SECOND–ORDER AND HIGHER–ORDER PERTURBATIONS OF TRAVEL TIME IN ISOTROPIC AND ANISOTROPIC MEDIA

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ABSTRACT

The partial derivatives of travel time with respect to model parameters are referred to as perturbations. Explicit equations for the second–order and higher–order perturbations of travel time in both isotropic and anisotropic media are derived. The perturbations of travel time and its spatial derivatives can be calculated by simple numerical quadratures along rays.

Keywords: Ray theory, travel time (action function), Hamilton–Jacobi equation, paraxial approximation, perturbation methods, inhomogeneous media, seismic anisotropy.

1. INTRODUCTION

The model of a smooth elastic medium for ray tracing is assumed to be specified by a set of smooth functions. This set of smooth functions is assumed to be an element of a linear normed space, hereinafter called the *model space*. We shall refer to the coordinates of the model with respect to a selected basis in the model space as *model parameters*. We shall then refer to the partial derivatives of travel time (action function) with respect to the model parameters as *perturbations of travel time*. Analogously, we shall refer to the partial derivatives of other quantities with respect to the model parameters as perturbations of the quantities. Note that the partial derivatives are generally defined as the Gâteaux variations in the directions of the corresponding basis functions.

This paper is devoted to the calculation of the second–order and higher–order perturbations of travel time. We have introduced the term "perturbations" in order to distinguish briefly the partial derivatives with respect to model parameters from the partial derivatives with respect to spatial or phase–space coordinates. In this way, we shall distinguish between the *partial phase–space derivatives* and perturbations of the Hamiltonian, and between the *spatial derivatives* and perturbations of travel time or other quantities.

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The travel time and its first–order spatial derivatives in a general smoothly heterogeneous model can be calculated by solving numerically a set of nonlinear ordinary differential equations called ray tracing equations. The second–order spatial derivatives of travel time can be calculated by solving numerically a set of linear ordinary differential equations called dynamic ray tracing equations, both in isotropic media (*Babich and Buldyrev, 1972*; *Arnaud, 1973*; *Červený and Hron, 1980*) and anisotropic media (*Červený, 1972*). For an overview of the ray theory and paraxial ray methods with their applications and relevant references refer to the book by *Červený* (*2001*). The third–order and higher–order spatial derivatives of travel time can be computed by simple numerical quadratures along rays, both in isotropic media (*Babich, Buldyrev and Molotkov, 1985*; *Červený, 2001*) and anisotropic media (*Klimeš, 1997, 1999*).

The equations for the second–order perturbations of travel time have already been derived by *Kravtsov and Orlov* (*1980, 1990*) and *Snieder and Sambridge* (*1992*) for isotropic media, and by *Farra* (*1999*) and *Červený* (*2001*) for generally anisotropic media. Whereas *Kravtsov and Orlov* (*1980, 1990*) perturbed the travel time at fixed spatial coordinates along unperturbed rays, *Snieder and Sambridge* (*1992*), *Farra* (*1999*) and *Červený* (*2001*) perturbed both rays and travel time and expressed the second–order perturbations of travel time in terms of the first–order perturbations of rays, which makes both the derivation and final equations more involved. For the comparison of their results with our equations refer to Section 6.

We follow the approach of *Kravtsov and Orlov* (*1980, 1990*) and calculate the *perturbations of travel time at fixed spatial coordinates* along unperturbed rays. Our approach considerably simplifies the derivation and yields the final equations for calculating the perturbations of travel time in a reasonably simple form. Our approach is a generalization of the method designed by *Babich, Buldyrev and Molotkov* (*1985*) for calculating the third–order and higher–order spatial derivatives of travel time.

We present the explicit equations for the second–order and higher–order perturbations of travel time in Cartesian coordinates. The perturbations of travel time are expressed in the form of integrals along the ray, with the proper initial values. The integrands are composed of spatial derivatives and perturbations of travel time, and of the partial phase–space derivatives and perturbations of the Hamiltonian. The aggregate orders of spatial derivatives and perturbations of travel time in the integrands are equal to or lower than the aggregate order of spatial derivatives and perturbations of travel time being computed. Simultaneously, the orders of perturbations of travel time in the integrands are lower than the order of perturbations of travel time or its spatial derivative being computed. The perturbations and spatial derivatives of the Hamiltonian contain perturbations and spatial derivatives of density–normalized elastic moduli (or of a power of the phase velocity in isotropic media) up to the order corresponding to that of the calculated perturbations and spatial derivatives of travel time.

The general explicit equations for the spatial derivatives and perturbations of travel time of all orders are derived in Section 2. Whereas Section 2 represents the essence of the paper, the remaining Sections 3 to 6 contain just particular specifications of the general equations, notes on their application and on their relation to previously published equations. The reader may stop reading at the end of Section 2 unless he is interested in special cases of general equations or their discussion.

In Section 3, the individual equations for the spatial derivatives and perturbations of travel time up to the third order are presented as examples, in order to illustrate the general equations of Section 2. Those, who are not fond of the general theory in Section 2 but wish to calculate the second–order or even third–order perturbations of travel time in anisotropic media, will directly find the particular equations in Section 3.

Section 4 contains various notes related to the derived equations. For example, mutual relations of various perturbative approximations corresponding to the various kinds of the Hamiltonian are discussed with a view to their accuracy, or a numerical algorithm of calculating the perturbations in the vicinities of caustics and pseudocaustics is proposed. The notes of Section 4 are meant for readers wishing to apply the derived equations theoretically or numerically.

In Section 5, the equations of Section 3 for the spatial derivatives and perturbations of travel time up to the third order are specified for isotropic media, using three kinds of the Hamiltonian, corresponding to the three most common kinds of the independent parameter along rays. Those who wish to calculate the second–order or even third–order perturbations of travel time in isotropic media may flick through Section 2 and then refer directly to Section 5.

Section 6, devoted to the comparison with previously published equations, is of little importance for most readers. Section 6 may be useful only to readers already familiar with the equations for the second–order perturbations of travel time derived in the previous papers by *Snieder and Sambridge* (*1992*), *Farra* (*1999*) or *Červený* (*2001*) in order to illustrate the differences in approaches and to compare the derived equations.

2. EQUATIONS FOR THE DERIVATIVES AND PERTURBATIONS OF TRAVEL TIME

In *Section 2.1*, we introduce the definitions and notation used throughout the paper. In *Section 2.2*, we express the eikonal equation in the general form of the stationary Hamilton–Jacobi equation and derive its consequence, identity (11), which is of principal importance in deriving the equations for the spatial derivatives and perturbations of travel time. In *Section 2.3*, we define ray parameters and recall the basics of dynamic ray tracing. The dynamic ray tracing equations are necessary for calculating the second–order spatial derivatives of travel time, and for introducing the covariant derivatives of travel time with respect to the ray parameters. In *Section 2.4*, we define the covariant derivatives of travel time with respect to the ray parameters and utilize identity (11) in deriving simple equations for calculating the covariant derivatives with respect to the ray parameters and perturbations of travel time. Section 2.4 constitutes the final result of the paper.

2.1. Basic definitions and notation

The model of a smooth elastic medium for calculating travel time is assumed to be specified by the set $f = f(x_i)$ of smooth functions. The smooth functions may represent, e.g., the spatial distributions of the individual density–normalized elastic moduli. This set of smooth functions is assumed to be an element of a linear normed space, called the *model space*. Assume that the model space is generated by a linearly independent set $\{b_\kappa\}$ of its elements, each element $b_\kappa = b_\kappa(x_i)$ being a set of smooth functions. Set $\{b_\kappa\}$ then represents the basis of the model space. We shall refer to the coordinates f_κ of *model* $f(x_i) = \sum_\kappa f_\kappa\, b_\kappa(x_i)$ with respect to the selected basis $\{b_\kappa\}$ in the model space as the *model parameters*.

We assume that the Hamiltonian is a function of *phase–space coordinates*, composed of spatial coordinates x_i and slowness–vector components p_j, and of model parameters f_κ,

$$H = H(x_i, p_j, f_\kappa) \quad . \tag{1}$$

Similarly, the travel time and other quantities calculated in the model are assumed to be functions of *spatial coordinates* x_i and of model parameters f_κ,

$$\tau = \tau(x_i, f_\kappa) \quad . \tag{2}$$

Note that, for a given model determined by model parameters f_κ, we may define a continuous set of the Hamiltonians, parametrized by several additional parameters f_κ. For example, there are two S–wave polarizations with the two respective Hamiltonians corresponding to the anisotropic ray theory in anisotropic media. Instead of selecting one of these two Hamiltonians, we may consider a one–parametric set of Hamiltonians, parametrized by f_μ, such that we obtain the Hamiltonian corresponding to one polarization for $f_\mu = -1$, the Hamiltonian corresponding to the other polarization for $f_\mu = +1$, and the averaged Hamiltonian of both S–wave polarizations corresponding to the anisotropic common ray approximation by *Bakker* (*2002*) for $f_\mu = 0$. We may also consider a two–parametric set of Hamiltonians, parametrized by f_μ and f_ν, such that we obtain the Hamiltonian corresponding to the isotropic common ray approximation in the reference isotropic medium for $(f_\mu, f_\nu) = (0, 0)$, the Hamiltonian corresponding to one anisotropic S–wave polarization for $(f_\mu, f_\nu) = (1, 0)$, the Hamiltonian corresponding to the other anisotropic S–wave polarization for $(f_\mu, f_\nu) = (0, 1)$, and the averaged Hamiltonian corresponding to the anisotropic common ray approximation by *Bakker* (*2002*) for $(f_\mu, f_\nu) = (\frac{1}{2}, \frac{1}{2})$. For the sake of simplicity, we shall also refer to these additional parameters f_κ, parametrizing the Hamiltonians in a given model, as the *model parameters*.

We shall refer to the partial derivatives with respect to model parameters f_κ as the *perturbations*.

We shall use the Einstein summation convention, and denote the partial derivatives with respect to spatial coordinates x_i by lower–case Roman subscripts following a comma, and the *perturbations by lower–case Greek subscripts* following a comma. In the phase space, we denote the partial derivatives with respect to components p_j

of the slowness vector by lower–case Roman superscripts following a comma. For instance,

$$H^{,ab\ldots f}_{,ij\ldots n\alpha\ldots\nu} = \frac{\partial}{\partial f_\alpha}\cdots\frac{\partial}{\partial f_\nu}\,\frac{\partial}{\partial x_i}\frac{\partial}{\partial x_j}\cdots\frac{\partial}{\partial x_n}\,\frac{\partial}{\partial p_a}\frac{\partial}{\partial p_b}\cdots\frac{\partial}{\partial p_f}H \tag{3}$$

denotes the perturbations of the partial *phase–space derivatives* of the Hamiltonian. The perturbations are taken at fixed phase–space coordinates x_i, p_j, and the partial phase–space derivatives are calculated at the fixed function $f(x_i)=\sum_\kappa f_\kappa\, b_\kappa(x_i)$ of the linear normed model space. Similarly,

$$\tau_{,ij\ldots n\alpha\ldots\nu} = \frac{\partial}{\partial f_\alpha}\cdots\frac{\partial}{\partial f_\nu}\,\frac{\partial}{\partial x_i}\frac{\partial}{\partial x_j}\cdots\frac{\partial}{\partial x_n}\tau \tag{4}$$

denotes the perturbations of the *spatial derivatives* of travel time τ. The perturbations are taken at fixed spatial coordinates x_i, and the partial spatial derivatives are calculated at the fixed function $f(x_i)=\sum_\kappa f_\kappa\, b_\kappa(x_i)$ of the linear normed model space.

We also introduce "multi–indices" in order to make the equations more concise and easy to survey. For example,

$$\begin{matrix}\tau_{,rij} & \tau_{,rk\alpha} \\ {}_{,rik} & {}_{,rj\alpha} \\ {}_{,rjk} & {}_{,ri\alpha}\end{matrix} \tag{5}$$

stands for

$$\tau_{,rij}\,\tau_{,rk\alpha} + \tau_{,rik}\,\tau_{,rj\alpha} + \tau_{,rjk}\,\tau_{,ri\alpha} \quad . \tag{6}$$

2.2. Eikonal equation and its consequences

In both isotropic and anisotropic media, we assume the *travel time* (action function) $\tau(x_i, f_\kappa)$ determined by the *eikonal equation* in the general form of the stationary *Hamilton–Jacobi equation*

$$H\big(x_i, \tau_{,j}(x_m, f_\mu), f_\kappa\big) = 0 \quad , \tag{7}$$

where the function $H(x_i, p_j, f_\kappa)$ of the phase–space coordinates and model parameters is the Hamiltonian, see (1). The corresponding ray tracing equations then have the form of Hamilton's equations

$$\frac{\mathrm{d}}{\mathrm{d}\gamma_3}x_i = \frac{\partial}{\partial p_i}H(x_q, p_r, f_\kappa) \quad , \qquad \frac{\mathrm{d}}{\mathrm{d}\gamma_3}p_i = -\frac{\partial}{\partial x_i}H(x_q, p_r, f_\kappa) \quad , \tag{8}$$

where parameter γ_3 along rays is determined by the form of the Hamiltonian.

If $\tau(x_i, f_\kappa)$ is the solution of eikonal equation (7), function

$$h(x_k, f_\kappa) = H\big(x_i, \tau_{,j}(x_m, f_\mu), f_\kappa\big) \tag{9}$$

is obviously constant (equal to zero) and all its perturbations and spatial derivatives thus vanish,

$$\frac{\partial}{\partial f_\alpha}\cdots\frac{\partial}{\partial f_\nu}\,\frac{\partial}{\partial x_i}\cdots\frac{\partial}{\partial x_n}\,h(x_q, f_\kappa) = 0 \quad . \tag{10}$$

In terms of the Hamiltonian, this equation reads

$$\left(\frac{\partial}{\partial f_\alpha}+\tau_{,s\alpha}\frac{\partial}{\partial p_s}\right)\cdots\left(\frac{\partial}{\partial f_\nu}+\tau_{,z\nu}\frac{\partial}{\partial p_z}\right)\left(\frac{\partial}{\partial x_i}+\tau_{,ia}\frac{\partial}{\partial p_a}\right)\cdots\left(\frac{\partial}{\partial x_n}+\tau_{,nf}\frac{\partial}{\partial p_f}\right)H=0\ . \quad (11)$$

Here the perturbations and partial phase–space derivatives are computed at point $(x_q,p_r)=(x_q,\tau_{,r}(x_s,f_\kappa))$ in the phase space.

2.3. Ray parameters and dynamic ray tracing

We define the matrices of the partial derivatives of coordinates x_i and of the slowness–vector components $\tau_{,i}$ with respect to 3 *ray parameters*: ray take–off parameters γ_1, γ_2, and independent parameter γ_3 along rays,

$$Q_{ia}=\frac{\partial x_i}{\partial\gamma_a}\quad ,\qquad P_{ia}=\frac{\partial\tau_{,i}}{\partial\gamma_a}\quad , \quad (12)$$

where $\frac{\partial}{\partial\gamma_3}$ is identical to $\frac{\mathrm{d}}{\mathrm{d}\gamma_3}$ used in other equations. Matrices Q_{ia} and P_{ia} describe, by definition, the properties of the orthonomic system of rays corresponding to the travel time under consideration. They may be expressed in terms of their initial values and the paraxial ray propagator matrix (*Červený, 2001*). Let us emphasize that the definition of matrices Q_{ia} and P_{ia} depends on the kind of parameter γ_3 along rays, which is in turn determined by the form of the Hamiltonian, refer to Section 5 for examples. The use of matrices Q_{ia} and P_{ia}, defined for a particular kind of γ_3, in the equations for the perturbations and spatial derivatives of travel time, derived from the Hamiltonian corresponding to different γ_3, has to be avoided. Matrices Q_{ia} and P_{ia} are often calculated for $\gamma_3=\tau$. The transformation of matrix Q_{ia} to the one defined for different γ_3 has been described by *Klimeš* (*1997, 1999*).

Equation

$$P_{ia}=\tau_{,ij}\ Q_{ja} \quad (13)$$

is a direct consequence of the above definitions. The dynamic ray tracing system

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\gamma_3}Q_{ia}&=\quad H^{,i}_{,j}(x_q,p_r)\ Q_{ja}+H^{,ij}(x_q,p_r)\ P_{ja}\\ \frac{\mathrm{d}}{\mathrm{d}\gamma_3}P_{ia}&=-H_{,ij}(x_q,p_r)\ Q_{ja}-H^{,j}_{,i}(x_q,p_r)\ P_{ja}\end{aligned} \quad (14)$$

can be obtained by differentiating the ray tracing system (8) with respect to γ_a (*Červený, 1972, 2001*; *Hanyga, 1982*; *Klimeš, 1994*). For more details on the dynamic ray tracing system, including the initial conditions, refer to the book by *Červený* (*2001*). After insertion of (13), the first equation of the dynamic ray tracing system (14) becomes

$$\frac{\mathrm{d}}{\mathrm{d}\gamma_3}Q_{ia}=Q_{ja}\left(\frac{\partial}{\partial x_j}+\tau_{,jk}\frac{\partial}{\partial p_k}\right)\frac{\partial}{\partial p_i}H\quad . \quad (15)$$

Let us emphasize once again that the matrices Q_{ia} and P_{ia} in this paper are defined by equation (12), and correspond to the orthonomic system of rays under consideration.

