SPATIAL DERIVATIVES AND PERTURBATION DERIVATIVES OF AMPLITUDE IN ISOTROPIC AND ANISOTROPIC MEDIA

L. Klimeš

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

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ABSTRACT

Explicit equations for the spatial derivatives and perturbation derivatives of amplitude in both isotropic and anisotropic media are derived. The spatial and perturbation derivatives of the logarithm of amplitude can be calculated by numerical quadratures along the rays.

The spatial derivatives of amplitude may be useful in calculating the higher–order terms in the ray series, in calculating the higher–order amplitude coefficients of Gaussian beams, in estimating the accuracy of zero–order approximations of both the ray method and Gaussian beams, in estimating the accuracy of the paraxial approximation of individual Gaussian beams, or in estimating the accuracy of the asymptotic summation of paraxial Gaussian beams. The perturbation derivatives of amplitude may be useful in perturbation expansions from elastic to viscoelastic media and in estimating the accuracy of the common–ray approximations of the amplitude in the coupling ray theory.

Key words: ray theory, amplitude, transport equation, paraxial approximation, perturbation methods, inhomogeneous media, seismic anisotropy

1. INTRODUCTION

The Hamiltonian in the *eikonal equation* (stationary Hamilton–Jacobi equation) for travel time is a function of phase–space coordinates, which are composed of spatial coordinates and of slowness–vector components. We assume that the Hamiltonian depends also on *perturbation parameters*, which parametrize the continuous system of Hamiltonians in the continuous system of eikonal equations. Each eikonal equation for travel time may be supplemented by a *transport equation* for amplitude. The transport equation depends on the Hamiltonian and may also depend on additional perturbation parameters. The rays traced using the Hamiltonian depend on the perturbation parameters. Travel time, amplitude and other quantities calculated along the rays are then functions of the spatial coordinates and of the perturbation parameters.

We shall refer to the partial derivatives of travel time, amplitude or other quantities with respect to the perturbation parameters as *perturbation derivatives* of these quantities. We have introduced the term perturbation derivatives in order to distinguish briefly the partial derivatives with respect to perturbation 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 perturbation derivatives of the Hamiltonian, and between the *spatial derivatives* and perturbation derivatives of travel time, amplitude or other quantities.

If the spatial and perturbation derivatives of a quantity are known, we may approximate the quantity by the *Taylor expansion* with respect to the spatial coordinates and perturbation parameters. The Taylor expansion with respect to the perturbation parameters is the simplest but very important special case of the *perturbation expansion* (*Murdock, 1999*).

This paper is devoted to the calculation of the spatial derivatives and perturbation derivatives of amplitude. In this paper, the transport equation for amplitude is formally attached to an orthonomic system of rays corresponding to a given eikonal equation for travel time. We follow the approach of *Kravtsov and Orlov (1980, 1990)*, *Klimeš (2002a)* and *Kravtsov (2005)*, and calculate the perturbation derivatives of all quantities at fixed spatial coordinates along unperturbed rays.

The second–order or higher–order spatial derivatives of amplitude are required in calculating or approximating the first–order or higher–order terms in the ray series or the first–order or higher–order amplitude coefficients of Gaussian beams. The first–order amplitude coefficients may then be useful in estimating the accuracy of the zero–order approximations of both the ray method and Gaussian beams. The first–order spatial derivatives of amplitude enable us to estimate the accuracy of the paraxial approximation of individual Gaussian beams, whereas the second–order spatial derivatives of amplitude may be useful in estimating the accuracy of the asymptotic summation of paraxial Gaussian beams. The first–order perturbation derivatives of amplitude may be useful in perturbation expansions from elastic to viscoelastic media and in estimating the accuracy of the common–ray approximations of the amplitude in the coupling ray theory.

The travel time and its first–order spatial derivatives in a general smoothly heterogeneous medium can be calculated by solving numerically a set of nonlinear ordinary differential equations called the ray tracing equations. The amplitude and the second–order spatial derivatives of travel time can be calculated by solving numerically a set of linear ordinary differential equations called the 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 the rays, both in isotropic media

(*Babich et al., 1985*; *Červený, 2001*) and anisotropic media (*Klimeš, 1997, 1999, 2002a*). The first–order and higher–order perturbation derivatives of travel time and of its spatial derivatives can also be computed by analogous numerical quadratures along the rays, both in isotropic media and anisotropic media (*Klimeš, 2002a*).

