Tracing real-valued reference rays in anisotropic viscoelastic media

Luděk Klimeš

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

Summary

The eikonal equation in an attenuating medium has the form of a complex–valued Hamilton–Jacobi equation and must be solved in terms of the complex–valued travel time. A very suitable approximate method for calculating the complex–valued travel time right in real space is represented by the perturbation from the reference travel time calculated along real–valued reference rays to the complex–valued travel time defined by the complex–valued Hamilton–Jacobi equation.

The real–valued reference rays are calculated using the reference Hamiltonian function. The reference Hamiltonian function is constructed using the complex–valued Hamiltonian function corresponding to a given complex–valued Hamilton–Jacobi equation.

The ray tracing equations and the corresponding equations of geodesic deviation are often formulated in terms of the eigenvectors of the Christoffel matrix. Unfortunately, a complex–valued Christoffel matrix need not have all three eigenvectors at an S–wave singularity. We thus formulate the ray tracing equations and the corresponding equations of geodesic deviation using the eigenvalues of a complex–valued Christoffel matrix, without the eigenvectors of the Christoffel matrix. The resulting equations for the real–valued reference P–wave rays and real–valued reference common S–wave rays are applicable everywhere, including S–wave singularities.

Keywords

Attenuation, anisotropy, heterogeneous media, wave propagation, ray theory, complex–valued travel time, complex–valued Hamilton–Jacobi equation, complex–valued eikonal equation, perturbation methods.

Seismic Waves in Complex 3–D Structures, **30** (2020), 77–94 (ISSN 2336–3827, online at http://sw3d.cz)

1. Introduction

Attenuation is a very important phenomenon in wave propagation, and is essential whenever the intensity of waves matters.

The eikonal equation in an attenuating medium has the form of a complex–valued Hamilton–Jacobi equation and must be solved in terms of the complex–valued travel time. The solution of the complex–valued Hamilton–Jacobi equation for complex–valued travel time by Hamilton's (1837) equations of rays would require complex–valued rays (complex–valued geodesics). Since the material properties are known in real space only, we cannot calculate complex–valued rays. We thus need to calculate the complex–valued travel time right in real space. A very suitable approximate method for this purpose is represented by the perturbation from the reference travel time calculated along real–valued reference rays to the complex–valued travel time defined by the complex–valued Hamilton–Jacobi equation.

For this perturbation from the reference travel time to the complex–valued travel time, we need a complex–valued perturbation Hamiltonian function, i.e., a family of complex–valued Hamiltonian functions smoothly parametrized by one or more perturbation parameters. The perturbation Hamiltonian function must smoothly connect the reference Hamiltonian function with the Hamiltonian function corresponding to a given complex–valued Hamilton–Jacobi equation, and Hamilton's equations corresponding to the reference Hamiltonian function must yield real–valued reference rays. The reference Hamiltonian function and the complex–valued perturbation Hamiltonian function are constructed using the complex–valued Hamiltonian function corresponding to a given complex–valued Hamilton–Jacobi equation according to Klimeš & Klimeš (2011).

When a perturbation Hamiltonian function is constructed, we can calculate the perturbation derivatives (derivatives with respect to perturbation parameters) of travel time according to equations by Klimeš (2002), and construct the perturbation expansion (Taylor expansion with respect to perturbation parameters) of travel time. For the calculation of the n^{th} order perturbation derivatives of travel time, we need the perturbation derivatives of the perturbation Hamiltonian function up to the $(n{-}1)^{\text{th}}$ order and the phase–space and mixed derivatives of the perturbation Hamiltonian function up to the n^{th} order at the real–valued reference rays. Under phase space, we understand a spatial manifold parametrized by coordinates x^i with cotangent spaces parametrized by slowness–vector components p_i. The perturbation derivatives of travel time of all orders are calculated by simple numerical quadratures along unperturbed reference rays.

The anisotropic–ray–theory S–wave rays are smoothly but very sharply bent in a vicinity of the S–wave singularity or when crossing the split intersection singularity, and cannot be used as the reference rays, which was demonstrated by Bulant & Klimeš (2018). This problem can be overcome by tracing the reference common S–wave rays for both S–wave polarizations. Both S–wave travel times are then approximated by the perturbation from the reference common S–wave rays. In this paper, we thus concentrate on real–valued reference common S–wave rays instead of reference anisotropic–ray–theory S–wave rays.