2.4. Equations for the spatial derivatives and perturbations of travel time

We now introduce the *covariant derivatives*

$$T_{ab\ldots f\alpha\ldots\nu} = \tau_{,ij\ldots n\alpha\ldots\nu}\, Q_{ia} Q_{jb} \cdots Q_{nf} \tag{16}$$

of travel time with respect to ray parameters γ_a. Let us differentiate covariant derivatives (16) along a ray with respect to γ_3, and insert equations (8) and (15) for $\frac{\mathrm{d}}{\mathrm{d}\gamma_3} x_i$ and $\frac{\mathrm{d}}{\mathrm{d}\gamma_3} Q_{ia}$, respectively,

$$\frac{\mathrm{d}}{\mathrm{d}\gamma_3}[\tau_{,ijk\ldots mn\alpha\ldots\nu} Q_{ia} Q_{jb} Q_{kc} \cdots Q_{me} Q_{nf}] = K_{ijk\ldots mn\alpha\ldots\nu} Q_{ia} Q_{jb} Q_{kc} \cdots Q_{me} Q_{nf} \ , \tag{17}$$

where

$$\begin{aligned} K_{ijk\ldots mn\alpha\ldots\nu} = \tau_{,rijk\ldots mn\alpha\ldots\nu} \frac{\partial}{\partial p_r} H + \tau_{,rjk\ldots mn\alpha\ldots\nu} & \left(\frac{\partial}{\partial x_i} + \tau_{,is} \frac{\partial}{\partial p_s} \right) \frac{\partial}{\partial p_r} H \\ + \tau_{,irk\ldots mn\alpha\ldots\nu} & \left(\frac{\partial}{\partial x_j} + \tau_{,js} \frac{\partial}{\partial p_s} \right) \frac{\partial}{\partial p_r} H \\ & \vdots \\ + \tau_{,ijk\ldots mr\alpha\ldots\nu} & \left(\frac{\partial}{\partial x_n} + \tau_{,ns} \frac{\partial}{\partial p_s} \right) \frac{\partial}{\partial p_r} H \ . \end{aligned} \tag{18}$$

The covariant derivatives with respect to the ray parameters and perturbations of travel time may thus be expressed in the form of the integral along the ray,

$$\boxed{T_{ab\ldots f\alpha\ldots\nu}(\gamma_3) = T_{ab\ldots f\alpha\ldots\nu}(\gamma_3^0) + \int_{\gamma_3^0}^{\gamma_3} \mathrm{d}\gamma_3\ K_{ij\ldots n\alpha\ldots\nu}\ Q_{ia} Q_{jb} \cdots Q_{nf} \quad ,} \tag{19}$$

with initial conditions $T_{ab\ldots f\alpha\ldots\nu}(\gamma_3^0)$ defined by equation (16). The initial conditions are also briefly mentioned at the end of this section.

The spatial derivatives in coordinates x_i and perturbations of travel time may then be expressed in terms of covariant derivatives (19),

$$\boxed{\tau_{,ij\ldots n\alpha\ldots\nu} = T_{ab\ldots f\alpha\ldots\nu}\ Q^{-1}_{ai} Q^{-1}_{bj} \cdots Q^{-1}_{fn} \quad ,} \tag{20}$$

where we have used Q^{-1}_{ai} to denote the components of the matrix inverse to matrix Q_{ia}. Matrix Q^{-1}_{ai} exists and is finite off caustics.

The perturbations and spatial derivatives of travel time on the right–hand side of equation (18) coincide with the corresponding terms on the left–hand side of equation (11), and are thus cancelled if subtracting (11) from (18),

$$\boxed{\begin{aligned} K_{ijk\dots mn\alpha\dots\nu} = \tau_{,rijk\dots mn\alpha\dots\nu}\frac{\partial}{\partial p_r}H + \tau_{,rjk\dots mn\alpha\dots\nu}\left(\frac{\partial}{\partial x_i}+\tau_{,is}\frac{\partial}{\partial p_s}\right)\frac{\partial}{\partial p_r}H \\ +\tau_{,irk\dots mn\alpha\dots\nu}\left(\frac{\partial}{\partial x_j}+\tau_{,js}\frac{\partial}{\partial p_s}\right)\frac{\partial}{\partial p_r}H \\ \vdots \qquad\qquad\qquad \\ +\tau_{,ijk\dots mr\alpha\dots\nu}\left(\frac{\partial}{\partial x_n}+\tau_{,ns}\frac{\partial}{\partial p_s}\right)\frac{\partial}{\partial p_r}H \\ -\left(\frac{\partial}{\partial f_\alpha}+\tau_{,s\alpha}\frac{\partial}{\partial p_s}\right)\dots\left(\frac{\partial}{\partial f_\nu}+\tau_{,z\nu}\frac{\partial}{\partial p_z}\right)\left(\frac{\partial}{\partial x_i}+\tau_{,ia}\frac{\partial}{\partial p_a}\right)\dots\left(\frac{\partial}{\partial x_n}+\tau_{,nf}\frac{\partial}{\partial p_f}\right)H \ , \quad (21)\end{aligned}}$$

for all integration kernels (21) except K, K_i and K_{ij} corresponding to τ, $\tau_{,i}$ and $\tau_{,ij}$. Travel time τ and its first–order spatial derivatives $\tau_{,i}$ are calculated by ray tracing (8), while the second–order spatial derivatives $\tau_{,ij}$ are calculated by means of dynamic ray tracing (14) and equation (13).

If we calculate the spatial derivatives and perturbations in the order $\tau_{,i}$ (ray tracing), $\tau_{,\alpha}$, $\tau_{,ij}$ (dynamic ray tracing), $\tau_{,i\alpha}$, $\tau_{,\alpha\beta}$, $\tau_{,ijk}$, $\tau_{,ij\alpha}$, $\tau_{,i\alpha\beta}$, $\tau_{,\alpha\beta\gamma}$, $\tau_{,ijkl}$, $\tau_{,ijk\alpha}$, $\tau_{,ij\alpha\beta}$, $\tau_{,i\alpha\beta\gamma}$, $\tau_{,\alpha\beta\gamma\delta}$, etc., the right–hand side of equation (21) contains only the previously calculated spatial derivatives and perturbations of travel time. The special cases of equation (21) corresponding to the first–order, second–order and third–order derivatives and perturbations of travel time are presented in Section 3 as examples.

Let us illustrate the order of calculating the spatial derivatives and perturbations of travel time graphically:

$$\begin{array}{ccccccc} (\tau_{,i}) & \tau_{,\alpha} & & & & & \\ (\tau_{,ij}) & \tau_{,i\alpha} & \tau_{,\alpha\beta} & & & & \\ \tau_{,ijk} & \tau_{,ij\alpha} & \tau_{,i\alpha\beta} & \tau_{,\alpha\beta\gamma} & & & \\ \tau_{,ijkl} & \tau_{,ijk\alpha} & \tau_{,ij\alpha\beta} & \tau_{,i\alpha\beta\gamma} & \tau_{,\alpha\beta\gamma\delta} & & \\ \tau_{,ijklm} & \tau_{,ijkl\alpha} & \tau_{,ijk\alpha\beta} & \tau_{,ij\alpha\beta\gamma} & \tau_{,i\alpha\beta\gamma\delta} & \tau_{,i\alpha\beta\gamma\delta\varepsilon} & \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{array}$$

To calculate the derivatives or perturbations of travel time of a selected order, the derivatives and perturbations of travel time situated on the left and above the selected ones must be known. The derivatives of travel time enclosed in parentheses are calculated by ray tracing and dynamic ray tracing.

Note that covariant derivatives $T_{\dots 3\dots}$, containing at least one index 3 in place of the lower–case subscripts corresponding to the covariant derivatives with respect to the ray parameters, can be expressed analytically. For instance, for $a = 3$, equation (16) with (12) and (8) reads

$$T_{3b\dots f\alpha\dots\nu} = \tau_{,ij\dots n\alpha\dots\nu}\,H^{,i}\,Q_{jb}\cdots Q_{nf} \quad . \tag{22}$$

Equation (18) then yields

$$\boxed{T_{3b\ldots f\alpha\ldots\nu} = [K_{j\ldots n\alpha\ldots\nu} - (H^{,s}_{\substack{,j\\ \vdots\\ ,n}} + H^{,rs}\tau_{\substack{,rj\\ \vdots\\ ,rn}})\,\tau_{\substack{,s\ldots n\alpha\ldots\nu\\ \vdots\\ ,j\ldots s\alpha\ldots\nu}}]\,Q_{jb}\cdots Q_{nf} \qquad (23)}$$

for all $T_{3\ldots}$ except T_3, T_{3b} and T_{3bc}. For the calculation of T_{3bc}, refer to equation (33) in the next section.

We thus need to calculate only $T_{A\ldots F\alpha\ldots\nu}$ with $A, ..., F = 1, 2$ (including $T_{A\ldots F}$ and $T_{\alpha\ldots\nu}$) by numerical quadrature (19). Initial conditions $T_{A\ldots F\alpha\ldots\nu}(\gamma_3^0)$ are defined by equation (16). The initial conditions for these covariant derivatives are zero at a point source, $T_{A\ldots F\alpha\ldots\nu}(\gamma_3^0) = 0$, see (16), but are generally finite for the finite initial value $Q_{ia}(\gamma_3^0)$ of the matrix of geometrical spreading.

3. EXAMPLES OF THE INTEGRANDS AND INTEGRALS IN GENERAL MEDIA

The special cases of the general results of Section 2 corresponding to the first–order, second–order and third–order perturbations of travel time are presented in Sections 3.1, 3.2, and 3.3, respectively, in order to illustrate somewhat abstract final equations (21) and (23).

The equations for calculating the perturbations of travel time of a particular order also include the equations for the spatial derivatives of travel time of equal order, and the equations for the mixed spatial derivatives and perturbations of travel time of equal aggregate order, because these derivatives and perturbations are required for calculating the perturbations of the respective order while they are not required for calculating the perturbations of lower orders.

3.1. First–order perturbations of travel time

For the first–order perturbations of travel time, integrand (21) of equation (19) takes the form of

$$K_\alpha = \tau_{,r\alpha}\frac{\partial}{\partial p_r}H - \left(\frac{\partial}{\partial f_\alpha} + \tau_{,s\alpha}\frac{\partial}{\partial p_s}\right)H \quad , \tag{24}$$

which reduces to integrand

$$K_\alpha = -H_{,\alpha} \tag{25}$$

of the well–known first–order perturbation equation for travel time (e.g., *Červený, 2001,* eq. 3.9.6).

3.2. Second–order perturbations of travel time

The second–order spatial derivatives $\tau_{,ij}$ are calculated using equation (13) from matrices Q_{ia} and P_{ia}, which are solutions of the dynamic ray tracing system (14).

For the first–order perturbations of the first–order spatial derivatives of travel time, equation (21) reads

$$K_{i\alpha} = \tau_{,ri\alpha}\frac{\partial}{\partial p_r}H + \tau_{,r\alpha}\left(\frac{\partial}{\partial x_i}+\tau_{,is}\frac{\partial}{\partial p_s}\right)\frac{\partial}{\partial p_r}H - \left(\frac{\partial}{\partial f_\alpha}+\tau_{,s\alpha}\frac{\partial}{\partial p_s}\right)\left(\frac{\partial}{\partial x_i}+\tau_{,ia}\frac{\partial}{\partial p_a}\right)H\ , \tag{26}$$

which reduces to

$$K_{i\alpha} = -H_{,i\alpha} - H_{,\alpha}^{,r}\,\tau_{,ri} \quad . \tag{27}$$

The value of the integral (19) of $K_{i\alpha}Q_{i3}$ is given by equations (23) and (25),

$$T_{3\alpha} = -H_{,\alpha} \quad . \tag{28}$$

For the second–order perturbations of travel time, equation (21) becomes

$$K_{\alpha\beta} = \tau_{,r\alpha\beta}\frac{\partial}{\partial p_r}H - \left(\frac{\partial}{\partial f_\alpha}+\tau_{,r\alpha}\frac{\partial}{\partial p_r}\right)\left(\frac{\partial}{\partial f_\beta}+\tau_{,s\beta}\frac{\partial}{\partial p_s}\right)H \quad , \tag{29}$$

which can be expressed as

$$K_{\alpha\beta} = -H_{,\alpha\beta} - H_{\substack{,\alpha\\,\beta}}^{,r}\,\tau_{\substack{,r\beta\\,r\alpha}} - H^{,rs}\tau_{,r\alpha}\,\tau_{,s\beta} \quad . \tag{30}$$

3.3. Third–order perturbations of travel time

For the third–order spatial derivatives of travel time, equation (21) is

$$K_{ijk} = \tau_{,rijk}\frac{\partial}{\partial p_r}H + \tau_{,rjk}\left(\frac{\partial}{\partial x_i}+\tau_{,is}\frac{\partial}{\partial p_s}\right)\frac{\partial}{\partial p_r}H + \tau_{,irk}\left(\frac{\partial}{\partial x_j}+\tau_{,js}\frac{\partial}{\partial p_s}\right)\frac{\partial}{\partial p_r}H$$

$$+\tau_{,ijr}\left(\frac{\partial}{\partial x_k}+\tau_{,ks}\frac{\partial}{\partial p_s}\right)\frac{\partial}{\partial p_r}H - \left(\frac{\partial}{\partial x_i}+\tau_{,ia}\frac{\partial}{\partial p_a}\right)\left(\frac{\partial}{\partial x_j}+\tau_{,jb}\frac{\partial}{\partial p_b}\right)\left(\frac{\partial}{\partial x_k}+\tau_{,kc}\frac{\partial}{\partial p_c}\right)H\ , \tag{31}$$

i.e.

$$K_{ijk} = -H_{,ijk} - H_{\substack{,ij\\,ik\\,jk}}^{,a}\,\tau_{\substack{,ak\\,aj\\,ai}} - H_{\substack{,i\\,j\\,k}}^{,ab}\,\tau_{\substack{,aj\\,ai\\,ai}}\,\tau_{\substack{,bk\\,bk\\,bj}} - H^{,abc}\,\tau_{,ai}\,\tau_{,bj}\,\tau_{,ck} \quad . \tag{32}$$

For the integral (19) of $K_{ijk}Q_{i3}Q_{jb}Q_{kc}$, equations (11) and (22) yield

$$T_{3bc} = -H_{,jk}Q_{jb}Q_{kc} - H_{\substack{,j\\,j}}^{,k}\,Q_{\substack{jb\\jc}}\,P_{\substack{kc\\kb}} - H^{,jk}P_{jb}P_{kc} \quad . \tag{33}$$

Note that $Q_{i3} = H^{,i}$ and $P_{i3} = -H_{,i}$ according to definition (12) and ray tracing system (8). For the first–order perturbations of the second–order spatial derivatives of travel time, equation (21) becomes

$$K_{ij\alpha} = \tau_{,rij\alpha}\frac{\partial}{\partial p_r}H + \tau_{,rj\alpha}\left(\frac{\partial}{\partial x_i} + \tau_{,is}\frac{\partial}{\partial p_s}\right)\frac{\partial}{\partial p_r}H + \tau_{,ir\alpha}\left(\frac{\partial}{\partial x_j} + \tau_{,js}\frac{\partial}{\partial p_s}\right)\frac{\partial}{\partial p_r}H$$
$$- \left(\frac{\partial}{\partial f_\alpha} + \tau_{,s\alpha}\frac{\partial}{\partial p_s}\right)\left(\frac{\partial}{\partial x_i} + \tau_{,ia}\frac{\partial}{\partial p_a}\right)\left(\frac{\partial}{\partial x_j} + \tau_{,jb}\frac{\partial}{\partial p_b}\right)H \quad , \tag{34}$$

i.e.

$$K_{ij\alpha} = -H_{,ij\alpha} - H^{,r}_{\substack{,ij\\,i\alpha\\,j\alpha}}\,\tau_{\substack{,r\alpha\\,rj\\,ri}} - H^{,r}_{,\alpha}\tau_{,rij} - H^{,rs}_{\substack{,i\\,j\\,\alpha}}\,\tau_{\substack{,rj\\,ri\\,ri}}\,\tau_{\substack{,s\alpha\\,s\alpha\\,sj}} - H^{,rs}\tau_{,rij}\tau_{,s\alpha} - H^{,rst}\tau_{,ri}\tau_{,sj}\tau_{,t\alpha} \ . \tag{35}$$

The value of the integral (19) of $K_{ij\alpha}Q_{i3}Q_{jb}$ is given by equations (23) and (27),

$$T_{3b\alpha} = -H_{,j\alpha}Q_{jb} - H^{,j}_{,\alpha}P_{jb} - (H^{,s}_{,j}Q_{jb} + H^{,sj}P_{jb})\,\tau_{,s\alpha} \quad . \tag{36}$$