We present the explicit equations for the first–order and higher–order spatial and perturbation derivatives of amplitude in Cartesian coordinates. The spatial and perturbation derivatives of the logarithm of amplitude are expressed in the form of integrals along the ray, with the proper initial values. The integrands are composed of the spatial and perturbation derivatives of travel time, of these derivatives of the logarithm of amplitude, as well as of the partial phase–space and perturbation derivatives of the Hamiltonian. The aggregate orders of the spatial and perturbation derivatives of amplitude in the integrands are equal to or lower than the aggregate order of the derivatives of amplitude being computed. Simultaneously, the orders of the perturbation derivatives of amplitude in the integrands are lower than the order of the perturbation derivatives of amplitude or its spatial derivative being computed. The aggregate orders of the spatial and perturbation derivatives of travel time in the integrands do not exceed the aggregate order of the derivatives of amplitude being computed by more than 2. Neither do the aggregate orders of the spatial and perturbation derivatives of the Hamiltonian in the integrands exceed the aggregate order of the derivatives of amplitude being computed by more than 2. The order of the perturbation derivatives of travel time and of the Hamiltonian is equal to or lower than the order of the perturbation derivatives of amplitude being computed.

Note that the equations for the polarization vectors depend considerably on the kind of high–frequency asymptotic ray theory. The equations for the spatial and perturbation derivatives of the anisotropic–ray–theory polarization vectors and of the isotropic–ray–theory P–wave polarization vector can be derived directly from the Christoffel equation (*Červený, 2001, eq. 2.2.20*) for the polarization vectors. The equations for the first–order spatial derivatives and first–order perturbation derivatives of the isotropic–ray–theory S–wave polarization vectors have been derived by *Coates and Chapman (1990)* and *Klimeš (2002b)*.

2. EQUATIONS FOR THE SPATIAL AND PERTURBATION DERIVATIVES OF AMPLITUDE

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, define the transport equation for amplitude, and derive its consequence, identity (16), which is of principal importance in deriving the equations for the spatial and perturbation derivatives of amplitude. In Section 2.3, we define the ray parameters and recall the basics of dynamic ray tracing. The dynamic ray tracing equations are necessary for calculating the amplitude, and for introducing the covariant derivatives of amplitude with respect to the ray parameters. In Section 2.4, we define the covariant derivatives of amplitude with respect to the ray parameters and utilize identity (16) in deriving the equations for calculating both the covariant derivatives with respect to the ray parameters and perturbation derivatives of amplitude. Section 2.4 constitutes the final result of the paper.

2.1. Basic definitions and notation

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 parameters f_κ,

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

Parameters f_α are called *perturbation parameters* (*Baumgärtel, 1985*; *Murdock, 1999*; *Klimeš and Bulant, 2004, 2006*) or model parameters (*Tarantola, 1987*; *Klimeš, 2002*). Perturbation parameters f_κ may parametrize the spatial distribution of the material properties of the medium (e.g., of the individual density–normalized elastic moduli in the case of an elastic wavefield), but some of them may also parametrize a continuous set of Hamiltonians in the given medium instead of parametrizing the medium. 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 $(f_\mu, f_\nu) = (\frac{1}{2}, \frac{1}{2})$.

The rays traced using Hamiltonian (1) depend on perturbation parameters f_κ. Travel time τ, amplitude A and other quantities calculated along the rays are then functions of spatial coordinates x_i and of perturbation parameters f_κ,

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

We shall refer to the partial derivatives with respect to perturbation parameters f_κ as the *perturbation derivatives.* Note that *Klimeš (2002a)* refers to the perturbation derivatives briefly 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 perturbation derivatives by lower–case *Greek subscripts* following a comma. In 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,

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

denotes the perturbation derivatives of the partial *phase–space derivatives* of the Hamiltonian. The perturbation derivatives are taken at fixed phase–space coordinates x_i, p_j, and the partial phase–space derivatives are calculated at fixed perturbation parameters f_κ. Similarly,

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

denotes the perturbation derivatives of the *spatial derivatives* of travel time τ. The perturbation derivatives are taken at fixed spatial coordinates x_i, and the partial spatial derivatives are calculated at fixed perturbation parameters f_κ.

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

$$\tau_{\substack{,rij \\ ,rik \\ ,rjk}} \; \tau_{\substack{,rk\alpha \\ ,rj\alpha \\ ,ri\alpha}} \tag{5}$$

stands for

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

2.2. Transport equation

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 perturbation 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 the rays is determined by the form of the Hamiltonian. The solution of the Hamilton–Jacobi equation (7), travel time τ, is then calculated by the quadrature of equation

$$\frac{\mathrm{d}}{\mathrm{d}\gamma_3} \tau = p_i \, \frac{\partial}{\partial p_i} H(x_q, p_r, f_\kappa) \tag{9}$$

along a ray.

We define the *transport equation* for amplitude $A = A(x_m, f_\kappa)$ as

$$\frac{\partial}{\partial x_i}(A^2 \varrho V_i) = 0 \quad , \tag{10}$$

where the *ray velocity vector* V_i is defined as the derivative of coordinates x_i with respect to travel time τ along a ray,

$$V_i = \frac{\mathrm{d}x_i}{\mathrm{d}\tau} = \frac{\mathrm{d}x_i}{\mathrm{d}\gamma_3}\left(\frac{\mathrm{d}\tau}{\mathrm{d}\gamma_3}\right)^{-1} \quad . \tag{11}$$

In our abstract formulation, function $\varrho = \varrho(x_m, f_\kappa)$ is a function, parametrizing the transport equation. If A is the amplitude of displacement of an elastic wavefield, ϱ is the density. We shall thus refer to function $\varrho = \varrho(x_m, f_\kappa)$ as the *density*.

