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THE RAY SERIES METHOD AND DYNAMIC RAY TRACING SYSTEM FOR THREE-DIMENSIONAL INHOMOGENEOUS MEDIA

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ABSTRACT

The ray series method is used to study propagation of seismic waves in the three-dimensional media consisting of generally inhomogeneous layers separated by curved interfaces. The investigation is carried out with the help of the so-called ray centered coordinate system which was proposed by Popov and Pšenčík (1978a). It is shown that in this system the principal components of the amplitude coefficients in the ray series for *S* waves do not rotate about the ray with respect to the basis vectors when the wave progresses, even though they rotate with respect to the unit vectors $\hat{n}$ and $\hat{b}$ along the direction of the normal and binormal to the ray, respectively. This considerably simplifies the final expressions for the amplitude coefficients for *S* waves, whose two principal components are decoupled in the ray-centered coordinate system. The ray-centered coordinate system is also applied to the eikonal equation in order to produce a dynamic ray tracing system consisting of three nonlinear ordinary differential equations of the first order determining the second derivatives of the time field and, in this manner, even the basic geometrical properties of the wave fronts (e.g., principal curvatures and geometrical spreading) along the ray. Several different modifications of the dynamic ray tracing system are presented. It is demonstrated that in the case of generally inhomogeneous two-dimensional media the dynamic ray tracing system reduces, under certain not too restrictive conditions, to the single first order differential equation of the Riccati type. Finally, the phase matching method is used to determine discontinuities of individual quantities in the dynamic ray tracing system when the wave is impinging on a curved interface separating two generally inhomogeneous media. Since all basic equations are presented in a computationally convenient matrix formulation, they can be readily employed for any numerical evaluation of dynamic properties of seismic waves propagating through structurally complicated media. As the paper describes all basic features of asymptotic ray theory (the name under which the ray series method is known on this continent), it can serve as a starting point for anyone wishing to develop computer programs for the computation of synthetic seismograms.

1. INTRODUCTION

The ray series method (also known as asymptotic ray theory in English literature) has recently enjoyed an increasing popularity among seismologists who have applied it successfully to various problems in crustal seismology and oil exploration (e.g., Belonosova *et al.*, 1967; Hron *et al.*, 1977; Červený *et al.*, 1977; May and Hron, 1978). The main advantage of the method rests in the fact that it can be used in studies dealing with the propagation of seismic body waves through complicated geological structures, such as laterally inhomogeneous layers with curved interfaces.

The ray series method was pioneered in seismology independently by Babich and Alekseyev (1958) and Karal and Keller (1959). A fairly detailed description of the method is also given by Hron (1968), Červený and Ravindra (1971), Hron and Kanasewich (1971), Červený *et al.* (1977), where comprehensive lists of literature

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can be found. Unfortunately, most of the authors could present only a rather concise review of the ray series method when applied to complicated structures because of the complexity of the basic elastodynamic equation for generally inhomogeneous elastic media. Sometimes this results in decreased clarity of the exposition of the theory especially if it is applied to the most general types of elastic media, where the results of vector analysis become slightly cumbersome.

It has been a commonly accepted practice that the amplitude coefficients of ray series applied to the basic elastodynamic equation are resolved at any point of the ray into three components corresponding to the unit vectors $\hat{t}$, $\hat{n}$, and $\hat{b}$ specifying positive orientation of the tangent, normal and binormal to the ray, respectively. Unfortunately, several difficulties of a purely numerical nature can be encountered here, at the very beginning of the application of the ray series method. First, determination of vectors $\hat{n}$ and $\hat{b}$ for the ray in three dimensions also implies computation of the curvature K and torsion T of the ray, which itself is not always an easy task. Furthermore, the formal expressions for the principal components of amplitude coefficients of S waves are rather complicated for $T \neq 0$, since these components rotate about the ray relative to the vectors $\hat{n}$ and $\hat{b}$ as the wave progresses. This, in turn, leads to the coupling between the components of displacement vector of S waves into both directions even in the zeroth order approximation of the ray series, which is the most frequently used.

In this paper an attempt is made to overcome all the above mentioned difficulties by replacing vectors $\hat{n}$ and $\hat{b}$ with another pair of unit vectors $\hat{e}_1$ and $\hat{e}_2$ [see equation (1)] also perpendicular to the ray but such that the displacement vector of S waves remains stationary with respect to them at all times. This not only results in the decoupling of the components of the S displacement vector in the directions of $\hat{e}_1$ and $\hat{e}_2$ but also considerably simplifies the whole theoretical development of all basic formulas so that a high degree of clarity can be maintained. The main advantage of the introduction of $\hat{e}_1$ and $\hat{e}_2$, however, rests with the fact that both vectors can be evaluated rather easily at any point of the ray following the method presented in the Appendix. Thus a new system of curvilinear coordinates with its basis formed by the triplet of mutually orthogonal vectors $\hat{t}$, $\hat{e}_1$, and $\hat{e}_2$ can be used for the ray tracing procedure and all related problems (Červený *et al.*, 1977; Popov and Pšenčík, 1978a, b) with great success. In this paper this system is called a ray-centered coordinate system and the related coordinates are denoted by $[s, q_1, q_2]$.

If $\vec{r} = \vec{r}(s)$ is a position vector of the ray taken as a function of the length s of the ray path from a fixed reference point at s_0, the set of vectors $\hat{t}$, $\hat{e}_1$, and $\hat{e}_2$ which forms the basis of the ray-centered coordinate system can be formally introduced with the help of normal vector $\hat{n}$, binormal vector $\hat{b}$, and torsion T of the ray as

$$\hat{e}_1 = \hat{n}\cos\theta - \hat{b}\sin\theta, \qquad \hat{e}_2 = \hat{n}\sin\theta + \hat{b}\cos\theta, \qquad \hat{t} = \frac{d\vec{r}}{ds} \tag{1}$$

with

$$\theta(s) = \int_{s_0}^{s} T(\xi)\, d\xi + \theta(s_0), \tag{2}$$

where the integral is taken along the ray. The value of $\theta(s_0)$ in (2) can be chosen arbitrarily, but once it is specified, the values of $\theta(s)$, $\hat{e}_1(s)$, and $\hat{e}_2(s)$ are determined uniquely by (1) and (2) for the remainder of the ray.

Direct application of the Frenet formulas $d\hat{n}/ds = T\hat{b} - K\hat{t}$ and $d\hat{b}/ds = -T\hat{n}$ reveals important properties of $\hat{e}_1$ and $\hat{e}_2$, namely

$$\frac{d\hat{e}_1}{ds} = -K\cos\theta\hat{t}, \qquad \frac{d\hat{e}_2}{ds} = -K\sin\theta\hat{t}. \tag{3}$$

They will be used later in the development of the set of three ordinary nonlinear differential equations (62) governing the variation of geometrical spreading of the ray tube along the ray.

Exploitation of sets of differential equations for the evaluation of geometrical spreading of the ray tube was first proposed by Belonosova *et al.* (1967) and various forms of these sets can be found in Červený *et al.* (1977). Although individual sets differ in the number of constituting differential equations and their complexity, all can be called *dynamic ray tracing systems* due to their role in the determination of ray amplitudes of seismic body waves.

A detailed study (see Červený *et al.*, 1977) would show that a certain trade-off exists between the complexity and the number of differential equations in the dynamic ray tracing systems: either eight ordinary linear differential equations of the first order in the system designed for the dynamic ray tracing in a generally inhomogeneous three-dimensional media (Popov and Pšenčík, 1978a, b) may be found or only three, but nonlinear, ordinary differential equations of the same order in an equivalent set (Červený and Pšenčík, 1979; Hubral, 1979). However, the minimum number of linear differential equations in the ray tracing system is still five (Červený, 1976).

The dynamic ray tracing systems which are presented in this paper [see, e.g., equation (76)] consist of three ordinary nonlinear equations of the first order. Although one of these systems corresponds to that of Hubral (1979) a fundamental difference exists in the way of its development: Hubral chose as a starting point in his derivations the set of eight differential equations presented by Popov and Pšenčík (1978a), whereas our dynamic ray tracing systems are obtained directly from the eikonal equation written in the ray-centered coordinates. This renders the derivation easy and straightforward. Since dynamic ray tracing systems may be used not only for the evaluation of geometrical spreading of the ray tube but also in various other problems, e.g. in certain inverse problems in seismic exploration, several equivalent forms of this dynamic ray tracing are presented in equation (76) so that the most suitable version of the system can be selected for a particular problem.

Obviously, application of the dynamic ray tracing system to wave propagation in layered media can be made only if the appropriate initial conditions at interfaces are imposed on the system. This is accomplished by the so-called phase matching method which requires that the phase functions of incident, reflected, and transmitted waves be equal on the curved interface at the vicinity of the point of incidence. Even though the phase matching method was already used in the past by several authors investigating the incidence of electromagnetic waves on curved interfaces separating homogeneous media (e.g., Deschamps, 1972; Lee, 1975; James, 1976), the present application of the theory is new in that sense that it is applied to the case of curved interfaces separating generally inhomogeneous media. Our results, which are obtained in a very straightforward manner, are in complete agreement with those obtained by other methods (Gel'chinskiy, 1961; Hubral, 1979).

Although it is hoped that this short account of some of the achievements brought about by the application of the ray-centered coordinate system is quite convincing,

it is felt that the field of possible applications of the system is far from being exhausted. Pšenčík (1979), for example, used the ray-centered coordinate system to develop a compact formula for the leading term of the ray series for multiply reflected seismic waves with an arbitrary number of conversions propagating in generally inhomogeneous media separated by curved interfaces. Also, the ray-centered coordinate system seems to be suitable for the studies of wave fields highly concentrated in the vicinity of ray.

2. The Basic System of Equations in the Ray Method

Let us consider a generally inhomogeneous, perfectly elastic medium, the properties of which are described by Lamé coefficients λ, μ, and volume density ρ, all of which are continuous functions of Cartesian coordinates x_i, $i = 1, 2, 3$, as are all their derivatives. If u_i denotes the components of the complex displacement vector $\vec{u}(x_i, t)$ and σ_{ij} are the components of stress tensor, the basic elastodynamic equation can be written

$$\rho u_{i,tt} = \sigma_{ij,j}, \qquad i = 1, 2, 3, \qquad j = 1, 2, 3, \quad (4)$$

if the Einstein summation rule is used together with commonly accepted notations for partial derivatives with respect to time

$$\left(u_{i,tt} = \frac{\partial^2 u_i}{\partial t^2}\right)$$

or coordinates

$$\left(\sigma_{ij,j} = \sum_{j=1}^{3} \frac{\partial \sigma_{ij}}{\partial x_j}\right).$$

In the following we shall use the same notation for partial derivatives of tensors of any order with respect to coordinates. Recalling that the Hooke's law for an isotropic medium can be written in the form $\sigma_{ij} = \lambda \delta_{ij} e_{kk} + 2\mu e_{ij}$, where $e_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i})$ are the components of the strain tensor and δ_{ij} is the Kronecker symbol, the basic elastodynamic equation (4) can be recast as

$$\rho u_{i,tt} = (\lambda + \mu) u_{j,ij} + \mu u_{i,jj} + \lambda_{,i} u_{j,j} + \mu_{,j} u_{i,j} + \mu_{,j} u_{j,i}. \quad (5)$$

The solution of this equation is sought in terms of functions which are nonanalytic along some moving surfaces called wave fronts. Generally, any wave front at time t can be implicitly described by the equation

$$t = \tau(x_i). \quad (6)$$

Then one can assume that the components of the displacement vector may be written in the form of a ray series

$$u_i(x_j, t) = \sum_{k=0}^{\infty} U_i^{(k)}(x_j) F_k[t - \tau(x_j)]. \quad (7)$$

Functions F_k are, in general, complex functions of real argument ξ satisfying relations

$$F_k' \equiv \frac{dF_k(\xi)}{d\xi} = F_{k-1}(\xi), \tag{8}$$

$$F_k(\xi) = f_k(\xi) + ig_k(\xi), \qquad g_k(\xi) = \pi^{-1} \int_{-\infty}^{+\infty} f_k(x)(x - \xi)^{-1}\, dx, \tag{9}$$

with real and imaginary parts f_k and g_k constituting Hilbert pairs of functions. Equation (8) asserts that the order of discontinuity of function F_{k+1} is less by one than that of F_k everywhere on the wave front. In this paper the vectorial complex function $\vec{U}^{(k)}(x_j)$ with scalar components $[U_1^{(k)}, U_2^{(k)}, U_3^{(k)}]$ is called a k-th amplitude coefficient (or the amplitude coefficient of the k-th order) in the ray series, whereas a scalar function $\tau(x_j)$ will be called a phase function or eikonal. A ray series similar to equation (7) can also be used for the studies of harmonic waves of a very high frequency ω. In that case, the displacement vector $\vec{u}$ is expanded in an asymptotic series in the inverse powers of frequency ω. This explains why the ray series expansion technique is generally known in English literature as asymptotic ray theory. Similarly, the above form of the ray series with F_k determined by (8) and (9) can also be used for high-frequency signals of short duration, as it is shown by Červený *et al.* (1977).