For the second–order perturbations of the spatial gradient of travel time, equation (21) takes the form of

$$K_{i\alpha\beta} = \tau_{,ri\alpha\beta}\frac{\partial}{\partial p_r}H + \tau_{,r\alpha\beta}\left(\frac{\partial}{\partial x_i} + \tau_{,is}\frac{\partial}{\partial p_s}\right)\frac{\partial}{\partial p_r}H$$
$$- \left(\frac{\partial}{\partial f_\alpha} + \tau_{,s\alpha}\frac{\partial}{\partial p_s}\right)\left(\frac{\partial}{\partial f_\beta} + \tau_{,t\beta}\frac{\partial}{\partial p_t}\right)\left(\frac{\partial}{\partial x_i} + \tau_{,ia}\frac{\partial}{\partial p_a}\right)H \ , \tag{37}$$

which may be expressed as

$$K_{i\alpha\beta} = -H_{,i\alpha\beta} - H^{,r}_{\substack{,i\alpha\\,i\beta\\,\alpha\beta}}\,\tau_{\substack{,r\beta\\,r\alpha\\,ri}} - H^{,r}_{\substack{,\alpha\\,\beta}}\,\tau_{\substack{,ri\beta\\,ri\alpha}} - H^{,rs}_{\substack{,i\\,\alpha\\,\beta}}\,\tau_{\substack{,r\alpha\\,ri\\,ri}}\,\tau_{\substack{,s\beta\\,s\beta\\,s\alpha}} - H^{,rs}\tau_{\substack{,ri\alpha\\,ri\beta}}\,\tau_{\substack{,s\beta\\,s\alpha}} - H^{,rst}\tau_{,ri}\tau_{,s\alpha}\tau_{,t\beta} \ . \tag{38}$$

For the integral (19) of $K_{i\alpha\beta}Q_{i3}$, equations (23) and (30) yield

$$T_{3\alpha\beta} = -H_{,\alpha\beta} - H^{,r}_{\substack{,\alpha\\,\beta}}\,\tau_{\substack{,r\beta\\,r\alpha}} - H^{,rs}\tau_{,r\alpha}\tau_{,s\beta} \quad . \tag{39}$$

For the third–order perturbations of travel time, equation (21) reads

$$K_{\alpha\beta\gamma} = \tau_{,r\alpha\beta\gamma}\frac{\partial}{\partial p_r}H - \left(\frac{\partial}{\partial f_\alpha} + \tau_{,r\alpha}\frac{\partial}{\partial p_r}\right)\left(\frac{\partial}{\partial f_\beta} + \tau_{,s\beta}\frac{\partial}{\partial p_s}\right)\left(\frac{\partial}{\partial f_\gamma} + \tau_{,t\gamma}\frac{\partial}{\partial p_t}\right)H \ , \tag{40}$$

i.e.

$$K_{\alpha\beta\gamma} = -H_{,\alpha\beta\gamma} - H^{,r}_{\substack{,\alpha\beta\\,\alpha\gamma\\,\beta\gamma}}\,\tau_{\substack{,r\gamma\\,r\beta\\,r\alpha}} - H^{,r}_{\substack{,\alpha\\,\beta\\,\gamma}}\,\tau_{\substack{,r\beta\gamma\\,r\alpha\gamma\\,r\alpha\beta}} - H^{,rs}_{\substack{,\alpha\\,\beta\\,\gamma}}\,\tau_{\substack{,r\beta\\,r\alpha\\,r\alpha}}\,\tau_{\substack{,s\gamma\\,s\gamma\\,s\beta}} - H^{,rs}\tau_{\substack{,r\alpha\beta\\,r\alpha\gamma\\,r\beta\gamma}}\,\tau_{\substack{,s\gamma\\,s\beta\\,s\alpha}} - H^{,rst}\tau_{,r\alpha}\tau_{,s\beta}\tau_{,t\gamma} \ . \tag{41}$$

4. SOME NOTES RELATED TO THE PERTURBATIONS OF TRAVEL TIME

Section 4 contains various notes related to the derived equations.

The integrands of numerical quadrature (19) often go to infinity at caustics, let us mention the second–order perturbations of travel time as the simplest example. In *Section 4.2*, a numerical algorithm of calculating the second–order perturbations of travel time in the vicinities of caustics and pseudocaustics is proposed. Analogous tricks may also be applied to other spatial derivatives and perturbations of travel time.

Various kinds of the Hamiltonian yield various kinds of parameter γ_3 along rays, and different kinds of parameter γ_3 yield different perturbations of travel time. It is well known that different kinds of the linearized approximation of travel time with respect to model parameters have considerably different accuracies (e.g., *Bulant, Klimeš and Pšenčík, 2000*; *Bulant and Klimeš, 2002*). As already suggested by *Snieder and Sambridge (1992)*, it may sometimes be useful to transform the equations for the perturbations of travel time into the ray–centred coordinate system, or in another words, into wavefront–normal and ray–normal components. This separation of the wavefront–normal and ray–normal components of the covariant spatial derivatives of travel time may be especially useful to study and control the accuracy of the various kinds of the Taylor expansion of travel time with respect to model parameters. The related problems are discussed in Sections 4.1, 4.3, 4.4 and 4.5. A possibility to apply differently accurate kinds of the linearized approximation of travel time with respect to model parameters, corresponding to the same Hamiltonian, is mentioned in *Section 4.1.* The decomposition of the covariant spatial derivatives of travel time into the wavefront–normal and ray–normal components is introduced in *Section 4.3.* The selection of the "optimal" form of the Hamiltonian for the perturbative approximation of travel times is discussed in *Section 4.4.* Equations for the ray–normal derivatives and perturbations of travel time are then briefly discussed in *Section 4.5.*

4.1. First–order approximations of travel time in a perturbed model

The linear Taylor expansion of travel time with respect to model parameters is determined by equations (19), (20) and (25),

$$\tau(x_k, f_\kappa) \approx \tau(x_k, f^0_\kappa) - \int_{\gamma_3^0}^{\gamma_3} \mathrm{d}\gamma_3 \sum_\alpha H_{,\alpha}(x_m, p_n, f^0_\kappa)\,(f_\alpha - f^0_\alpha) \quad , \tag{42}$$

where $x_k = x_k(\gamma_3)$ and $p_k = p_k(\gamma_3)$ are the phase–space coordinates of the ray in the background model $f^0(x_i) = \sum_\kappa f^0_\kappa b_\kappa(x_i)$. The second–order and higher–order terms of the Taylor expansion represent the inaccuracy of the linear Taylor expansion (42).

We may also define the new, perturbed travel time $\overline{\tau}(x_k, f_\kappa)$ by equation

$$\overline{\tau}(x_k, f_\kappa) = \tau(x_k, f^0_\kappa) - \int_{\gamma_3^0}^{\gamma_3} \mathrm{d}\gamma_3\,[H(x_m, p_n, f_\kappa) - H(x_m, p_n, f^0_\kappa)] \quad , \tag{43}$$

where the integral is calculated along rays in the background model $f^0(x_i) = \sum_\kappa f_\kappa^0 b_\kappa(x_i)$. The perturbations of $\overline{\tau}(x_k, f_\kappa)$ are given by equations (19) and (20) with $K_{\alpha\ldots\nu}$ replaced by

$$\overline{K}_{\alpha\ldots\nu} = -H_{,\alpha\ldots\nu} \quad . \tag{44}$$

Both approximations (42) and (43) are equivalent with respect to the first–order perturbations, but approximation (43) also includes the small parts of higher–order perturbations, the terms corresponding to $-H_{,\alpha\ldots\nu}$, see (30), (41), and also (21) in general. The Taylor expansion of error $\tau(x_k, f_\kappa) - \overline{\tau}(x_k, f_\kappa)$ of approximation (43) is given by equations (19) and (20) with $K_{\alpha\ldots\nu}$ replaced by $K_{\alpha\ldots\nu} - \overline{K}_{\alpha\ldots\nu}$. If the Hamiltonian is linearly dependent on model parameters f_κ, its second–order and higher–order perturbations $H_{,\alpha\beta}$, $H_{,\alpha\beta\gamma}$, ..., vanish and approximations (42) and (43) become identical, which may sometimes be favourable, e.g., for linearized inversion of travel times.

4.2. Numerical calculation of the second–order perturbations of travel time

Numerical calculation of the first–order perturbations of the gradient of travel time by quadrature (19) with (27) should represent no problem. On the other hand, if we insert (20) into integration kernel (30) for the second–order perturbations of travel time,

$$K_{\alpha\beta} = -H_{,\alpha\beta} - H^{,r}_{\substack{,\alpha\\ ,\beta}} Q^{-1}_{\substack{ar\\ ar}} T_{\substack{a\beta\\ a\alpha}} - H^{,rs} Q^{-1}_{ar} Q^{-1}_{bs} T_{a\alpha} T_{b\beta} \quad , \tag{45}$$

we see that we cannot integrate (45) numerically in the vicinities of caustics where $H^{,rs}$ and $T_{a\alpha}$ are finite while Q_{ia} is singular. Fortunately, we may use equation (19) with (27) and identity

$$\frac{\mathrm{d}}{\mathrm{d}\gamma_3}\left(P^{-1}_{ar} Q^{-1}_{br}\right) = H_{,rs}\, P^{-1}_{ar} P^{-1}_{bs} - H^{,rs} Q^{-1}_{ar} Q^{-1}_{bs} \quad , \tag{46}$$

following from dynamic ray tracing equations (14), to express $K_{\alpha\beta}$ in an alternative form,

$$K_{\alpha\beta} = -H_{,\alpha\beta} + H_{\substack{,r\alpha\\ ,r\beta}} P^{-1}_{\substack{ar\\ ar}} T_{\substack{a\beta\\ a\alpha}} - H_{,rs}\, P^{-1}_{ar} P^{-1}_{bs} T_{a\alpha}\, T_{b\beta} + \frac{\mathrm{d}}{\mathrm{d}\gamma_3}\left(P^{-1}_{ar} Q^{-1}_{br} T_{a\alpha}\, T_{b\beta}\right) \; . \tag{47}$$

The last term may be integrated analytically, whereas the other terms are continuous in the vicinities of caustics and may be numerically integrated everywhere, with the exception of the vicinities of pseudocaustics where P_{ia} is singular. Since equation (47) is valid for complex–valued ray fields with the slightly imaginary and thus everywhere regular matrix Q_{ia} of geometrical spreading, the analytical integral of the last term is applicable also to the limiting case of real–valued rays touching the caustics. Combining equations (45) and (47) enables the optimization of calculating the second–order perturbations of travel time by numerical quadrature (19).

Similar tricks have also to be applied to many other perturbations and spatial derivatives of travel time.

4.3. Covariant derivatives of travel time in ray–centred coordinates

Ray–centred coordinates (Riemannian normal coordinates) were applied to the polarization of electromagnetic waves by *Luneburg (1944)* and to dynamic ray tracing in isotropic media by *Babich and Buldyrev (1972)* and *Popov and Pšenčík (1978a, 1978b)*, and then to dynamic ray tracing in anisotropic media by *Hanyga (1982)* and *Klimeš (1994)*. The first two basis vectors of the ray–centred coordinate system are tangent to the wavefront, the third basis vector is tangent to the ray. The covariant derivatives of travel time with respect to the first two basis vectors correspond to the projection of the spatial derivatives of travel time onto the plane perpendicular to the ray, covariant derivatives of travel time with respect to the third basis vector correspond to the projection of the spatial derivatives of travel time onto the wavefront normal. Since the basis vectors tangent to the wavefront may be chosen in various ways (*Hanyga, 1982*; *Klimeš, 1994*), we shall not introduce covariant derivatives with respect to the individual basis vectors, but restrict our equations to the decomposition of the spatial derivatives into the ray–normal and wavefront–normal components. The transformation of the ray–normal and wavefront–normal components into covariant derivatives with respect to the individual basis vectors of the ray–centred coordinate system is straightforward.

The spatial gradient $\tau_{,i\ldots}$ of travel time or its spatial derivatives and perturbations can be decomposed into the component $E^{\parallel}_{ia}\tau_{,a\ldots}$ normal to the wavefront and component $E^{\perp}_{ia}\tau_{,a\ldots}$ normal to the ray. The projection matrix onto the wavefront normal is

$$E^{\parallel}_{ia} = (p_r H^{,r})^{-1} p_i H^{,a} \quad , \tag{48}$$

and the projection matrix onto the plane perpendicular to the ray is

$$E^{\perp}_{ia} = \delta_{ia} - E^{\parallel}_{ia} \quad , \tag{49}$$

see *Snieder and Sambridge (1992,* eq. 28) for an isotropic case. Hence,

$$\tau_{,ij\ldots n\alpha\ldots\nu} = E^{\parallel}_{ia}\tau_{,aj\ldots n\alpha\ldots\nu} + E^{\perp}_{ia}\tau_{,aj\ldots n\alpha\ldots\nu} \quad . \tag{50}$$

Component $E^{\parallel}_{ia}\tau_{,a\ldots}$ corresponds to the covariant derivative with respect to the ray–centred coordinate parallel to the ray, whereas component $E^{\perp}_{ia}\tau_{,a\ldots}$ corresponds to the covariant derivatives with respect to the ray–centred coordinates parallel to the wavefront.

Wavefront–normal component $E^{\parallel}_{ia}\tau_{,a\ldots}$ need not be calculated by numerical quadrature (19). The equations for the wavefront–normal component of the second–order and third–order spatial derivatives $\tau_{,ij}$, $\tau_{,ijk}$ follow from equations (48) and (11),

$$E^{\parallel}_{ia}\tau_{,aj} = -(H^{,q}p_q)^{-1} p_i H_{,j} \quad , \tag{51}$$

$$E^{\parallel}_{ia}\tau_{,ajk} = -(H^{,q}p_q)^{-1} p_i \left[H_{,jk} + H^{,s}_{,j}{}_{,k}\tau_{,sk} + H^{,rs}\tau_{,rj}\,\tau_{,sk}\right] \quad . \tag{52}$$

The equations for the wavefront–normal components of spatial derivatives $\tau_{,i\alpha}$, $\tau_{,ij\alpha}$, $\tau_{,i\alpha\beta}$, $\tau_{,ijkl}$, ..., follow from equations (48) and (18),

$$E^{\parallel}_{ia}\,\tau_{,aj\dots n\alpha\dots\nu} = (H^{,q}p_q)^{-1}p_i\,[K_{j\dots n\alpha\dots\nu} - (H^{,s}_{\substack{,j\\ \vdots\\ ,n}} + H^{,rs}\tau_{\substack{,rj\\ \vdots\\ ,rn}})\;\tau_{\substack{,s\dots n\alpha\dots\nu\\ \vdots\\ ,j\dots s\alpha\dots\nu}}] \quad . \tag{53}$$

Equations (52) and (53) may be used to express the wavefront–normal components $E^{\parallel}_{ia}\,\tau_{,a\dots}$ of spatial derivatives $\tau_{,a\dots}$ in terms of the partial phase–space derivatives and perturbations of the Hamiltonian and in terms of lower–order spatial derivatives and perturbations $\tau_{,\dots}$ of travel time.

Let us introduce projections

$$\tau^{\perp}_{,ij\dots n\alpha\dots\nu} = E^{\perp}_{ia}\,E^{\perp}_{jb}\cdots E^{\perp}_{nf}\;\tau_{,ab\dots f\alpha\dots\nu} \tag{54}$$

of spatial derivatives of travel time or its perturbations onto the plane perpendicular to the ray, and refer to them as the *ray–normal derivatives* and perturbations of travel time. For pure perturbations we formally put $\tau^{\perp}_{,\alpha\dots\nu} = \tau_{,\alpha\dots\nu}$. To calculate the ray–normal derivatives and perturbations of travel time, we need to evaluate quadratures (19) numerically.

Equations (52) and (53) may iteratively be used to express integration kernels (21) and spatial derivatives and perturbations (50) of travel time in terms of the partial phase–space derivatives and perturbations of the Hamiltonian and in terms of the ray–normal derivatives and perturbations (54) of travel time.

For example, we may use equations (25), (50), (53) and (54) to express the first–order perturbations of the gradient of travel time as

$$\tau_{,i\alpha} = -(H^{,q}p_q)^{-1}p_i\,H_{,\alpha} + \tau^{\perp}_{,i\alpha} \quad . \tag{55}$$

Inserting (55) into (30), we obtain the integration kernel for the second–order perturbations of travel time in the form of

$$\begin{aligned} K_{\alpha\beta} = &- H_{,\alpha\beta} + (H^{,q}p_q)^{-1}H^{,r}_{\substack{,\alpha\\ ,\beta}}\,p_r\,H_{\substack{,\beta\\ ,\alpha}} - (H^{,q}p_q)^{-2}H^{,rs}p_r\,p_s\,H_{,\alpha}H_{,\beta} \\ &- H^{,r}_{\substack{,\alpha\\ ,\beta}}\,\tau^{\perp}_{\substack{,r\beta\\ ,r\alpha}} + (H^{,q}p_q)^{-1}H_{\substack{,\alpha\\ ,\beta}}\,H^{,rs}p_r\,\tau^{\perp}_{\substack{,s\beta\\ ,s\alpha}} - H^{,rs}\tau^{\perp}_{,r\alpha}\,\tau^{\perp}_{,s\beta} \quad . \end{aligned} \tag{56}$$

4.4. Special forms of the Hamiltonian

Integration kernels $K_{\alpha\dots\nu}$ for the perturbations of travel time are composed of the partial phase–space derivatives and perturbations of the Hamiltonian and of the perturbations of the spatial gradient of travel time. Using the approach of Section 4.3, we may express integration kernels $K_{\alpha\dots\nu}$ in terms of the partial phase–space derivatives and perturbations of the Hamiltonian and in terms of the first–order ray–normal derivatives of the perturbations of travel time, see (56) for example.