Transport equation (10) is formally attached to an orthonomic system of rays corresponding to stationary Hamilton–Jacobi equation (7). For a particular choice of the Hamiltonian, transport equation (10) may have a relevant physical meaning. For example, if the Hamilton–Jacobi equation defines the anisotropic–ray–theory travel time corresponding to a selected eigenvalue of the Christoffel matrix, transport equation (10) describes the amplitude A of the zero–order anisotropic–ray–theory solution of the elastodynamic equation (*Červený, 2001, eq. 2.4.47*).

We express amplitude $A = A(x_i, f_\kappa)$ in terms of *amplitude exponent* $\beta = \beta(x_i, f_\kappa)$,

$$A = \sqrt{\frac{1}{\varrho}\frac{\mathrm{d}\tau}{\mathrm{d}\gamma_3}}\ \exp(\beta) \quad . \tag{12}$$

Transport equation (10) with (11) and (12) reads

$$\frac{\partial}{\partial x_i}\left[\exp(2\beta)\frac{\mathrm{d}x_i}{\mathrm{d}\gamma_3}\right] = 0 \quad , \tag{13}$$

and after differentiating the product,

$$\frac{\partial\beta}{\partial x_i}\frac{\mathrm{d}x_i}{\mathrm{d}\gamma_3} + \frac{1}{2}\frac{\partial}{\partial x_i}\frac{\mathrm{d}x_i}{\mathrm{d}\gamma_3} = 0 \quad . \tag{14}$$

Inserting $\mathrm{d}x_i/\mathrm{d}\gamma_3$ from ray tracing equations (8), we may express transport equation (14) in terms of the Hamiltonian,

$$\left[\beta_{,i} + \frac{1}{2}\left(\frac{\partial}{\partial x_i} + \tau_{,ik}\frac{\partial}{\partial p_k}\right)\right]\frac{\partial}{\partial p_i}H = 0 \quad . \tag{15}$$

The spatial and perturbation derivatives of transport equation (15) yield

$$\begin{aligned}&\left(\frac{\partial}{\partial f_\alpha} + \tau_{,s\alpha}\frac{\partial}{\partial p_s}\right)\cdots\left(\frac{\partial}{\partial f_\nu} + \tau_{,z\nu}\frac{\partial}{\partial p_z}\right)\\ \times&\left(\frac{\partial}{\partial x_i} + \tau_{,ia}\frac{\partial}{\partial p_a}\right)\cdots\left(\frac{\partial}{\partial x_n} + \tau_{,nf}\frac{\partial}{\partial p_f}\right)\left[\beta_{,r} + \frac{1}{2}\left(\frac{\partial}{\partial x_r} + \tau_{,rk}\frac{\partial}{\partial p_k}\right)\right]\frac{\partial}{\partial p_r}H = 0 \ .\end{aligned} \tag{16}$$

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

$$Q_{ia} = \frac{\partial x_i}{\partial \gamma_a} \quad , \qquad P_{ia} = \frac{\partial \tau_{,i}}{\partial \gamma_a} \quad , \tag{17}$$

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 of 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 the rays, which is in turn determined by the form of the Hamiltonian. The use of matrices Q_{ia} and P_{ia}, defined for a particular kind of γ_3, in the equations for the spatial and perturbation derivatives of amplitude, 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

$$P_{ia} = \tau_{,ij}\; Q_{ja} \tag{18}$$

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

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}\gamma_3} Q_{ia} &= \quad H_{,j}^{,i}\, Q_{ja} + H^{,ij} P_{ja} \quad , \\ \frac{\mathrm{d}}{\mathrm{d}\gamma_3} P_{ia} &= -H_{,ij}\, Q_{ja} - H_{,i}^{,j}\, P_{ja} \; . \end{aligned} \tag{19}$$

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 (18), the first equation of the dynamic ray tracing system (19) becomes

$$\frac{\mathrm{d}}{\mathrm{d}\gamma_3} Q_{ia} = Q_{ja} \left(\frac{\partial}{\partial x_j} + \tau_{,jk} \frac{\partial}{\partial p_k} \right) \frac{\partial}{\partial p_i} H \quad . \tag{20}$$

Let us emphasize once again that the matrices Q_{ia} and P_{ia} in this paper are defined by equation (17), and correspond to the orthonomic system of rays under consideration.