The desired solution of the basic elastodynamic equation (5) in the form of the ray series (7) is formally obtained by inserting (7) into (5). Realizing that

$$u_{i,j} = \sum_{k=0}^{\infty} (U_{i,j}^{(k)} F_k - U_i^{(k)} \tau_{,j} F_k'),$$

$$u_{i,jm} = \sum_{k=0}^{\infty} (U_{i,jm}^{(k)} F_k - U_{i,j}^{(k)} \tau_{,m} F_k' - U_{i,m}^{(k)} \tau_{,j} F_k' - U_i^{(k)} \tau_{,jm} F_k' + U_i^{(k)} \tau_{,j} \tau_{,m} F_k''),$$

$$u_{i,tt} = \sum_{k=0}^{\infty} U_i^{(k)} F_k'',$$

we get

$$\sum_{k=0}^{\infty} \{F_k'' N_i[\vec{U}^{(k)}] - F_k' M_i[\vec{U}^{(k)}] + F_k L_i[\vec{U}^{(k)}]\} = 0,$$

where three new vector operators $\vec{N}(\vec{U}^{(k)})$, $\vec{M}(\vec{U}^{(k)})$, and $\vec{L}(\vec{U}^{(k)})$ are defined in terms of their components as

$$N_i(\vec{U}^{(k)}) = -\rho U_i^{(k)} + (\lambda + \mu) U_j^{(k)} \tau_{,i} \tau_{,j} + \mu U_i^{(k)} \tau_{,j} \tau_{,j}, \tag{10}$$

$$M_i(\vec{U}^{(k)}) = (\lambda + \mu)[U_{j,i}^{(k)} \tau_{,j} + U_{j,j}^{(k)} \tau_{,i} + U_j^{(k)} \tau_{,ij}] + \mu[2U_{i,j}^{(k)} \tau_{,j} + U_i^{(k)} \tau_{,jj}] + \lambda_{,i} U_j^{(k)} \tau_{,j} + \mu_{,j} U_i^{(k)} \tau_{,j} + \mu_{,j} U_j^{(k)} \tau_{,i}, \tag{10'}$$

$$L_i(\vec{U}^{(k)}) = (\lambda + \mu) U_{j,ij}^{(k)} + \mu U_{i,jj}^{(k)} + \lambda_{,i} U_{j,j}^{(k)} + \mu_{,j} U_{i,j}^{(k)} + \mu_{,j} U_{j,i}^{(k)} \tag{10''}$$

with $F_k' = dF_k(\xi)/d\xi$ and $F_k'' = d^2F_k(\xi)/d\xi^2$. The above series may be further rewritten if the basic property of the functions F_k, namely $F_k' = F_{k-1}$ [equation (8)], is used. Then we can write equation (5) as

$$\sum_{k=0}^{\infty} \{F_{k-2}N_i[\vec{U}^{(k)}] - F_{k-1}M_i[\vec{U}^{(k)}] + F_kL_i[\vec{U}^{(k)}]\} = 0$$

or, after collecting the coefficients of F_k, in the equivalent form

$$F_{-2}\{N_i[\vec{U}^{(0)}]\} + F_{-1}\{N_i[\vec{U}^{(1)}] - M_i[\vec{U}^{(0)}]\} + \sum_{k=0}^{\infty} F_k\{N_i[\vec{U}^{(k+2)}] - M_i[\vec{U}^{(k+1)}] + L_i[\vec{U}^{(k)}]\} = 0.$$

Equation (5) will be satisfied identically if the terms inside of all three pairs of braces { } are equal to zero. This leads to a new system of equations

$$\left.\begin{aligned} N_i(\vec{U}^{(0)}) &= 0, \\ N_i(\vec{U}^{(1)}) - M_i(\vec{U}^{(0)}) &= 0, \\ N_i(\vec{U}^{(k)}) - M_i(\vec{U}^{(k-1)}) + L_i(\vec{U}^{(k-2)}) &= 0, \qquad k \geqq 2, \end{aligned}\right\} \tag{11}$$

which, due to its linearity, can be recast as

$$N_i[\vec{U}^{(k)}] - M_i[\vec{U}^{(k-1)}] + L_i[\vec{U}^{(k-2)}] = 0, \; k = 0, 1, 2, \ldots, \tag{12}$$

provided that $\vec{U}^{(-1)} = 0 = \vec{U}^{(-2)}$.

The recurrent system (12) represents the basic system of equations in the ray method that can be used for the determination of all amplitude coefficients $\vec{U}^{(k)}$, $k = 0, 1, 2, \ldots$ as well as phase function τ.

3. Existence Conditions for a Nontrivial Solution of the First Equation in the Basic System. Eikonal Equations

In this section, the first equation in system (11)

$$\vec{N}(\vec{U}^{(0)}) = 0 \tag{13}$$

shall be considered. Equation (13) represents a system of three linear equations for three unknown components of the amplitude coefficient $\vec{U}^{(0)}$, namely, $U_j^{(0)}$, $j = 1, 2, 3$, which can be written with the help of equation (10) as

$$U_j^{(0)}\{-\rho\delta_{ij} + (\lambda + \mu)\tau_{,i}\tau_{,j} + \mu\delta_{ij}\tau_{,k}\tau_{,k}\} = 0, \qquad i = 1, 2, 3. \tag{14}$$

The nontrivial solution of this system requires that the determinant of the system be equal to zero

$$\begin{vmatrix} -\rho + (\lambda+\mu)\tau_{,1}^2 + \mu\tau_{,k}\tau_{,k} & (\lambda+\mu)\tau_{,1}\tau_{,2} & (\lambda+\mu)\tau_{,1}\tau_{,3} \\ (\lambda+\mu)\tau_{,1}\tau_{,2} & -\rho + (\lambda+\mu)\tau_{,2}^2 + \mu\tau_{,k}\tau_{,k} & (\lambda+\mu)\tau_{,2}\tau_{,3} \\ (\lambda+\mu)\tau_{,1}\tau_{,3} & (\lambda+\mu)\tau_{,2}\tau_{,3} & -\rho + (\lambda+\mu)\tau_{,3}^2 + \mu\tau_{,k}\tau_{,k} \end{vmatrix} = 0. \quad (15)$$

After some simple rearrangements, this constraint can be conveniently recast as

$$-\rho^3 + (\tau_{,k}\tau_{,k})\rho^2[(\lambda+2\mu)+2\mu] - (\tau_{,k}\tau_{,k})^2\rho\mu[2(\lambda+2\mu)+\mu] + (\tau_{,k}\tau_{,k})^3\mu^2(\lambda+2\mu) = 0. \quad (16)$$

If we denote

$$\alpha = \sqrt{\frac{\lambda+2\mu}{\rho}}, \qquad \beta = \sqrt{\frac{\mu}{\rho}}, \quad (17)$$

equation (16) then reduces to

$$\left(\tau_{,k}\tau_{,k} - \frac{1}{\alpha^2}\right)\left(\tau_{,k}\tau_{,k} - \frac{1}{\beta^2}\right)^2 = 0. \quad (18)$$

Thus, the system (14) has a nontrivial solution if and only if one of the two following conditions is satisfied

$$\tau_{,k}\tau_{,k} = \frac{1}{\alpha^2} \quad (19)$$

$$\tau_{,k}\tau_{,k} = \frac{1}{\beta^2}. \quad (20)$$

These equations are generally known as the eikonal equations. In this paper the corresponding waves are called a compressional (P) or shear (S) wave, depending on whether it satisfies equation (19) or (20).

Methods of the solution of the eikonal equation are also well known, and can be found in many books dealing with partial differential equations. One of the most frequently used techniques is the method of characteristic curves that enables us to solve a partial differential equation by means of a system of ordinary differential equations, numerical solutions of which are well developed. The characteristic curves of the eikonal equation represent *rays* and the corresponding set of six ordinary differential equations ("ray tracing sytem") can be written as (see Červený *et al.*, 1977, for details)

$$\frac{dx_i}{d\tau} = v^2 p_i, \qquad \frac{dp_i}{d\tau} = -v^{-1}\frac{\partial v}{dx_i}, \qquad i = 1, 2, 3,$$

where $p_i = \partial\tau/\partial x_i$ are the components of the slowness vector and v is the phase velocity of the wave ($v = \alpha$ for P waves, $v = \beta$ for S waves).

4. Higher Order Equations in the Basic System. Transport Equations

In this section we are concerned mainly with the amplitude coefficient $\vec{U}^{(k)}$ in the ray series (7). Since we have shown in the previous section that in case of high frequency signals, P and S waves propagate independently in elastic media, the amplitude coefficient $\vec{U}^{(k)}$ pertaining to different kinds of elastic waves (P or S) can be studied separately. In both cases each amplitude coefficient $\vec{U}^{(k)}$ will be resolved into components using our ray centered coordinate system (1) in the same way, namely

$$\vec{U}^{(k)} = U_p^{(k)}\hat{t} + U_{s1}^{(k)}\hat{e}_1 + U_{s2}^{(k)}\hat{e}_2 = \vec{U}_{\parallel}^{(k)} + \vec{U}_{\perp}^{(k)}, \tag{21}$$

with two vector components

$$\vec{U}_{\parallel}^{(k)} = U_p^{(k)}\hat{t}, \qquad \vec{U}_{\perp}^{(k)} = U_{s1}^{(k)}\hat{e}_1 + U_{s2}^{(k)}\hat{e}_2, \tag{21'}$$

indicating the polarization of the displacement in the directions parallel and perpendicular to the ray, respectively.

In accordance with the widely accepted terminology, which takes into account polarization of elastic waves in a homogeneous perfectly elastic medium, we will call $\vec{U}_{\parallel}^{(k)}$ and $\vec{U}_{\perp}^{(k)}$ principal and additional components of the amplitude coefficient $\vec{U}^{(k)}$, respectively, if the wave propagates with the speed of P waves $\alpha = \sqrt{(\lambda + 2\mu)/\rho}$. In the other case, when the wave speed is equal to that of S waves $\beta = \sqrt{\mu/\rho}$, the principal and additional components will be represented by $\vec{U}_{\perp}^{(k)}$ and $\vec{U}_{\parallel}^{(k)}$, respectively.

The same terminology will be used even for the scalar components of amplitude coefficients $\vec{U}^{(k)}$: there will be one principal component, $U_p^{(k)}$, in the case of P waves and two, $U_{s1}^{(k)}$ and $U_{s2}^{(k)}$, in the case of S waves. The remaining scalar components in both cases will be called additional.

It should be noted that this way of resolving amplitude coefficients given by (21) differs from the traditional resolution

$$\vec{U}^{(k)} = U_p^{(k)}\hat{t} + U_n^{(k)}\hat{n} + U_b^{(k)}\hat{b}$$

with $\hat{n}$ and $\hat{b}$ being unit vectors of the principal normal and binormal, respectively. Advantage of our resolution of $\vec{U}^{(k)}$ using (21) rests in a higher degree of simplicity and symmetry of the final formulas.