The terms in $K_{\alpha\dots\nu}$ containing the first–order ray–normal derivatives (54) of the perturbations of travel time are related to the perturbations of the ray path and vanish if the ray path is not affected by small changes in model parameters. The other terms in $K_{\alpha\ldots\nu}$ are the results of the choice of the independent variable γ_3 along a ray, which is in turn determined by the form of the Hamiltonian.

Terms $-H_{,\alpha\ldots\nu}$ in $K_{\alpha\ldots\nu}$ may be fitted by travel time (43). We shall now search for the forms of the Hamiltonian, for which integration (43) yields the exact travel time if the ray path is not affected by small changes in model parameters.

For this purpose, we shall consider the Hamiltonian in the form of

$$H(x_q,p_r,f_\kappa) = \overline{H}(x_q,p_r,f_\kappa) - V(x_q,f_\kappa) \quad , \tag{57}$$

where $\overline{H}(x_q,p_r,f_\kappa)$ is a *homogeneous function* of the N^{th} degree with respect to slowness vector p_k. Then

$$\overline{H}^{,a} p_a = N\,\overline{H} \tag{58}$$

according to Euler's theorem on homogeneous functions, and also

$$H^{,a}_{,\ldots}\, p_a = N\,\overline{H}_{,\ldots} \quad . \tag{59}$$

Differentiating (59) with respect to p_b yields

$$H^{,ab}_{,\ldots} p_a = (N{-}1)\,\overline{H}^{,b}_{,\ldots}\,, \quad H^{,abc}_{,\ldots} p_a = (N{-}2)\,\overline{H}^{,bc}_{,\ldots}\,, \quad H^{,abcd}_{,\ldots} p_a = (N{-}3)\,\overline{H}^{,bcd}_{,\ldots}\,, \tag{60}$$

etc., subsequently

$$H^{,ab}_{,\ldots} p_a p_b = (N{-}1)N\,\overline{H}_{,\ldots}\,, \quad H^{,abc}_{,\ldots} p_a p_b p_c = (N{-}2)(N{-}1)N\,\overline{H}_{,\ldots}\,, \tag{61}$$

and so forth. Note that function $V(x_q,f_\kappa)$ determines independent parameter γ_3 along a ray through relation

$$\mathrm{d}\gamma_3 = N\,V(x_q,f_\kappa)\,\mathrm{d}\tau \quad . \tag{62}$$

An example of Hamiltonian (57) for anisotropic media is Hamiltonian

$$H(x_q,p_r,f_\kappa) = V(x_q,f_\kappa)\,[G(x_q,p_r,f_\kappa)]^{\frac{N}{2}} - V(x_q,f_\kappa) \quad , \tag{63}$$

where $G(x_q,p_r,f_\kappa)$ is the eigenvalue of the Christoffel matrix.

Equation (56) with (57), (59), (60) and (61) reads

$$K_{\alpha\beta} = -H_{,\alpha\beta} + \frac{N{+}1}{N\overline{H}}\overline{H}_{,\alpha}\overline{H}_{,\beta} - \frac{1}{N\overline{H}}\overline{H}_{\substack{,\alpha\\,\beta}} V_{\substack{,\beta\\,\alpha}} - \frac{N{-}1}{N\overline{H}} V_{,\alpha}V_{,\beta} - \overline{H}^{,r}_{\substack{,\alpha\\,\beta}}\tau^{\perp}_{\substack{,r\beta\\,r\alpha}} - \overline{H}^{,rs}\tau^{\perp}_{,r\alpha}\tau^{\perp}_{,s\beta}\,. \tag{64}$$

Terms $(N{+}1)\overline{H}_{,\alpha}\overline{H}_{,\beta}$, $\overline{H}_{\substack{,\alpha\\,\beta}} V_{\substack{,\beta\\,\alpha}}$ and $(N{-}1)V_{,\alpha}V_{,\beta}$ vanish if $N=-1$ and $V_{,\alpha}=0$, or if $N=1$ and $\overline{H}_{,\alpha}=0$.

In the first case, $\overline{H}(x_q,p_r,f_\kappa)$ is a homogeneous function of degree $N=-1$ with respect to slowness vector p_k and V is a constant. Such a Hamiltonian is

$$H(x_q,p_r,f_\kappa) = -[G(x_q,p_r,f_\kappa)]^{-\frac{1}{2}} + 1 \tag{65}$$

in anisotropic media, where $G(x_q,p_r,f_\kappa)$ is the eigenvalue of the Christoffel matrix, and

$$H(x_q,p_r,f_\kappa) = -[p_r p_r]^{-\frac{1}{2}}\,v^{-1}(x_q,f_\kappa) + 1 \tag{66}$$

in isotropic media, where $v(x_q,f_\kappa)$ is the phase velocity. The independent parameter γ_3 along a ray is then the travel time. Note that *Bulant and Klimeš (2002)* suggested the perturbative approximation (43) of travel time with Hamiltonian (65) as the optimal option for the coupling ray theory by *Coates and Chapman (1990)*.

In the second case, $\overline{H}$ is independent of the model space and, consequently, of the spatial coordinates,

$$H(x_q, p_r, f_\kappa) = \overline{H}(p_r) - V(x_q, f_\kappa) \quad , \tag{67}$$

where $\overline{H}(p_r)$ is a homogeneous function of degree $N = 1$. Hamiltonian (67) is not possible in a general anisotropic medium, where the anisotropy is spatially dependent. However, it may be selected in a *factorized anisotropic medium* (*Červený, 1989*) or *isotropic medium*. In an isotropic medium, such a Hamiltonian is

$$H(x_q, p_r, f_\kappa) = \sqrt{p_r p_r} - v^{-1}(x_q, f_\kappa) \quad , \tag{68}$$

where $v(x_q, f_\kappa)$ is the phase velocity. For Hamiltonian (68), independent parameter γ_3 is the arclength along the ray.

Although Hamiltonians (65), (66), (67) and (68) have been derived using the expressions for the first–order and second–order perturbations of travel time only, integration (43) yields the exact travel time for these Hamiltonians if the ray path is not affected by small changes in model parameters. For the Hamiltonians of forms (65), (66), (67) and (68), integration kernels $K_{\alpha\ldots\nu}$ are thus composed of terms $-H_{,\alpha\ldots\nu}$ and of terms containing the first–order ray–normal derivatives of the perturbations of travel time only.

4.5. Calculation of the ray–normal derivatives of travel time

In Sections 4.3 and 4.4 we have seen that it may sometimes be useful to express integration kernels $K_{\alpha\ldots\nu}$ for the perturbations of travel time in terms of the partial phase–space derivatives and perturbations of the Hamiltonian and in terms of the ray–normal derivatives and perturbations (54) of travel time. We shall now discuss the properties of the ray–normal derivatives and possibilities of calculating them.

Analogously to equation (16), we define the *covariant ray–normal derivatives*

$$T^{\perp}_{ab\ldots f\alpha\ldots\nu} = \tau^{\perp}_{,ij\ldots n\alpha\ldots\nu}\, Q_{ia} Q_{jb} \cdots Q_{nf} \tag{69}$$

of travel time with respect to ray parameters γ_a. Since

$$E^{\perp}_{ri}\, Q_{r3} = 0 \quad , \tag{70}$$

all covariant ray–normal derivatives $T^{\perp}_{ab\ldots f\alpha\ldots\nu}$ containing index 3 among the Roman subscripts vanish,

$$T^{\perp}_{3b\ldots f\alpha\ldots\nu} = 0 \quad . \tag{71}$$

Only covariant ray–normal derivatives $T^{\perp}_{AB\ldots F\alpha\ldots\nu}$, where the upper–case Roman subscripts take values $A, B, ..., F = 1, 2$, may be non–zero. The first two columns of matrix Q^{τ}_{iA} defined for $\gamma_3 = \tau$ are related to the first two columns of matrix Q_{iA} defined for general γ_3 through equation (*Klimeš, 1997, 1999*)

$$Q^{\tau}_{iA} = E^{\perp}_{ri}\, Q_{rA} \quad . \tag{72}$$

We may then express the non–zero covariant ray–normal derivatives (69) in terms of matrix Q^{τ}_{iA} defined for $\gamma_3 = \tau$,

$$T^{\perp}_{AB...F\alpha...\nu} = \tau_{,ij...n\alpha...\nu}\, Q^{\tau}_{iA} Q^{\tau}_{jB} \cdots Q^{\tau}_{nF} \quad . \tag{73}$$

Covariant ray–normal derivatives $T^{\perp}_{ab...f\alpha...\nu}$ are thus, unlike $T_{ab...f\alpha...\nu}$, independent of the kind of γ_3 used in definition (12) of matrix Q_{ia}. In this way, covariant ray–normal derivatives $T^{\perp}_{ab...f\alpha...\nu}$ are independent of the choice of the form of the Hamiltonian. As a consequence, equation

$$\tau^{\perp}_{,ij...n\alpha...\nu} = T^{\perp}_{AB...F\alpha...\nu}\, Q^{-1}_{Ai} Q^{-1}_{Bj} \cdots Q^{-1}_{Fn} \tag{74}$$

inverse to (69), see (71), is valid for matrix Q_{ia} defined with respect to arbitrary γ_3, i.e. defined for an arbitrary Hamiltonian. Here Q^{-1}_{Ai} are the first two rows of of the matrix inverse to Q_{ia}.

We define *ray–normal integration kernels* $K^{\perp}_{ij...n\alpha...\nu}$ for the ray–normal derivatives by equation

$$T^{\perp}_{ab...f\alpha...\nu}(\gamma_3) = T^{\perp}_{ab...f\alpha...\nu}(\gamma^0_3) + \int_{\gamma^0_3}^{\gamma_3} \mathrm{d}\gamma_3\, \frac{\partial\tau}{\partial\gamma_3}\, K^{\perp}_{ij...n\alpha...\nu}\, Q_{ia} Q_{jb} \cdots Q_{nf} \ , \tag{75}$$

analogous to equation (19) except for factor $\partial\tau/\partial\gamma_3$. To make this definition unique, we impose additional conditions

$$E^{\parallel}_{ar}\, K^{\perp}_{i...r...n\alpha...\nu} = 0 \tag{76}$$

on the ray–normal integration kernels, based on identities (70) and (71). The ray–normal integration kernels $K^{\perp}_{ij...n\alpha...\nu}$ defined in this way are independent of the kind of γ_3 and of the choice of the form of the Hamiltonian.

If the Hamiltonian has a form yielding $\gamma_3 = \tau$, i.e. if

$$H^{,r} p_r = 1 \tag{77}$$

along rays, covariant ray–normal derivatives (73) are the results of quadrature (19) with $Q_{iA} = Q^{\tau}_{iA}$ and $K_{i...f\alpha...\nu} = K^{\tau}_{i...f\alpha...\nu}$. Then considering (70), (71) and (72), we see that

$$K^{\perp}_{ij...n\alpha...\nu} = E^{\perp}_{ia}\, E^{\perp}_{jb} \cdots E^{\perp}_{nf}\, K^{\tau}_{ab...f\alpha...\nu} \quad , \tag{78}$$

where $K^{\tau}_{ij...n\alpha...\nu}$ is the integration kernel $K_{ij...n\alpha...\nu}$ corresponding to a Hamiltonian yielding $\gamma_3 = \tau$. Unfortunately, the relation of $K^{\perp}_{ij...n\alpha...\nu}$ to integration kernels $K_{ij...n\alpha...\nu}$ corresponding to other forms of the Hamiltonian (yielding $\gamma_3 \neq \tau$) is considerably more complex, with the exception of relation

$$K^{\perp}_{\alpha...\nu} = (H^{,r} p_r)^{-1}\, K_{\alpha...\nu} \tag{79}$$

resulting from definition (75) for any form of the Hamiltonian.

For example, if the Hamiltonian corresponds to $\gamma_3 = \tau$ and thus satisfies condition (77) along rays, equations (27), (50), (51) and (78) yield the ray–normal integration kernel for the perturbations of the travel–time gradient in the form

$$K^{\perp}_{i\alpha} = E^{\perp}_{ia}\,(-H_{,a\alpha} + H_{,a}\, H^{,r}_{,\alpha}\, p_r) - H^{,r}_{,\alpha}\, \tau^{\perp}_{,ri} \quad , \tag{80}$$

and ray–normal integration kernel $K^{\perp}_{\alpha\beta} = K_{\alpha\beta}$ for the second–order perturbations of the travel–time gradient is given by equation (56).

5. EXAMPLES OF THE INTEGRANDS IN ISOTROPIC MEDIA

In Section 5, the equations of Section 3 for the spatial derivatives and perturbations of travel time up to the third order are specified for isotropic media, using three kinds of the Hamiltonian, corresponding to the three most common kinds of the independent parameter along rays.

The integration kernels $K_{i...n\alpha...\nu}$ corresponding to equal travel times $\tau(x_i, f_\kappa)$ and equal kinds of γ_3 are equal. Yet the equal integration kernels $K_{i...n\alpha...\nu}$ may still be expressed in considerably different forms. Different Hamiltonians corresponding to the same travel time $\tau(x_i, f_\kappa)$ and the same kind of γ_3 yield equal integration kernels in different forms, and these forms may further be converted using various identities, such as (11).

There are many forms of the Hamiltonian for isotropic media. The general form of the Hamiltonian considered hereinafter is a special case of Hamiltonian (57) with its slowness–vector dependent part $\overline{H}$ independent of the model, $\overline{H}(x_q, p_r, f_\kappa) = \overline{H}(p_r)$, which results in vanishing partial derivatives $H^{;a...}_{,i...}$, $H^{;a...}_{,\alpha...}$ with respect to p_a mixed with spatial derivatives or perturbations. This considerably simplifies many equations. The general form of the Hamiltonian considered here includes Hamiltonian (68). For a more detailed discussion of this and other forms of the Hamiltonian, refer to *Červený (2001)*.

In this section, we consider a general form of the Hamiltonian for isotropic media, which is the above–mentioned special case of Hamiltonian (57),

$$H(x_q, p_r, f_\kappa) = N^{-1}p^N - V(x_q, f_\kappa) \quad , \tag{81}$$

with

$$p = \sqrt{p_r p_r} \tag{82}$$

and

$$V(x_q, f_\kappa) = N^{-1}v^{-N}(x_q, f_\kappa) \quad , \tag{83}$$

where $v(x_q, f_\kappa)$ is the phase velocity (*Červený, 2001,* eq. 3.1.6). The limiting case of Hamiltonian (81) for $N=0$, obtained by the l'Hospital rule with respect to N, is

$$H(x_q, p_r, f_\kappa) = \ln(p) - V(x_q, f_\kappa) \quad , \tag{84}$$

with

$$V(x_q, f_\kappa) = -\ln[v(x_q, f_\kappa)] \tag{85}$$

(*Červený, 2001,* eq. 3.1.7). The independent parameter along a ray corresponding to Hamiltonian (81) is

$$\gamma_3 = \gamma_3^0 + \int_{s^0}^{s} v^{N-1}\mathrm{d}s \quad , \tag{86}$$

where s is the arclength along the ray.

