel time have the same form as the equations for the transformation of spatial derivatives of travel time. We thus unify spatial coordinates x^i with perturbation parameters f^α and denote these extended coordinates by $x^{\underline{i}}$,

$$x^{\underline{i}} = (x^i, f^\alpha) \ . \tag{6}$$

Extended coordinate $x^{\underline{i}}$ represents both x^i and f^α. Derivative $H_{,\underline{i}}$ represents both $H_{,i}$ and $H_{,\alpha}$, derivative $H_{,\underline{ij}}$ represents $H_{,ij}$, $H_{,\alpha j}$, $H_{,i\beta}$ and $H_{,\alpha\beta}$, etc., and analogously for other functions.

3. TRANSFORMATION OF THE FIRST–ORDER DERIVATIVES OF TRAVEL TIME

Condition (4) means that interface (1) should simultaneously represent the zero isosurface of function $\tau(x^i, f^\alpha) - \widetilde{\tau}(x^i, f^\alpha)$, whose gradient should thus be a multiple of the gradient of function $F(x^i, f^\alpha)$. We shall refer to the corresponding factor as the Lagrange multiplier.

We differentiate condition (4) with respect to x^i and f^α under constraint (1). We obtain Snell's law (*Hamilton, 1837, Eq.* C[7])

$$\tau_{,i} = \widetilde{\tau}_{,i} + F_{,i}\,\lambda \tag{7}$$

and analogous law

$$\tau_{,\alpha} = \widetilde{\tau}_{,\alpha} + F_{,\alpha}\,\lambda \tag{8}$$

for perturbation derivatives. Here $\lambda = \lambda(x^m, f^\mu)$ is the Lagrange multiplier defined for x^i satisfying constraint (1). Note that perturbation derivatives $F_{,\alpha}$ describe perturbations of the interface.

Since the transformed travel time τ must satisfy Hamilton–Jacobi equation (3), the Lagrange multiplier can be calculated from non–linear, usually algebraic, equation

$$\boxed{H\big(x^i, \widetilde{\tau}_{,j} + F_{,j}\,\lambda, f^\mu\big) = C \ .} \tag{9}$$

Note that the Hamiltonian function used in Eq. equation (9) is often different from the Hamiltonian function used in Hamilton's equations for rays, especially in anisotropic or bianisotropic media. In this way, the Hamiltonian function used in Eq. (9) is often different from the Hamiltonian function used in all other transformation equations for the spatial and perturbation derivatives of travel time.

For example, in wave propagation in anisotropic or bianisotropic media, various functions of the eigenvalues of the Kelvin–Christoffel matrix may be used as the Hamiltonian function in Hamilton's equations and in the transformation equations for the derivatives of travel time, whereas the determinant of the Kelvin–Christoffel matrix is used as the Hamiltonian function in Eq. (9).

Equation (9) usually has several solutions λ, which correspond to different kinds of the transformed travel time. Only half of the solutions usually correspond to the given side of the interface, i.e. to the correct sign of $H^{,q}F_{,q}$. The Lagrange multiplier should be properly selected from the solutions of Eq. (9). The selection should be prescribed uniquely by the ray code (*Červený et al., 1988, Sec. 4*; *Červený, 2001, Sec. 3.2.2*). Note that the ray code may even prescribe termination of tracing rays and calculating travel time in some cases, e.g., for imaginary solution λ in real–valued coordinates x^i.

The selected Lagrange multiplier λ can then be inserted into Snell's law (7) and transformation equation (8), which may be expressed in common form

$$\boxed{\tau_{,\underline{i}} = \widetilde{\tau}_{,\underline{i}} + F_{,\underline{i}}\,\lambda \ , \qquad (10)}$$

where the underlined lower–case subscripts represent both the lower–case and Greek subscripts.

4. TRANSFORMATION OF THE SECOND–ORDER DERIVATIVES OF TRAVEL TIME

We apply an analogous approach to that in the previous section, but now to condition (10) rather than to condition (4). For each subscript $\underline{i}$, we differentiate condition (10) with respect to $x^{\underline{j}}$ under constraint (1) and obtain condition (*Hamilton, 1837, Eq.* R^7)

$$\tau_{,\underline{i}\underline{j}} = \widetilde{\tau}_{,\underline{i}\underline{j}} + F_{,\underline{i}\underline{j}}\,\lambda + F_{,\underline{i}}\,\lambda_{,\underline{j}} + F_{,\underline{j}}\,\lambda_{\underline{i}} \ , \tag{11}$$

where $\lambda_{\underline{i}} = \lambda_{\underline{i}}(x^m, f^\mu)$ is the corresponding Lagrange multiplier. These Lagrange multipliers are defined for x^m satisfying constraint (1).

We introduce projection operator

$$N_{\underline{i}\underline{j}} = (F_{,\underline{r}}F_{,\underline{r}})^{-1}F_{,\underline{i}}F_{,\underline{j}} \tag{12}$$

onto the normal to the interface, and projection operator

$$E_{\underline{i}\underline{j}} = \delta_{\underline{i}\underline{j}} - N_{\underline{i}\underline{j}} \tag{13}$$

onto the plane tangent to the interface. Since $\tau_{,\underline{i}\underline{j}}$ is symmetric with respect to its subscripts,

$$N_{\underline{a}\underline{i}}E_{\underline{b}\underline{j}}\tau_{,\underline{i}\underline{j}} = N_{\underline{a}\underline{i}}E_{\underline{b}\underline{j}}\tau_{,\underline{j}\underline{i}} \ . \tag{14}$$

We insert Eq. (11) into Eq. (14), and arrive at

$$E_{\underline{a}\underline{j}}\lambda_{,\underline{j}} = E_{\underline{a}\underline{j}}\lambda_{\underline{j}} \ . \tag{15}$$

Since $N_{\underline{a}\underline{j}}\lambda_{,\underline{j}}$ is not defined by Eq. (9), we may put

$$N_{\underline{a}\underline{j}}\lambda_{,\underline{j}} = N_{\underline{a}\underline{j}}\lambda_{\underline{j}} \ . \tag{16}$$

The summation of Eqs (15) and (16) yields

$$\lambda_{,\underline{i}} = \lambda_{\underline{i}} \ , \tag{17}$$

and condition (11) reads

$$\boxed{\tau_{,\underline{i}\underline{j}} = T_{\underline{i}\underline{j}} + F_{,\underline{i}}\,\lambda_{\underline{j}} + F_{,\underline{j}}\,\lambda_{\underline{i}} \ ,} \tag{18}$$

where the values of

$$\boxed{T_{\underline{i}\underline{j}} = \widetilde{\tau}_{,\underline{i}\underline{j}} + F_{,\underline{i}\underline{j}}\,\lambda} \tag{19}$$

are known. Lagrange multiplier λ is determined by Eq. (9), and is used in transformation relation (10) for the first–order derivatives.

We differentiate Hamilton–Jacobi equation (3) with respect to $x^{\underline{i}}$ (*Hamilton, 1837, Eq.* T[7]),

$$H_{,\underline{i}} + H^{,r}\tau_{,r\underline{i}} = 0 \ . \tag{20}$$

We insert Eg. (18) into Eq. (20), and arrive at (*Hamilton, 1837, Eq.* U[7])

$$H_{,\underline{i}} + H^{,r}T_{r\underline{i}} + F_{,\underline{i}}H^{,r}\lambda_r + H^{,r}F_{,r}\,\lambda_{\underline{i}} = 0 \ . \tag{21}$$

We formally define

$$H^{,\alpha} = 0 \ , \tag{22}$$

and express identity (21) as

$$\big(H^{,r}F_{,r}\delta^{\underline{a}}_{\underline{i}} + F_{,\underline{i}}H^{,\underline{a}}\big)\lambda_{\underline{a}} = -S_{\underline{i}} \ , \tag{23}$$

where

$$\boxed{S_{\underline{i}} = H_{,\underline{i}} + H^{,r}T_{r\underline{i}} \ .} \tag{24}$$