4.1. Computation of amplitude coefficients for P waves

Let's consider additional components for P waves $U_{s1}^{(k)}$ and $U_{s2}^{(k)}$ first. Multiplication of equation (10) by vectors $\hat{e}_1$ and $\hat{e}_2$ yields two scalar products

$$N_i(\vec{U}^{(k)})e_{1i} = (-\rho + \mu\alpha^{-2})U_{s1}^{(k)}, \qquad N_i(\vec{U}^{(k)})e_{2i} = (-\rho + \mu\alpha^{-2})U_{s2}^{(k)}.$$

Thus the scalar products of equation (12) with $\hat{e}_1$ and $\hat{e}_2$ lead to the final expressions for the additional components of P waves $U_{s1}^{(k)}$ and $U_{s2}^{(k)}$

$$\left.\begin{aligned} U_{s1}^{(k)} &= (-\rho + \mu\alpha^{-2})^{-1}[M_i(\vec{U}^{(k-1)}) - L_i(\vec{U}^{(k-2)})]e_{1i}, \\ U_{s2}^{(k)} &= (-\rho + \mu\alpha^{-2})^{-1}[M_i(\vec{U}^{(k-1)}) - L_i(\vec{U}^{(k-2)})]e_{2i}, \end{aligned}\right\} \tag{22}$$

or, in vectorial notation

$$\vec{U}_{\perp}^{(k)} = (-\rho + \mu\alpha^{-2})^{-1}[\vec{M}(\vec{U}^{(k-1)}) - \vec{L}(\vec{U}^{(k-2)})]. \tag{22'}$$

Hence the additional components for P waves are obtained as a result of differentiation carried on the amplitude coefficients of lower order $\vec{U}^{(k-1)}$ and $\vec{U}^{(k-2)}$ in the form of vectorial operators $\vec{M}$ and $\vec{L}$ given in equations (10). Equations (22) and (22') are also valid, of course, for the first two amplitude coefficients ($k = 0$, $k = 1$) due to our definition $\vec{U}^{(-1)} = \vec{U}^{(-2)} = 0$ made earlier. Thus, for $k = 0$, the additional components $U_{s1}^{(k)}$ and $U_{s2}^{(k)}$ for P waves vanish.

The determination of principal components for P waves is a little more complicated. Since $N_i\tau_{,i} = 0$, the scalar multiplication of equation (12) by the gradient of phase function τ, gives a new vector equation, which in our component notation is written as

$$M_i(\vec{U}^{(k)})\tau_{,i} = L_i(\vec{U}^{(k-1)})\tau_{,i}.$$

Due to the linearity of the vector operator $\vec{M}$ this equation may be further recast into a more convenient form,

$$M_i(\vec{U}_{\parallel}^{(k)})\tau_{,i} = [L_i(\vec{U}^{(k-1)}) - M_i(\vec{U}_{\perp}^{(k)})]\tau_{,i}, \tag{23}$$

if the vector components of $\vec{U}^{(k)}$ [equation (21')] are used. Here all functions on the right side of the equation are already known due to the recurrent character of the basic system (12) and equation (22').

Let us now pay attention to the left side of equation (23). Since the components of $\hat{t}$ can be expressed in terms of the gradient of phase function τ we have

$$\left.\begin{aligned} U_{\parallel j}^{(k)} &= U_p^{(k)} t_j = U_p^{(k)} \alpha\tau_{,j}, \\ U_{\parallel j,i}^{(k)} &= U_{p,i}^{(k)} \alpha\tau_{,j} + U_p^{(k)}(\alpha_{,i}\tau_{,j} + \alpha\tau_{,ji}). \end{aligned}\right\} \tag{24}$$

Consequently, the left side of equation (23) after some arrangements leads to the expression

$$M_i(U_p^{(k)}\hat{t})\tau_{,i} = 2\alpha\rho(U_{p,i}^{(k)}\tau_{,i}) + U_p^{(k)}[\alpha\rho\tau_{,jj} + \alpha(\rho_{,j}\tau_{,j}) + 4\rho(\alpha_{,j}\tau_{,j}) + 2\alpha^3\rho\tau_{,ij}\tau_{,i}\tau_{,j}].$$

This may be further simplified if the following identities are employed

$$U_{p,j}^{(k)}\tau_{,j} = \alpha^{-2}\frac{dU_p^{(k)}}{d\tau}, \qquad \rho_{,j}\tau_{,j} = \alpha^{-2}\frac{d\rho}{d\tau}, \qquad \alpha_{,j}\tau_{,j} = \alpha^{-2}\frac{d\alpha}{d\tau},$$

$$\tau_{,ij}\tau_{,i}\tau_{,j} = \frac{1}{2}(\tau_{,i}\tau_{,i})_{,j}\tau_{,j} = \frac{1}{2}\alpha^{-2}\frac{d\alpha^{-2}}{d\tau},$$

resulting in

$$M_i(U_p^{(k)}\hat{t})\tau_{,i} = \frac{2\rho}{\alpha}\frac{dU_p^{(k)}}{d\tau} + U_p^{(k)}\left(\alpha\rho\tau_{,ii} + \frac{\rho}{\alpha}\frac{d\ln(\rho\alpha^2)}{d\tau}\right). \tag{25}$$

It means that equation (23) can be recast in a final form

$$\frac{dU_P^{(k)}}{d\tau} + \frac{1}{2} U_P^{(k)} \left(\alpha^2 \tau_{,jj} + \frac{d \ln(\rho\alpha^2)}{d\tau} \right) = g_0^{(k)}(\tau), \tag{26}$$

with

$$g_0^{(k)}(\tau) = \frac{\alpha}{2\rho} [L_i(\vec{U}^{(k-1)}) - M_i(\vec{U}_\perp^{(k)})]\tau_{,i}, \tag{27}$$

from which the principal component for P waves, $U_P^{(k)}$, is obtained. Equation (26) is generally known in the literature as a transport equation and it will be referred to as such throughout this paper.

4.2. Computation of amplitude coefficients for S waves

Analogically to the case of P waves, additional components of S waves can be determined rather easily provided that all previous amplitude coefficients of lower order have been determined in accordance with the recurrent character of the basic system (12).

Let us carry out multiplication of equation (12) by the vector $\hat{t}$ tangent to the ray. The left side of the resulting equation

$$N_i(\vec{U}^{(k)})t_i = [M_i(\vec{U}^{(k-1)}) - L_i(\vec{U}^{(k-2)})]t_i$$

can be conveniently expressed as

$$N_i(\vec{U}^{(k)})t_i = (\lambda + \mu)\beta^{-2} U_P^{(k)},$$

if we realize that $U_i^{(k)} t_i = U_P^{(k)}$. Thus the final formula for the additional component of S waves can be immediately written as

$$U_P^{(k)} = \frac{\beta^2}{\lambda + \mu} [M_i(\vec{U}^{(k-1)}) - L_i(\vec{U}^{(k-2)})]t_i \tag{28}$$

indicating that the additional component is again obtained as a result of differentiation of the amplitude coefficients of lower order.

Derivation of differential equations for the principal components of S waves, $U_{S1}^{(k)}$ and $U_{S2}^{(k)}$, is once again more involved, but similar in nature to the way the principal components of P waves, $U_P^{(k)}$, were obtained. Because $N_i(\vec{U}^{(k)})e_{1i} = 0$ and $N_i(\vec{U}^{(k)})e_{2i} = 0$, the scalar multiplication of (12) by $\hat{e}_1$ and $\hat{e}_2$ produces

$$M_i(\vec{U}^{(k)})e_{1i} = L_i(\vec{U}^{(k-1)})e_{1i}, \qquad M_i(\vec{U}^{(k)})e_{2i} = L_i(\vec{U}^{(k-1)})e_{2i}.$$

Due to the linearity of vector operator $\vec{M}$ both equations can be rewritten as

$$\left.\begin{aligned} M_i(\vec{U}_\perp^{(k)})e_{1i} &= [L_i(\vec{U}^{(k-1)}) - M_i(\vec{U}_\parallel^{(k)})]e_{1i}, \\ M_i(\vec{U}_\perp^{(k)})e_{2i} &= [L_i(\vec{U}^{(k-1)}) - M_i(\vec{U}_\parallel^{(k)})]e_{2i}, \end{aligned}\right\} \tag{29}$$

where $\vec{U}_\perp^{(k)}$ and $\vec{U}_\parallel^{(k)}$ are given in (21′).

The left sides of both equations can be evaluated easily according to (10′). Thus the first of the above equations becomes

$$M_i(\vec{U}_\perp{}^{(k)})e_{1i} = [(\lambda + \mu)\tau_{,j}e_{1i} + 2\mu\tau_{,i}e_{1j}]U^{(k)}_{\perp j,i} + [(\lambda + \mu)\tau_{,ij}e_{1i} + \mu\tau_{,ii}e_{1j} + \lambda_{,i}\tau_{,j}e_{1i} + \mu_{,i}\tau_{,i}e_{1j}]U^{(k)}_{\perp j}. \quad (30)$$

The second equation in (29) can be treated in exactly the same way producing the result that can be obtained directly from (30) by replacing components of $\hat{e}_1$ by those of $\hat{e}_2$. Seeing that

$$\left.\begin{aligned} U^{(k)}_{\perp i} &= U^{(k)}_{s1}e_{1i} + U^{(k)}_{s2}e_{2i}, \\ U^{(k)}_{\perp i,j} &= U^{(k)}_{s1,j}e_{1i} + U^{(k)}_{s2,j}e_{2i} + U^{(k)}_{s1}e_{1i,j} + U^{(k)}_{s2}e_{2i,j}, \end{aligned}\right\} \quad (31)$$

equation (30) becomes

$$\begin{aligned} M_i(\vec{U}_\perp{}^{(k)})e_{1i} = {} & 2\mu\tau_{,i}U^{(k)}_{s1,i} + U^{(k)}_{s1}[(\lambda + \mu)e_{1i}(\tau_{,j}e_{1j,i} + \tau_{,ij}e_{1j}) \\ & + \mu_{,i}\tau_{,i} + \mu(\tau_{,ii} + 2\tau_{,i}e_{1j}e_{1j,i})] + U^{(k)}_{s2}[2\mu\tau_{,i}e_{1j}e_{2j,i} \\ & + (\lambda + \mu)e_{1i}(\tau_{,j}e_{2j,i} + \tau_{,ij}e_{2j})]. \end{aligned}$$

Realizing that

$$(e_{1j}\tau_{,j})_{,i} = e_{1j,i}\tau_{,j} + e_{1j}\tau_{,ji} = 0,$$

$$(e_{2j}\tau_{,j})_{,i} = e_{2j,i}\tau_{,j} + e_{2j}\tau_{,ji} = 0,$$

$$\tau_{,i}U^{(k)}_{s1,i} = \beta^{-2}\frac{dU^{(k)}_{s1}}{d\tau},$$

$$e_{1j}\tau_{,i}e_{1j,i} = e_{1j}\beta^{-2}\frac{de_{1j}}{d\tau} = -K\cos\theta e_{1j}\tau_{,j} = 0,$$

$$e_{1j}\tau_{,i}e_{2j,i} = e_{1j}\beta^{-2}\frac{de_{2j}}{d\tau} = -K\sin\theta e_{1j}\tau_{,j} = 0,$$

equation (30) finally reduces to

$$M_i(\vec{U}_\perp{}^{(k)})e_{1i} = 2\rho\left[\frac{dU^{(k)}_{s1}}{d\tau} + \frac{1}{2}U^{(k)}_{s1}\left(\beta^2\tau_{,ii} + \frac{d\ln(\rho\beta^2)}{d\tau}\right)\right]. \quad (32)$$

Replacing e_{1i} and $U^{(k)}_{s1}$ in (32) by e_{2i} and $U^{(k)}_{s2}$ produces an expression valid for the left side of the second equation in (29)

$$M_i(\vec{U}_\perp{}^{(k)})e_{2i} = 2\rho\left[\frac{dU^{(k)}_{s2}}{d\tau} + \frac{1}{2}U^{(k)}_{s2}\left(\beta^2\tau_{,ii} + \frac{d\ln(\rho\beta^2)}{d\tau}\right)\right]. \quad (32')$$

Consequently, transport equations for S waves can be written finally as

$$\left.\begin{aligned} \frac{dU^{(k)}_{s1}}{d\tau} + \frac{1}{2}U^{(k)}_{s1}\left(\beta^2\tau_{,ii} + \frac{d\ln(\rho\beta^2)}{d\tau}\right) &= g_1{}^{(k)}(\tau), \\ \frac{dU^{(k)}_{s2}}{d\tau} + \frac{1}{2}U^{(k)}_{s2}\left(\beta^2\tau_{,ii} + \frac{d\ln(\rho\beta^2)}{d\tau}\right) &= g_2{}^{(k)}(\tau), \end{aligned}\right\} \quad (33)$$

with

$$\left.\begin{aligned} g_1^{(k)}(\tau) &= (2\rho)^{-1}[L_i(\tilde{U}^{(k-1)}) - M_i(\tilde{U}_\parallel^{(k)})]e_{1i}, \\ g_2^{(k)}(\tau) &= (2\rho)^{-1}[L_i(\tilde{U}^{(k-1)}) - M_i(\tilde{U}_\parallel^{(k)})]e_{2i}. \end{aligned}\right\} \tag{34}$$

Simple comparison of differential equations (26) and (33) reveals that the transport equations, which determine the principal components for both P and S waves, have an identical form. Furthermore, the transport equations for both principal components of S waves are independent of one another in this derivation, thereby enormously simplifying amplitude computations for the rays in three dimensions.