The Hamiltonians of general form (81) simplify the equations because all their partial derivatives with respect to p_a mixed with spatial derivatives or perturbations vanish,

$$H^{,a\dots}_{,i\dots} = 0 \quad , \qquad H^{,a\dots}_{,\alpha\dots} = 0 \quad . \tag{87}$$

The spatial derivatives and perturbations of the Hamiltonian are

$$H_{,i\dots\alpha} = -V_{,i\dots\alpha} \quad , \tag{88}$$

where V is defined by (83) or (85). Equations (25), (27), (28), (30), (32), (33), (35), (36), (38), (39), (41) then simplify to

$$K_{\alpha} = V_{,\alpha} \quad , \tag{89}$$

$$K_{i\alpha} = V_{,i\alpha} \quad , \tag{90}$$

$$T_{3\alpha} = V_{,\alpha} \quad , \tag{91}$$

$$K_{\alpha\beta} = V_{,\alpha\beta} - H^{,rs}\tau_{,r\alpha}\tau_{,s\beta} \quad , \tag{92}$$

$$K_{ijk} = V_{,ijk} - H^{,abc}\tau_{,ai}\,\tau_{,bj}\,\tau_{,ck} \quad , \tag{93}$$

$$T_{3bc} = V_{,jk}Q_{jb}Q_{kc} - H^{,jk}P_{jb}P_{kc} \quad , \tag{94}$$

$$K_{ij\alpha} = V_{,ij\alpha} - H^{,rs}\tau_{,rij}\,\tau_{,s\alpha} - H^{,rst}\tau_{,ri}\,\tau_{,sj}\,\tau_{,t\alpha} \quad , \tag{95}$$

$$T_{3b\alpha} = V_{,j\alpha}Q_{jb} - H^{,sj}\tau_{,s\alpha}\,P_{jb} \quad , \tag{96}$$

$$K_{i\alpha\beta} = V_{,i\alpha\beta} - H^{,rs}\underset{,ri\beta}{\tau_{,ri\alpha}}\underset{,s\alpha}{\tau_{,s\beta}} - H^{,rst}\tau_{,ri}\,\tau_{,s\alpha}\tau_{,t\beta} \quad , \tag{97}$$

$$T_{3\alpha\beta} = V_{,\alpha\beta} - H^{,rs}\tau_{,r\alpha}\tau_{,s\beta} \quad , \tag{98}$$

$$K_{\alpha\beta\gamma} = V_{,\alpha\beta\gamma} - H^{,rs}\underset{\substack{,r\beta\\ ,r\gamma}}{\tau_{,r\alpha}}\underset{\substack{,s\alpha\gamma\\ ,s\alpha\beta}}{\tau_{,s\beta\gamma}} - H^{,rst}\tau_{,r\alpha}\tau_{,s\beta}\,\tau_{,t\gamma} \quad . \tag{99}$$

The homogeneous derivatives of Hamiltonians (81) or (84) with respect to the slowness vector are

$$H^{,a} = p^{N-2}p_a \quad , \tag{100}$$

$$H^{,ab} = p^{N-2}\delta_{ab} + (N{-}2)\;p^{N-4}p_a p_b \quad , \tag{101}$$

$$H^{,abc} = (N{-}2)\big[p^{N-4}\underset{\substack{b\\ c}}{p_a}\underset{\substack{ac\\ ab}}{\delta_{bc}} + (N{-}4)\;p^{N-6}p_a p_b p_c\big] \quad , \tag{102}$$

and so on. The projection matrix (49) onto the plane perpendicular to the ray reads

$$E^{\perp}_{ia} = \delta_{ia} - p^{-2}p_i p_a \quad . \tag{103}$$

Identity matrix δ_{ia} in equations (101), (102) may also be expressed in terms of projection matrix (103),

$$H^{,ab} = p^{N-2}E^{\perp}_{ab} + (N{-}1)\;p^{N-4}p_a p_b \quad , \tag{104}$$

$$H^{,abc} = (N{-}2)\big[p^{N-4}\underset{\substack{b\\ c}}{p_a}\underset{\substack{ac\\ ab}}{E^{\perp}_{bc}} + (N{-}1)\;p^{N-6}p_a p_b p_c\big] \quad . \tag{105}$$

Identity (11) with (88) and (100) yields

$$p^{N-2} p_r \tau_{,ri} = V_{,i} \quad , \qquad p^{N-2} p_r \tau_{,r\alpha} = V_{,\alpha} \quad , \tag{106}$$

see also equation (51) with (88) and (100). Inserting definition (83) or (85) of V into (106), we obtain the wavefront–normal projections of $\tau_{,ij}$ and $\tau_{,i\alpha}$ in the first index onto vector $p^{-1}p_r$,

$$p^{-1} p_r \tau_{,ri} = -v^{-2} v_{,i} \quad , \qquad p^{-1} p_r \tau_{,r\alpha} = -v^{-2} v_{,\alpha} \quad , \tag{107}$$

which are naturally independent of N. Conditions (87) also allow the equation for the wavefront–normal component of spatial derivative $\tau_{,ijk}$ to be simplified. For the third–order spatial derivatives of travel time identity (11) with (87), (88) and (100) yields

$$p^{-1} p_i \tau_{,ijk} = v^{N-1} [V_{,jk} - H^{,rs} \tau_{,rj} \, \tau_{,sk}] \quad , \tag{108}$$

see also equation (52) with (87), (88) and (100). Conditions (87) analogously allow the equations for the wavefront–normal components of spatial derivatives $\tau_{,i\alpha}$, $\tau_{,ij\alpha}$, $\tau_{,i\alpha\beta}$, ..., following from equations (18) and (100), to be simplified,

$$p^{-1} p_i \tau_{,ij\dots n\alpha\dots\nu} = v^{N-1} [K_{j\dots n\alpha\dots\nu} - H^{,rs} \underset{\underset{,rn}{\vdots}}{\tau_{,rj}} \, \underset{\underset{,j\dots s\alpha\dots\nu}{\vdots}}{\tau_{,s\dots n\alpha\dots\nu}}] \quad , \tag{109}$$

see also equation (53) with (100).

At least three special cases of Hamiltonian (81) are interesting:

For $\underline{N=0}$, the independent parameter along the ray is the travel time, $\gamma_3 = \tau$. Hamiltonian (84) is very suitable for deriving integration kernels $K^{\tau}_{i\dots n\alpha\dots\nu}$ corresponding to the travel time and for their conversion into ray–normal integration kernels $K^{\perp}_{i\dots n\alpha\dots\nu}$ using equation (78).

For $\underline{N=1}$, we obtain Hamiltonian (68) optimizing the first–order perturbation correction of travel time. The independent parameter along the ray is the arclength, $\gamma_3 = s$. The equations for the perturbations of travel time derived using this Hamiltonian enable the wavefront–normal derivatives to be separated more simply than with other kinds of the Hamiltonian, see factor $(N{-}1)$ in equations (104) and (105). This is especially useful for expressing ray–normal integration kernels $K^{\perp}_{\alpha\dots\nu}$ in terms of the ray–normal derivatives and perturbations of travel time.

If we select $\underline{N=2}$, all third–order and higher–order derivatives $H^{,abc\dots}_{,\dots}$ of the Hamiltonian with respect to the slowness vector vanish, see factor $(N{-}2)$ in equation (102). This enables the derivation of equations for integration kernels $K_{i\dots n\alpha\dots\nu}$ to be considerably simplified. The derivation of the equations for ray–normal integration kernels $K^{\perp}_{\alpha\dots\nu}$, corresponding to pure perturbations, using equation (79) and Hamiltonian (81) with $N=2$, is usually simpler than with other forms of the Hamiltonian. The independent parameter along the ray is natural variable $\gamma_3 = \sigma$.

5.1. Integration with respect to the natural variable

We shall refer to parameter

$$\sigma = \sigma^0 + \int_{s^0}^{s} v \, \mathrm{d}s = \sigma^0 + \int_{\tau^0}^{\tau} v^2 \mathrm{d}\tau \tag{110}$$

as the *natural variable along the ray*. If we choose the Hamiltonian in Cartesian coordinates in the form

$$H(x_q, p_r, f_\kappa) = \tfrac{1}{2} p_k p_k - \tfrac{1}{2} v^{-2}(x_q, f_\kappa) \quad , \tag{111}$$

then $\gamma_3 = \sigma$. The homogeneous partial derivatives of Hamiltonian (111) with respect to the slowness vector are

$$H^{,a} = p_a \quad , \qquad H^{,ab} = \delta_{ab} \quad , \qquad H^{,abc\ldots} = 0 \quad , \tag{112}$$

see also equations (100) to (102) with $N = 2$. Equations (89) to (99) then simplify to

$$K^{\sigma}_{\alpha} = \big(\tfrac{1}{2}v^{-2}\big)_{,\alpha} \quad , \tag{113}$$
$$K^{\sigma}_{i\alpha} = \big(\tfrac{1}{2}v^{-2}\big)_{,i\alpha} \quad , \tag{114}$$
$$T^{\sigma}_{3\alpha} = \big(\tfrac{1}{2}v^{-2}\big)_{,\alpha} \quad , \tag{115}$$
$$K^{\sigma}_{\alpha\beta} = \big(\tfrac{1}{2}v^{-2}\big)_{,\alpha\beta} - \tau_{,r\alpha}\tau_{,r\beta} \quad , \tag{116}$$
$$K^{\sigma}_{ijk} = \big(\tfrac{1}{2}v^{-2}\big)_{,ijk} \quad , \tag{117}$$
$$T^{\sigma}_{3bc} = \big(\tfrac{1}{2}v^{-2}\big)_{,jk} Q_{jb} Q_{kc} - P_{rb} P_{rc} \quad , \tag{118}$$
$$K^{\sigma}_{ij\alpha} = \big(\tfrac{1}{2}v^{-2}\big)_{,ij\alpha} - \tau_{,rij}\tau_{,r\alpha} \quad , \tag{119}$$
$$T^{\sigma}_{3b\alpha} = \big(\tfrac{1}{2}v^{-2}\big)_{,j\alpha} Q_{jb} - \tau_{,j\alpha} P_{jb} \quad , \tag{120}$$
$$K^{\sigma}_{i\alpha\beta} = \big(\tfrac{1}{2}v^{-2}\big)_{,i\alpha\beta} - \tau_{\substack{,ri\alpha \\ ,ri\beta}} \tau_{\substack{,r\beta \\ ,r\alpha}} \quad , \tag{121}$$
$$T^{\sigma}_{3\alpha\beta} = \big(\tfrac{1}{2}v^{-2}\big)_{,\alpha\beta} - \tau_{,r\alpha}\tau_{,r\beta} \quad , \tag{122}$$
$$K^{\sigma}_{\alpha\beta\gamma} = \big(\tfrac{1}{2}v^{-2}\big)_{,\alpha\beta\gamma} - \tau_{\substack{,r\alpha \\ ,r\beta \\ ,r\gamma}} \tau_{\substack{,r\beta\gamma \\ ,r\alpha\gamma \\ ,r\alpha\beta}} \quad . \tag{123}$$

Equations (113) to (123) are very simple compared to the equations corresponding to other kinds of parameter γ_3 along a ray. On the other hand, equations (113) to (123) are designed for calculation of all components of spatial derivatives and perturbations of travel time along a ray. In this way, equations (113) to (123) are not suitable for the separate calculation of the ray–normal derivatives and perturbations (54) of travel time. Integration kernels (113) and (116) have been derived by *Kravtsov and Orlov* (*1980,* eqs. 9.8 and 9.9; *1990,* eqs. 2.9.8 and 2.9.9) for the case of $\big(\tfrac{1}{2}v^{-2}\big)_{,\alpha\beta} = 0$. Unfortunately, *Kravtsov and Orlov* (*1980, 1990*) have disregarded integration kernel (114), although it is required for calculating the perturbation of travel–time gradient, which in turn should be inserted into integration kernel (116). Integration kernel (117) has been derived together with the integration kernels for higher–order spatial derivatives of travel time by *Červený* (*2001,* eq. 4.7.40).

5.2. Integration with respect to the arclength

Hamiltonian (68) is a special case of Hamiltonian (81) for $N=1$. Equations (104) and (105) then simplify to

$$H^{,ab} = p^{-1} E^{\perp}_{ab} \quad , \tag{124}$$

$$H^{,abc} = -p^{-3} \underset{\substack{b\\c}}{p_a} \underset{\substack{ac\\ab}}{E^{\perp}_{bc}} \quad . \tag{125}$$

Equations (89) to (99) with (124), (125) and (107) then yield

$$K^s_{\alpha} = (v^{-1})_{,\alpha} \quad , \tag{126}$$

$$K^s_{i\alpha} = (v^{-1})_{,i\alpha} \quad , \tag{127}$$

$$T^s_{3\alpha} = (v^{-1})_{,\alpha} \quad , \tag{128}$$

$$K^s_{\alpha\beta} = (v^{-1})_{,\alpha\beta} - v\, \tau^{\perp}_{,r\alpha} \tau^{\perp}_{,r\beta} \quad , \tag{129}$$

$$K^s_{ijk} = (v^{-1})_{,ijk} - \underset{\substack{,j\\,k}}{v_{,i}} \underset{\substack{rs\\rs}}{E^{\perp}_{rs}} \underset{\substack{,ri\\,ri}}{\tau_{,rj}} \underset{\substack{,sk\\,sj}}{\tau_{,sk}} \quad , \tag{130}$$

$$T^s_{3bc} = (v^{-1})_{,jk} Q_{jb} Q_{kc} - v\, E^{\perp}_{jk} P_{jb} P_{kc} \quad , \tag{131}$$

$$K^s_{ij\alpha} = (v^{-1})_{,ij\alpha} - v\, E^{\perp}_{rs} \tau_{,rij} \tau_{,s\alpha} - \underset{\substack{,j\\,\alpha}}{v_{,i}} \underset{\substack{rs\\rs}}{E^{\perp}_{rs}} \underset{\substack{,ri\\,ri}}{\tau_{,rj}} \underset{\substack{,s\alpha\\,sj}}{\tau_{,s\alpha}} \quad , \tag{132}$$

$$T^s_{3b\alpha} = (v^{-1})_{,j\alpha} Q_{jb} - v\, \tau^{\perp}_{,j\alpha} P_{jb} \quad , \tag{133}$$

$$K^s_{i\alpha\beta} = (v^{-1})_{,i\alpha\beta} - v\, \underset{rs}{E^{\perp}_{rs}} \underset{,ri\beta}{\tau_{,ri\alpha}} \underset{,s\alpha}{\tau_{,s\beta}} - \underset{\substack{,\alpha\\,\beta}}{v_{,i}} \underset{\substack{rs\\rs}}{E^{\perp}_{rs}} \underset{\substack{,ri\\,ri}}{\tau_{,r\alpha}} \underset{\substack{,s\beta\\,s\alpha}}{\tau_{,s\beta}} \quad , \tag{134}$$

$$T^s_{3\alpha\beta} = (v^{-1})_{,\alpha\beta} - v\, \tau^{\perp}_{,r\alpha} \tau^{\perp}_{,s\beta} \quad , \tag{135}$$

$$K^s_{\alpha\beta\gamma} = (v^{-1})_{,\alpha\beta\gamma} - v\, \underset{\substack{,r\beta\\,r\gamma}}{\tau^{\perp}_{,r\alpha}} \underset{\substack{,r\alpha\gamma\\,r\alpha\beta}}{\tau^{\perp}_{,r\beta\gamma}} - \underset{\substack{,\beta\\,\gamma}}{v_{,\alpha}} \underset{\substack{,r\alpha\\,r\alpha}}{\tau^{\perp}_{,r\beta}} \underset{\substack{,r\gamma\\,r\beta}}{\tau^{\perp}_{,r\gamma}} \quad . \tag{136}$$

5.3. Integration with respect to travel time

If independent parameter γ_3 along a ray is travel time τ, equation (78) can be used to derive the equations for the ray–normal integration kernels $K^{\perp}_{...}$ from integration kernels $K^{\tau}_{...}$ corresponding to travel time. To derive the equations for the integration kernels corresponding to $\gamma_3 = \tau$, we use Hamiltonian (84), $H(x_q, p_r, f_\kappa) = \ln(p) + \ln[v(x_q, f_\kappa)]$, which is a special limiting case of Hamiltonian (81) for $N=0$. Equations (104) and (105) then become

$$H^{,ab} = p^{-2} E^{\perp}_{ab} - p^{-4} p_a p_b \quad , \tag{137}$$

$$H^{,abc} = -2\, p^{-4} \underset{\substack{b\\c}}{p_a} \underset{\substack{ac\\ab}}{E^{\perp}_{bc}} + 2\, p^{-6} p_a p_b p_c \quad . \tag{138}$$

Compared to other Hamiltonians corresponding to $\gamma_3 = \tau$, the great advantage of this Hamiltonian (84) are vanishing partial derivatives $H_{,i\dots}^{,a\dots} = 0$ and $H_{,\alpha\dots}^{,a\dots} = 0$ with respect to p_a mixed with spatial derivatives or perturbations.

The equation for integration kernel K_α for the first–order perturbations of travel time is very simple for any Hamiltonian. Equation (89) with $V_{,\alpha} = -(\ln v)_{,\alpha}$ reads

$$K_\alpha^\tau = K_\alpha^\perp = -(\ln v)_{,\alpha} \quad . \tag{139}$$

The integration kernel for the first–order perturbations of the gradient of travel time is similarly given by equation (90),

$$K_{i\alpha}^\tau = -(\ln v)_{,i\alpha} \quad , \tag{140}$$

and may be converted into the corresponding ray–normal integration kernel using equation (78),

$$K_{i\alpha}^\perp = -E_{ia}^\perp \, (\ln v)_{,a\alpha} \quad . \tag{141}$$

Equation (91) with $V_{,\alpha} = -(\ln v)_{,\alpha}$ reads

$$T_{3\alpha}^\tau = -(\ln v)_{,\alpha} \quad . \tag{142}$$

The integration kernel $K_{\alpha\beta}$, given by equation (30), can be calculated for any Hamiltonian and then converted to $K_{\alpha\beta}^\tau = K_{\alpha\beta}^\perp$. The integration kernel for the second–order perturbations of travel time can be expressed in terms of the first–order perturbations of the complete slowness vector using conversion (79) of expression (116) for $K_{\alpha\beta}^\sigma$,

$$K_{\alpha\beta}^\tau = K_{\alpha\beta}^\perp = v^2 \left(\tfrac{1}{2} v^{-2}\right)_{,\alpha\beta} - v^2 \, \tau_{,r\alpha} \tau_{,r\beta} \quad , \tag{143}$$

or expressed in terms of the first–order perturbations of the first–order ray–normal derivatives of travel time using conversion (79) of expression (129) for $K_{\alpha\beta}^s$,

$$K_{\alpha\beta}^\tau = K_{\alpha\beta}^\perp = v \left(v^{-1}\right)_{,\alpha\beta} - v^2 \, \tau_{,r\alpha}^\perp \tau_{,r\beta}^\perp \quad . \tag{144}$$

Equation (144) may also be obtained from equation (92) with (85), (137) and (107).