The inverse matrix to

$$\big(H^{,r}F_{,r}\delta^{\underline{a}}_{\underline{i}} + F_{,\underline{i}}H^{,\underline{a}}\big) \tag{25}$$

is

$$(H^{,q}F_{,q})^{-1}\big[\delta^{\underline{i}}_{\underline{a}} - (2H^{,s}F_{,s})^{-1}F_{,\underline{a}}H^{,\underline{i}}\big] \ . \tag{26}$$

Then

$$\lambda_{\underline{a}} = -(H^{,q}F_{,q})^{-1}\big[\delta^{\underline{i}}_{\underline{a}} - (2H^{,s}F_{,s})^{-1}F_{,\underline{a}}H^{,\underline{i}}\big]S_{\underline{i}} \ , \tag{27}$$

which may also be expressed as

$$\lambda_{\underline{i}} = -(H^{,q}F_{,q})^{-1}S_{\underline{i}} + \tfrac{1}{2}(H^{,q}F_{,q})^{-2}F_{,\underline{i}}\,H^{,r}S_r \ . \tag{28}$$

We normalize $F_{,\underline{i}}$ so that its scalar product with $H^{,i}$ is unity,

$$\boxed{N_{\underline{i}} = (H^{,q}F_{,q})^{-1}F_{,\underline{i}} \ .} \tag{29}$$

Relation (28) then reads

$$\boxed{\lambda_{\underline{i}} = (H^{,q}F_{,q})^{-1}\left(-S_{\underline{i}} + \tfrac{1}{2}N_{\underline{i}}\,H^{,r}S_r\right) \; . \qquad (30)}$$

Relation (18) with Eqs (19) and (28) represents the explicit equation for the transformation of the second–order derivatives of travel time at a curved interface between two arbitrary media.

Transformation relation (18) with inserted Lagrange multipliers (28) reads

$$\tau_{,\underline{i}\underline{j}} = T_{\underline{i}\underline{j}} - (H^{,q}F_{,q})^{-1}\left[F_{,\underline{i}}S_{\underline{j}} + F_{,\underline{j}}S_{\underline{i}} - (H^{,p}F_{,p})^{-1}F_{,\underline{i}}F_{,\underline{j}}\,H^{,r}S_r\right] \qquad (31)$$

(*Hamilton, 1837, Eq.* V^7), where $S_{\underline{i}}$ is given by Eq. (24). Transformation relation (31) may be expressed more concisely in terms of normalized gradient (29),

$$\tau_{,\underline{i}\underline{j}} = T_{\underline{i}\underline{j}} - N_{\underline{i}}S_{\underline{j}} - N_{\underline{j}}S_{\underline{i}} + N_{\underline{i}}N_{\underline{j}}\,H^{,r}S_r \; . \qquad (32)$$

This transformation relation could also be obtained directly from transformation relation (18) with Eqs (29) and (30).

5. TRANSFORMATION OF THE THIRD–ORDER DERIVATIVES OF TRAVEL TIME

We differentiate condition (11) with respect to $x^{\underline{k}}$ under constraint (1) and obtain condition

$$\tau_{,\underline{i}\underline{j}\underline{k}} = \widetilde{\tau}_{,\underline{i}\underline{j}\underline{k}} + F_{,\underline{i}\underline{j}\underline{k}}\,\lambda + F_{,\underline{i}\underline{j}}\,\lambda_{,\underline{k}} + F_{,\underline{i}\underline{k}}\,\lambda_{,\underline{j}} + F_{,\underline{j}\underline{k}}\,\lambda_{\underline{i}} + F_{,\underline{i}}\,\lambda_{,\underline{j}\underline{k}} + F_{,\underline{j}}\,\lambda_{\underline{i},\underline{k}} + F_{,\underline{k}}\,\lambda_{\underline{i}\underline{j}} \; , \quad (33)$$

where $\lambda_{\underline{i}\underline{j}} = \lambda_{\underline{i}\underline{j}}(x^m, f^\mu)$ is the corresponding Lagrange multiplier. These Lagrange multipliers are defined for x^m satisfying constraint (1).

Since $\tau_{,\underline{i}\underline{j}\underline{k}}$ is symmetric with respect to its subscripts,

$$N_{\underline{a}\underline{j}}E_{\underline{b}\underline{k}}\tau_{,\underline{i}\underline{j}\underline{k}} = N_{\underline{a}\underline{j}}E_{\underline{b}\underline{k}}\tau_{,\underline{i}\underline{k}\underline{j}} \; . \qquad (34)$$

We insert condition (33) into relation (34), and arrive at

$$E_{\underline{a}\underline{k}}\lambda_{\underline{i},\underline{k}} = E_{\underline{a}\underline{k}}\lambda_{\underline{i}\underline{k}} \; . \qquad (35)$$

Since $N_{\underline{a}\underline{k}}\lambda_{\underline{i},\underline{k}}$ is not defined, we may put

$$N_{\underline{a}\underline{k}}\lambda_{\underline{i},\underline{k}} = N_{\underline{a}\underline{k}}\lambda_{\underline{i}\underline{k}} \; . \qquad (36)$$

The summation of conditions (35) and (36) yields

$$\lambda_{\underline{i},\underline{j}} = \lambda_{\underline{i}\underline{j}} \; . \qquad (37)$$

We insert Eqs (17) and (37) into condition (33),

$$\boxed{\tau_{,\underline{i}\underline{j}\underline{k}} = T_{\underline{i}\underline{j}\underline{k}} + F_{,\underline{i}}\lambda_{\underline{j}\underline{k}} + F_{,\underline{j}}\lambda_{\underline{i}\underline{k}} + F_{,\underline{k}}\lambda_{\underline{i}\underline{j}} \; , \qquad (38)}$$

where the values of

$$\boxed{T_{\underline{i}\underline{j}\underline{k}} = \widetilde{\tau}_{,\underline{i}\underline{j}\underline{k}} + F_{,\underline{i}\underline{j}\underline{k}}\,\lambda + F_{,\underline{i}\underline{j}}\,\lambda_{\underline{k}} + F_{,\underline{i}\underline{k}}\,\lambda_{\underline{j}} + F_{,\underline{j}\underline{k}}\,\lambda_{\underline{i}} \qquad (39)}$$

are known. Lagrange multiplier λ is determined by Eq. (9), and is used in transformation relation (10) for the first–order derivatives. Lagrange multipliers $\lambda_{\underline{i}}$ are given by relation (30), and are used in transformation relation (18) for the second–order derivatives.

We differentiate identity (20) with respect to $x^{\underline{j}}$,

$$H_{,\underline{i}\underline{j}} + H_{\underline{i}}^{;r}\tau_{,r\underline{j}} + H_{\underline{j}}^{;r}\tau_{,r\underline{i}} + H^{,rs}\tau_{,r\underline{i}}\tau_{,s\underline{j}} + H^{,r}\tau_{,r\underline{i}\underline{j}} = 0 \ . \tag{40}$$

We insert Eq. (38) into Eq. (40), and arrive at

$$H_{,\underline{i}\underline{j}}+H_{\underline{i}}^{;r}\tau_{,r\underline{j}}+H_{\underline{j}}^{;r}\tau_{,r\underline{i}}+H^{,rs}\tau_{,r\underline{i}}\tau_{,s\underline{j}}+H^{,r}T_{r\underline{i}\underline{j}}+F_{,\underline{i}}H^{,r}\,\lambda_{r\underline{j}}+F_{,\underline{j}}H^{,r}\,\lambda_{r\underline{i}}+H^{,r}F_{,r}\,\lambda_{\underline{i}\underline{j}} = 0 \ . \tag{41}$$

We express identity (41) as

$$H^{,r}F_{,r}\,\lambda_{\underline{i}\underline{j}} + F_{,\underline{i}}\,H^{,r}\lambda_{r\underline{j}} + F_{,\underline{j}}\,H^{,r}\lambda_{r\underline{i}} = -S_{\underline{i}\underline{j}} \ , \tag{42}$$

where

$$\boxed{S_{\underline{i}\underline{j}} = H_{,\underline{i}\underline{j}} + H_{\underline{i}}^{;r}\tau_{,r\underline{j}} + H_{\underline{j}}^{;r}\tau_{,r\underline{i}} + H^{,rs}\tau_{,r\underline{i}}\tau_{,s\underline{j}} + H^{,r}T_{r\underline{i}\underline{j}} \ .} \tag{43}$$