2.4. Equations for the spatial and perturbation derivatives of the amplitude exponent

The spatial and perturbation derivatives of amplitude (12) can be composed of these derivatives of amplitude exponent $\beta = \beta(x_m, f_\kappa)$, density $\varrho = \varrho(x_m, f_\kappa)$ and function

$$\frac{\mathrm{d}\tau}{\mathrm{d}\gamma_3} = H^{,r}(x_m, \tau_{,n}(x_k, f_\mu), f_\kappa)\ \tau_{,r}(x_n, f_\nu) \quad . \tag{21}$$

The spatial and perturbation derivatives of function $\mathrm{d}\tau/\mathrm{d}\gamma_3$ are composed of these derivatives of functions $H^{,i}(x_m, \tau_{,n}(x_k, f_\mu), f_\kappa)$ and $\tau_{,i}(x_n, f_\kappa)$. The spatial and perturbation derivatives of travel time $\tau(x_n, f_\kappa)$ can be calculated using the equations derived by *Klimeš (2002a)*. It is thus sufficient to derive the equations for calculating the spatial and perturbation derivatives of amplitude exponent $\beta = \beta(x_m, f_\kappa)$.

We introduce the *covariant derivatives*

$$B_{ab\ldots f\alpha\ldots\nu} = \beta_{,ij\ldots n\alpha\ldots\nu}\, Q_{ia} Q_{jb} \cdots Q_{nf} \tag{22}$$

of the amplitude exponent with respect to ray parameters γ_a. Let us differentiate covariant derivatives (22) along a ray with respect to γ_3, and insert equations (8) and (20) for $\frac{\mathrm{d}}{\mathrm{d}\gamma_3} x_i$ and $\frac{\mathrm{d}}{\mathrm{d}\gamma_3} Q_{ia}$, respectively,

$$\frac{\mathrm{d}}{\mathrm{d}\gamma_3}[\beta_{,ijk\ldots mn\alpha\ldots\nu} Q_{ia} Q_{jb} Q_{kc} \cdots Q_{me} Q_{nf}] = C_{ijk\ldots mn\alpha\ldots\nu} Q_{ia} Q_{jb} Q_{kc} \cdots Q_{me} Q_{nf} \ , \tag{23}$$

where

$$\begin{aligned} C_{ijk\ldots mn\alpha\ldots\nu} = \beta_{,rijk\ldots mn\alpha\ldots\nu} \frac{\partial}{\partial p_r} H + \beta_{,rjk\ldots mn\alpha\ldots\nu} & \left(\frac{\partial}{\partial x_i} + \tau_{,is} \frac{\partial}{\partial p_s} \right) \frac{\partial}{\partial p_r} H \\ + \beta_{,irk\ldots mn\alpha\ldots\nu} & \left(\frac{\partial}{\partial x_j} + \tau_{,js} \frac{\partial}{\partial p_s} \right) \frac{\partial}{\partial p_r} H \\ & \vdots \\ + \beta_{,ijk\ldots mr\alpha\ldots\nu} & \left(\frac{\partial}{\partial x_n} + \tau_{,ns} \frac{\partial}{\partial p_s} \right) \frac{\partial}{\partial p_r} H \quad . \end{aligned} \tag{24}$$

The covariant derivatives with respect to the ray parameters and perturbation derivatives of the amplitude exponent may thus be expressed in the form of the integral along the ray,

$$\boxed{B_{ab\ldots f\alpha\ldots\nu}(\gamma_3) = B_{ab\ldots f\alpha\ldots\nu}(\gamma_3^0) + \int_{\gamma_3^0}^{\gamma_3} \mathrm{d}\gamma_3\ C_{ij\ldots n\alpha\ldots\nu}\ Q_{ia} Q_{jb} \cdots Q_{nf} \quad ,} \tag{25}$$

with initial conditions $B_{ab\ldots f\alpha\ldots\nu}(\gamma_3^0)$ defined by equation (22). The initial conditions for the amplitude exponent and for its covariant derivatives (22) are generally finite for the finite initial value $Q_{ia}(\gamma_3^0)$ of the matrix of geometrical spreading. At a point or linear source, at which matrix $Q_{ia}(\gamma_3^0)$ is singular, initial values $\beta_{ab\ldots f\alpha\ldots\nu}(\gamma_3^0)$ and even $B_{ab\ldots f\alpha\ldots\nu}(\gamma_3^0)$ may be infinite. Point or linear sources thus require a separate treatment. Calculation of integral (25) through caustic points may also require separate treatment.