The integration kernel for the third–order derivatives of travel time can be obtained from equation (93) with (85), (138) and (107),

$$K_{ijk}^\tau = -(\ln v)_{,ijk} + 2\, v^{-3} v_{,i} v_{,j} v_{,k} - 2\, v \; v_{\substack{,i\\,j\\,k}} \, E^\perp_{\substack{rs\\rs\\rs}} \, \tau_{\substack{,rj\\,ri\\,ri}} \, \tau_{\substack{,sk\\,sk\\,sj}} \quad , \tag{145}$$

and may be converted into the corresponding ray–normal integration kernel using equation (78),

$$K_{ijk}^\perp = E_{ia}^\perp \, E_{jb}^\perp \, E_{kc}^\perp \left[-(\ln v)_{,abc} + 2\, v^{-3} v_{,a} v_{,b} v_{,c}\right] - 2\, v \; E^\perp_{\substack{ir\\jr\\kr}} \, v_{\substack{,r\\,r\\,r}} \, \tau^\perp_{\substack{,sj\\,si\\,si}} \, \tau^\perp_{\substack{,sk\\,sk\\,sj}} \; . \tag{146}$$

Equation (94), with $V_{,bc} = -(\ln v)_{,bc}$ and $H^{,rs}$ given by (137), reads

$$T_{3bc}^\tau = -(\ln v)_{,jk} Q_{jb} Q_{kc} - v^2 (E_{jk}^\perp - p^{-2} p_j p_k) \, P_{jb} P_{kc} \quad . \tag{147}$$

Inserting expression (107) for $p^{-1} p_r \tau_{,ri}$ into equation (147), we obtain

$$T_{3bc}^\tau = v \left(v^{-1}\right)_{,jk} Q_{jb} Q_{kc} - v^2 \, E_{jk}^\perp \, P_{jb} P_{kc} \quad . \tag{148}$$

Equation (95) for integration kernel $K_{ij\alpha}$ with (137), (138) and (107) yields

$$K^{\tau}_{ij\alpha} = -(\ln v)_{,ij\alpha} + 2\,v^{-3} v_{,i} v_{,j} v_{,\alpha} - v^2 (E^{\perp}_{rs} - p^{-2} p_r p_s)\,\tau_{,rij}\tau_{,s\alpha} - 2\,v\,v_{\substack{,i\\,j\\,\alpha}}\,E^{\perp}_{\substack{rs\\rs\\rs}}\,\tau_{\substack{,rj\\,ri\\,ri}}\tau_{\substack{,s\alpha\\,s\alpha\\,sj}}\ . \tag{149}$$

Equation (108) with $N=1$, $V_{,jk}=(v^{-1})_{,jk}$ and $H^{,rs}$ given by (124) reads

$$p^{-1} p_i \tau_{,ijk} = \left(v^{-1}\right)_{,jk} - v\,E^{\perp}_{rs}\,\tau_{,rj}\tau_{,sk} \quad . \tag{150}$$

Inserting expressions (107) and (150) into equation (149) and applying conversion (78), we arrive at

$$\begin{aligned} K^{\perp}_{ij\alpha} = {} & E^{\perp}_{ia}\,E^{\perp}_{jb}\left[-(\ln v)_{,ab\alpha} + 2\,v^{-3} v_{,a} v_{,b} v_{,\alpha}\right] - v^2 \tau^{\perp}_{,rij}\,\tau^{\perp}_{,r\alpha} \\ & - \left[E^{\perp}_{ia}\,E^{\perp}_{jb}\,\left(v^{-1}\right)_{,ab} - v\,\tau^{\perp}_{,ri}\tau^{\perp}_{,rj}\right] v_{,\alpha} - 2\,v\,E^{\perp}_{\substack{ir\\jr}}\,v_{\substack{,r\\,r}}\tau^{\perp}_{\substack{,sj\\,si}}\,\tau^{\perp}_{\substack{,s\alpha\\,s\alpha}} - 2\,v\,v_{,\alpha}\tau^{\perp}_{,si}\,\tau^{\perp}_{,sj}\ , \end{aligned} \tag{151}$$

which may be rearranged to read

$$K^{\perp}_{ij\alpha} = E^{\perp}_{ia}\,E^{\perp}_{jb}\left[-(\ln v)_{,ab\alpha} + v^{-2} v_{,ab} v_{,\alpha}\right] - v^2 \tau^{\perp}_{,rij}\,\tau^{\perp}_{,r\alpha} - 2v\,E^{\perp}_{\substack{ir\\jr}}\,v_{\substack{,r\\,r}}\,\tau^{\perp}_{\substack{,sj\\,si}}\,\tau^{\perp}_{\substack{,s\alpha\\,s\alpha}} - v\,v_{,\alpha}\tau^{\perp}_{,si}\,\tau^{\perp}_{,sj}\ . \tag{152}$$

Equation (96), with $V_{,b\alpha} = -(\ln v)_{,b\alpha}$ and $H^{,rs}$ given by (137), reads

$$T^{\tau}_{3b\alpha} = -(\ln v)_{,j\alpha} Q_{jb} - v^2 (E^{\perp}_{js} - p^{-2} p_j p_s)\,\tau_{,s\alpha} P_{jb} \quad . \tag{153}$$

Inserting expressions (107) for $p^{-1} p_r \tau_{,ri}$ and $p^{-1} p_r \tau_{,r\alpha}$ into equation (153), we obtain

$$T^{\tau}_{3b\alpha} = v\left(v^{-1}\right)_{,j\alpha} Q_{jb} - v^2\,\tau^{\perp}_{,j\alpha} P_{jb} \quad . \tag{154}$$

Equation (97) for integration kernel $K_{i\alpha\beta}$ with (137), (138) and (107) reads

$$K^{\tau}_{i\alpha\beta} = -(\ln v)_{,i\alpha\beta} + 2\,v^{-3} v_{,i} v_{,\alpha} v_{,\beta} - v^2 (E^{\perp}_{\substack{rs\\rs}} - p^{-2} p_{\substack{r\\r}} p_{\substack{s\\s}})\,\tau_{\substack{,ri\alpha\\,ri\beta}}\tau_{\substack{,s\beta\\,s\alpha}} - 2\,v\,v_{\substack{,i\\,\alpha\\,\beta}}\,E^{\perp}_{\substack{rs\\rs\\rs}}\,\tau_{\substack{,r\alpha\\,ri\\,ri}}\tau_{\substack{,s\beta\\,s\beta\\,s\alpha}}\ . \tag{155}$$

Equation (109), with $N=1$, $H^{,rs}$ given by (124) and $K_{j\alpha}$ given by (127), yields

$$p^{-1} p_i\,\tau_{,ij\alpha} = \left(v^{-1}\right)_{,j\alpha} - v\,E^{\perp}_{rs}\,\tau_{,rj}\tau_{,s\alpha} \quad . \tag{156}$$

Inserting expressions (107) and (156) into equation (155) and applying conversion (78), we arrive at

$$\begin{aligned} K^{\perp}_{i\alpha\beta} = {} & E^{\perp}_{ia}\left[-(\ln v)_{,a\alpha\beta} + 2\,v^{-3} v_{,a} v_{,\alpha} v_{,\beta}\right] - v^2 \tau^{\perp}_{\substack{,ri\alpha\\,ri\beta}}\,\tau^{\perp}_{\substack{,r\beta\\,r\alpha}} \\ & - \left[E^{\perp}_{ia}\,\left(v^{-1}\right)_{\substack{,a\alpha\\,a\beta}} - v\,\tau^{\perp}_{\substack{,ri\\,ri}}\,\tau^{\perp}_{\substack{,r\alpha\\,r\beta}}\right] v_{\substack{,\beta\\,\alpha}} - 2\,v\,E^{\perp}_{ir}\,v_{,r}\,\tau^{\perp}_{,s\alpha}\tau^{\perp}_{,s\beta} - 2\,v\,v_{\substack{,\alpha\\,\beta}}\tau^{\perp}_{\substack{,si\\,si}}\,\tau^{\perp}_{\substack{,s\beta\\,s\alpha}} \quad , \end{aligned} \tag{157}$$

which may be further rearranged to read

$$K^{\perp}_{i\alpha\beta} = E^{\perp}_{ia}\left[v\left(v^{-1}\right)_{,\alpha\beta}\right]_{,a} - v^2 \tau^{\perp}_{\substack{,ri\alpha\\,ri\beta}}\,\tau^{\perp}_{\substack{,r\beta\\,r\alpha}} - 2\,v\,E^{\perp}_{ir}\,v_{,r}\,\tau^{\perp}_{,s\alpha}\tau^{\perp}_{,s\beta} - v\,v_{\substack{,\alpha\\,\beta}}\tau^{\perp}_{\substack{,si\\,si}}\,\tau^{\perp}_{\substack{,s\beta\\,s\alpha}} \quad . \tag{158}$$

Equation (98), with $V_{,\alpha\beta} = -(\ln v)_{,\alpha\beta}$ and $H^{,rs}$ given by (137), reads

$$T^{\tau}_{3\alpha\beta} = -(\ln v)_{,\alpha\beta} - v^2 (E^{\perp}_{rs} - p^{-2} p_r p_s)\,\tau_{,r\alpha}\tau_{,s\beta} \quad . \tag{159}$$

Inserting expression (107) for $p^{-1}p_r\tau_{,r\alpha}$ into equation (159), we obtain

$$T^{\tau}_{3\alpha\beta} = v\left(v^{-1}\right)_{,\alpha\beta} - v^2\,\tau^{\perp}_{,r\alpha}\,\tau^{\perp}_{,r\beta} \quad . \tag{160}$$

Integration kernel $K_{\alpha\beta\gamma}$ for the third–order perturbations of travel time, given by equation (41), can be calculated for any Hamiltonian and then converted to $K^{\tau}_{\alpha\beta\gamma} = K^{\perp}_{\alpha\beta\gamma}$. To express the integration kernel in terms of the second–order perturbations of the complete slowness vector, we shall convert expression (123) for $K^{\sigma}_{\alpha\beta\gamma}$ using equation (79),

$$K^{\tau}_{\alpha\beta\gamma} = K^{\perp}_{\alpha\beta\gamma} = v^2\left(\tfrac{1}{2}v^{-2}\right)_{,\alpha\beta\gamma} - v^2\,\tau_{\substack{,r\alpha\\,r\beta\\,r\gamma}}\,\tau_{\substack{,r\beta\gamma\\,r\alpha\gamma\\,r\alpha\beta}} \quad . \tag{161}$$

To express the integration kernel in terms of the first–order ray–normal derivatives of the second–order perturbations of travel time, we shall convert expression (136) for $K^{s}_{\alpha\beta\gamma}$ by means of equation (79),

$$K^{\tau}_{\alpha\beta\gamma} = K^{\perp}_{\alpha\beta\gamma} = v\left(v^{-1}\right)_{,\alpha\beta\gamma} - v^2\tau^{\perp}_{\substack{,r\alpha\\,r\beta\\,r\gamma}}\,\tau^{\perp}_{\substack{,r\beta\gamma\\,r\alpha\gamma\\,r\alpha\beta}} - v\,v_{\substack{,\alpha\\,\beta\\,\gamma}}\,\tau^{\perp}_{\substack{,r\beta\\,r\alpha\\,r\alpha}}\,\tau^{\perp}_{\substack{,r\gamma\\,r\gamma\\,r\beta}} \quad . \tag{162}$$

6. COMPARISON WITH EQUATIONS OF OTHER AUTHORS

Various equations for the second–order perturbations of travel time in smooth models were derived, e.g., by *Kravtsov and Orlov* (*1980, 1990*), *Snieder and Sambridge* (*1992*), *Farra* (*1999*) and *Červený* (*2001*). We shall compare their equations with our equations in this section.

The approach of *Kravtsov and Orlov* (*1980, 1990*) is identical to our approach and their equations can thus be directly compared with our equations. *Kravtsov and Orlov* assumed an isotropic medium with Hamiltonian (111) and derived integration kernels (113) and (116) for the case of vanishing second–order perturbations $\left(\frac{1}{2}v^{-2}\right)_{,\alpha\beta} = 0$ (*Kravtsov and Orlov, 1980,* eqs. 9.8 and 9.9; *1990,* eqs. 2.9.8 and 2.9.9).

In contrast with our approach, *Snieder* (*1990*), *Snieder and Sambridge* (*1992*), *Farra* (*1999*) and *Červený* (*2001*) also perturbed the positions of rays. *Snieder and Sambridge* (*1992*) perturbed rays as geometrical objects, independently of their parametrization, assuming all perturbations of the points of rays to be perpendicular to the unperturbed rays. *Snieder and Sambridge* (*1992*) assumed an isotropic medium with vanishing second–order perturbations $\left(v^{-1}\right)_{,\alpha\beta} = 0$. *Snieder* (*1990*) derived the special case of equations by *Snieder and Sambridge* (*1992*) for a homogeneous background.

Farra (*1999*) and *Červený* (*2001*) perturbed the points of rays according to the perturbed ray tracing equations. They considered a general Hamiltonian, including generally anisotropic media.

We shall compare the results of *Farra* (*1999*) and *Červený* (*2001*) with our equations in Sections 6.1 and 6.2, and the results of *Snieder and Sambridge* (*1992*) with our equations in Section 6.3. These sections are structured in a similar way. We briefly recall the corresponding results of the other authors in the first paragraph of the section, and then demonstrate the relation to our equations. Note that the results of *Snieder and Sambridge* (*1992*) or *Farra* (*1999*) can be expressed in many forms. In each of Sections 6.1, 6.2 and 6.3, the author selected the form which he considered to be the best suitable for comparison with our equations.

6.1. Comparison of the second–order perturbations of travel time with the equations by Farra (1999) and Červený (2001)

Let us briefly recall the results of *Farra* (*1999*) and *Červený* (*2001*) for the second–order perturbations of travel time in this paragraph, and show their relation to our equations in the rest of Section 6.1. In contrast with our approach, *Farra* (*1999*) and *Červený* (*2001*) also perturbed positions $x_i = x_i(\gamma_a, f_\kappa)$ of the rays and corresponding slowness vectors

$$p_i = \tau_{,i}\big(x_i(\gamma_a, f_\kappa), f_\nu\big) \quad , \tag{163}$$

considering the relevant second–order Taylor expansions with respect to small changes $f_\kappa - f_\kappa^0$ in the model parameters in forms

$$x_i \approx x_i^0 + \varepsilon\, x_i^1 + \varepsilon^2 x_i^2 \tag{164}$$

and

$$p_i \approx p_i^0 + \varepsilon\, p_i^1 + \varepsilon^2 p_i^2 \quad . \tag{165}$$

Here

$$x_i^0(\gamma_a) = x_i(\gamma_a, f_\kappa^0) \tag{166}$$

and

$$p_i^0 = \tau_{,i}(x_i^0, f_\kappa^0) \tag{167}$$

are the phase–space coordinates of the unperturbed ray in the background model $f^0(x_i) = \sum_\kappa f_\kappa^0\, b_\kappa(x_i)$. The perturbed rays are defined by the perturbed ray tracing equations (*Farra and Madariaga, 1987,* eq. 11; *Farra, 1999,* eq. 11; *Červený, 2001,* eq. 4.7.20). The linear term in the second–order Taylor expansion (164) of the positions of rays with respect to small changes $f_\kappa - f_\kappa^0$ in the model parameters is

$$\varepsilon\, x_i^1(\gamma_a) = \sum_\alpha x_{i,\alpha}(\gamma_a, f_\kappa^0)\, (f_\alpha - f_\alpha^0) \quad . \tag{168}$$

The linear term in the second–order Taylor expansion (165) of slowness vector (163) is

$$\varepsilon\, p_i^1 = \tau_{,ij}(x_m^0, f_\kappa^0)\, \varepsilon\, x_j^1 + \sum_\alpha \tau_{,i\alpha}(x_m^0, f_\kappa^0)\, (f_\alpha - f_\alpha^0) \quad . \tag{169}$$

The second–order approximation of the perturbed travel time from point $x_i(\gamma_a^0, f_\kappa)$ to point $x_i(\gamma_a, f_\kappa)$ reads (*Farra, 1999,* eq. 20; *Červený, 2001,* eq. 4.7.29)

$$\Big[\tau(x_k, f_\kappa)\Big]_{\gamma_3^0}^{\gamma_3} \approx \int_{\gamma_3^0}^{\gamma_3} \mathrm{d}\gamma_3 \Big[H^{0,i}\, p_i^0 - \varepsilon\, H^1 - \varepsilon^2\big(H^2 + \tfrac{1}{2} H^1_{,i}\, x_i^1 + \tfrac{1}{2} H^{1,i}\, p_i^1\big)\Big] + \Big[\varepsilon\, p_i^0 x_i^1 + \varepsilon^2 p_i^0 x_i^2 + \tfrac{1}{2}\varepsilon^2 p_i^1 x_i^1\Big]_{\gamma_3^0}^{\gamma_3} \quad , \tag{170}$$

where

$$H^0 = H(x^0_m, p^0_n, f^0_\kappa) \quad , \tag{171}$$

$$\varepsilon\, H^1 = \sum_\alpha H_{,\alpha}(x^0_m, p^0_n, f^0_\kappa)\,(f_\alpha - f^0_\alpha) \quad , \tag{172}$$

and

$$\varepsilon^2 H^2 = \tfrac{1}{2}\sum_\alpha\sum_\beta H_{,\alpha\beta}(x^0_m, p^0_n, f^0_\kappa)\,(f_\alpha - f^0_\alpha)(f_\beta - f^0_\beta) \quad . \tag{173}$$

Quadrature (170) is performed along an unperturbed ray in the background model. The unperturbed ray, given by fixed ray take–off parameters $\gamma_1 = \gamma^0_1$ and $\gamma_2 = \gamma^0_2$, is parametrized by γ_3.