Analogously to solution (28) of Eq. (23), which has the form of

$$\lambda_{\underline{i}} = -(H^{,q}F_{,q})^{-1}S_{\underline{i}}+F_{,\underline{i}}A \ , \tag{44}$$

we shall search for the solution of Eq. (42) in the form

$$\lambda_{\underline{i}\underline{j}} = -(H^{,q}F_{,q})^{-1}S_{\underline{i}\underline{j}} + F_{,\underline{i}}A_{\underline{j}} + F_{,\underline{j}}A_{\underline{i}} + F_{,\underline{i}}F_{,\underline{j}}A \ . \tag{45}$$

Here we use unknowns A and $A_{\underline{i}}$ in Eq. (45) only locally, and A has no relation to A in Eq. (44). We insert Eq. (45) into Eq. (42),

$$\begin{aligned} &-S_{\underline{i}\underline{j}} - (H^{,q}F_{,q})^{-1}\big(F_{,\underline{i}}\,H^{,r}S_{r\underline{j}} + F_{,\underline{j}}\,H^{,r}S_{r\underline{i}}\big) \\ &\quad + 2H^{,r}F_{,r}\big(F_{,\underline{i}}A_{\underline{j}} + F_{,\underline{j}}A_{\underline{i}}\big) + F_{,\underline{i}}F_{,j}\,H^{,r}A_r + 3H^{,r}F_{,r}\,F_{,\underline{i}}F_{,j}A = -S_{\underline{i}\underline{j}} \ . \end{aligned} \tag{46}$$

We fit the terms with single gradient $F_{,i}$ by

$$A_{\underline{i}} = \tfrac{1}{2}(H^{,q}F_{,q})^{-2}H^{,r}S_{r\underline{i}} \ , \tag{47}$$

and then the terms with dyadic product $F_{,\underline{i}}F_{,\underline{j}}$ by

$$A = -\tfrac{2}{3}(H^{,q}F_{,q})^{-1}H^{,r}A_r = -\tfrac{1}{3}(H^{,q}F_{,q})^{-3}H^{,r}S_{rs}H^{,s} \ . \tag{48}$$

We insert Eqs (47) and (48) into Eq. (45) and obtain solution

$$\begin{aligned} \lambda_{\underline{i}\underline{j}} = -(H^{,q}F_{,q})^{-1}S_{\underline{i}\underline{j}} &+ \tfrac{1}{2}(H^{,s}F_{,s})^{-2}\big(F_{,\underline{i}}\,H^{,r}S_{r\underline{j}} + F_{,\underline{j}}\,H^{,r}S_{r\underline{i}}\big) \\ &- \tfrac{1}{3}(H^{,q}F_{,q})^{-3}F_{,\underline{i}}F_{,\underline{j}}\,H^{,r}S_{rs}H^{,s} \end{aligned} \tag{49}$$

of Eq. (42). Relation (49) may be expressed more concisely in terms of normalized gradient (29),

$$\boxed{\lambda_{\underline{i}\underline{j}} = (H^{,q}F_{,q})^{-1}\left[-\,S_{\underline{i}\underline{j}} + \tfrac{1}{2}\big(N_{\underline{i}}\,H^{,r}S_{r\underline{j}} + N_{\underline{j}}\,H^{,r}S_{r\underline{i}}\big) - \tfrac{1}{3}N_{\underline{i}}N_{\underline{j}}\,H^{,r}S_{rs}H^{,s}\right] \ ,} \tag{50}$$

where $S_{\underline{i}\underline{j}}$ is given by definition (43). Relation (38) with Eqs (39) and (50) represents the explicit equation for the transformation of the third–order derivatives of travel time at a curved interface between two arbitrary media.

Note that transformation relation (38) with inserted Lagrange multipliers (50) reads

$$\begin{aligned}\tau_{,\underline{i}\underline{j}\underline{k}} = T_{\underline{i}\underline{j}\underline{k}} &- N_{\underline{i}} S_{\underline{j}\underline{k}} - N_{\underline{j}} S_{\underline{i}\underline{k}} - N_{\underline{k}} S_{\underline{i}\underline{j}} \\ &+ N_{\underline{i}} N_{\underline{j}} H^{,r} S_{r\underline{k}} + N_{\underline{i}} N_{\underline{k}} H^{,r} S_{r\underline{j}} + N_{\underline{j}} N_{\underline{k}} H^{,r} S_{r\underline{i}} \\ &- N_{\underline{i}} N_{\underline{j}} N_{\underline{k}} H^{,r} S_{rs} H^{,s} \ .\end{aligned} \tag{51}$$

6. TRANSFORMATION OF THE FOURTH–ORDER DERIVATIVES OF TRAVEL TIME

We differentiate condition (33) with respect to x^l under constraint (1) and obtain condition

$$\begin{aligned}\tau_{,\underline{i}\underline{j}\underline{k}\underline{l}} = \widetilde{\tau}_{,\underline{i}\underline{j}\underline{k}\underline{l}} &+ F_{,\underline{i}\underline{j}\underline{k}\underline{l}}\,\lambda \\ &+ F_{,\underline{i}\underline{j}\underline{k}}\,\lambda_{,\underline{l}} + F_{,\underline{i}\underline{j}\underline{l}}\,\lambda_{,\underline{k}} + F_{,\underline{i}\underline{k}\underline{l}}\,\lambda_{,\underline{j}} + F_{,\underline{j}\underline{k}\underline{l}}\,\lambda_{\underline{i}} \\ &+ F_{,\underline{i}\underline{j}}\,\lambda_{,\underline{k}\underline{l}} + F_{,\underline{i}\underline{k}}\,\lambda_{,\underline{j}\underline{l}} + F_{,\underline{j}\underline{k}}\,\lambda_{\underline{i},\underline{l}} + F_{,\underline{i}\underline{l}}\,\lambda_{,\underline{j}\underline{k}} + F_{,\underline{j}\underline{l}}\,\lambda_{\underline{i},\underline{k}} + F_{,\underline{k}\underline{l}}\,\lambda_{\underline{i}\underline{j}} \\ &+ F_{,\underline{i}}\,\lambda_{,\underline{j}\underline{k}\underline{l}} + F_{,\underline{j}}\,\lambda_{\underline{i},\underline{k}\underline{l}} + F_{,\underline{k}}\,\lambda_{\underline{i}\underline{j},\underline{l}} + F_{,\underline{l}}\,\lambda_{\underline{i}\underline{j}\underline{k}} \ ,\end{aligned} \tag{52}$$

where $\lambda_{\underline{i}\underline{j}\underline{k}} = \lambda_{\underline{i}\underline{j}\underline{k}}(x^m, f^\mu)$ is the corresponding Lagrange multiplier. These Lagrange multipliers are defined for x^m satisfying constraint (1).

Since $\tau_{,\underline{i}\underline{j}\underline{k}\underline{l}}$ is symmetric with respect to its subscripts,

$$N_{\underline{a}\underline{k}} E_{\underline{b}\underline{l}} \tau_{,\underline{i}\underline{j}\underline{k}\underline{l}} = N_{\underline{a}\underline{k}} E_{\underline{b}\underline{l}} \tau_{,\underline{i}\underline{j}\underline{l}\underline{k}} \ . \tag{53}$$

We insert condition (52) into relation (53), and arrive at

$$E_{\underline{a}\underline{l}} \lambda_{\underline{i}\underline{j},\underline{l}} = E_{\underline{a}\underline{l}} \lambda_{\underline{i}\underline{j}\underline{l}} \ . \tag{54}$$

Since $N_{\underline{a}\underline{l}} \lambda_{\underline{i}\underline{j},\underline{l}}$ is not defined, we may put

$$N_{\underline{a}\underline{l}} \lambda_{\underline{i}\underline{j},\underline{l}} = N_{\underline{a}\underline{l}} \lambda_{\underline{i}\underline{j}\underline{l}} \ . \tag{55}$$

The summation of conditions (54) and (55) yields

$$\lambda_{\underline{i}\underline{j},\underline{k}} = \lambda_{\underline{i}\underline{j}\underline{k}} \ . \tag{56}$$