It should be noted that the decoupling of principal components $U_{s1}^{(0)}$ and $U_{s2}^{(0)}$ for the leading term in the ray series for S waves was first achieved by Pšenčík (1979).

In this paper, success in the decoupling of principal components of S waves for all amplitude coefficients in the ray series, regardless of their order, has been achieved. [After submitting the article to press, the authors read a paper by Hubral: "On the computation of shear waves by the ray method", *Geophys. J.* **57,** 445–449 (1979), in which Hubral also obtained decoupled transport equations for the principal shear wave components.]

4.3. Solution of transport equations

It was shown in two previous subsections that the transport equations for all three basic components $U_p^{(k)}$, $U_{s1}^{(k)}$, and $U_{s2}^{(k)}$ can be written in one simple form [see equations (26) and (33)]

$$\frac{dU^{(k)}}{d\tau} + \frac{1}{2}U^{(k)}\left(v^2\tau_{,ii} + \frac{d\ln(\rho v^2)}{d\tau}\right) = g^{(k)}(\tau) \tag{35}$$

provided that $U^{(k)} = U_p^{(k)}$, $v = \alpha$, $g^{(k)} = g_0^{(k)}$ in the case of P waves and $U^{(k)} = U_{s1}^{(k)}$ (or $U^{(k)} = U_{s2}^{(k)}$), $v = \beta$, $g^{(k)} = g_1^{(k)}$, (or $g^{(k)} = g_2^{(k)}$) for S waves. The solution of equation (35) is easy if one realizes (see Červený and Ravindra, 1971) that

$$\tau_{,ii} = \frac{1}{Jv}\frac{d}{d\tau}\frac{J}{(v)}$$

with J standing for the Jacobian of the transformation from the Cartesian coordinates into ray coordinates $[s, \gamma_1, \gamma_2]$. Here the ray coordinates γ_1 and γ_2 specify a particular ray, the position on which is characterized by the remaining coordinate s. The ray coordinates γ_1, γ_2 can be regarded as curvilinear coordinates on the wave front at some specified time, or, in case of a point source, as takeoff angles from the source. They are also called "ray parameters".

The function J plays a basic role in the evaluation of dynamic properties of seismic waves by ray methods since it is closely related to the geometrical expansion of the ray tube. Useful formulas expressing the geometrical spreading of the ray tube in terms of J are given by Červený *et al.* (1977).

Implementing the above formulas, equation (35) leads to a rather simple ordinary differential equation of the first order

$$\frac{d}{d\tau}(\sqrt{Jv\rho}\,U^{(k)}) = \sqrt{Jv\rho}\,g^{(k)}(\tau) \tag{36}$$

the solution of which is

$$U^{(k)}(\tau) = [J(\tau)v(\tau)\rho(\tau)]^{-1/2}\left\{\phi^{(k)}(\gamma_1, \gamma_2) + \int_{\tau_0}^{\tau} [J(\xi)v(\xi)\rho(\xi)]^{1/2} g^{(k)}(\xi)\, d\xi\right\}. \quad (37)$$

Here the constant of integration $\phi^{(k)}(\gamma_1, \gamma_2)$ is independent of τ being the function of two ray parameters γ_1 and γ_2 only. It depends on the mode of wave propagation, having generally different values for different basic components: $\phi^{(k)} = \phi_p^{(k)}$, $\phi^{(k)} = \phi_{s1}^{(k)}$ and $\phi^{(k)} = \phi_{s2}^{(k)}$ for $U^{(k)} = U_p^{(k)}$, $U^{(k)} = U_{s1}^{(k)}$ and $U^{(k)} = U_{s2}^{(k)}$, respectively. The integration in (37) is carried along the ray starting at some point of reference corresponding to $\tau = \tau_0$, with $d\xi$ denoting a time element along the ray. Note that the choice of τ_0 in (37) must be consistent with the selection of the constant of integration $\phi^{(k)}(\gamma_1, \gamma_2)$.

Equation (37) can be rewritten in an equivalent form

$$U^{(k)}(\tau) = U^{(k)}(\tau_0)\sqrt{\frac{J(\tau_0)\rho(\tau_0)v(\tau_0)}{J(\tau)\rho(\tau)v(\tau)}} + \frac{1}{\sqrt{J(\tau)\rho(\tau)v(\tau)}} \cdot \int_{\tau_0}^{\tau} \sqrt{J(\xi)v(\xi)\rho(\xi)}\, g^{(k)}(\xi)\, d\xi \quad (38)$$

provided that $U^{(k)}$ is known at some point on the ray corresponding to $\tau = \tau_0$.

Obviously equations (37) and (38) hold for any of the three principal components $U_p^{(k)}$, $U_{s1}^{(k)}$, or $U_{s2}^{(k)}$ if appropriate values of v, $\phi^{(k)}$, and $g^{(k)}$ are used.

In case of the zero order approximation of the ray series ($k = 0$) we have $g^{(0)} \equiv 0$. The expression for any principal component then reduces to

$$\left.\begin{aligned} U^{(0)}(\tau) &= \frac{\phi^{(0)}(\gamma_1, \gamma_2)}{\sqrt{J(\tau)v(\tau)\rho(\tau)}} \\ \text{or} \qquad U^{(0)}(\tau) &= U^{(0)}(\tau_0)\sqrt{\frac{J(\tau_0)\rho(\tau_0)v(\tau_0}{J(\tau)\rho(\tau)v(\tau)}} \end{aligned}\right\} \quad (39)$$

which are the special cases of (37) and (38) corresponding to $k = 0$ and $g^{(k)} = 0$.

It should be noted that the equation (39) for the principal components can be generalized to include any type of multiply reflected and transmitted converted wave in inhomogeneous layered media with curved interfaces. In order to solve the problem of reflection and transmission at any individual curved interface, the amplitude coefficients $\vec{U}^{(0)}$ corresponding to incident, reflected, and transmitted waves are usually decomposed into three components in the local coordinate system on the interface with its origin at the point of incidence O and z-axis oriented along the normal to the interface at O. After decomposition, the solution of the problem is the same, regardless of basic vectors $[(\hat{t}, \hat{e}_1, \hat{e}_2)$ or $(\hat{t}, \hat{n}, \hat{b})]$ actually used along the ray. Therefore, even when ray-centered coordinate systems are used along the ray, standard procedures at the points of incidence can be applied on curved interfaces. The details about the procedures can be found, for example, in Červený and Ravindra (1971), Pšenčík (1979).

The most complicated part in the computation of the principal components of amplitude coefficients is the evaluation of function J, which characterizes the geometrical expansion of the ray tube. This applies even to the zero-order approximation of the ray theory [see equation (39)]. In the next section, the determination of the function J shall be dealt with in detail.

5. Derivation of Function J From the Eikonal Equation in the Ray-Centered Coordinate System

5.1. Some properties of the ray-centered coordinate system

Let us select an arbitrary ray that will be called *a central ray*. If the ray-centered coordinate system $[s, q_1, q_2]$ with the basis vectors $\hat{t}$, $\hat{e}_1$, $\hat{e}_2$ satisfying equations (1) to (3), is introduced for the ray, q_1, q_2 represent length coordinates in the plane perpendicular to the central ray, with s standing for the length of the central ray from some reference point on the ray.

Thus, a position vector of any point at the vicinity of the central ray can be written as

$$\vec{r}(s, q_1, q_2) = \vec{r}(s, 0, 0) + q_1\hat{e}_1(s) + q_2\hat{e}_2(s). \tag{40}$$

We shall now show that the ray-centered coordinate system is orthogonal and find expressions for the length element dr. From (40) we have

$$(dr)^2 = d\vec{r}\cdot d\vec{r} =$$

$$\left[\left(\frac{\partial\vec{r}(s, 0, 0)}{\partial s} + q_1\frac{d\hat{e}_1}{ds} + q_2\frac{d\hat{e}_2}{ds}\right)ds + \hat{e}_1(s)\,dq_1 + \hat{e}_2(s)\,dq_2\right]^2. \tag{41}$$

Taking into account equation (3) and relation $\partial\vec{r}(s, 0, 0)/\partial s = \hat{t}$, expression (41) yields

$$(dr)^2 = h^2ds^2 + dq_1^2 + dq_2^2,$$

where the scale factor h is given by

$$h = 1 - K(q_1\cos\theta + q_2\sin\theta). \tag{42}$$

This enables us to write length of the infinitesimal vector $d\vec{r}$ as

$$dr = \sqrt{h^2ds^2 + dq_1^2 + dq_2^2}. \tag{43}$$

Formula (43) shows that the ray-centered coordinate system $[s, q_1, q_2]$ is orthogonal, with the scale factors h, 1, 1.

5.2. Eikonal equation in the ray-centered coordinate system

Since the gradient of phase function τ in the ray-centered coordinate system is

$$\nabla\tau = \frac{1}{h}\frac{\partial\tau}{\partial s}\hat{t} + \frac{\partial\tau}{\partial q_1}\hat{e}_1 + \frac{\partial\tau}{\partial q_2}\hat{e}_2, \tag{44}$$

the eikonal equations (19) and (20) can be written in the ray-centered coordinate system, as

$$\nabla\tau\cdot\nabla\tau = \frac{1}{h^2}\tau_{,s}^2 + \tau_{,1}^2 + \tau_{,2}^2 = \frac{1}{v^2} \tag{45}$$

where v represents the velocity of the wave, $\tau_{,s} = \partial\tau/\partial s$, $\tau_{,1} = \partial\tau/\partial q_1$, $\tau_{,2} = \partial\tau/\partial q_2$, and h is a scale factor given by (42). It is convenient to recast equation (45) into the form

$$\tau_{,s} = \frac{h}{v}\sqrt{1 - v^2(\tau_{,1}^2 + \tau_{,2}^2)} \tag{46}$$

equivalent to the Hamilton-Jacobi equation for the functional $\int_{M_0}^{M} v^{-1}\,dr$ with the length element given in equation (43). The corresponding Hamiltonian is

$$H(q_i, p_i) = -\frac{h}{v}\sqrt{1 - v^2(p_1^2 + p_2^2)}, \tag{47}$$

where q_i are generalized coordinates and p_i generalized momenta.