Note that the values of εx^1_i and εp^1_i have to be calculated and inserted into equation (170). The expressions for εx^1_i and εp^1_i derived by *Farra and Madariaga* (*1987,* eq. 13), *Farra* (*1999,* eq. 12) or *Červený* (*2001,* eq. 4.7.22) contain the whole paraxial ray propagator matrix and their relation to the orthonomic system of rays under perturbation is not clear. That is why the comparison of equation (170) with our equations is not trivial. On the other hand, if we calculate the first–order perturbations $\tau_{,i\alpha}$ of the travel–time gradient at the unperturbed ray from the perturbations $x_{i,\alpha}$, $p_{i,\alpha}$ of the phase–space ray coordinates, the components of the paraxial ray propagator matrix vanish due to the symplectic property, and we arrive at quadrature (19) with integration kernel (27), as shown in Section 6.2. In the rest of Section 6.1, we shall demonstrate that equation (170) is equivalent to equations (19) and (20), with integration kernel K_α given by equation (25) and integration kernel $K_{\alpha\beta}$ given by equation (30).

Equation (170) includes, in addition to the perturbations of the travel time between points $x_i(\gamma^0_a, f^0_\kappa)$ and $x_i(\gamma_a, f^0_\kappa)$, also the second–order paraxial approximations of the travel time from point $x_i(\gamma^0_a, f^0_\kappa)$ to point $x_i(\gamma^0_a, f_\kappa)$ and from point $x_i(\gamma_a, f^0_\kappa)$ to point $x_i(\gamma_a, f_\kappa)$ in the perturbed model. To avoid possible confusion, let us emphasize that superscript ^{0} of γ_a has no relation to superscript ^{0} of f_κ. Superscript ^{0} of γ_a denotes the values of ray parameters at the initial point of a ray, whereas superscript ^{0} of f_κ denotes the background model. The linear and quadratic terms of the paraxial approximation of travel time from point $x^0_i = x_i(\gamma_a, f^0_\kappa)$ to point $x_i = x_i(\gamma_a, f_\kappa)$ are

$$\begin{aligned}\tau^{\mathrm{PRA}} = {}&\tau_{,i}(x^0_m, f^0_\kappa)\,\varepsilon\, x^1_i + \tau_{,i}(x^0_m, f^0_\kappa)\,\varepsilon^2 x^2_i + \tfrac{1}{2}\tau_{,ij}(x^0_m, f^0_\kappa)\,\varepsilon^2 x^1_i\, x^1_j \\ &+ \sum_\alpha \tau_{,i\alpha}(x^0_m, f^0_\kappa)\,\varepsilon\, x^1_i\,(f_\alpha - f^0_\alpha) \quad ,\end{aligned} \tag{174}$$

where we have approximated the first–order spatial derivatives of travel time by (169) and the second–order spatial derivatives by the unperturbed ones. The argument of the last term in equation (170), with p^0_i and εp^1_i replaced by expressions (167) and (169), reads

$$\begin{aligned}\varepsilon\, p^0_i\, x^1_i + \varepsilon^2 p^0_i\, x^2_i + \tfrac{1}{2}\varepsilon^2 p^1_i\, x^1_i = {}&\tau_{,i}(x^0_m, f^0_\kappa)\,(\varepsilon\, x^1_i + \varepsilon^2 x^2_i) + \tfrac{1}{2}\tau_{,ij}(x^0_m, f^0_\kappa)\,\varepsilon^2 x^1_i\, x^1_j \\ &+ \tfrac{1}{2}\sum_\alpha \tau_{,i\alpha}(x^0_m, f^0_\kappa)\,\varepsilon\, x^1_i\,(f_\alpha - f^0_\alpha) \quad .\end{aligned} \tag{175}$$

We may now compare the argument of the last term of equation (170) with the linear and quadratic terms of paraxial approximation (174),

$$\varepsilon\, p_i^0\, x_i^1 + \varepsilon^2 p_i^0\, x_i^2 + \tfrac{1}{2}\varepsilon^2 p_i^1\, x_i^1 = \tau^{\mathrm{PRA}} - \tfrac{1}{2} \sum_\alpha \tau_{,i\alpha}(x_m^0, f_\kappa^0)\; \varepsilon\, x_i^1\, (f_\alpha - f_\alpha^0) \quad . \tag{176}$$

We may thus separate, in equation (170), the perturbations at fixed spatial coordinates from the linear and quadratic terms of the paraxial ray approximation,

$$\begin{aligned}\Big[\tau(x_k, f_\kappa)\Big]_{\gamma_3^0}^{\gamma_3} \approx \int_{\gamma_3^0}^{\gamma_3} \mathrm{d}\gamma_3 \Big[& H^{0,i}\, p_i^0 - \varepsilon\, H^1 - \varepsilon^2 \big(H^2 + \tfrac{1}{2} H^1_{,i}\, x_i^1 + \tfrac{1}{2} H^{1,i}\, p_i^1\big) \\ & - \frac{\mathrm{d}}{\mathrm{d}\gamma_3} \Big(\tfrac{1}{2} \sum_\alpha \tau_{,i\alpha}(x_m^0, f_\kappa^0)\; \varepsilon\, x_i^1\, (f_\alpha - f_\alpha^0) \Big) \Big] + \Big[\tau^{\mathrm{PRA}}\Big]_{\gamma_3^0}^{\gamma_3} \quad . \end{aligned} \tag{177}$$

Inserting expressions (168) and (169) for εx_i^1 and εp_i^1, equation (177) with (172) and (173) reads

$$\begin{aligned}\Big[\tau(x_k, f_\kappa)\Big]_{\gamma_3^0}^{\gamma_3} \approx & \int_{\gamma_3^0}^{\gamma_3} \mathrm{d}\gamma_3\; H^{0,i}\, p_i^0 + \sum_\alpha \tau_{,\alpha}(x_m^0, f_\kappa^0)\; (f_\alpha - f_\alpha^0) \\ & + \tfrac{1}{2} \sum_\alpha \sum_\beta \tau_{,\alpha\beta}(x_m^0, f_\kappa^0)\; (f_\alpha - f_\alpha^0)(f_\beta - f_\beta^0) + \Big[\tau^{\mathrm{PRA}}\Big]_{\gamma_3^0}^{\gamma_3} \quad , \end{aligned} \tag{178}$$

where $\tau_{,\alpha}$ and $\tau_{,\alpha\beta}$ are given by equations (19) and (20), with integration kernel K_α given by equation (25) and symmetric integration kernel $K_{\alpha\beta}$ given by equation

$$K_{\alpha\beta} = -H_{,\alpha\beta} - \tfrac{1}{2} H_{\substack{,i\alpha \\ ,i\beta}} x_{\substack{i,\beta \\ i,\alpha}} - \tfrac{1}{2} H^{,i}_{\substack{,\alpha \\ ,\beta}} \tau_{\substack{,i\beta \\ ,i\alpha}} - \tfrac{1}{2} H^{,i}_{\substack{,\alpha \\ ,\beta}} \tau_{\substack{,ij \\ ,ij}}\, x_{\substack{j,\beta \\ j,\alpha}} - \frac{\mathrm{d}}{\mathrm{d}\gamma_3} \Big(\tfrac{1}{2} \tau_{\substack{,i\alpha \\ ,i\beta}}\, x_{\substack{i,\beta \\ i,\alpha}} \Big) \quad . \tag{179}$$

We shall now show that integration kernel (179) is identical to (30).

Perturbing ray tracing system (8), we obtain equation (*Farra and Madariaga, 1987,* eq. 11; *Farra, 1999,* eq. 11)

$$\frac{\mathrm{d}}{\mathrm{d}\gamma_3} x_{i,\alpha} = H^{,i}_{,j}\, x_{j,\alpha} + H^{,ij} p_{j,\alpha} + H^{,i}_{,\alpha} \quad , \tag{180}$$

where we may express $p_{j,\alpha}$ in terms of $x_{j,\alpha}$ and $\tau_{,j\alpha}$,

$$\frac{\mathrm{d}}{\mathrm{d}\gamma_3} x_{i,\alpha} = H^{,i}_{,j}\, x_{j,\alpha} + H^{,ij}\, (\tau_{,jk}\, x_{k,\alpha} + \tau_{,j\alpha}) + H^{,i}_{,\alpha} \quad . \tag{181}$$

Equation (11) yields

$$\frac{\mathrm{d}}{\mathrm{d}\gamma_3} \tau_{,i\alpha} = -H_{,i\alpha} - H^{,r}_{\substack{,i \\ ,\alpha}}\, \tau_{\substack{,r\alpha \\ ,ri}} - H^{,rs}\, \tau_{,ri}\, \tau_{,s\alpha} \quad . \tag{182}$$

Equations (181) and (182) yield

$$\frac{\mathrm{d}}{\mathrm{d}\gamma_3} \Big(\tau_{,i\alpha}\, x_{i,\beta} \Big) = -H_{,i\alpha} x_{i,\beta} - H^{,r}_{,\alpha} \tau_{,ri}\, x_{i,\beta} + H^{,rs} \tau_{,r\alpha} \tau_{,s\beta} + H^{,i}_{,\beta} \tau_{,i\alpha} \quad . \tag{183}$$

Inserting identity (183) into equation (179), the terms containing $x_{i,\beta}$ cancel out and we obtain equation (30) for integration kernel $K_{\alpha\beta}$.

6.2. Comparison of the first–order perturbations of the travel–time gradient with the equations by Farra and Madariaga (1987), Farra (1999) and Červený (2001)

Let us briefly recall the equations for the first–order perturbations $x_{i,\alpha}$, $p_{i,\alpha}$ of the phase–space ray coordinates in this paragraph, and show their relation to our equations for the first–order perturbations $\tau_{,i\alpha}$ of the travel–time gradient at the unperturbed ray in the rest of Section 6.2. The expressions for the first–order perturbations $x_{i,\alpha}$, $p_{i,\alpha}$ of the phase–space ray coordinates read (*Farra and Madariaga, 1987,* eq. 13; *Farra, 1999,* eq. 12; *Červený, 2001,* eq. 4.7.22)

$$\begin{aligned} x_{i,\alpha}(\gamma_3) = {} & Q^{(1)}_{ij}(\gamma_3,\gamma_3^0)\; x_{j,\alpha}(\gamma_3^0) + Q^{(2)}_{ij}(\gamma_3,\gamma_3^0)\; p_{j,\alpha}(\gamma_3^0) \\ & + \int_{\gamma_3^0}^{\gamma_3} \mathrm{d}\gamma_3' \Big[Q^{(1)}_{ij}(\gamma_3,\gamma_3')\; H^{\,;j}_{,\alpha}(\gamma_3') - Q^{(2)}_{ij}(\gamma_3,\gamma_3')\; H_{,j\alpha}(\gamma_3') \Big] \quad , \end{aligned} \tag{184}$$

$$\begin{aligned} p_{i,\alpha}(\gamma_3) = {} & P^{(1)}_{ij}(\gamma_3,\gamma_3^0)\; x_{j,\alpha}(\gamma_3^0) + P^{(2)}_{ij}(\gamma_3,\gamma_3^0)\; p_{j,\alpha}(\gamma_3^0) \\ & + \int_{\gamma_3^0}^{\gamma_3} \mathrm{d}\gamma_3' \Big[P^{(1)}_{ij}(\gamma_3,\gamma_3')\; H^{\,;j}_{,\alpha}(\gamma_3') - P^{(2)}_{ij}(\gamma_3,\gamma_3')\; H_{,j\alpha}(\gamma_3') \Big] \quad , \end{aligned} \tag{185}$$

where $Q^{(1)}_{ij}$, $P^{(1)}_{ij}$, $Q^{(2)}_{ij}$ and $P^{(2)}_{ij}$ are 3×3 submatrices of the 6×6 paraxial ray propagator matrix

$$\begin{pmatrix} Q^{(1)}_{ij}(\gamma_3,\gamma_3') & Q^{(2)}_{ij}(\gamma_3,\gamma_3') \\ P^{(1)}_{ij}(\gamma_3,\gamma_3') & P^{(2)}_{ij}(\gamma_3,\gamma_3') \end{pmatrix} \quad , \tag{186}$$

which is the solution of dynamic ray tracing system (14) with unit initial conditions

$$Q^{(1)}_{ij}(\gamma_3',\gamma_3') = \delta_{ij} \ , \quad P^{(1)}_{ij}(\gamma_3',\gamma_3') = 0 \ , \quad Q^{(2)}_{ij}(\gamma_3',\gamma_3') = 0 \ , \quad P^{(2)}_{ij}(\gamma_3',\gamma_3') = \delta_{ij} \ . \tag{187}$$

Quadratures (184) and (185) are performed along an unperturbed ray in the background model. We are thus suppressing arguments γ_1, γ_2 and f^0_κ, which are constant along the ray, and are expressing explicitly only parameter γ_3 along the ray in this section.

The first–order perturbations $\tau_{,i\alpha}$ of the travel–time gradient at the unperturbed ray are related to perturbations (184) and (185) of the phase–space ray coordinates through equation

$$\tau_{,i\alpha}(\gamma_3) = p_{i,\alpha}(\gamma_3) - \tau_{,ij}(\gamma_3)\; x_{i,\alpha}(\gamma_3) \quad , \tag{188}$$

see (169). The corresponding covariant derivatives (16) of travel time with respect to ray parameters are

$$T_{a\alpha}(\gamma_3) = Q_{ia}(\gamma_3)\; p_{i,\alpha}(\gamma_3) - P_{ia}(\gamma_3)\; x_{i,\alpha}(\gamma_3) \quad , \tag{189}$$

where matrices Q_{ia} and P_{ia}, defined by (12), correspond to the orthonomic system of rays under consideration and satisfy equation (13). Inserting (184) and (185) into (189), we arrive at

$$
\begin{aligned}
T_{a\alpha}(\gamma_3) = & \left[Q_{ia}(\gamma_3)\, P^{(1)}_{ij}(\gamma_3,\gamma_3^0) - P_{ia}(\gamma_3)\, Q^{(1)}_{ij}(\gamma_3,\gamma_3^0)\right] x_{j,\alpha}(\gamma_3^0) \\
& + \left[Q_{ia}(\gamma_3)\, P^{(2)}_{ij}(\gamma_3,\gamma_3^0) - P_{ia}(\gamma_3)\, Q^{(2)}_{ij}(\gamma_3,\gamma_3^0)\right] p_{j,\alpha}(\gamma_3^0) \\
& + \int_{\gamma_3^0}^{\gamma_3} \mathrm{d}\gamma_3' \Big\{ \left[Q_{ia}(\gamma_3)\, P^{(1)}_{ij}(\gamma_3,\gamma_3') - P_{ia}(\gamma_3)\, Q^{(1)}_{ij}(\gamma_3,\gamma_3')\right] H^{;j}_{,\alpha}(\gamma_3') \\
& \qquad - \left[Q_{ia}(\gamma_3)\, P^{(2)}_{ij}(\gamma_3,\gamma_3') - P_{ia}(\gamma_3)\, Q^{(2)}_{ij}(\gamma_3,\gamma_3')\right] H_{,j\alpha}(\gamma_3') \Big\} \; . \qquad (190)
\end{aligned}
$$

The symplectic property (*Červený, 2001*) then yields

$$
\begin{aligned}
T_{a\alpha}(\gamma_3) = & \left[Q_{ia}(\gamma_3^0)\, P^{(1)}_{ij}(\gamma_3^0,\gamma_3^0) - P_{ia}(\gamma_3^0)\, Q^{(1)}_{ij}(\gamma_3^0,\gamma_3^0)\right] x_{j,\alpha}(\gamma_3^0) \\
& + \left[Q_{ia}(\gamma_3^0)\, P^{(2)}_{ij}(\gamma_3^0,\gamma_3^0) - P_{ia}(\gamma_3^0)\, Q^{(2)}_{ij}(\gamma_3^0,\gamma_3^0)\right] p_{j,\alpha}(\gamma_3^0) \\
& + \int_{\gamma_3^0}^{\gamma_3} \mathrm{d}\gamma_3' \Big\{ \left[Q_{ia}(\gamma_3')\, P^{(1)}_{ij}(\gamma_3',\gamma_3') - P_{ia}(\gamma_3')\, Q^{(1)}_{ij}(\gamma_3',\gamma_3')\right] H^{;j}_{,\alpha}(\gamma_3') \\
& \qquad - \left[Q_{ia}(\gamma_3')\, P^{(2)}_{ij}(\gamma_3',\gamma_3') - P_{ia}(\gamma_3')\, Q^{(2)}_{ij}(\gamma_3',\gamma_3')\right] H_{,j\alpha}(\gamma_3') \Big\} \; . \qquad (191)
\end{aligned}
$$

Inserting unit initial conditions (187) for the paraxial ray propagator matrix, and considering relation (189) at initial point $\gamma_3 = \gamma_3^0$, we obtain equation

$$
T_{a\alpha}(\gamma_3) = T_{a\alpha}(\gamma_3^0) - \int_{\gamma_3^0}^{\gamma_3} \mathrm{d}\gamma_3' \left[P_{ia}(\gamma_3')\, H^{;i}_{,\alpha}(\gamma_3') + Q_{ia}(\gamma_3')\, H_{,i\alpha}(\gamma_3')\right] \; . \qquad (192)
$$

Considering relation (13), we see that equation (192) is identical to equation (19) with integration kernel $K_{i\alpha}$ given by equation (27).

Whereas the whole paraxial ray propagator matrix is required to calculate the first–order perturbations $x_{i,\alpha}$ and $p_{i,\alpha}$ of the phase–space ray coordinates using equations (184) and (185), only matrices Q_{ia} and P_{ia} corresponding to the orthonomic system of rays under consideration are required to calculate the first–order perturbations $\tau_{,i\alpha}$ of the travel–time gradient at the unperturbed ray using equation (192).