The Hamiltonian function and its first–order phase–space derivatives are required in ray tracing. The second–order phase–space derivatives of the Hamiltonian function are required in solving the equations of geodesic deviation. The Hamiltonian function and its phase–space derivatives are usually calculated in terms of the eigenvectors of the Christoffel matrix (Klimeš, 2006; Vavryčuk, 2008; 2010). In this formulation, we need the S–wave eigenvectors of the Christoffel matrix even for calculating the geodesic deviation of P–wave rays.

Unfortunately, a complex–valued Christoffel matrix need not have all three eigenvectors at an S–wave singularity (Klimeš, 2020). In this paper, we thus follow Červený (1972) and formulate the ray tracing equations and the corresponding equations of geodesic deviation using the eigenvalues of a complex–valued Christoffel matrix, without the eigenvectors of the Christoffel matrix. The resulting equations for the real–valued reference P–wave rays and real–valued reference common S–wave rays are applicable everywhere, including S–wave singularities.

In Section 3, we summarize the equations for the Hamiltonian function and for its first–order and second–order phase–space derivatives. The equations were derived for a real–valued Hamiltonian function by Klimeš (2006) and are applicable to a complex–valued Hamiltonian function if the Christoffel matrix has three orthonormal eigenvectors.

In Section 4, we convert the equations for the Hamiltonian function and for its first–order and second–order phase–space derivatives into the corresponding equations formulated without the eigenvectors.

In Section 5, we summarize the construction of the reference Hamiltonian function and of its first–order and second–order phase–space derivatives for tracing the real–valued reference rays according to Klimeš & Klimeš (2011).

In Section 6, we mention the transformation of the real–valued reference rays at structural interfaces.

In Section 7, we summarize the perturbation expansion of complex–valued travel time along real–valued reference rays.

Although we present the equations for homogeneous Hamiltonian functions of various degrees, we propose to prefer homogeneous Hamiltonian functions of degree $N = -1$ with respect to the slowness vector. Homogeneous Hamiltonian functions of degree $N = -1$ usually yield the most accurate linear perturbations of travel time, which was theoretically explained by Klimeš (2002, sec. 4.4), numerically demonstrated by Bulant & Klimeš (2008) in examples of perturbations from isotropic reference rays and common anisotropic reference rays in an anisotropic elastic medium, and also numerically demonstrated by Vavryčuk (2012) in examples of perturbations from real–valued reference rays to the complex–valued travel time in two isotropic attenuating media.

We use the componental notation for vectors and matrices. For example, p_i stands for the covariant vector with components p_i. The Einstein summation over repetitive lower–case Roman indices is used throughout the paper. The summation does not apply to subscripts α corresponding to the derivatives with respect to the perturbation parameter and to subscripts in parentheses corresponding to the eigenvectors of the Christoffel matrix.

2. Complex–valued Christoffel matrix

2.1. Complex–valued frequency–domain stiffness tensor

The 3×3×3×3 frequency–domain stiffness tensor (elastic tensor, tensor of elastic moduli) $c_{ijkl} = c_{ijkl}(x^m, \omega)$ is complex–valued in viscoelastic media. It is symmetric with respect to the first pair of indices

$$c_{ijkl} = c_{jikl} \tag{1}$$

and with respect to the second pair of indices

$$c_{ijkl} = c_{ijlk} \quad . \tag{2}$$

It is thus frequently expressed in the form of the 6×6 stiffness matrix which lines correspond to the first pair of indices and columns to the second pair of indices.

We assume in this paper that the stiffness tensor is symmetric with respect to the exchange of the first pair of indices and the second pair of indices,

$$c_{ijkl} = c_{klij} \quad , \tag{3}$$

i.e., that the 6×6 stiffness matrix is symmetric.

Hereinafter, we shall consider the $3 \times 3 \times 3 \times 3$ frequency–domain density–reduced stiffness tensor

$$a_{ijkl} = c_{klij}\, \varrho^{-1} \quad , \tag{4}$$

where ϱ is a real–valued density. Density–reduced stiffness tensor (4) obviously obeys symmetry relations (1)–(3).

2.2. Complex–valued Christoffel matrix and its eigenvalues

The Christoffel matrix reads

$$\Gamma_{ij}(x^m, p_n) = a_{ikjl}(x^m)\, p_k p_l \quad , \tag{5}$$

where x^m are the Cartesian coordinates, $a_{ijkl}(x^m)$ the density–normalized elastic moduli, and p_i the components of the slowness vector.