We will restrict our attention to the immediate vicinity of the central ray characterized by very small values of q_1 and q_2. As $\partial\tau(s, q_1, q_2)/\partial q_1 = \partial\tau(s, q_1, q_2)/\partial q_2 = 0$ on the central ray (i.e., for $q_1 = q_2 = 0$), the Taylor expansion for the phase function τ valid in the surrounding part of the central ray consisting of terms up to the second order, is easily recognized to be

$$\tau(s, q_1, q_2) \doteq \tau(s, 0, 0) + \frac{1}{2}\left\{\left[\frac{\partial^2\tau(s, q_1, q_2)}{\partial q_1^2}\right]^{q_1^2}_{q_1=q_2=0} + \left[\frac{\partial^2\tau(s, q_1, q_2)}{\partial q_2^2}\right]^{q_2^2}_{q_1=q_2=0} + 2\left[\frac{\partial^2\tau(s, q_1, q_2)}{\partial q_1\partial q_2}\right]^{q_1q_2}_{q_1=q_2=0}\right\}. \tag{48}$$

Let us denote

$$\mathbf{M} = \begin{bmatrix} M_{11} & M_{12} \\ M_{12} & M_{22} \end{bmatrix}, \qquad M_{ij} = \left[\frac{\partial^2\tau(s, q_1, q_2)}{\partial q_i\partial q_j}\right]_{q_1=q_2=0}, \qquad q = \begin{bmatrix} q_i \\ q_2 \end{bmatrix} \tag{49}$$

The symmetrix matrix $\mathbf{M}$ will be called here a matrix of the second derivatives of the time field. The notation (49) enables us to rewrite Taylor's expansion (48) in a more compact form, namely

$$\tau(s, q_1, q_2) \doteq \tau(s, 0, 0) + \tfrac{1}{2}\, q^T\mathbf{M}q \tag{50}$$

with q^T denoting the transposed matrix of q. This leads directly to

$$\tau_{,s} = \frac{\partial\tau(s, q_1, q_2)}{\partial s} \doteq v^{-1} + \frac{1}{2}(M'_{11}q_1^2 + M'_{22}q_2^2 + 2M'_{12}q_1q_2) = v^{-1} + \frac{1}{2}q^T\mathbf{M}'q, \tag{51}$$

and

$$\tau_{,1} = \frac{\partial \tau(s, q_1, q_2)}{\partial q_1} \doteq M_{11} q_1 + M_{12} q_2, \qquad \tau_{,2} = \frac{\partial \tau(s, q_1, q_2)}{\partial q_2} = M_{22} q_2 + M_{12} q_1, \tag{52}$$

where the prime denotes differentiation with respect to s.

Now we will seek an expansion for the right-hand side of equation (46) valid in the immediate neighborhood of the central ray. We will use the notation introduced in equation (47). If we limit expansion to terms up to the second order in q_i and $\tau_{,i}$ we obtain

$$H(q_1, q_2, \tau_{,1}, \tau_{,2}) = H(0, 0, 0, 0) + \frac{1}{2} v(\tau_{,1}^2 + \tau_{,2}^2) + \left.\frac{\partial H}{\partial q_1}\right|_0 q_1 + \left.\frac{\partial H}{\partial q_2}\right|_0 q_2 + \frac{1}{2}\left\{\left.\frac{\partial^2 H}{\partial q_1^{\,2}}\right|_0 q_1^{\,2} + \left.\frac{\partial^2 H}{\partial q_2^{\,2}}\right|_0 q_2^{\,2} + 2\left.\frac{\partial^2 H}{\partial q_1 \partial q_2}\right|_0 q_1 q_2\right\} \tag{53}$$

with all partial derivatives taken on the central ray. For $\partial H/\partial q_i$ we obtain easily from (47)

$$\frac{\partial H}{\partial q_i} = \frac{h v_{,i} - v h_{,i}[1 - v^2(\tau_{,1}^2 + \tau_{,2}^2)]}{v^2[1 - v^2(\tau_{,1}^2 + \tau_{,2}^2)]^{1/2}}. \tag{54}$$

On the central ray, however, $(\partial H/\partial q_i)\,|_0 = 0$ since (53), (51), and (46) must be compatible. Therefore, on the central ray, $v_{,i} h = v h_{,i}$ yielding [see equation (42)]

$$h_{,1} = \frac{\partial h(s, q_1, q_2)}{\partial q_1} = -K \cos\theta = \frac{v_{,1}}{v}, \qquad h_{,2} = \frac{\partial h(s, q_1, q_2)}{\partial q_2} = -K \sin\theta = \frac{v_{,2}}{v}, \tag{55}$$

with v, $v_{,1} = \partial v/\partial q_1$ and $v_{,2} = \partial v/\partial q_2$ evaluated on the central ray where $q_1 = q_2 = 0$. The formulas (55) indicate that $h_{,1}$ and $h_{,2}$ do not depend on coordinates q_1 and q_2, but only on s. The above relations bring about a very convenient expression for the scale factor h, namely

$$h = 1 + v^{-1}(q_1 v_{,1} + q_2 v_{,2}) \tag{56}$$

which is no longer explicitly dependent on the curvature K of the ray and on θ, linked through equation (2) to the torsion T of the ray.

The direct differentiation of (54) produces

$$\left.\frac{\partial^2 H}{\partial q_1^{\,2}}\right|_0 = \frac{v_{,11}}{v^2}, \qquad \left.\frac{\partial^2 H}{\partial q_2^{\,2}}\right|_0 = \frac{v_{,22}}{v^2}, \qquad \left.\frac{\partial^2 H}{\partial q_1 \partial q_2}\right|_0 = \frac{v_{,12}}{v^2} \tag{57}$$

where

$$v_{,ij} = \left[\frac{\partial^2 v}{\partial q_1 \partial q_2}\right]_{q_1 = q_2 = 0}. \tag{58}$$

In this manner, the Hamiltonian can be approximated in the vicinity of the central ray, where q_1, q_2, $\tau_{,1}$, and $\tau_{,2}$ are sufficiently small, as

$$H(q_1, q_2, \tau_{,1}, \tau_{,2}) = -v^{-1} + \tfrac{1}{2} v(\tau_{,1}^2 + \tau_{,2}^2) + \tfrac{1}{2} v^{-2}(v_{,11}q_1^2 + v_{,22}q_2^2 + 2v_{,12}q_1q_2), \quad (59)$$

where v and $v_{,ij}$ are taken on the central ray. Consequently, the eikonal equation (46) yields

$$\tau_{,s} + \tfrac{1}{2} v(\tau_{,1}^2 + \tau_{,2}^2) = v^{-1} - \tfrac{1}{2} v^{-2}(v_{,11}q_1^2 + v_{,22}q_2^2 + 2v_{,12}q_1q_2). \quad (60)$$

This can be further rearranged with the help of equations (51) and (52) into the final form

$$\tfrac{1}{2}[M'_{11} + v(M_{11}^2 + M_{12}^2) + v^{-2}v_{,11}]q_1^2 + \tfrac{1}{2}[M'_{22} + v(M_{22}^2 + M_{12}^2) + v^{-2}v_{,22}]q_2^2 + [M'_{12} + vM_{12}(M_{11} + M_{22}) + v^{-2}v_{,12}]q_1q_2 = 0 \quad (61)$$

by collecting terms with equal powers of q_iq_j. Here, as before, the prime indicates differentiation with respect to the length of ray s. Equation (61) will serve as a starting point for the derivation of the dynamic ray tracing system presented in the next subsection.

5.3. Dynamic ray tracing in three-dimensional inhomogeneous media

We showed in subsection 4.3 that the ray amplitude cannot be computed without the evaluation of function J. The evaluation of function J and some other geometrical characteristics of the wave front in the vicinity of the central ray will be carried out during the procedure termed *Dynamic Ray Tracing*. It is based on the system of three ordinary nonlinear differential equations of the first order that follow from the eikonal equation written in terms of the ray-centered coordinates in the form (61), namely

$$\left.\begin{aligned} \frac{dM_{11}}{ds} + v(M_{11}^2 + M_{12}^2) &= -v^{-2}v_{,11}, \\ \frac{dM_{22}}{ds} + v(M_{22}^2 + M_{12}^2) &= -v^{-2}v_{,22}, \\ \frac{dM_{12}}{ds} + vM_{12}(M_{11} + M_{22}) &= -v^{-2}v_{,12}. \end{aligned}\right\} \quad (62)$$

Numerical values of M_{11}, M_{22}, and M_{12} can be calculated along the ray by solving the dynamic ray tracing system (62) provided that their values are known at some point on the ray.

Simple inspection of the system (62) reveals that it may be rewritten using a convenient matrix formulation

$$\frac{d\mathbf{M}}{ds} + v\mathbf{M}^2 = -v^{-2}\mathbf{V} \quad (63)$$

by introducing a new symmetric matrix of the second derivatives of wave velocity

with respect to the ray centered coordinates q_1 and q_2, $\mathbf{V}$, as

$$\mathbf{V} = \begin{bmatrix} v_{,11} & v_{,12} \\ v_{,12} & v_{,22} \end{bmatrix} \tag{64}$$

where $v_{,ij}$ are given by (58).

From a mathematical point of view (63) is an ordinary nonlinear differential equation of the first order of the Riccati type in the matrix form that, in general, cannot be solved by elementary analytical methods. It can, of course, be solved numerically by standard techniques.

The use of the matrix of second derivatives of the time field, $\mathbf{M}$, given in our dynamic ray tracing system (63), considerably simplifies formal expressions of several functions needed for amplitude computation based on the ray series approach. This is best seen on function J linked to the phase function τ through the relation

$$\nabla^2\tau = \tau_{,ii} = \frac{1}{Jv}\frac{d}{d\tau}\left(\frac{J}{v}\right). \tag{65}$$

Expressing $\nabla^2\tau$ in the ray-centered coordinates $[s, q_1, q_2]$ and using (42), this is recognized as

$$\nabla^2\tau = \frac{\partial^2\tau}{\partial s^2} + \frac{\partial^2\tau}{\partial q_1{}^2} + \frac{\partial^2\tau}{\partial q_2{}^2} = \frac{\partial}{\partial s}\left(\frac{1}{v}\right) + M_{11} + M_{22} \tag{66}$$

for $q_1 = q_2 = 0$, enabling us to write the solution of (65) in the form of

$$J(\tau) = J(\tau_0)\exp\left\{\int_{\tau_0}^{\tau} v^2(M_{11} + M_{22})\,d\tau\right\} = J(\tau_0)\exp\left\{\int_{\tau_0}^{\tau} v^2 tr\,\mathbf{M}\,d\tau\right\}, \tag{67}$$

with the trace of matrix $\mathbf{M}$ optionally given as the sum of its eigenvalues $\mathrm{tr}\,\mathbf{M} = M_1 + M_2$.

The dynamic ray tracing system (63) can be easily rewritten in terms of curvatures of the wave front. This requires recognition of the direct connection between $\mathbf{M}$ and so-called curvature matrix of the wave front, $\mathbf{K}$ (see Deschampes, 1972; Lee, 1975; James, 1976), namely

$$\mathbf{M} = \frac{1}{v}\mathbf{K} \tag{68}$$

with

$$\mathbf{K} = \begin{bmatrix} K_{11} & K_{12} \\ K_{12} & K_{22} \end{bmatrix} \tag{69}$$

being symmetric, too. From (63) and (68) we easily get

$$v\frac{d\mathbf{K}}{ds} - v_{,s}\mathbf{K} + v\mathbf{K}^2 = -\mathbf{V}, \tag{70}$$

with v and $v_{,s} = (\partial v/\partial s)$ evaluated on the central ray. The same equation was obtained by Hubral (1979), who derived it from eight differential equations of the first order presented by Popov and Pšenčík (1978a) and discussed earlier in the Introduction. Obviously, equation (67) for the function J can be easily recast in terms of elements of matrix **K**, namely

$$J(\tau) = J(\tau_0) \exp\left\{\int_{\tau_0}^{\tau} v(K_{11} + K_{22})d\tau\right\}. \tag{71}$$

As $K_{11} + K_{22} = K_1 + K_2$, where K_1 and K_2 are the eigenvalues of matrix **K**, representing the principal curvatures of the wave front, formula (71) gives a well-known expression for J in terms of the principal curvatures of the wave front (see, e.g., Červený and Ravindra, 1971). Note that the sum, $K_1 + K_2 = \text{tr } \mathbf{K} = 2H$, equals twice the mean curvature H.