6.3. Comparison with the equations by Snieder and Sambridge (1992)

Let us briefly recall the results of *Snieder and Sambridge* (*1992*) in this paragraph, and show their relation to our equations in the rest of Section 6.3. *Snieder and Sambridge* (*1992*) considered an isotropic medium and parametrized rays by the arclength, $\gamma_3 = s$, which corresponds to Hamiltonian (68). They assumed vanishing second–order perturbations of the spatial slowness distribution, $u_{,\alpha\beta} = \left(v^{-1}\right)_{,\alpha\beta} = 0$. *Snieder and Sambridge* (*1992*) perturbed rays as geometrical objects, independently of their parametrization, assuming all perturbations of the points of rays to be perpendicular to the unperturbed rays,

$$
x_i \approx x_i^0 + \varepsilon\, r_i^1 + \varepsilon^2 r_i^2 \quad , \qquad (193)
$$

where the perturbations of the positions are restricted to the wavefront tangent plane,

$$r_i^1 p_i = 0 \quad , \qquad r_i^2 p_i = 0 \quad . \tag{194}$$

Coordinates $x_i^0 = x_i^0(\gamma_a)$ of unperturbed rays are defined by (166). The linear term in the second–order Taylor expansion (193) of the positions of rays with respect to small changes $f_\kappa - f_\kappa^0$ in the model parameters can be expressed in the form

$$\varepsilon\, r_i^1(\gamma_a) = \sum_\alpha r_{i,\alpha}(\gamma_a, f_\kappa^0)\,(f_\alpha - f_\alpha^0) \quad , \tag{195}$$

analogous to (168). The second–order approximation of the perturbed travel time from point $x_i(\gamma_a^0, f_\kappa)$ to point $x_i(\gamma_a, f_\kappa)$ reads (*Snieder and Sambridge, 1992,* eqs. 12, 13a, 20a and 61)

$$\Big[\tau(x_k, f_\kappa)\Big]_{s^0}^{s} \approx \int_{s^0}^{s} \mathrm{d}s \Big[u^0 + \varepsilon\, u^1 + \varepsilon^2 \tfrac{1}{2} r_i^1 \Big(u_{,i}^1 - u^1 \frac{u_{,i}^0}{u^0}\Big)\Big] + \Big[\tfrac{1}{2}\varepsilon^2 u^0 r_i^1 \frac{\mathrm{d}}{\mathrm{d}s} r_i^1\Big]_{s^0}^{s} \; , \tag{196}$$

where $s^0 = \gamma_3^0$ and $s = \gamma_3$. Here $u = v^{-1}$ is used to denote the slowness distribution in general, with u^0 being the background slowness along the unperturbed ray and εu^1 the linear part of the Taylor expansion of the slowness with respect to small changes $f_\kappa - f_\kappa^0$ in the model parameters,

$$u^0 = u(x_i^0, f_\kappa^0) \quad , \qquad \varepsilon\, u^1 = \sum_\alpha u_{,\alpha}(x_i^0, f_\kappa^0)\,(f_\alpha - f_\alpha^0) \quad . \tag{197}$$

Quadrature (196) is performed along an unperturbed ray in the background model. Note that the values of εr_i^1 have to be calculated and inserted into equation (196). In the rest of Section 6.3, we shall demonstrate that equation (196) is equivalent to equations (19) and (20), with integration kernel K_α given by equation (126) and integration kernel $K_{\alpha\beta}$ given by equation (129) with $\big(v^{-1}\big)_{,\alpha\beta} = 0$.

Considering constraints (194), the first–order coordinate perturbations $r_{i,\alpha}$ in (195) are the ray–normal projections

$$r_{i,\alpha} = E_{ij}^{\perp}\, x_{j,\alpha} \tag{198}$$

of the coordinate perturbations $x_{i,\alpha}$ defined by the perturbed ray tracing equations. Here the ray–normal projection matrix $E_{ij}^{\perp}$ is given by (103). For Hamiltonian (68), equation (181) with (124) reads

$$\frac{\mathrm{d}}{\mathrm{d}s} x_{i,\alpha} = p^{-1} E_{ij}^{\perp}\,(\tau_{,jk} x_{k,\alpha} + \tau_{,j\alpha}) \quad . \tag{199}$$

Equations (198) and (199) with (103) yield

$$\frac{\mathrm{d}}{\mathrm{d}s} r_{i,\alpha} = p^{-1} E_{ij}^{\perp}\,(\tau_{,jk} x_{k,\alpha} + \tau_{,j\alpha}) - p^{-3}(E_{ir}^{\perp}\, p_j + p_i\, E_{jr}^{\perp})\,\tau_{,rs}\, p_s\, x_{j,\alpha} \quad , \tag{200}$$

where we may use equation (198) to transform $x_{j,\alpha}$ into $r_{j,\alpha}$,

$$\frac{\mathrm{d}}{\mathrm{d}s} r_{i,\alpha} = p^{-1} E_{ij}^{\perp}\,(\tau_{,jk}\, r_{k,\alpha} + \tau_{,j\alpha}) - p^{-3} p_i\, p_j\, \tau_{,jk}\, r_{k,\alpha} \quad . \tag{201}$$

All quantities in equation (201), including the derivatives and perturbations of travel time, are taken at the unperturbed ray.

Equation (196) includes, in addition to the perturbations of the travel time between points $x_i(\gamma_a^0, f_\kappa^0)$ and $x_i(\gamma_a, f_\kappa^0)$, also the second–order paraxial approximations of the travel time from point $x_i(\gamma_a^0, f_\kappa^0)$ to point $x_i(\gamma_a^0, f_\kappa)$ and from point $x_i(\gamma_a, f_\kappa^0)$ to point $x_i(\gamma_a, f_\kappa)$ in the perturbed model. The linear and quadratic terms of the paraxial approximation of travel time from point $x_i^0 = x_i(\gamma_a, f_\kappa^0)$ to point $x_i = x_i(\gamma_a, f_\kappa)$ are given by equation (174). Considering coordinate perturbations (193) constrained by (194), paraxial approximation (174) takes the form

$$\tau^{\mathrm{PRA}} = \tfrac{1}{2}\tau_{,ij}(x_m^0, f_\kappa^0)\,\varepsilon^2 r_i^1 r_j^1 + \sum_\alpha \tau_{,i\alpha}(x_m^0, f_\kappa^0)\,\varepsilon\, r_i^1\,(f_\alpha - f_\alpha^0) \quad . \tag{202}$$

The argument of the last term in equation (196), with εr_i^1 replaced by expression (195), reads

$$\tfrac{1}{2}\varepsilon^2 u^0 r_i^1 \frac{\mathrm{d}}{\mathrm{d}s} r_i^1 = \tfrac{1}{2}\sum_\alpha \sum_\beta u^0 r_{i,\alpha} \frac{\mathrm{d}r_{i,\beta}}{\mathrm{d}s}\,(f_\alpha - f_\alpha^0)\,(f_\beta - f_\beta^0) \quad , \tag{203}$$

which may be converted into

$$\tfrac{1}{2}\varepsilon^2 u^0 r_i^1 \frac{\mathrm{d}}{\mathrm{d}s} r_i^1 = \tfrac{1}{2}\sum_\alpha \sum_\beta r_{i,\alpha}\,(\tau_{,ij} r_{j,\beta} + \tau_{,i\beta})\,(f_\alpha - f_\alpha^0)\,(f_\beta - f_\beta^0) \tag{204}$$

using (201). We may now compare the argument of the last term of equation (196) with the linear and quadratic terms of paraxial approximation (202),

$$\tfrac{1}{2}\varepsilon^2 u^0 r_i^1 \frac{\mathrm{d}}{\mathrm{d}s} r_i^1 = \tau^{\mathrm{PRA}} - \tfrac{1}{2}\sum_\alpha \sum_\beta r_{i,\alpha}\tau_{,i\beta}\,(f_\alpha - f_\alpha^0)\,(f_\beta - f_\beta^0) \quad . \tag{205}$$

In equation (196), we may thus separate the perturbations at fixed spatial coordinates from the linear and quadratic terms of the paraxial ray approximation,

$$\begin{aligned}\Big[\tau(x_k, f_\kappa)\Big]_{s^0}^{s} \approx \int_{s^0}^{s} \mathrm{d}s \Big[& u^0 + \varepsilon\, u^1 + \varepsilon^2 \tfrac{1}{2} r_i^1 \left(u_{,i}^1 - u^1 \frac{u_{,i}^0}{u^0} \right) \\ & - \tfrac{1}{2}\sum_\alpha \sum_\beta \frac{\mathrm{d}}{\mathrm{d}s}\Big(r_{i,\alpha}\tau_{,i\beta}\Big)\,(f_\alpha - f_\alpha^0)\,(f_\beta - f_\beta^0)\Big] + \Big[\tau^{\mathrm{PRA}}\Big]_{s^0}^{s} \; .\end{aligned} \tag{206}$$

Inserting expressions (195) and (197) for εr_i^1 and εu^1, equation (206) becomes

$$\begin{aligned}\Big[\tau(x_k, f_\kappa)\Big]_{s^0}^{s} \approx \int_{s^0}^{s} \mathrm{d}s\, u^0 & + \sum_\alpha \tau_{,\alpha}(x_m^0, f_\kappa^0)\,(f_\alpha - f_\alpha^0) \\ & + \tfrac{1}{2}\sum_\alpha \sum_\beta \tau_{,\alpha\beta}(x_m^0, f_\kappa^0)\,(f_\alpha - f_\alpha^0)\,(f_\beta - f_\beta^0) + \Big[\tau^{\mathrm{PRA}}\Big]_{s^0}^{s} \; ,\end{aligned} \tag{207}$$

where $\tau_{,\alpha}$ and $\tau_{,\alpha\beta}$ are given by equations (19) and (20), with integration kernel K_α given by equation (126) and symmetric integration kernel $K_{\alpha\beta}$ given by equation

$$K_{\alpha\beta}^{s} = \tfrac{1}{2} r_{\substack{i,\alpha \\ i,\beta}} u_{\substack{,i\beta \\ ,i\alpha}} - \tfrac{1}{2} r_{\substack{i,\alpha \\ i,\beta}} u_{\substack{,\beta \\ ,\alpha}} u_{\substack{,i \\ ,i}} u^{-1} - \frac{\mathrm{d}}{\mathrm{d}s}\Big(\tfrac{1}{2} \tau_{\substack{,i\alpha \\ ,i\beta}} r_{\substack{i,\beta \\ i,\alpha}} \Big) \quad . \tag{208}$$

We shall now show that integration kernel (208) is identical to (129) with $(v^{-1})_{,\alpha\beta}=0$.

For Hamiltonian (68), equation (182) with (124) reads

$$\frac{\mathrm{d}}{\mathrm{d}s}\tau_{,i\alpha} = u_{,i\alpha} - p^{-1}\tau_{,ir}\,E^{\perp}_{,rs}\,\tau_{,s\alpha} \quad . \tag{209}$$

Equations (201) and (209) yield

$$\frac{\mathrm{d}}{\mathrm{d}s}\Big(\tau_{,i\alpha}r_{i,\beta}\Big) = u_{,i\alpha}r_{i,\beta} + p^{-1}\tau_{,i\alpha}E^{\perp}_{,ij}\,\tau_{,j\beta} - p^{-3}\tau_{,i\alpha}\,p_i\,p_j\,\tau_{,jk}\,r_{k,\alpha} \quad , \tag{210}$$

which may be converted using identities (107) into

$$\frac{\mathrm{d}}{\mathrm{d}s}\Big(\tau_{,i\alpha}r_{i,\beta}\Big) = u_{,i\alpha}\,r_{i,\beta} + p^{-1}\tau^{\perp}_{,i\alpha}\,\tau^{\perp}_{,i\beta} - p^{-1}u_{,\alpha}\,u_{,k}\,r_{k,\alpha} \quad . \tag{211}$$

Inserting identity (211) into equation (208), the terms containing $r_{i,\alpha}$ cancel out and we obtain equation (129) for integration kernel $K^{s}_{\alpha\beta}$, but without term $(v^{-1})_{,\alpha\beta}$, because *Snieder and Sambridge (1992)* assumed vanishing second–order slowness perturbations $u_{,\alpha\beta}=(v^{-1})_{,\alpha\beta}$.

7. CONCLUSIONS

The spatial derivatives and perturbations of travel time in isotropic or anisotropic media can be calculated using equation (20), with the covariant derivatives with respect to ray parameters and perturbations of travel time given partly explicitly by equation (23) and partly by numerical quadratures (19). The general form of the integration kernels of quadratures (19) is given by equation (21). The special cases of integration kernels (21), corresponding to the individual spatial derivatives and perturbations of travel time up to the third order in generally anisotropic media, are shown in Section 3. The equations for calculating the individual spatial derivatives and perturbations of travel time up to the third order in isotropic media are presented in Section 5.

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References

Arnaud J.A., 1973. Hamiltonian theory of beam mode propagation. In: Wolf E. (ed.): *Progress in Optics, Vol. 11*, North–Holland publ. Co.

Babich V.M. and Buldyrev N.J., 1972. *Asymptotic Methods in Problems of Diffraction of Short Waves* (in Russian). Nauka, Moscow.

Babich V.M., Buldyrev N.J. and Molotkov I.A., 1985. *Space–time Ray Method. Linear and Non–linear Waves* (in Russian). Leningrad Univ. Press, Leningrad.

Bakker P.M., 2002. Coupled anisotropic shear wave raytracing in situations where associated slowness sheets are almost tangent. *Pure Appl. Geophys.*, **159**, in press.

Bulant P. and Klimeš L., 2002. Numerical algorithm of the coupling ray theory in weakly anisotropic media. *Pure Appl. Geophys.*, **159**, in press, online at "http://sw3d.mff.cuni.cz".

Bulant P., Klimeš L. and Pšenčík I., 2000. Comparison of ray methods with the exact solution in the 1-D anisotropic "twisted crystal" model. *Expanded Abstracts of 70th Annual Meeting (Calgary)*, pp. 2289–2292, Soc. Explor. Geophysicists, Tulsa, online at "http://sw3d.mff.cuni.cz".

Červený V., 1972. Seismic rays and ray intensities in inhomogeneous anisotropic media. *Geophys. J. R. Astr. Soc.*, **29**, 1–13.

Červený V., 1989. Ray tracing in factorized anisotropic inhomogeneous media. *Geophys. J. Int.*, **99**, 91–100.

Červený V., 2001. *Seismic Ray Theory.* Cambridge Univ. Press, Cambridge.

Červený V. and Hron F., 1980. The ray series method and dynamic ray tracing system for three–dimensional inhomogeneous media. *Bull. Seismol. Soc. Am.*, **70**, 47–77.

Coates R.T. and Chapman C.H., 1990. Quasi–shear wave coupling in weakly anisotropic 3-D media. *Geophys. J. Int.*, **103**, 301–320.

Farra V., 1999. Computation of second–order traveltime perturbation by Hamiltonian ray theory. *Geophys. J. Int.*, **136**, 205–217.

Farra V. and Madariaga R., 1987. Seismic waveform modeling in heterogeneous media by ray perturbation theory. *J. Geophys. Res.*, **92B**, 2697–2712.

Hanyga A., 1982. Dynamic ray tracing in an anisotropic medium. *Tectonophysics*, **90**, 243–251.

Klimeš L., 1994. Transformations for dynamic ray tracing in anisotropic media. *Wave Motion*, **20**, 261–272.

Klimeš L., 1997. Calculation of the third and higher travel–time derivatives in isotropic and anisotropic media. In: *Seismic Waves in Complex 3-D Structures, Report 6*, pp. 157–166, Dep. Geophys., Charles Univ., Prague, online at "http://sw3d.mff.cuni.cz".

Klimeš L., 1999. Calculation of the third and higher travel–time derivatives in isotropic and anisotropic media. *Expanded Abstracts of 69th Annual Meeting (Houston)*, pp. 1751–1754, Soc. Explor. Geophysicists, Tulsa, online at "http://sw3d.mff.cuni.cz".

Kravtsov Yu.A. and Orlov Yu.I., 1980. *Geometrical Optics of Inhomogeneous Media* (in Russian). Nauka, Moscow.

Kravtsov Yu.A. and Orlov Yu.I., 1990. *Geometrical Optics of Inhomogeneous Media.* Springer–Verlag, Heidelberg.

Luneburg R.K., 1944. *Mathematical Theory of Optics.* Lecture notes, Brown University, Providence, Rhode Island. Reedition: University of California Press, Berkeley and Los Angeles, 1964.

Popov M.M. and Pšenčík I., 1978a. Ray amplitudes in inhomogeneous media with curved interfaces. *Travaux Instit. Géophys. Acad. Tchécosl. Sci. No. 454, Geofys. Sborník*, **24**, 111–129, Academia, Praha.

Popov M.M. and Pšenčík I., 1978b. Computation of ray amplitudes in inhomogeneous media with curved interfaces. *Stud. Geophys. Geod.*, **22**, 248–258.

Snieder R., 1990. A perturbative analysis of non–linear inversion. *Geophys. J. Int.*, **101**, 545–556.

Snieder R. and Sambridge M., 1992. Ray perturbation theory for travel times and ray paths in 3-D heterogeneous media. *Geophys. J. Int.*, **109**, 294–322.