The Christoffel matrix is a symmetric real–valued matrix for real–valued stiffness tensor $a_{ikjl}(x^m)$ and slowness vector p_i. The Christoffel matrix a symmetric complex–valued matrix for complex–valued stiffness tensor $a_{ikjl}(x^m)$. The Christoffel matrix is a quadratic function of the slowness vector, and its three eigenvalues are then homogeneous functions of the second degree with respect to the slowness vector.

The 3×3 Christoffel matrix Γ_{ij} has three eigenvalues $G_{(a)}$, $a = 1, 2, 3$. The eigenvalues are the solutions of the cubic characteristic equation

$$G^3 - G^2 \operatorname{tr}(\Gamma_{ij}) + G \operatorname{tr}(\widetilde{\Gamma}_{ij}) - \det(\Gamma_{ij}) = 0 \quad , \tag{6}$$

where

$$\operatorname{tr}(\widetilde{\Gamma}_{ij}) = (\Gamma_{11})^2 + (\Gamma_{22})^2 + (\Gamma_{33})^2 - (\Gamma_{12})^2 - (\Gamma_{13})^2 - (\Gamma_{23})^2 \tag{7}$$

is the trace of the matrix $\widetilde{\Gamma}_{ij}$ of the cofactors of 3×3 Christoffel matrix Γ_{ij}. We shall use $G_{(3)}$ for the eigenvalue with the largest real part, which corresponds to the P wave. We shall use $G_{(1)}$ and $G_{(2)}$ for two other eigenvalues corresponding to S waves.

In a vicinity of the S–wave singularity, the relative rounding errors of S–wave eigenvalues $G_{(1)}$ and $G_{(2)}$ may approach 0.001 for single–precision coefficients of cubic characteristic equation (6). However, the numerical error of the average value of S–wave eigenvalues $G_{(1)}$ and $G_{(2)}$ corresponds to machine precision even in this case, independently on the kind of averaging. The numerical error of P–wave eigenvalue $G_{(3)}$ corresponds to machine precision.

We assume in this paper that P–wave eigenvalue $G_{(3)}$ is different from S–wave eigenvalues $G_{(1)}$ and $G_{(2)}$, because P–wave eigenvalue $G_{(3)}$ may approach one of the S–wave eigenvalues just for extremely strong anisotropy.

2.3. Phase–space derivatives of the Christoffel matrix

As we need to handle both the derivatives with respect to x^m and p_n, we denote any partial phase–space derivative by $'$ or *. Both Γ'_{ij} and $\Gamma^\star_{ij}$ then stand for the first–order partial phase–space derivatives

$$\Gamma_{ij,k} \equiv \frac{\partial \Gamma_{ij}}{\partial x^k} = \frac{\partial a_{imjn}}{\partial x^k} p_m p_n \tag{8}$$

or

$$\Gamma_{ij}^{,k} \equiv \frac{\partial \Gamma_{ij}}{\partial p_k} = (a_{ikjm} + a_{imjk}) p_m \quad . \tag{9}$$

Analogously, $\Gamma'^\star_{ij}$ stands for the second–order partial phase–space derivatives

$$\Gamma_{ij,kl} \equiv \frac{\partial^2 \Gamma_{ij}}{\partial x^k \partial x^l} = \frac{\partial^2 a_{imjn}}{\partial x^k \partial x^l} p_m p_n \tag{10}$$

or

$$\Gamma_{ij,k}^{,l} \equiv \frac{\partial^2 \Gamma_{ij}}{\partial x^k \partial p_l} = \frac{\partial (a_{iljm} + a_{imjl})}{\partial x^k} p_m \tag{11}$$

or

$$\Gamma_{ij}^{,kl} \equiv \frac{\partial^2 \Gamma_{ij}}{\partial p_k \partial p_l} = a_{ikjl} + a_{iljk} \tag{12}$$

(Červený, 2001, eq. 4.14.8).

3. Complex–valued Hamiltonian function expressed in terms of the eigenvectors of the Christoffel matrix

If all three eigenvalues of the Christoffel matrix are different, the complex–valued Christoffel matrix has three complex–valued unit eigenvectors $g_{i(a)}$ corresponding to eigenvalues $G_{(a)}$ defined by equations

$$g_{i(a)} G_{(a)} = \Gamma_{ij} g_{j(a)} \tag{13}$$

and

$$g_{i(a)} g_{i(a)} = 1 \tag{14}$$

(no summation over $_{(a)}$). These eigenvectors are mutually orthogonal,

$$g_{i(a)} g_{i(b)} = 0 \quad \text{for} \quad b \neq a \quad . \tag{15}$$

If the Christoffel matrix is real–valued, its eigenvectors $g_{i(a)}$ are real–valued.