We insert Eqs (17), (37) and (56) into relation (52),

$$\boxed{\tau_{,\underline{i}\underline{j}\underline{k}\underline{l}} = T_{\underline{i}\underline{j}\underline{k}\underline{l}} + F_{,\underline{i}}\,\lambda_{\underline{j}\underline{k}\underline{l}} + F_{,\underline{j}}\,\lambda_{\underline{i}\underline{k}\underline{l}} + F_{,\underline{k}}\,\lambda_{\underline{i}\underline{j}\underline{l}} + F_{,\underline{l}}\,\lambda_{\underline{i}\underline{j}\underline{k}} \ ,} \tag{57}$$

where the values of

$$\boxed{\begin{aligned}T_{\underline{i}\underline{j}\underline{k}\underline{l}} = \widetilde{\tau}_{,\underline{i}\underline{j}\underline{k}\underline{l}} &+ F_{,\underline{i}\underline{j}\underline{k}\underline{l}}\,\lambda \\ &+ F_{,\underline{i}\underline{j}\underline{k}}\,\lambda_{\underline{l}} + F_{,\underline{i}\underline{j}\underline{l}}\,\lambda_{\underline{k}} + F_{,\underline{i}\underline{k}\underline{l}}\,\lambda_{\underline{j}} + F_{,\underline{j}\underline{k}\underline{l}}\,\lambda_{\underline{i}} \\ &+ F_{,\underline{i}\underline{j}}\,\lambda_{\underline{k}\underline{l}} + F_{,\underline{i}\underline{k}}\,\lambda_{\underline{j}\underline{l}} + F_{,\underline{j}\underline{k}}\,\lambda_{\underline{i}\underline{l}} + F_{,\underline{i}\underline{l}}\,\lambda_{\underline{j}\underline{k}} + F_{,\underline{j}\underline{l}}\,\lambda_{\underline{i}\underline{k}} + F_{,\underline{k}\underline{l}}\,\lambda_{\underline{i}\underline{j}}\end{aligned}} \tag{58}$$

are known. Lagrange multiplier λ is determined by Eq. (9), and is used in transformation relation (10) for the first–order derivatives. Lagrange multipliers $\lambda_{\underline{i}}$ are given by relation (30), and are used in transformation relation (18) for the second–order derivatives. Lagrange multipliers $\lambda_{\underline{i}\underline{j}}$ are given by relation (50), and are used in transformation relation (38) for the third–order derivatives.

We differentiate identity (40) with respect to $x^{\underline{k}}$,

$$\begin{aligned} &H_{,\underline{i}\underline{j}\underline{k}} + H_{\underline{i}\underline{j}}^{;r}\tau_{,r\underline{k}} + H_{\underline{i}\underline{k}}^{;r}\tau_{,r\underline{j}} + H_{\underline{j}\underline{k}}^{;r}\tau_{,r\underline{i}} \\ &\quad + H_{\underline{i}}^{;rs}\tau_{,r\underline{j}}\tau_{,s\underline{k}} + H_{\underline{j}}^{;rs}\tau_{,r\underline{i}}\tau_{,s\underline{k}} + H_{\underline{k}}^{;rs}\tau_{,r\underline{i}}\tau_{,s\underline{j}} + H^{,rst}\tau_{,r\underline{i}}\tau_{,s\underline{j}}\tau_{,t\underline{k}} \\ &\quad + H_{\underline{i}}^{;r}\tau_{,r\underline{j}\underline{k}} + H_{\underline{j}}^{;r}\tau_{,r\underline{i}\underline{k}} + H_{\underline{k}}^{;r}\tau_{,r\underline{i}\underline{j}} \\ &\quad + H^{,rs}\tau_{,r\underline{i}}\tau_{,s\underline{j}\underline{k}} + H^{,rs}\tau_{,r\underline{j}}\tau_{,s\underline{i}\underline{k}} + H^{,rs}\tau_{,r\underline{k}}\tau_{,s\underline{i}\underline{j}} + H^{,r}\tau_{,r\underline{i}\underline{j}\underline{k}} = 0 \ . \end{aligned} \tag{59}$$

We insert Eq. (57) into Eq. (59), and arrive at

$$H^{,r}F_{,r}\,\lambda_{\underline{i}\underline{j}\underline{k}} + F_{,\underline{i}}\,H^{,r}\lambda_{r\underline{j}\underline{k}} + F_{,\underline{j}}\,H^{,r}\lambda_{r\underline{i}\underline{k}} + F_{,\underline{k}}\,H^{,r}\lambda_{r\underline{i}\underline{j}} = -S_{\underline{i}\underline{j}\underline{k}} \ , \tag{60}$$

where

$$\boxed{\begin{aligned} S_{\underline{i}\underline{j}\underline{k}} = {} & H_{,\underline{i}\underline{j}\underline{k}} + H_{\underline{i}\underline{j}}^{;r}\tau_{,r\underline{k}} + H_{\underline{i}\underline{k}}^{;r}\tau_{,r\underline{j}} + H_{\underline{j}\underline{k}}^{;r}\tau_{,r\underline{i}} \\ & + H_{\underline{i}}^{;rs}\tau_{,r\underline{j}}\tau_{,s\underline{k}} + H_{\underline{j}}^{;rs}\tau_{,r\underline{i}}\tau_{,s\underline{k}} + H_{\underline{k}}^{;rs}\tau_{,r\underline{i}}\tau_{,s\underline{j}} + H^{,rst}\tau_{,r\underline{i}}\tau_{,s\underline{j}}\tau_{,t\underline{k}} \\ & + H_{\underline{i}}^{;r}\tau_{,r\underline{j}\underline{k}} + H_{\underline{j}}^{;r}\tau_{,r\underline{i}\underline{k}} + H_{\underline{k}}^{;r}\tau_{,r\underline{i}\underline{j}} \\ & + H^{,rs}\tau_{,r\underline{i}}\tau_{,s\underline{j}\underline{k}} + H^{,rs}\tau_{,r\underline{j}}\tau_{,s\underline{i}\underline{k}} + H^{,rs}\tau_{,r\underline{k}}\tau_{,s\underline{i}\underline{j}} + H^{,r}T_{,r\underline{i}\underline{j}\underline{k}} \ . \end{aligned} \quad (61)}$$

Analogously to Eq. (45), we shall search for the solution of Eq. (60) in the form

$$\begin{aligned} \lambda_{\underline{i}\underline{j}\underline{k}} = {} & -(H^{,q}F_{,q})^{-1}S_{\underline{i}\underline{j}\underline{k}} + F_{,\underline{i}}A_{\underline{j}\underline{k}} + F_{,\underline{j}}A_{\underline{i}\underline{k}} + F_{,\underline{k}}A_{\underline{i}\underline{j}} \\ & + F_{,\underline{i}}F_{,\underline{j}}A_{\underline{k}} + F_{,\underline{i}}F_{,\underline{k}}A_{\underline{j}} + F_{,\underline{j}}F_{,\underline{k}}A_{\underline{i}} + F_{,\underline{i}}F_{,\underline{j}}F_{,\underline{k}}A \ . \end{aligned} \tag{62}$$

Here we use unknowns A, $A_{\underline{i}}$ and $A_{\underline{i}\underline{j}}$ in expression (62) only locally: they have no relation to A and $A_{\underline{i}}$ used locally in the previous section. We insert Eq. (62) into Eq. (60),

$$\begin{aligned} & -S_{\underline{i}\underline{j}\underline{k}} - (H^{,q}F_{,q})^{-1}\big(F_{,\underline{i}}\,H^{,r}S_{r\underline{j}\underline{k}} + F_{,\underline{j}}\,H^{,r}S_{r\underline{i}\underline{k}} + F_{,\underline{k}}\,H^{,r}S_{r\underline{i}\underline{j}}\big) \\ &\quad + 2H^{,r}F_{,r}\big(F_{,\underline{i}}A_{\underline{j}\underline{k}} + F_{,\underline{j}}A_{\underline{i}\underline{k}} + F_{,\underline{k}}A_{\underline{i}\underline{j}}\big) \\ &\quad + 2\big(F_{,\underline{i}}F_{,\underline{j}}H^{,r}A_{r\underline{k}} + F_{,\underline{i}}F_{,\underline{k}}H^{,r}A_{r\underline{j}} + F_{,\underline{j}}F_{,\underline{k}}H^{,r}A_{r\underline{i}}\big) \\ &\quad + 3H^{,r}F_{,r}\big(F_{,\underline{i}}F_{,\underline{j}}A_{\underline{k}} + F_{,\underline{i}}F_{,\underline{k}}A_{\underline{j}} + F_{,\underline{j}}F_{,\underline{k}}A_{\underline{i}}\big) \\ &\quad + 3F_{,\underline{i}}F_{,\underline{j}}F_{,\underline{k}}\,H^{,r}A_r + 4H^{,r}F_{,r}\,F_{,\underline{i}}F_{,\underline{j}}F_{,\underline{k}}A = -S_{\underline{i}\underline{j}\underline{k}} \ . \end{aligned} \tag{63}$$