Knowing that $\mathbf{M}^{-1} = 0$, $\mathbf{K}^{-1} = 0$ at the point source, both equations (63) and (70) are not too suitable for the numerical solution if we start computations just from a point source. In such a case two new matrices, **N** and **R**, defined as $\mathbf{N} = \mathbf{M}^{-1}$ and $\mathbf{R} = \mathbf{K}^{-1}$, could be used instead.

$$\mathbf{N} = \frac{1}{\tau_{,11}\tau_{,22} - \tau_{,12}^2}\begin{bmatrix} \tau_{,22} & -\tau_{,12} \\ -\tau_{,12} & \tau_{,11} \end{bmatrix} \tag{72}$$

transforms (63) into

$$\frac{d\mathbf{N}}{ds} - v^{-2}\mathbf{NVN} = v\mathbf{I}, \tag{73}$$

with **I** being an identity matrix and $\mathbf{N} = 0$ at the point source.

The second matrix **R**, frequently called the matrix of radii of curvature of the wave front, is also closely related to **N** since

$$\mathbf{R} = \mathbf{K}^{-1} = v^{-1}\mathbf{N}. \tag{74}$$

Inserting (74) into (73) or (70) yields

$$v\frac{d\mathbf{R}}{ds} + v_{,s}\mathbf{R} - \mathbf{RVR} = v\mathbf{I}. \tag{75}$$

The eigenvalues of **R**, R_1, and R_2, are known as the principal radii of curvature of the wave front and they are linked to the corresponding principal curvatures K_1 and K_2 via $R_1 = 1/K_1$, $R_2 = 1/K_2$.

A simple comparison of (63) with (70) and of (73) with (75) reveals that the equations (63) and (73) are slightly simpler than equations (70) and (75). It seems, therefore, more convenient to use equations (63) or (73) for the numerical integration, even when we are interested in **K** or **R**. After this, the appropriate values of matrices **K** and **R** can be evaluated with the help of (68) and (74), respectively.

It is worth mentioning that equations (63), (70), (73), and (75) can be rewritten if

travel time, τ, is used as a parameter along the ray instead of the length of the ray, s. Then the above equations transform into the following equivalent forms

$$\left.\begin{aligned} \frac{d\mathbf{M}}{d\tau} + v^2\mathbf{M}^2 &= -v^{-1}\mathbf{V}, & \frac{d\mathbf{K}}{d\tau} - v^{-1}v_{,\tau}\mathbf{K} + v\mathbf{K}^2 &= -\mathbf{V}, \\ \frac{d\mathbf{N}}{d\tau} - v^{-1}\mathbf{N}\mathbf{V}\mathbf{N} &= v^2\mathbf{I}, & \frac{d\mathbf{R}}{d\tau} + v^{-1}v_{,\tau}\mathbf{R} - \mathbf{R}\mathbf{V}\mathbf{R} &= v\mathbf{I}, \end{aligned}\right\} \tag{76}$$

where v and $v_{,\tau} = \partial v/\partial\tau$ are taken on the central ray.

Despite our rather detailed discussion of various forms of the dynamic ray tracing system presented so far, we shall mention two other forms of the system that may prove useful under special circumstances.

In the first case, the system for $\mathbf{N}$ in (76) will be used as a starting point. Denoting the trace and determinant of $\mathbf{N}$, $T_N = \text{tr } \mathbf{N}$ and $D_N = \det \mathbf{N}$, respectively, equation (76) leads to

$$\frac{dT_N}{d\tau} + v^{-1}T_V D_N - v^{-1}T_N B_N = 2v^2, \qquad \frac{dD_N}{d\tau} - v^{-1}D_N B_N = v^2 T_N, \tag{77}$$

where $T_V = \text{tr } \mathbf{V}$ denotes the trace of $\mathbf{V}$ defined in (64) and

$$B_N = V_{11}N_{11} + V_{22}N_{22} + 2V_{12}N_{12} = tr(\mathbf{VN}). \tag{78}$$

This, combined with the differential equation for J [see equation (65)],

$$\frac{dJ}{d\tau} = v^2 T_N D_N{}^{-1} J, \tag{79}$$

results in

$$\frac{d}{d\tau}\left(\frac{J}{D_N}\right) = -v^{-1}D_N{}^{-1}JB_N, \tag{80}$$

which in turn gives

$$J(\tau) = C_1 D_N \exp\left\{-\int_{\tau_0}^{\tau} v^{-1}B_N d\tau\right\}, \tag{81}$$

where C_1 is some constant of proportionality. The last formula, under special conditions, such as $B_N = 0$, can be simplified even further. Thus assuming $B_N = 0$, equation (81) reduces to

$$J(\tau) = C_1 \det \mathbf{N} = C_1 \det (v\,\mathbf{R}) \tag{82}$$

which, in the case of homogeneous media, becomes

$$J(\tau) = C_2 G^{-1},$$

with G representing the Gaussian curvature of the wave front, defined with the help of $\mathbf{R}$ as $G = (\det \mathbf{R})^{-1}$, and C_2 being some constant of proportionality. It is possible to show that equation (82) is valid even for rays in inhomogeneous media for which the velocity structure is a linear function of Cartesian coordinates.

The second special form of the dynamic ray tracing system will be derived from equation (76) involving matrix $\mathbf{M}$. It is seen that by introducing a new matrix $\mathbf{J}$ related to $\mathbf{M}$ via

$$\mathbf{M} = \frac{1}{v^2}\frac{d\mathbf{J}}{d\tau}\mathbf{J}^{-1}, \tag{83}$$

the original differential equation for $\mathbf{M}$ transforms into a linear differential equation of the second order for $\mathbf{J}$

$$v\frac{d^2\mathbf{J}}{d\tau^2} - 2v_{,\tau}\frac{d\mathbf{J}}{d\tau} = -v^2\,\mathbf{V}\mathbf{J}. \tag{84}$$

According to (67), however, function J must satisfy

$$\frac{dJ}{d\tau} = v^2 T_M J, \tag{85}$$

where T_M stands for the trace of $\mathbf{M}$. In accordance with (83) T_M has the value

$$T_M = \operatorname{tr}\mathbf{M} = \frac{1}{v^2}\frac{d}{d\tau}[ln(\det \mathbf{J})], \tag{86}$$

allowing us to write the solution to equation (85) finally as

$$J(\tau) = C \det(\mathbf{J}), \tag{87}$$

with C representing a constant of proportionality.

Undoubtedly, more special forms of the dynamic ray tracing system, similar to equation (84), could be derived but they are left as an exercise to interested readers.

5.4. Special cases of dynamic ray tracing

The dynamic ray tracing systems (76) derived for generally inhomogeneous three-dimensional structures can be simplified considerably under special conditions, which are often used in practical applications.

It is known that the majority of models used nowadays in seismology and oil exploration for seismic numerical modeling are essentially two-dimensional, since their elastic and geometrical characteristics do not change in one fixed direction. In such cases the propagation of seismic waves is frequently investigated only in the plane perpendicular to this fixed direction which is then parallel to the direction of binormals of all rays.

The situation, when a point symmetric source is located in a two-dimensional medium described above, can be regarded as a special case of a more general problem which is characterized by the following two conditions: (1) $v_{,12} = 0$ along the whole ray between some two points $\tau = \tau_1$ and $\tau = \tau_2$; (2) $M_{12} = 0$ at least at one

point τ_0, $\tau_1 \leqq \tau_0 \leqq \tau_2$. The second condition, for example, is satisfied if at the point $\tau = \tau_0$ both principal directions of curvature of the wave front lay in the coordinate planes $q_1 = \text{const}$, and $q_2 = \text{const}$.

A brief inspection of equations (62) reveals that the two previous conditions assure the zero values of all off-diagonal terms in **M** and **V**, thereby reducing the system (62) to two independent differential equations for M_{11}, M_{22}

$$\frac{dM_{11}}{d\tau} + v^2 M_{11}^2 = -v^{-1} v_{,11} \qquad \frac{dM_{22}}{d\tau} + v^2 M_{22}^2 = -v^{-1} v_{,22}. \tag{88}$$

Hence we can rewrite (67) for function J as

$$J(\tau) = J_1(\tau) \cdot J_2(\tau), \tag{89}$$

where

$$J_1(\tau) = J_1(\tau_0) \exp\left\{\int_{\tau_0}^{\tau} v^2 M_{11}\, d\tau\right\}, \qquad J_2(\tau) = J_2(\tau_0) \exp\left\{\int_{\tau_0}^{\tau} v^2 M_{22}\, d\tau\right\} \tag{90}$$

writing $J(\tau_0) = J_1(\tau_0) J_2(\tau_0)$. Obviously $J_1(\tau)$ now characterizes the geometrical expansion of the ray tube in the direction of $\hat{e}_1$ whereas $J_2(\tau)$ does the same for the direction $\hat{e}_2$. Consequently, we will restrict ourselves to the presentations of formulas concerning $J_1(\tau)$ knowing that the similar set exists for $J_2(\tau)$ as well.

Four different formulas can be written for $J_1(\tau)$, each of them corresponding to a different equation in the system (76) that for this special case are also written below

$$J_1(\tau) = J_1(\tau_0) \exp\left\{\int_{\tau_0}^{\tau} v^2 M_{11}\, d\tau\right\}, \qquad \frac{dM_{11}}{d\tau} + v^2 M_{11}^2 = -v^{-1} v_{,11}, \tag{91}$$

$$J_1(\tau) = J_1(\tau_0) \exp\left\{\int_{\tau_0}^{\tau} v K_{11}\, d\tau\right\}, \qquad \frac{dK_{11}}{d\tau} - v^{-1} v_{,\tau} K_{11} + v K_{11}^2 = -v_{,11}, \tag{92}$$

$$J_1(\tau) = J_1(\tau_0) \exp\left\{\int_{\tau_0}^{\tau} v^2 N_{11}^{-1}\, d\tau\right\}, \qquad \frac{dN_{11}}{d\tau} - v^{-1} v_{,11} N_{11}^2 = v^2, \tag{93}$$

$$J_1(\tau) = J_1(\tau_0) \exp\left\{\int_{\tau_0}^{\tau} v R_{11}^{-1}\, d\tau\right\}, \qquad \frac{dR_{11}}{d\tau} + v^{-1} v_{,\tau} R_{11} - v_{,11} R_{11}^2 = v. \tag{94}$$

Here $v_{,\tau} = (\partial v/\partial \tau)$ denotes a derivative along the ray, whereas K_{11} and R_{11} represent in this case principal curvature and radius of curvature of the wave front, respectively.

Let it be noted that the equations corresponding to $J_2(\tau)$ (which characterizes the geometrical expansion of the ray tube in the direction of $\hat{e}_2$) can be simply solved analytically in many practical applications important in oil exploration and crustal seismology. This applies, e.g., to the cases of a point source and a line source parallel to $\hat{e}_2$ (see details in Červený and Pšenčík, 1979). Thus, in these applications the

dynamic ray tracing reduces to one nonlinear ordinary differential equation of the first order and Riccati type, see (91) to (94).

5.5. Dynamic ray tracing across curved interfaces

Whenever the ray impinges on a boundary between two different media its direction changes abruptly resulting in the discontinuity of the matrix of second derivatives of the time field **M**. Understandably, this jump in values of **M** for reflected and transmitted rays must be known before the dynamic ray tracing system can be solved along the ray of reflected or transmitted waves.