The spatial derivatives in coordinates x_i and perturbation derivatives of the amplitude exponent may then be expressed in terms of covariant derivatives (25),

$$\boxed{\beta_{,ij\ldots n\alpha\ldots\nu} = B_{ab\ldots f\alpha\ldots\nu}\, Q^{-1}_{ai} Q^{-1}_{bj} \cdots Q^{-1}_{fn} \quad ,} \tag{26}$$

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 terms on the right–hand side of equation (24) coincide with the corresponding terms on the left–hand side of equation (16). All of the terms on the right–hand side of (24) are thus cancelled if (16) is subtracted from (24),

$$\begin{aligned}
C_{ijk\ldots mn\alpha\ldots\nu} = \beta_{,rijk\ldots mn\alpha\ldots\nu}\,\frac{\partial}{\partial p_r}H &+ \beta_{,rjk\ldots mn\alpha\ldots\nu}\left(\frac{\partial}{\partial x_i}+\tau_{,is}\frac{\partial}{\partial p_s}\right)\frac{\partial}{\partial p_r}H \\
&+ \beta_{,irk\ldots mn\alpha\ldots\nu}\left(\frac{\partial}{\partial x_j}+\tau_{,js}\frac{\partial}{\partial p_s}\right)\frac{\partial}{\partial p_r}H \\
&\;\;\vdots \\
&+ \beta_{,ijk\ldots mr\alpha\ldots\nu}\left(\frac{\partial}{\partial x_n}+\tau_{,ns}\frac{\partial}{\partial p_s}\right)\frac{\partial}{\partial p_r}H \\
-\left(\frac{\partial}{\partial f_\alpha}+\tau_{,u\alpha}\frac{\partial}{\partial p_u}\right)\cdots\left(\frac{\partial}{\partial f_\nu}+\tau_{,z\nu}\frac{\partial}{\partial p_z}\right)& \\
\times\left(\frac{\partial}{\partial x_i}+\tau_{,ia}\frac{\partial}{\partial p_a}\right)\cdots\left(\frac{\partial}{\partial x_n}+\tau_{,nf}\frac{\partial}{\partial p_f}\right)&\left[\beta_{,r}+\frac{1}{2}\left(\frac{\partial}{\partial x_r}+\tau_{,rs}\frac{\partial}{\partial p_s}\right)\right]\frac{\partial}{\partial p_r}H \ ,
\end{aligned} \tag{27}$$

for all integration kernels (27), including C corresponding to amplitude exponent β.

If we calculate the spatial and perturbation derivatives in the order $\beta_{,i}$, $\beta_{,\alpha}$, $\beta_{,ij}$, $\beta_{,i\alpha}$, $\beta_{,\alpha\beta}$, $\beta_{,ijk}$, $\beta_{,ij\alpha}$, $\beta_{,i\alpha\beta}$, $\beta_{,\alpha\beta\gamma}$, $\beta_{,ijkl}$, $\beta_{,ijk\alpha}$, $\beta_{,ij\alpha\beta}$, $\beta_{,i\alpha\beta\gamma}$, $\beta_{,\alpha\beta\gamma\delta}$, etc., the right–hand side of equation (27) contains only the previously calculated spatial and perturbation derivatives of the amplitude exponent. The special cases of equation (27) corresponding to the zero–order, first–order and second–order spatial and perturbation derivatives of the amplitude exponent are presented in Section 3 as examples.

Let us illustrate the order of calculating the spatial and perturbation derivatives of the amplitude exponent graphically:

$$\begin{array}{lllllll}
\beta_{,i} & \beta_{,\alpha} & & & & & \\
\beta_{,ij} & \beta_{,i\alpha} & \beta_{,\alpha\beta} & & & & \\
\beta_{,ijk} & \beta_{,ij\alpha} & \beta_{,i\alpha\beta} & \beta_{,\alpha\beta\gamma} & & & \\
\beta_{,ijkl} & \beta_{,ijk\alpha} & \beta_{,ij\alpha\beta} & \beta_{,i\alpha\beta\gamma} & \beta_{,\alpha\beta\gamma\delta} & & \\
\beta_{,ijklm} & \beta_{,ijkl\alpha} & \beta_{,ijk\alpha\beta} & \beta_{,ij\alpha\beta\gamma} & \beta_{,i\alpha\beta\gamma\delta} & \beta_{,i\alpha\beta\gamma\delta\varepsilon} & \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots
\end{array}$$

To calculate the spatial and perturbation derivatives of the amplitude exponent of a selected order, the spatial and perturbation derivatives of the amplitude exponent situated on the left and above the selected ones must be known, with the exception of $\beta_{,\alpha}$ which is not present in the equations for other perturbation derivatives of the amplitude exponent.