We fit the terms with single gradient $F_{,i}$ by

$$A_{\underline{i}\underline{j}} = \tfrac{1}{2}(H^{,q}F_{,q})^{-2}H^{,r}S_{r\underline{i}\underline{j}} \ , \tag{64}$$

then the terms with dyadic product $F_{,\underline{i}}F_{,\underline{j}}$ by

$$A_{\underline{i}} = -\tfrac{2}{3}(H^{,q}F_{,q})^{-1}H^{,r}A_{r\underline{i}} = -\tfrac{1}{3}(H^{,q}F_{,q})^{-3}H^{,r}H^{,s}S_{rs\underline{i}} \ , \tag{65}$$

and then the terms with triadic product $F_{,\underline{i}}F_{,\underline{j}}F_{,\underline{k}}$ by

$$A = -\tfrac{3}{4}(H^{,q}F_{,q})^{-1}H^{,r}A_r = \tfrac{1}{4}(H^{,q}F_{,q})^{-4}H^{,r}H^{,s}H^{,t}S_{rst} \ . \tag{66}$$

We insert Eqs (64), (65) and (66) into Eq. (62) and obtain solution

$$\begin{aligned}\lambda_{\underline{i}\underline{j}\underline{k}} = -(H^{,q}F_{,q})^{-1}S_{\underline{i}\underline{j}\underline{k}} &+ \tfrac{1}{2}(H^{,q}F_{,q})^{-2}\big(F_{,\underline{i}}\,H^{,r}S_{r\underline{j}\underline{k}} + F_{,\underline{j}}\,H^{,r}S_{r\underline{i}\underline{k}} + F_{,\underline{k}}\,H^{,r}S_{r\underline{j}\underline{k}}\big)\\ &- \tfrac{1}{3}(H^{,q}F_{,q})^{-3}H^{,r}H^{,s}\big(F_{,\underline{i}}F_{,\underline{j}}S_{rs\underline{k}} + F_{,\underline{i}}F_{,\underline{k}}S_{rs\underline{j}} + F_{,\underline{j}}F_{,\underline{k}}S_{rs\underline{i}}\big)\\ &+ \tfrac{1}{4}(H^{,q}F_{,q})^{-4}F_{,\underline{i}}F_{,\underline{j}}F_{,\underline{k}}\,H^{,r}H^{,s}H^{,t}S_{rst}\end{aligned} \tag{67}$$

of Eq. (60). Relation (67) may be expressed more concisely in terms of normalized gradient (29),

$$\boxed{\begin{aligned}\lambda_{\underline{i}\underline{j}\underline{k}} = (H^{,q}F_{,q})^{-1}\big[-S_{\underline{i}\underline{j}\underline{k}} &+ \tfrac{1}{2}\big(N_{\underline{i}}\,H^{,r}S_{r\underline{j}\underline{k}} + N_{\underline{j}}\,H^{,r}S_{r\underline{i}\underline{k}} + N_{\underline{k}}\,H^{,r}S_{r\underline{j}\underline{k}}\big)\\ &- \tfrac{1}{3}H^{,r}H^{,s}\big(N_{\underline{i}}N_{\underline{j}}S_{rs\underline{k}} + N_{\underline{i}}N_{\underline{k}}S_{rs\underline{j}} + N_{\underline{j}}N_{\underline{k}}S_{rs\underline{i}}\big)\\ &+ \tfrac{1}{4}N_{\underline{i}}N_{\underline{j}}N_{\underline{k}}\,H^{,r}H^{,s}H^{,t}S_{rst}\big] \ ,\end{aligned}} \tag{68}$$

where $S_{\underline{i}\underline{j}\underline{k}}$ is given by definition (61). Relation (57) with Eqs (58) and (68) represents the explicit relation for the transformation of the fourth–order derivatives of travel time at a curved interface between two arbitrary media.

Note that transformation relation (57) with inserted Lagrange multipliers (68) reads

$$\begin{aligned}\tau_{,\underline{i}\underline{j}\underline{k}\underline{l}} = T_{\underline{i}\underline{j}\underline{k}\underline{l}} &- N_{\underline{i}}S_{\underline{j}\underline{k}\underline{l}} - N_{\underline{j}}S_{\underline{i}\underline{k}\underline{l}} - N_{\underline{k}}S_{\underline{i}\underline{j}\underline{l}} - N_{\underline{l}}S_{\underline{i}\underline{j}\underline{k}}\\ &+ N_{\underline{i}}N_{\underline{j}}H^{,r}S_{r\underline{k}\underline{l}} + N_{\underline{i}}N_{\underline{k}}H^{,r}S_{r\underline{j}\underline{l}} + N_{\underline{i}}N_{\underline{l}}H^{,r}S_{r\underline{j}\underline{k}}\\ &+ N_{\underline{j}}N_{\underline{k}}H^{,r}S_{r\underline{i}\underline{l}} + N_{\underline{j}}N_{\underline{l}}H^{,r}S_{r\underline{i}\underline{k}} + N_{\underline{k}}N_{\underline{l}}H^{,r}S_{r\underline{i}\underline{j}}\\ &- H^{,r}H^{,s}\big(N_{\underline{i}}N_{\underline{j}}N_{\underline{k}}S_{rs\underline{l}} + N_{\underline{i}}N_{\underline{j}}N_{\underline{l}}S_{rs\underline{k}} + N_{\underline{i}}N_{\underline{k}}N_{\underline{l}}S_{rs\underline{j}} + N_{\underline{j}}N_{\underline{k}}N_{\underline{l}}S_{rs\underline{i}}\big)\\ &+ N_{\underline{i}}N_{\underline{j}}N_{\underline{k}}N_{\underline{l}}\,H^{,r}H^{,s}H^{,t}S_{rst} \ .\end{aligned} \tag{69}$$

7. TRANSFORMATION OF HIGHER–ORDER DERIVATIVES OF TRAVEL TIME

For higher–order derivatives, we obtain transformation relation

$$\boxed{\tau_{,\underline{i}\underline{j}\ldots\underline{m}\underline{n}} = T_{,\underline{i}\underline{j}\ldots\underline{m}\underline{n}} + \sum_{\substack{\{\underline{a}\}\subset\{\underline{i}\underline{j}\ldots\underline{m}\underline{n}\}\\ \{\underline{b}\ldots\underline{h}\}=\{\underline{i}\underline{j}\ldots\underline{m}\underline{n}\}\setminus\{\underline{a}\}}} F_{,\underline{a}}\,\lambda_{\underline{b}\ldots\underline{h}}} \tag{70}$$

analogous to Eqs (18), (38) and (57). Here $\{\underline{i}\underline{j}...\underline{m}\underline{n}\}$ represents the set of indices $\underline{i}$, $\underline{j}$, ..., $\underline{m}$, $\underline{n}$, and $\sum_{\{\underline{a}\}\subset\{\underline{i}\underline{j}...\underline{m}\underline{n}\}}$ implies the summation over all single–element subsets of set $\{\underline{i}\underline{j}...\underline{m}\underline{n}\}$, i.e. over the subscripts of $\tau_{,\underline{i}\underline{j}...\underline{m}\underline{n}}$. Notation $\{\underline{b}...\underline{h}\} = \{\underline{i}\underline{j}...\underline{m}\underline{n}\}\backslash\{\underline{a}\}$ means that $\underline{b}...\underline{h}$ represents all indices other than $\underline{a}$.