Before using the phase matching method, an expansion of the phase function $\tau(s, q_1, q_2)$ at an arbitrary point $s = s_0$ on the ray must be found. We denote the point $[s_0, 0, 0]$ by O. Neglecting all higher terms than $(s - s_0)^2$, q_1^2, q_2^2, we can write [see (50)]

$$\tau(s, q_1, q_2) \doteq \tau(s_0, 0, 0) + \left.\frac{\partial \tau}{\partial s}\right|_0 (s - s_0) + \frac{1}{2}\left.\frac{\partial^2 \tau}{\partial s^2}\right|_0 (s - s_0)^2 + \frac{1}{2} q^T \mathbf{M} q, \tag{95}$$

where the derivatives of τ and values of **M** are taken at O and q^T once again denotes a transposed matrix of $\begin{bmatrix} q_1 \\ q_2 \end{bmatrix}$. According to (51), however

$$\left.\frac{\partial \tau}{\partial s}\right|_0 = \frac{1}{v(s_0)}, \qquad \left.\frac{\partial^2 \tau}{\partial s^2}\right|_0 = -\frac{1}{v^2(s_0)} v_{,s}, \tag{96}$$

so that (95) becomes

$$\tau(s, q_1, q_2) \doteq \tau_0 + v^{-1}(s - s_0) - \tfrac{1}{2} v^{-2} v_{,s} (s - s_0)^2 + \tfrac{1}{2} q^T \mathbf{M} q, \tag{97}$$

where $\tau_0 = \tau(s_0, 0, 0)$. All quantities v, $v_{,s}$ and **M** are taken at O.

Now, transform equation (97) for the phase function $\tau(s, q_1, q_2)$ into a new auxiliary Cartesian coordinate system $[l, q_1, q_2]$ with the basis $\hat{t}$, $\hat{e}_1$, $\hat{e}_2$ at O. The new system has the same basis vectors at O as the ray-centered coordinate system $[s, q_1, q_2]$. The only difference is that the system $[l, q_1, q_2]$ is Cartesian, whereas the ray-centered coordinate system $[s, q_1, q_2]$ is curvilinear (albeit orthogonal). The length element, dr, in the ray-centered coordinate system $[s, q_1, q_2]$ is given by (43) and in the Cartesian coordinate system by $dr = \sqrt{dl^2 + dq_1^2 + dq_2^2}$. Thus, for fixed q_1 and q_2, element dl in the Cartesian system is related to the element ds by the formula $dl = h\,ds$ (see section 5.1). It means that it can be written, according to (56), for small $s - s_0$,

$$s - s_0 \doteq h^{-1} l = l - v^{-1}(q_1 v_{,1} + q_2 v_{,2})\, l.$$

Inserting this into (97) we finally get

$$\tau(l, q_1, q_2) \doteq \tau_0 + v^{-1} l - v^{-2}(q_1 v_{,1} + q_2 v_{,2}) l - \tfrac{1}{2} v^{-2} v_{,s} l^2 + \tfrac{1}{2} q^T \mathbf{M}\, q. \tag{98}$$

All quantities τ_0, v, $v_{,1}$, $v_{,2}$, $v_{,s}$, and **M** are again taken at O, i.e., at the point $[s_0, 0, 0]$.

Until now, the point O has been an arbitrary point on the ray. Next, assume that the ray under consideration strikes a curved interface S, which separates two generally inhomogeneous media, at the point O. As it is well known, four new waves are then generated at the interface, namely, reflected and transmitted P and S waves. The phase matching method requires that the phase function of incident, reflected and transmitted waves be equal on S in the vicinity of O. The phase functions of all these waves can be described in the neighborhood of O by the formula (98). However, the direct application of (98) to the phase matching is not yet possible, as they are written in different Cartesian coordinate systems for different waves. Therefore, we will introduce a new local Cartesian coordinate system, on the interface S at O, and express the phase functions of all relevant waves in this coordinate system. The new local Cartesian coordinate system $[n, d_1, d_2]$ can be introduced at the point O in such a way that the corresponding basis vectors $\hat{n}$, $\hat{d}_1$, $\hat{d}_2$ are oriented in the following manner

- $\hat{n}$ is a normal vector to the curved interface at O, pointed into the medium containing the incident wave;
- $\hat{d}_1$ is oriented along the intersection of the plane of incidence with the tangent plane to the interface at O in such a way that it makes an acute angle with the unit tangent $\hat{t}$ to the ray of incident wave at O;
- $\hat{d}_2$ is a tangent vector to the interface at O being defined as a cross-product $\hat{d}_2 = \hat{n} \times \hat{d}_1$. (Note that $\hat{d}_2$ is perpendicular to the plane of incidence.)

Let it now be assumed that the basis vector $\hat{e}_2$ in the auxiliary Cartesian coordinate system pertinent to the incident ray coincides with the basis vector $\hat{d}_2$. (If this is not true, the auxiliary Cartesian coordinate system connected with the ray must be rotated at O about the vector $\hat{t}$ in such a way that $\hat{e}_2$ coincides with $\hat{d}_2$; this situation will be considered later.) The Cartesian coordinate system $[l, q_1, q_2]$ is linked to the local Cartesian coordinate system $[n, d_1, d_2]$ through the transform

$$\begin{aligned} q_1 &= \pm d_1 \cos i - n \sin i, \\ q_2 &= d_2, \\ l &= d_1 \sin i \pm n \cos i, \end{aligned} \tag{99}$$

where i is an acute angle between the tangent to the ray at O and $\hat{n}$. The upper sign in (99) corresponds to the reflected rays, whereas the lower sign is to be taken for the incident and transmitted rays. Inserting (99) into (98), we obtain a new expression for the phase function $\tau(n, d_1, d_2)$ in the coordinates $[n, d_1, d_2]$ in the vicinity of O, with the accuracy up to the second order in n, d_1, and d_2.

Now we shall look for the values of the phase function $\tau(n, d_1, d_2)$ on the interface S in the vicinity of O. In the local coordinate system $[n, d_1, d_2]$ interface S can be described by the equation

$$n = n(d_1, d_2).$$

In the neighborhood of O, with the accuracy up to the second order in d_1 and d_2, this reduces to

$$n = -\tfrac{1}{2}\, d^T \mathbf{D}\, d, \tag{100}$$

where d^T is the transposed matrix of $d = \begin{bmatrix} d_1 \\ d_2 \end{bmatrix}$ and $\mathbf{D}$ is the curvature matrix of the interface S at O. The sign "$-$" indicates that the positive curvatures were chosen for those parts of the interface that are seen as convex by an observer located in the medium containing incident wave.

It follows from (99) and (100) that

$$q = \mathbf{H}\, d + 0(d^2), \qquad \mathbf{H} = \begin{bmatrix} \pm\cos i & 0 \\ 0 & 1 \end{bmatrix}. \tag{101}$$

We denote by $\tau_I(d_1, d_2)$ the values of τ along the interface

$$\tau_I(d_1, d_2) = \tau[n(d_1, d_2), d_1, d_2].$$

They are obtained from the expression for the phase function $\tau(n, d_1, d_2)$ by using equation (100). Inserting (99), (100), (101) into (98), we obtain $\tau_I(d_1, d_2)$ in the vicinity of O, with the accuracy up to the second order in d_1 and d_2, the following formula

$$\begin{aligned} \tau_I(d_1, d_2) \doteq\ & \tau_0 + v^{-1} \sin i\, d_1 \mp \tfrac{1}{2} v^{-1} \cos i\, d^T \mathbf{D}\, d \\ & - v^{-2}(\pm d_1 \cos i\, v_{,1} + d_2 v_{,2}) d_1 \sin i - \tfrac{1}{2} v^{-2} v_{,s} d_1^2 \sin^2 i \\ & + \tfrac{1}{2} d^T \mathbf{HMH}\, d. \end{aligned} \tag{102}$$

This can be written in a more compact matrix form

$$\tau_I(d_1, d_2) \doteq \tau_0 + v^{-1} \sin i\, d_1 + \tfrac{1}{2} d^T \mathbf{F}\, d, \tag{103}$$

where

$$\mathbf{F} = \mathbf{HMH} \mp v^{-1} \cos i\, \mathbf{D} - v^{-2} \sin i \begin{bmatrix} \pm 2 v_{,1} \cos i & v_{,2} \\ v_{,2} & 0 \end{bmatrix} - \frac{\sin^2 i}{v^2} \begin{bmatrix} v_{,s} & 0 \\ 0 & 0 \end{bmatrix}. \tag{104}$$

As before, the upper signs in (102) and (104) correspond to the reflected waves, while the lower signs are related to the incident and transmitted waves. The values of v, $v_{,i}$, $v_{,s}$, and $\mathbf{F}$ are taken at 0; $v_{,i} = \partial v/\partial q_i$, $v_{,s} = \partial v/\partial s$. (These derivatives can, of course, be expressed in terms of the derivatives $\partial v/\partial d_1$, $\partial v/\partial d_2$, and $\partial v/\partial n$.)

Only now, having derived a general expression (103) for the phase function τ_I in the neighborhood of the point of incidence O, the initial conditions for the dynamic ray tracing system of the reflected and transmitted waves are easily obtained by the phase matching method. In order to distinguish between the symbols related to the incident, reflected, and transmitted waves, the following notation is used: the tilde above the symbol will denote quantities pertinent to the reflected and transmitted waves, whereas the plain symbols v, $v_{,1}$, $v_{,2}$, $v_{,s}$, and $\mathbf{M}$ will refer to the incident wave. The requirement of equal phase on the interface expressed as $\tau_I = \tilde{\tau}_I$ results in the Snell's law

$$v^{-1} \sin i = \tilde{v}^{-1} \sin \tilde{i}$$

and the equation

$$\mathbf{F} = \tilde{\mathbf{F}} \tag{105}$$

that can be rewritten using equation (104) as

$$\tilde{\mathbf{M}} = \mathbf{SMS} + u\,\mathbf{GDG} + \frac{\sin i}{v}\,\mathbf{GEG} \tag{106}$$

with

$$\left.\begin{aligned} \mathbf{S} &= \begin{bmatrix} \mp\dfrac{\cos i}{\cos \tilde{i}} & 0 \\ 0 & 1 \end{bmatrix}, \qquad \mathbf{G} = \begin{bmatrix} \pm\dfrac{1}{\cos \tilde{i}} & 0 \\ 0 & 1 \end{bmatrix}, \\ \mathbf{E} &= \begin{bmatrix} E_{11} & E_{12} \\ E_{12} & 0 \end{bmatrix}, \qquad u = \left[\frac{\cos i}{v} \pm \frac{\cos i}{\tilde{v}}\right], \\ E_{11} &= 2\left(\frac{v_{,1}}{v}\cos i \pm \frac{\tilde{v}_{,1}}{\tilde{v}}\cos \tilde{i}\right) - \frac{\sin i}{v}\,(v_{,s} - \tilde{v}_{,s}), \\ E_{12} &= E_{21} = -\frac{v_{,2}}{v} + \frac{\tilde{v}_{,2}}{\tilde{v}}, \end{aligned}\right\} \tag{107}$$

evaluated at the point of incidence O. In this manner all matrices $\tilde{\mathbf{M}}$ for the reflected and transmitted waves are fully determined at O, provided that the velocity structure in both layers is known at the vicinity of the point of incidence together with the geometrical shape of the interface (see matrix **D**), and the matrix **M** of the incident wave.

Physical interpretation of the last two terms in (106) is rather easy: since **D** and **E** vanish for the plane interface and homogeneous media, respectively, the second term characterizes the influence of the curvature of the interface, while the third term represents a correction accounting for any inhomogeneity in the medium along the interface. This means that in the case of two homogeneous layers separated by a plane interface equation (106) reduces to

$$\tilde{\mathbf{M}} = \mathbf{SMS} \tag{108}$$

that can also be obtained by elementary means based on geometrical reasoning.

It should be noted that the first two terms in (106) are well known in electromagnetic wave propagation and can be found in Deschamps (1972), Lee (1975), or James (1976), among others. In seismology, a similar expression written in terms of radii of curvature has also become popular in recent times. It was first derived by Gel'chinskiy (1961) and discussed in detail by Červený and Ravindra (1971). The Gel'chinskiy formula follows directly from our expression (106) with the help of equation (68) according to which $\mathbf{M} = 1/v\ \mathbf{K}$. In this way we get the curvature matrix in the form

$$\tilde{\mathbf{K}} = \tilde{v}\,v^{-1}\,\mathbf{SKS} + \tilde{v}\,u\,\mathbf{GDG} + \frac{\tilde{v}}{v}\sin i\,\mathbf{GEG} \tag{109}$$

that can be transformed to that originally derived by Gel'chinskiy by means of the differential geometry of surfaces. Similar expressions have also been derived recently by Hubral (1979).