Note that covariant derivatives $B_{\ldots 3\ldots}$, containing at least one index 3 in place of the lower–case Roman subscripts corresponding to the covariant derivatives with respect to the ray parameters, can be expressed analytically. For instance, for $a=3$, equation (22) with (17) and (8) reads

$$B_{3b\ldots f\alpha\ldots\nu} = \beta_{,ij\ldots n\alpha\ldots\nu}\, H^{,i}\, Q_{jb}\cdots Q_{nf} \quad . \tag{28}$$

Equation (24) inserted into (28) then yields

$$\boxed{B_{3b\ldots f\alpha\ldots\nu} = \Big[C_{j\ldots n\alpha\ldots\nu} - \big(\underset{\substack{\vdots\\ ,n}}{H^{,s}_{,j}} + H^{,rs}\underset{\substack{\vdots\\ ,rn}}{\tau_{,rj}}\big)\,\underset{\substack{\vdots\\ ,j\ldots s\alpha\ldots\nu}}{\beta_{,s\ldots n\alpha\ldots\nu}}\Big]\, Q_{jb}\cdots Q_{nf} \quad .} \tag{29}$$

We thus need to calculate only $B_{A\ldots F\alpha\ldots\nu}$ with $A,\ldots,F=1,2$ (including $B_{A\ldots F}$ and $B_{\alpha\ldots\nu}$) by numerical quadrature (25). Initial conditions $B_{A\ldots F\alpha\ldots\nu}(\gamma_3^0)$ are defined by equation (22).

3. EXAMPLES OF THE INTEGRANDS AND INTEGRALS IN GENERAL MEDIA

The special cases of the general results of Section 2 corresponding to the zero–order, first–order and second–order spatial and perturbation derivatives of the amplitude exponent are presented in Sections 3.1, 3.2, and 3.3, respectively, in order to illustrate the somewhat abstract final equations (27) and (29).

3.1. Amplitude

For the amplitude exponent itself, integrand (27) of equation (25) takes the form of

$$C = \beta_{,r}\frac{\partial}{\partial p_r}H - \left[\beta_{,r} + \frac{1}{2}\left(\frac{\partial}{\partial x_r} + \tau_{,rs}\frac{\partial}{\partial p_s}\right)\right]\frac{\partial}{\partial p_r}H \quad , \tag{30}$$

which reduces to

$$C = -\tfrac{1}{2}\left(H^{,r}_{,r} + H^{,rs}\tau_{,rs}\right) \quad . \tag{31}$$

Inserting equation (20) into the right–hand side of expression

$$\frac{\mathrm{d}}{\mathrm{d}\gamma_3}\ln\left[\det(Q_{ia})\right] = Q^{-1}_{bj}\frac{\mathrm{d}}{\mathrm{d}\gamma_3}Q_{jb} \tag{32}$$

for the derivative of the logarithm of a determinant, and comparing the result with equation (31), we see that

$$C = -\frac{1}{2}\,\frac{\mathrm{d}}{\mathrm{d}\gamma_3}\ln\left[\det(Q_{ia})\right] \quad , \tag{33}$$

and

$$\beta(\gamma_3) = \beta(\gamma_3^0) + \tfrac{1}{2}\ln\big[\det(Q_{ia})\big](\gamma_3^0) - \tfrac{1}{2}\ln\big[\det(Q_{ia})\big](\gamma_3) \quad . \tag{34}$$

This is the generally known expression for the logarithm of amplitude (*Babich, 1961, eq. 3.7*). The amplitude is thus obtained by dynamic ray tracing (19), without any additional numerical quadrature.

3.2. First–order spatial and perturbation derivatives of amplitude

For the first–order spatial derivatives of the amplitude exponent, integrand (27) of equation (25) takes the form of

$$\begin{aligned} C_i =& \beta_{,ri}\frac{\partial}{\partial p_r}H + \beta_{,r}\left(\frac{\partial}{\partial x_i} + \tau_{,is}\frac{\partial}{\partial p_s}\right)\frac{\partial}{\partial p_r}H \\ & - \left(\frac{\partial}{\partial x_i} + \tau_{,ia}\frac{\partial}{\partial p_a}\right)\left[\beta_{,r} + \frac{1}{2}\left(\frac{\partial}{\partial x_r} + \tau_{,rs}\frac{\partial}{\partial p_s}\right)\right]\frac{\partial}{\partial p_r}H \quad , \end{aligned} \tag{35}$$

which reduces to integrand

$$C_i = -\tfrac{1}{2}\big[H_{,ri}^{,r} + H_{,i}^{,rs}\tau_{,rs} + H_{,r}^{,rs}\tau_{,si} + H^{,rst}\tau_{,rs}\tau_{,ti} + H^{,rs}\tau_{,rsi}\big] \quad . \tag{36}$$

The value of the integral (25) of $C_i Q_{i3}$ is given by equations (29) and (31),

$$B_3 = -\tfrac{1}{2}(H_{,r}^{,r} + H^{,rs}\tau_{,rs}) \quad . \tag{37}$$

For the first–order perturbation derivatives of the amplitude exponent, integrand (27) of equation (25) takes the form of

$$C_\alpha = \beta_{,r\alpha}\frac{\partial}{\partial p_r}H - \left(\frac{\partial}{\partial f_\alpha} + \tau_{,a\alpha}\frac{\partial}{\partial p_a}\right)\left[\beta_{,r} + \frac{1}{2}\left(\frac{\partial}{\partial x_r} + \tau_{,rs}\frac{\partial}{\partial p_s}\right)\right]\frac{\partial}{\partial p_r}H \quad , \tag{38}$$

which reduces to

$$C_\alpha = -\beta_{,r}\big[H_{,\alpha}^{,r} + H^{,rs}\tau_{,s\alpha}\big] - \tfrac{1}{2}\big[H_{,r\alpha}^{,r} + H_{,\alpha}^{,rs}\tau_{,rs} + H_{,r}^{,rs}\tau_{,s\alpha} + H^{,rst}\tau_{,rs}\tau_{,t\alpha} + H^{,rs}\tau_{,rs\alpha}\big] \; . \tag{39}$$