In transformation relation (70), we have put

$$\boxed{\begin{aligned} T_{,\underline{i}\underline{j}...\underline{m}\underline{n}} = \widetilde{\tau}_{,\underline{i}\underline{j}...\underline{m}\underline{n}} &+ F_{,\underline{i}\underline{j}...\underline{m}\underline{n}}\,\lambda \\ &+ \sum_{\substack{\{\underline{a}\}\subset\{\underline{i}\underline{j}...\underline{m}\underline{n}\}\\ \{\underline{b}...\underline{h}\}=\{\underline{i}\underline{j}...\underline{m}\underline{n}\}\backslash\{\underline{a}\}}} F_{,\underline{b}...\underline{h}}\,\lambda_{\underline{a}} \\ &+ \sum_{\substack{\{\underline{a}\underline{b}\}\subset\{\underline{i}\underline{j}...\underline{m}\underline{n}\}\\ \{\underline{c}...\underline{h}\}=\{\underline{i}\underline{j}...\underline{m}\underline{n}\}\backslash\{\underline{a}\underline{b}\}}} F_{,\underline{c}...\underline{h}}\,\lambda_{\underline{a}\underline{b}} \\ &+ \sum_{\substack{\{\underline{a}\underline{b}\underline{c}\}\subset\{\underline{i}\underline{j}...\underline{m}\underline{n}\}\\ \{\underline{d}...\underline{h}\}=\{\underline{i}\underline{j}...\underline{m}\underline{n}\}\backslash\{\underline{a}\underline{b}\underline{c}\}}} F_{,\underline{d}...\underline{h}}\,\lambda_{\underline{a}\underline{b}\underline{c}} \\ &\;\vdots \\ &+ \sum_{\substack{\{\underline{g}\underline{h}\}\subset\{\underline{i}\underline{j}...\underline{m}\underline{n}\}\\ \{\underline{a}...\underline{f}\}=\{\underline{i}\underline{j}...\underline{m}\underline{n}\}\backslash\{\underline{g}\underline{h}\}}} F_{,\underline{g}\underline{h}}\,\lambda_{\underline{a}...\underline{f}} \end{aligned}} \tag{71}$$

analogously to definitions (19), (39) and (58). Here $\sum_{\{\underline{a}\underline{b}\}\subset\{\underline{i}\underline{j}...\underline{m}\underline{n}\}}$ implies the summation over all two–element subsets of set $\{\underline{i}\underline{j}...\underline{m}\underline{n}\}$, and $\{\underline{c}...\underline{h}\} = \{\underline{i}\underline{j}...\underline{m}\underline{n}\}\backslash\{\underline{a}\underline{b}\}$ means that $\underline{c}...\underline{h}$ represents all indices other than $\underline{a}$ and $\underline{b}$. The values of all Lagrange multipliers in relation (71) are known from the transformations of the derivatives of orders lower than $\tau_{,\underline{i}\underline{j}...\underline{m}\underline{n}}$.

We then differentiate Hamilton–Jacobi equation (3) with respect to $x^{\underline{i}}$, $x^{\underline{j}}$, ..., $x^{\underline{m}}$, insert transformation relation (70) for $\tau_{,\underline{i}\underline{j}...\underline{m}r}$, and obtain identity

$$H^{,r}F_{,r}\,\lambda_{\underline{i}\underline{j}...\underline{m}} + \sum_{\substack{\{\underline{a}\}\subset\{\underline{i}\underline{j}...\underline{m}\}\\ \{\underline{b}...\underline{h}\}=\{\underline{i}\underline{j}...\underline{m}\}\backslash\{\underline{a}\}}} F_{,\underline{a}}\,\lambda_{\underline{b}...\underline{h}r}H^{,r} = -S_{\underline{i}\underline{j}...\underline{m}} \tag{72}$$

for Lagrange multipliers $\lambda_{\underline{i}\underline{j}...\underline{m}}$, where

$$\boxed{\begin{aligned} S_{\underline{i}\underline{j}...\underline{m}} = \left(\frac{\partial}{\partial x^{\underline{i}}}+\tau_{,\underline{i}r}\frac{\partial}{\partial p_r}\right)\left(\frac{\partial}{\partial x^{\underline{j}}}+\tau_{,\underline{j}s}\frac{\partial}{\partial p_s}\right)...\left(\frac{\partial}{\partial x^{\underline{m}}}+\tau_{,\underline{m}z}\frac{\partial}{\partial p_z}\right)H \\ -\tau_{,\underline{i}\underline{j}...\underline{m}r}H^{,r} + T_{,\underline{i}\underline{j}...\underline{m}r}H^{,r} \end{aligned}} \tag{73}$$

represents the generalization of definitions (24), (43) and (61) to higher–order derivatives. Definition (73) contains the derivatives of orders lower than $\tau_{,\underline{i}\underline{j}...\underline{m}\underline{n}}$ only.

The Lagrange multipliers in relation (70) for the transformation of the higher–order derivatives of travel time at a curved interface between two arbitrary media then read

$$\boxed{\begin{aligned}\lambda_{\underline{i}\underline{j}\ldots\underline{m}} = (H^{,q}F_{,q})^{-1}\Big[& - S_{\underline{i}\underline{j}\ldots\underline{m}} \\ & + \tfrac{1}{2} \sum_{\substack{\{\underline{a}\}\subset\{\underline{i}\underline{j}\ldots\underline{m}\} \\ \{\underline{b}\ldots\underline{h}\}=\{\underline{i}\underline{j}\ldots\underline{m}\}\setminus\{\underline{a}\}}} N_{\underline{a}}\, H^{,r} S_{r\underline{b}\ldots\underline{h}} \\ & - \tfrac{1}{3} \sum_{\substack{\{\underline{a}\underline{b}\}\subset\{\underline{i}\underline{j}\ldots\underline{m}\} \\ \{\underline{c}\ldots\underline{h}\}=\{\underline{i}\underline{j}\ldots\underline{m}\}\setminus\{\underline{a}\underline{b}\}}} N_{\underline{a}} N_{\underline{b}}\, H^{,r} H^{,s} S_{rs\underline{c}\ldots\underline{h}} \\ & + \tfrac{1}{4} \sum_{\substack{\{\underline{a}\underline{b}\underline{c}\}\subset\{\underline{i}\underline{j}\ldots\underline{m}\} \\ \{\underline{d}\ldots\underline{h}\}=\{\underline{i}\underline{j}\ldots\underline{m}\}\setminus\{\underline{a}\underline{b}\underline{c}\}}} N_{\underline{a}} N_{\underline{b}} N_{\underline{c}}\, H^{,r} H^{,s} H^{,t} S_{rst\underline{d}\ldots\underline{h}} \\ & \;\vdots \\ & + \tfrac{(-1)^K}{K} N_{\underline{i}} N_{\underline{j}} \ldots N_{\underline{m}}\, H^{,r} H^{,s} \ldots H^{,z} S_{rs\ldots z}\Big] \; ,\end{aligned}} \tag{74}$$

where K is the order of derivative $\tau_{,\underline{i}\underline{j}\ldots\underline{m}\underline{n}}$. We may easily check that Lagrange multipliers (74) satisfy identity (72). Relation (74) represents the generalization of relations (30), (50) and (68) to the higher–order derivatives.