Note that the Gel'chinskiy formula could be used as the starting point for the derivation of the dynamic ray tracing system for generally inhomogeneous three-dimensional media. This procedure was used by Gol'din (personal communication).

During the derivation of the above formulas, the unit vector $\hat{e}_2$ in the ray-centered coordinate system was assumed to be equal to the unit vector $\hat{d}_2$ in the local coordinate system at the point of incidence O. In a three-dimensional inhomogeneous medium, however, vector $\hat{e}_2$ generally makes an angle $\Omega \neq 0$ with $\hat{d}_2$ (in the sense that $\hat{e}_1 \cdot \hat{d}_2 = \sin \Omega$). Hence an initial rotation of $\hat{e}_1$ and $\hat{e}_2$ about $\hat{t}$ is necessary to secure the assumed parallelity of $\hat{e}_2$ and $\hat{d}_2$. Because the second term in equations (106) and (109) is independent of any such rotation by angle Ω, the nonzero value of Ω will result only in the appropriate transform of matrix $\mathbf{M}$ related to the incident wave and the matrix $\mathbf{E}$. Consequently, denoting the matrix of rotation by

$$\mathbf{W} = \begin{bmatrix} \cos \Omega & \sin \Omega \\ -\sin \Omega & \cos \Omega \end{bmatrix}, \tag{110}$$

equations (106) and (109) are transformed into

$$\tilde{\mathbf{M}} = \mathbf{S}\mathbf{W}^T\mathbf{M}\mathbf{W}\mathbf{S} + u\,\mathbf{G}\mathbf{D}\mathbf{G} + \frac{\sin i}{v}\,\mathbf{G}\bar{\mathbf{E}}\mathbf{G} \tag{106'}$$

and

$$\tilde{\mathbf{K}} = \frac{\tilde{v}}{v}\,\mathbf{S}\mathbf{W}^T\mathbf{K}\mathbf{W}\mathbf{S} + \tilde{v}u\,\mathbf{G}\mathbf{D}\mathbf{G} + \frac{\tilde{v}}{v}\sin i\,\mathbf{G}\bar{\mathbf{E}}\mathbf{G}, \tag{109'}$$

respectively. The matrix $\bar{\mathbf{E}}$ in these formulas is obtained from (107) if $v_{,1}$ is replaced by $(v_{,1} \cos \Omega + v_{,2} \sin \Omega)$ and $v_{,2}$ by $(v_{,2} \cos \Omega - v_{,1} \sin \Omega)$, respectively. The matrix of the second derivatives of the time field, $\mathbf{M}$, and the curvature matrix, $\mathbf{K}$, in (106') and (109'), respectively, are related to the incident wave at the point of incidence O, where the unit vector $\hat{e}_2$ makes the angle Ω with the vector $\hat{d}_2$ of the local coordinate system centered at that location. Similarly, the matrices $\tilde{\mathbf{M}}$ and $\tilde{\mathbf{K}}$ are related to the reflected and transmitted waves at O; their unit vectors $\hat{e}_2$ are assumed to coincide with the vector $\hat{d}_2$ at O. The meaning of remaining quantities in both expressions remains unchanged.

Conclusions

Basic formulas of the ray series method (also known in English literature as the asymptotic ray theory) were developed for generally inhomogeneous three-dimensional media using the ray-centered coordinate system. Introduction of this system resulted in a considerable simplification of the evaluation of amplitude coefficients for S waves, whose two principal components decoupled.

The ray-centered coordinate system was also used for the derivation of so-called dynamic ray tracing system which governs the second derivatives of the time field and all basic geometric characteristics (e.g., curvature and geometrical spreading) of

the wave fronts. The dynamic ray tracing system for three-dimensional generally inhomogeneous media is formed by the three nonlinear ordinary differential equations of the first order that can be conveniently written in matrix formulation with the help of the matrix of second derivatives of the time field. Several different modifications of the dynamic ray tracing system, involving matrices of curvatures or radii of curvatures, were also presented.

The phase matching method was implemented to determine discontinuities of individual quantities in the dynamic ray tracing system assuming that the wave was impinging on a curved interface separating two generally inhomogeneous media.

Special care was given to all aspects of evaluating the function J that plays a crucial role in the determination of geometrical spreading of the ray tube.

All final formulas were cast in a computationally convenient form that can be easily coded in any high level programming language.

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Appendix

Determination of basis vectors in the ray-centered coordinate system

In this section a simple method of practical determination of the right-handed basis $(\hat{t}, \hat{e}_1, \hat{e}_2)$ of the ray-centered coordinate system is presented. It is based on the technique originally proposed by Popov and Pšenčík (1978b) and recently modified by Pšenčík (1979). As it is presented here for the sake of completeness only, we will restrict ourselves to a rather concise exposition of the method, referring any interested reader to the above mentioned papers, where all details are thoroughly discussed.

Let it be assumed that the computation of rays is carried out in a Cartesian coordinate system $[x_1, x_2, x_3]$ with the help of the ray tracing system consisting of six ordinary differential equations of the first order (see section 3)

$$\frac{dx_i}{d\tau} = v^2 p_i, \qquad \frac{dp_i}{d\tau} = -\frac{\partial \ln v}{\partial x_i}, \qquad i = 1, 2, 3 \quad \text{(A1)}$$

that represent the characteristics of the eikonal equation

$$p_1^2 + p_2^2 + p_3^2 = \frac{1}{v^2}, \quad \text{(A2)}$$

with $p_i = \partial\tau/\partial x_i$. Once the ray has been computed, the components of tangent vector to the ray, t_i, are easily expressible in terms of velocity v and components of slowness vector, p_i, as

$$\hat{t} = (vp_1, vp_2, vp_3). \quad \text{(A3)}$$

Thus, the determination of $\hat{t}$ is straightforward. In the following, therefore, only the determination of the basis vectors $\hat{e}_1$, $\hat{e}_2$ will be discussed. They are determined in the following two steps: First, introduce a new auxiliary triplet of unit vectors ($\hat{t}$, $\hat{\epsilon}_1$, $\hat{\epsilon}_2$), which can be easily determined at any point of the ray. Second, find a relation between ($\hat{t}$, $\hat{\epsilon}_1$, $\hat{\epsilon}_2$) and ($\hat{t}$, $\hat{e}_1$, $\hat{e}_2$).

First step. Introduction of unit vectors $\hat{\epsilon}_1$, $\hat{\epsilon}_2$ satisfying the following two conditions: (a) the unit vectors $\hat{t}$, $\hat{\epsilon}_1$, $\hat{\epsilon}_2$ are mutually orthogonal and form a right-handed system; (b) the unit vector $\hat{\epsilon}_2$ lies in the plane $x_3 = 0$. This is easily done by choosing

$$\left.\begin{aligned} \hat{\epsilon}_1 &= (vL^{-1}p_1p_3,\ vL^{-1}p_2p_3,\ -vL) \\ \hat{\epsilon}_2 &= (-L^{-1}p_2,\ L^{-1}p_1,\ 0), \end{aligned}\right\} \tag{A4}$$

where $L = \sqrt{p_1^2 + p_2^2} \neq 0$. (A special case, when $p_1 = p_2 = 0$, can be handled by renumbering the coordinates axes x_i.) It can be seen that the vectors $\hat{\epsilon}_1$, $\hat{\epsilon}_2$ in (A4) satisfy the above conditions, and that they can be easily determined at any point of the ray.

Second step. Now, express the unit vectors $\hat{e}_1$, $\hat{e}_2$ in terms of $\hat{\epsilon}_1$, $\hat{\epsilon}_2$. As they all lie in the same plane (perpendicular to the ray), it can be written

$$\hat{e}_1 = \cos\Phi\hat{\epsilon}_1 - \sin\Phi\hat{\epsilon}_2, \qquad \hat{e}_2 = \sin\Phi\hat{\epsilon}_1 + \cos\Phi\hat{\epsilon}_2. \tag{A5}$$

Inserting (A4) into (A5) we get

$$\left.\begin{aligned} \hat{e}_1 &= (L^{-1}[vp_1p_3\cos\Phi + p_2\sin\Phi],\ L^{-1}[vp_2p_3\cos\Phi - p_1\sin\Phi],\ -vL\cos\Phi) \\ \hat{e}_2 &= (L^{-1}[vp_1p_3\sin\Phi - p_2\cos\Phi],\ L^{-1}[vp_2p_3\sin\Phi + p_1\cos\Phi\ ],\ -vL\sin\Phi). \end{aligned}\right\} \tag{A6}$$

Thus, the problem of determining $\hat{e}_1$ and $\hat{e}_2$ reduces to the determination of angle $\Phi(\tau)$ made by $\hat{\epsilon}_1$, and $\hat{e}_1$; all other quantities in (A6) are known. We determine $\Phi(\tau)$ by finding two independent expressions for $d\hat{e}_1(\tau)/d\tau$; their comparison gives a simple differential equation for $\Phi(\tau)$.

Differentiating the unit vector $\hat{e}_1$ with respect to τ, we get from (A5) the first formula for $d\hat{e}_1/d\tau$

$$\frac{d\hat{e}_1}{d\tau} = \frac{d\hat{\epsilon}_1}{d\tau}\cos\Phi - \frac{d\hat{\epsilon}_2}{d\tau}\sin\Phi - (\hat{\epsilon}_1\sin\Phi + \hat{\epsilon}_2\cos\Phi)\frac{d\Phi}{d\tau}. \tag{A7}$$

From (3) and (55) we obtain an alternate expression for $d\hat{e}_1/d\tau$

$$\frac{d\hat{e}_1}{d\tau} = (\nabla v\cdot\hat{e}_1)\hat{t}. \tag{A8}$$

Inserting (A6) into (A8) yields

$$\frac{d\hat{e}_1}{d\tau} = \left\{\cos\Phi\left[L^{-1}vp_3\left(p_1\frac{\partial v}{\partial x_1} + p_2\frac{\partial v}{\partial x_2}\right) - vL\frac{\partial v}{\partial x_3}\right] + \sin\Phi L^{-1}\left[p_2\frac{\partial v}{\partial x_1} - p_1\frac{\partial v}{\partial x_2}\right]\right\}\hat{t}. \tag{A9}$$

As the left-hand sides of (A7) and (A9) are the same, the right-hand sides must also be the same. It will be sufficient in this paper to compare only the third components of these expressions. After some manipulations

$$\frac{d\Phi}{d\tau} = \frac{p_3\left(p_2 \dfrac{\partial v}{\partial x_1} - p_1 \dfrac{\partial v}{\partial x_2}\right)}{p_1^2 + p_2^2} \tag{A10}$$

is obtained. In the derivation of (A10), the eikonal equation (A2) and the formula

$$\frac{d(vL)}{d\tau} = -L^{-1}v^2 p_3{}^2\left(p_1 \frac{\partial v}{\partial x_1} + p_2 \frac{\partial v}{\partial x_2}\right) + v^2 L p_3 \frac{\partial v}{\partial x_3}$$

have been considered, which follows directly from the ray tracing system (A1).

The equation (A10) can be integrated along the ray to produce

$$\Phi(\tau) = \int_{\tau_0}^{\tau} \frac{p_3\left(p_2 \dfrac{\partial v}{\partial x_1} - p_1 \dfrac{\partial v}{\partial x_2}\right)}{p_1^2 + p_2^2}\, d\tau + \Phi(\tau_0). \tag{A11}$$

This is the final formula for $\Phi(\tau)$. Inserting it into (A6) we obtain the desired simple expressions for $\hat{e}_1$ and $\hat{e}_2$. The computation of the torsion and the curvature of the ray is not necessary in this procedure.

Formula (A11) can be simply generalized for layered media with curved interfaces, when we take into account the jumps in Φ across the interface.

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