3.3. Second–order spatial and perturbation derivatives of amplitude

For the second-order spatial derivatives of the amplitude exponent, equation (27) reads

$$\begin{aligned} C_{ij} =& \beta_{,rij}\frac{\partial}{\partial p_r}H + \beta_{,rj}\left(\frac{\partial}{\partial x_i} + \tau_{,is}\frac{\partial}{\partial p_s}\right)\frac{\partial}{\partial p_r}H + \beta_{,ir}\left(\frac{\partial}{\partial x_j} + \tau_{,js}\frac{\partial}{\partial p_s}\right)\frac{\partial}{\partial p_r}H \\ & - \left(\frac{\partial}{\partial x_i} + \tau_{,ia}\frac{\partial}{\partial p_a}\right)\left(\frac{\partial}{\partial x_j} + \tau_{,jb}\frac{\partial}{\partial p_b}\right)\left[\beta_{,r} + \frac{1}{2}\left(\frac{\partial}{\partial x_r} + \tau_{,rs}\frac{\partial}{\partial p_s}\right)\right]\frac{\partial}{\partial p_r}H \quad , \end{aligned} \tag{40}$$

which reduces to integrand

$$
\begin{aligned}
C_{ij} = & -\beta_{,r}\left[H^{,r}_{,ij}+H^{,rs}_{\substack{,i\\,j}}\tau_{\substack{,sj\\,si}}+H^{,rst}\tau_{,si}\tau_{,tj}+H^{,rs}\tau_{,sij}\right] \\
& -\tfrac{1}{2}\left[H^{,r}_{,rij}+H^{,rs}_{,ij}\tau_{,rs}+H^{,rs}_{\substack{,ri\\,rj}}\tau_{\substack{,sj\\,si}}+H^{,rst}_{\substack{,i\\,j}}\tau_{,rs}\tau_{\substack{,tj\\,ti}}+H^{,rst}_{,r}\tau_{,si}\tau_{,tj}+H^{,rstu}\tau_{,rs}\tau_{,ti}\tau_{,uj}\right. \\
& \left.+H^{,rs}_{\substack{,i\\,j}}\tau_{\substack{,rsj\\,rsi}}+H^{,rs}_{,r}\tau_{,sij}+H^{,rst}\tau_{,rs}\tau_{,tij}+H^{,rs}\tau_{,rsij}\right] \quad .
\end{aligned} \tag{41}
$$

The value of the integral (25) of $C_{ij}Q_{i3}Q_{jb}$ is determined by equation (29),

$$
B_{3b} = \left[C_j - \beta_{,r}(H^{,r}_{,j}+H^{,rs}\tau_{,sj})\right]Q_{jb} \quad , \tag{42}
$$

where C_j is given by equation (36). For the first–order perturbation derivatives of the first–order spatial derivatives of the amplitude exponent, equation (27) reads

$$
\begin{aligned}
C_{i\alpha} = & \beta_{,ri\alpha}\frac{\partial}{\partial p_r}H + \beta_{,r\alpha}\left(\frac{\partial}{\partial x_i}+\tau_{,is}\frac{\partial}{\partial p_s}\right)\frac{\partial}{\partial p_r}H \\
& -\left(\frac{\partial}{\partial f_\alpha}+\tau_{,a\alpha}\frac{\partial}{\partial p_a}\right)\left(\frac{\partial}{\partial x_i}+\tau_{,ib}\frac{\partial}{\partial p_b}\right)\left[\beta_{,r}+\frac{1}{2}\left(\frac{\partial}{\partial x_r}+\tau_{,rs}\frac{\partial}{\partial p_s}\right)\right]\frac{\partial}{\partial p_r}H \ ,
\end{aligned} \tag{43}
$$