Note that transformation relation (70) with inserted Lagrange multipliers (74) reads

$$\begin{aligned}\tau_{,\underline{i}\underline{j}\ldots\underline{m}\underline{n}} = T_{\underline{i}\underline{j}\ldots\underline{m}\underline{n}} & - \sum_{\substack{\{\underline{a}\}\subset\{\underline{i}\underline{j}\ldots\underline{m}\underline{n}\} \\ \{\underline{b}\ldots\underline{h}\}=\{\underline{i}\underline{j}\ldots\underline{m}\underline{n}\}\setminus\{\underline{a}\}}} N_{\underline{a}}\, S_{\underline{b}\ldots\underline{h}} \\ & + \sum_{\substack{\{\underline{a}\underline{b}\}\subset\{\underline{i}\underline{j}\ldots\underline{m}\underline{n}\} \\ \{\underline{c}\ldots\underline{h}\}=\{\underline{i}\underline{j}\ldots\underline{m}\underline{n}\}\setminus\{\underline{a}\underline{b}\}}} N_{\underline{a}} N_{\underline{b}}\, H^{,r} S_{r\underline{c}\ldots\underline{h}} \\ & - \sum_{\substack{\{\underline{a}\underline{b}\underline{c}\}\subset\{\underline{i}\underline{j}\ldots\underline{m}\underline{n}\} \\ \{\underline{d}\ldots\underline{h}\}=\{\underline{i}\underline{j}\ldots\underline{m}\underline{n}\}\setminus\{\underline{a}\underline{b}\underline{c}\}}} N_{\underline{a}} N_{\underline{b}} N_{\underline{c}}\, H^{,r} H^{,s} S_{rs\underline{d}\ldots\underline{h}} \\ & + \sum_{\substack{\{\underline{a}\underline{b}\underline{c}\underline{d}\}\subset\{\underline{i}\underline{j}\ldots\underline{m}\underline{n}\} \\ \{\underline{e}\ldots\underline{h}\}=\{\underline{i}\underline{j}\ldots\underline{m}\underline{n}\}\setminus\{\underline{a}\underline{b}\underline{c}\underline{d}\}}} N_{\underline{a}} N_{\underline{b}} N_{\underline{c}} N_{\underline{d}}\, H^{,r} H^{,s} H^{,t} S_{rst\underline{e}\ldots\underline{h}} \\ & \;\vdots \\ & + (-1)^K N_{\underline{i}} N_{\underline{j}} \ldots N_{\underline{m}} N_{\underline{n}}\, H^{,r} H^{,s} \ldots H^{,z} S_{rs\ldots z} \; ,\end{aligned} \tag{75}$$

where K is the order of derivative $\tau_{,\underline{ij}\ldots\underline{mn}}$. Transformation relation (75) represents the generalization of transformation relations (32), (51) and (69) to the higher–order derivatives.

8. EXAMPLES

In order to elucidate the notation used in this paper, let us present three very simple applications of the first–order perturbation derivatives of travel time, the imaginary first–order perturbation derivatives of the spatial gradient of travel time, and the fourth–order and higher–order spatial derivatives of travel time.

8.1. Misplacement of the interface due to an incorrectly known medium

We assume a ray corresponding to a wave reflected or refracted at an interface. We assume that the total travel time from the source to the receiver is given. We denote by $\widetilde{\tau}$ the travel time from the source to point x^i of the interface, and by τ' the travel time from point x^i of the interface to the receiver. We consider perturbation derivatives $\widetilde{\tau}_{,\alpha}$ and $\tau'_{,\alpha}$ of these travel times due to the inaccurately known media in which travel times $\widetilde{\tau}$ and τ' are calculated. The inaccurately known media then result in the perturbation of the correct position of the interface in order to preserve the total travel time from the source to the receiver. The displacement of the interface specified by constraint (1) is expressed in terms of perturbation derivative $F_{,\alpha}$.

The perturbation derivative of the given total travel time from the source to the receiver, which is composed of $\widetilde{\tau}_{,\alpha}$, $\tau'_{,\alpha}$ and term $\tau_{,\alpha}-\widetilde{\tau}_{,\alpha}$, determined by law (8), has to vanish,

$$\widetilde{\tau}_{,\alpha} + \tau'_{,\alpha} + F_{,\alpha}\,\lambda = 0\ . \tag{76}$$

Then

$$F_{,\alpha} = -(\widetilde{\tau}_{,\alpha} + \tau'_{,\alpha})\,\lambda^{-1}\ . \tag{77}$$

We wish to determine perturbation derivative $x^i_{,\alpha}$ of the displacement of point x^i in the direction perpendicular to the interface,

$$x^i_{,\alpha} = const\, F_{,i}\ . \tag{78}$$

Perturbation derivative of constraint (1) yields

$$F_{,i}\, x^i_{,\alpha} + F_{,\alpha} = 0\ . \tag{79}$$

The above two relations result in expression

$$x^i_{,\alpha} = -F_{,\alpha}\, F_{,i}\,(F_{,k}F_{,k})^{-1}\ . \tag{80}$$

We insert relation (77) into Eq. (80) and obtain

$$x^i_{,\alpha} = (\widetilde{\tau}_{,\alpha} + \tau'_{,\alpha})\,\lambda^{-1} F_{,i}\,(F_{,k}F_{,k})^{-1}\ . \tag{81}$$

We insert consequence

$$F_{,i} = (\tau_{,i} - \widetilde{\tau}_{,i})\,\lambda^{-1} \tag{82}$$

of Snell's law (7) into Eq. (81) and arrive at

$$x^i_{,\alpha} = (\widetilde{\tau}_{,\alpha} + \tau'_{,\alpha})(\tau_{,i} - \widetilde{\tau}_{,i})\,\lambda^{-2}(F_{,k}F_{,k})^{-1} \; . \tag{83}$$

Lagrange multiplier λ can be calculated from incident travel–time gradient $\widetilde{\tau}_{,i}$ and transformed travel–time gradient $\tau_{,i}$ using Snell's law (7) as

$$\lambda^2 = (\tau_{,j} - \widetilde{\tau}_{,j})(\tau_{,j} - \widetilde{\tau}_{,j})\,(F_{,k}F_{,k})^{-1} \; . \tag{84}$$

We insert relation (84) into Eq. (83), and obtain expression

$$x^i_{,\alpha} = (\widetilde{\tau}_{,\alpha} + \tau'_{,\alpha})\,(\tau_{,i} - \widetilde{\tau}_{,i})\,[(\tau_{,k} - \widetilde{\tau}_{,k})(\tau_{,k} - \widetilde{\tau}_{,k})]^{-1} \tag{85}$$

for the perturbation derivative of the displacement of point x^i of the interface in the direction perpendicular to the interface.

8.2. Perturbation expansion of complex–valued travel time along real–valued reference rays

We consider a complex–valued Hamiltonian function $\mathcal{H}(x^m, p_n)$ of real–valued spatial coordinates x^m and of complex–valued slowness vector p_n. We assume that $\mathcal{H}(x^m, p_n)$ is a holomorphic function of p_n in the domain of our interest. The rays corresponding to complex–valued Hamiltonian function $\mathcal{H}(x^m, p_n)$ are complex–valued. Unfortunately, in most practical applications, we are not able to evaluate Hamiltonian function $\mathcal{H}(x^m, p_n)$ and its phase–space derivatives at imaginary positions x^m. We thus need real–valued reference rays yielding real–valued reference travel time, and the perturbation expansion from the real–valued reference travel time to the complex–valued travel time corresponding to Hamiltonian function $\mathcal{H}(x^m, p_n)$.

We choose the reference Hamiltonian function $H(x^m, p_n)$ for tracing the real–valued reference rays according to *Klimeš and Klimeš (2011, Eq. 7)*. The corresponding one–parametric perturbation Hamiltonian function $H(x^m, p_n, f^\alpha)$ is linear with respect to perturbation parameter f^α, for $f^\alpha = 0$ is equal to the reference Hamiltonian function $H(x^m, p_n)$,

$$H(x^m, p_n, 0) = H(x^m, p_n) \; , \tag{86}$$

and for $f^\alpha = 1$ yields

$$H(x^m, p_n, 1) = \mathcal{H}(x^m, p_n) \; . \tag{87}$$

The values of the reference Hamiltonian function and its phase–space derivatives for real–valued slowness vector p_n read (*Klimeš and Klimeš, 2011, Eqs 10–11*)

$$H^{,a\ldots h}_{,i\ldots n}(x^r, p_s, 0) = \mathrm{Re}\big[\mathcal{H}^{,a\ldots h}_{,i\ldots n}(x^r, p_s)\big] \; . \tag{88}$$

The values of the first–order perturbation derivatives of the reference Hamiltonian function and its phase–space derivatives for real–valued slowness vector p_n read (*Klimeš and Klimeš, 2011, Eqs 12–13*)

$$H^{,a\ldots h}_{,i\ldots n\alpha}(x^r, p_s, 0) = \mathrm{i}\,\mathrm{Im}\big[\mathcal{H}^{,a\ldots h}_{,i\ldots n}(x^r, p_s)\big] \; . \tag{89}$$

All second–order and higher–order perturbation derivatives of the reference Hamiltonian function and its phase–space derivatives vanish (*Klimeš and Klimeš, 2011, Eqs 14–15*). The first–order phase–space derivatives

$$H_{,i}(x^r, p_s, 0) = \mathrm{Re}\big[\mathcal{H}_{,i}(x^r, p_s)\big] \tag{90}$$

and

$$H^{,a}(x^r, p_s, 0) = \mathrm{Re}\big[\mathcal{H}^{,a}(x^r, p_s)\big] \tag{91}$$

are used to trace the reference rays (*Klimeš and Klimeš, 2011, Eqs 19–20*). The first–order perturbation derivative

$$H_{,\alpha}(x^r, p_s, 0) = \mathrm{i}\,\mathrm{Im}\big[\mathcal{H}(x^r, p_s)\big] \tag{92}$$

is required for calculating the linear term $\tau_{,\alpha}$ in the perturbation expansion of the complex–valued travel time along real–valued rays.