which reduces to

$$
\begin{aligned}
C_{i\alpha} = & -\beta_{,ri}\left[H^{,r}_{,\alpha}+H^{,rs}\tau_{,s\alpha}\right] - \beta_{,r}\left[H^{,r}_{,i\alpha}+H^{,rs}_{\substack{,i\\,\alpha}}\tau_{\substack{,s\alpha\\,si}}+H^{,rst}\tau_{,si}\tau_{,t\alpha}+H^{,rs}\tau_{,si\alpha}\right] \\
& -\tfrac{1}{2}\left[H^{,r}_{,ri\alpha}+H^{,rs}_{,i\alpha}\tau_{,rs}+H^{,rs}_{\substack{,ri\\,r\alpha}}\tau_{\substack{,s\alpha\\,si}}+H^{,rst}_{\substack{,i\\,\alpha}}\tau_{,rs}\tau_{\substack{,t\alpha\\,ti}}+H^{,rst}_{,r}\tau_{,si}\tau_{,t\alpha}+H^{,rstu}\tau_{,rs}\tau_{,ti}\tau_{,u\alpha}\right. \\
& \left.+H^{,rs}_{\substack{,i\\,\alpha}}\tau_{\substack{,rs\alpha\\,rsi}}+H^{,rs}_{,r}\tau_{,si\alpha}+H^{,rst}\tau_{,rs}\tau_{,ti\alpha}+H^{,rs}\tau_{,rsi\alpha}\right] \quad .
\end{aligned} \tag{44}
$$

The value of the integral (25) of $C_{i\alpha}Q_{i3}$ is determined by equation (29),

$$
B_{3\alpha} = C_\alpha \quad , \tag{45}
$$

where C_α is given by equation (39). For the second–order perturbation derivatives of the amplitude exponent, equation (27) becomes

$$
\begin{aligned}
C_{\alpha\beta} = & \beta_{,r\alpha\beta}\frac{\partial}{\partial p_r}H \\
& -\left(\frac{\partial}{\partial f_\alpha}+\tau_{,a\alpha}\frac{\partial}{\partial p_a}\right)\left(\frac{\partial}{\partial f_\beta}+\tau_{,b\beta}\frac{\partial}{\partial p_b}\right)\left[\beta_{,r}+\frac{1}{2}\left(\frac{\partial}{\partial x_r}+\tau_{,rs}\frac{\partial}{\partial p_s}\right)\right]\frac{\partial}{\partial p_r}H \quad ,
\end{aligned} \tag{46}
$$

which can be expressed as

$$
\begin{aligned}
C_{\alpha\beta} = & -\beta_{\substack{,r\alpha\\,r\beta}}\left[H^{,r}_{\substack{,\beta\\,\alpha}}+H^{,rs}\tau_{\substack{,s\beta\\,s\alpha}}\right] - \beta_{,r}\left[H^{,r}_{,\alpha\beta}+H^{,rs}_{\substack{,\alpha\\,\beta}}\tau_{\substack{,s\beta\\,s\alpha}}+H^{,rst}\tau_{,s\alpha}\tau_{,t\beta}+H^{,rs}\tau_{,s\alpha\beta}\right] \\
& -\tfrac{1}{2}\left[H^{,r}_{,r\alpha\beta}+H^{,rs}_{,\alpha\beta}\tau_{,rs}+H^{,rs}_{\substack{,r\alpha\\,r\beta}}\tau_{\substack{,s\beta\\,s\alpha}}+H^{,rst}_{\substack{,\alpha\\,\beta}}\tau_{,rs}\tau_{\substack{,t\beta\\,t\alpha}}+H^{,rst}_{,r}\tau_{,s\alpha}\tau_{,t\beta}+H^{,rstu}\tau_{,rs}\tau_{,t\alpha}\tau_{,u\beta}\right. \\
& \left.+H^{,rs}_{\substack{,\alpha\\,\beta}}\tau_{\substack{,rs\beta\\,rs\alpha}}+H^{,rs}_{,r}\tau_{,s\alpha\beta}+H^{,rst}\tau_{,rs}\tau_{,t\alpha\beta}+H^{,rs}\tau_{,rs\alpha\beta}\right] \quad .
\end{aligned} \tag{47}
$$

4. CONCLUSIONS

The spatial and perturbation derivatives of amplitude can be composed of the spatial and perturbation derivatives of the Hamiltonian, density, travel time and amplitude exponent defined by equation (12). The spatial and perturbation derivatives of the amplitude exponent in isotropic or anisotropic media can be calculated using equation (26), in which the covariant derivatives with respect to ray parameters and perturbation derivatives of the amplitude exponent are given partly explicitly by equation (29) and partly by numerical quadratures (25). The general form of the integration kernels of quadratures (25) is given by equation (27). The special cases of integration kernels (27), corresponding to the individual spatial and perturbation derivatives of the amplitude exponent up to the second order in generally anisotropic media, are shown in Section 3.

The derived equations are applicable only along ray segments touching no caustics. Numerical quadratures (25), required for calculating the spatial and perturbation derivatives of the amplitude exponent, cannot be performed through caustic points. Simultaneously, equation (22) cannot be used to define the initial conditions at point or line sources. These singularities thus require separate treatment, postponed for future investigation.

For additional information, including various papers, computer codes and data, refer to the consortium research project "Seismic Waves in Complex 3–D Structures" ("http://sw3d.mff.cuni.cz").

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