The interface is assumed to be independent of the perturbation parameter f^α,

$$F_{,\alpha} = 0 \tag{93}$$

and

$$F_{,i\alpha} = 0 \ . \tag{94}$$

Transformation relation (8) then yields $\tau_{,\alpha} = \widetilde{\tau}_{,\alpha}$ for the linear term in the perturbation expansion of the complex–valued travel time along real–valued rays.

We shall now study the transformation of the linear term $\tau_{,i\alpha}$ in the perturbation expansion of the complex–valued travel–time gradient along real–valued reference rays. When we insert

$$N_\alpha = 0 \tag{95}$$

resulting from definition (29) with assumption (93), transformation relation (32) simplifies to

$$\tau_{,i\alpha} = T_{i\alpha} - N_i S_\alpha \ . \tag{96}$$

Definition (19) with assumption (94) reads

$$T_{i\alpha} = \widetilde{\tau}_{,i\alpha} \ . \tag{97}$$

Definition (24) with relation (97) reads

$$S_\alpha = H_{,\alpha} + H^{,r}\widetilde{\tau}_{,r\alpha} \ . \tag{98}$$

Transformation relation (96) with relations (97) and (98) reads

$$\tau_{,i\alpha} = \widetilde{\tau}_{,i\alpha} - N_i\left(H_{,\alpha} + H^{,r}\widetilde{\tau}_{,r\alpha}\right) \ , \tag{99}$$

which represents the final transformation relation for the linear term $\tau_{,i\alpha}$ in the perturbation expansion of the complex–valued travel–time gradient along real–valued reference rays. Here $H^{,r}$ is determined by definition (91) and $H_{,\alpha}$ by definition (92).

If we consider any vector t^i tangent to the interface,

$$N_i\, t^i = 0 \ , \tag{100}$$

we observe that

$$t^i\,\tau_{,i\alpha} = t^i\,\widetilde{\tau}_{,i\alpha} \ , \tag{101}$$

which is a direct consequence of condition (4). We also observe that

$$H^{,i}\,\tau_{,i\alpha} = -H_{,\alpha}\ , \tag{102}$$

see definition (29), which directly follows from differentiating Hamilton–Jacobi equation (3) with respect to f^α, see identity (20). Note that transformation relation (99) could also be obtained directly from identities (101) and (102).

8.3. Paraxial Super–Gaussian beams

Paraxial Super–Gaussian beams of the N^{th} order, $N = 4, 6, 8, ...$, have real–valued spatial derivatives of travel time up to the $(N\text{–}1)^{\mathrm{st}}$ order, and complex–valued spatial derivatives of travel time of the N^{th} order in smooth media (*Klimeš, 2013*).

We assume that the central rays of paraxial Super–Gaussian beams are real–valued and correspond to real–valued Hamiltonian functions of real–valued coordinates and real–valued slowness vectors, with real–valued phase–space derivatives of the Hamiltonian functions.

Let us now inspect the transformation of paraxial Super–Gaussian beams of the N^{th} order at a smooth interface. For this study, we consider the spatial derivatives of travel time only. All spatial derivatives of function F describing the interface are real–valued.

For the transformation of the derivatives of travel time up to the $(N-1)^{\mathrm{st}}$ order, the right–hand sides of definition (73) contain just the real–valued spatial derivatives of travel time, and thus

$$\mathrm{Im}(S_{ij...m}) = 0\ . \tag{103}$$

As a consequence, relation (74) yields

$$\mathrm{Im}(\lambda_{ij...m}) = 0\ . \tag{104}$$

Relation (71) then yields

$$\mathrm{Im}(T_{,ij...mn}) = 0\ . \tag{105}$$

Transformation relation (70) with identities (104) and (105) finally yields

$$\mathrm{Im}(\tau_{,ij...mn}) = 0\ . \tag{106}$$

We observe that Super–Gaussian beams of the N^{th} order remain Super–Gaussian beams of the N^{th} order after the transformation at a smooth interface.

Let us now study the transformation of the imaginary parts of the spatial derivatives of travel time of the N^{th} order. In this case, definition (73) yields

$$\mathrm{Im}(S_{ij...m}) = \mathrm{Im}(T_{,ij...mr})\,H^{,r}\ . \tag{107}$$

Considering identities (104), relation (71) yields

$$\mathrm{Im}(T_{,ij...mn}) = \mathrm{Im}(\widetilde{\tau}_{,ij...mn})\ . \tag{108}$$

Identity (107) with relation (108) reads

$$\mathrm{Im}(S_{ij...m}) = \mathrm{Im}(\widetilde{\tau}_{,ij...mr})\,H^{,r}\ . \tag{109}$$

We insert identities (108) and (109) into transformation relation (75) and obtain relation

$$\mathrm{Im}(\tau_{,ij...mn}) = (\delta^r_i - N_i H^{,r})(\delta^s_j - N_j H^{,s})...(\delta^y_m - N_m H^{,y})(\delta^z_n - N_n H^{,z})\,\mathrm{Im}(\widetilde{\tau}_{,rs...yz}) \tag{110}$$

for the transformation of paraxial Super–Gaussian beams of the N^{th} order at a smooth interface.

Considering definition (29), we observe that

$$\mathrm{Im}(\tau_{,ij...mn})\,H^{,n} = 0 \ , \tag{111}$$

which also directly follows from differentiating Hamilton–Jacobi equation (3) with respect to x^i, x^j, ..., x^m. If we consider N arbitrary vectors t^i_1, t^j_2, ..., t^m_{N-1}, t^n_N tangent to the interface,

$$N_i\,t^i_a = 0 \ , \tag{112}$$

we also observe that

$$\mathrm{Im}(\tau_{,ij...mn})\,t^i_1 t^j_2 ... t^m_{N-1} t^n_N = \mathrm{Im}(\widetilde{\tau}_{,ij...mn})\,t^i_1 t^j_2 ... t^m_{N-1} t^n_N \ , \tag{113}$$

which is a direct consequence of condition (4). Note that transformation relation (110) could also be obtained directly from identities (111) and (113).

9. CONCLUSIONS

In smooth media, the third–order and higher–order spatial derivatives of travel time and all perturbation derivatives of travel time can be calculated along unperturbed rays by simple numerical quadratures using the equations derived by *Klimeš (2002a)*.

If the structure contains smooth interfaces between layers or blocks, these derivatives of travel time have to be transformed at the interfaces. In this paper, we have derived explicit equations for transforming all these derivatives of travel time at the interfaces. The equations are applicable to both real–valued and complex–valued travel time. The equations are expressed in terms of a general Hamiltonian function and are applicable to travel–time derivatives of arbitrary orders in smooth heterogeneous media, both isotropic and arbitrarily anisotropic or bianisotropic. The interface represents the surface at which the Hamiltonian function or its partial derivatives of an arbitrary order may be discontinuous. The interface is specified by an implicit equation. No local coordinates are needed for the transformation of travel–time derivatives.

The derived equations may have many applications. Let us mention two examples. The spatial fourth–order derivatives of travel time are necessary for calculating the first–order term of the ray series in order to estimate the accuracy of the zero–order ray theory. The fourth–order and higher–order derivatives of travel time are essential for studying the paraxial Super–Gaussian beams (*Klimeš, 2013*).

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