Note that the numerical errors of the S–wave eigenvalues in a vicinity of the S–wave singularity calculated by solving equations (13) are considerably smaller than the numerical errors when solving characteristic equation (6). However, this better accuracy probably implies no practical advantage in applying ray methods.

If the S–wave eigenvalues of the real–valued Christoffel matrix are equal, the corresponding orthonormal S–wave eigenvectors $g_{i(1)}$ and $g_{i(2)}$ can be selected arbitrarily in the plane orthogonal to the P–wave eigenvector $g_{i(3)}$.

If the S–wave eigenvalues of the complex–valued Christoffel matrix are equal, the corresponding S–wave eigenvectors $g_{i(1)}$ and $g_{i(2)}$ need not exist (Klimeš, 2020).

We summarize the equations for the Hamiltonian function in this section. The equations were derived for a real–valued Hamiltonian function by Klimeš (2006) and are applicable to a complex–valued Hamiltonian function if the Christoffel matrix has three orthonormal eigenvectors.

In the next Section 4, we convert these equations into the corresponding equations formulated without the eigenvectors.

3.1. Phase–space derivatives of the eigenvalues of the Christoffel matrix

If all three eigenvectors of the complex–valued Christoffel matrix exist, we transform Christoffel matrix (5), its first–order phase–space derivatives (8), (9), and second–order phase–space derivatives (10), (11), (12) into the eigenvectors,

$$\Gamma_{(ab)} = g_{i(a)}\Gamma_{ij}g_{j(b)} \quad , \tag{16}$$

$$\Gamma'_{(ab)} = g_{i(a)}\Gamma'_{ij}g_{j(b)} \quad , \tag{17}$$

$$\Gamma'^{\star}_{(ab)} = g_{i(a)}\Gamma'^{\star}_{ij}g_{j(b)} \quad . \tag{18}$$

The eigenvalue of the Christoffel matrix may then be expressed as (Klimeš, 2006, eq. 21)

$$G_{(a)} = \Gamma_{(aa)} \quad . \tag{19}$$

The first–order phase–space derivatives of the eigenvalue of the Christoffel matrix may be expressed as (Klimeš, 2006, eq. 22)

$$G'_{(a)} = \Gamma'_{(aa)} \quad , \tag{20}$$

and the second–order phase–space derivatives of the eigenvalue of the Christoffel matrix may be expressed as (Klimeš, 2006, eq. 23)

$$G'^{\star}_{(a)} = \Gamma'^{\star}_{(aa)} + 2\sum_{b\neq a}\frac{\Gamma'_{(ab)}\Gamma^{\star}_{(ab)}}{G_{(a)} - G_{(b)}} \quad . \tag{21}$$

Equations (8)–(12), (17), (18), (20) and (21) are suitable for the numerical calculation of the first–order and second–order partial phase–space derivatives of the eigenvalues of the Christoffel matrix.

3.2. Reference anisotropic–ray–theory rays

The P–wave eigenvector $g_{i(3)}$ of the Christoffel matrix is usually well defined. S–wave eigenvectors $g_{i(1)}$ and $g_{i(2)}$ are reasonably defined if the relative difference

$$2\,|G_{(1)} - G_{(2)}|/|G_{(1)} + G_{(2)}| \tag{22}$$

of the S–wave eigenvalues is sufficiently greater than a given minimum relative difference. The angular numerical error of the S–wave eigenvectors in radians roughly corresponds to the relative rounding error divided by relative difference (22). A typical given minimum relative difference in single precision is about 0.00001. If the relative difference (22) is smaller than a given minimum relative difference, the first–order phase space derivatives of the S–wave eigenvalues are considerably inaccurate, the second–order phase space derivatives of the S–wave eigenvalues are meaningless, the KMAH index and the matrix of geometrical spreading may be considerably erroneous, and we have to terminate tracing anisotropic–ray–theory S–wave rays.

We consider here Hamiltonian functions homogeneous of arbitrary degree N with respect to slowness vector p_i. According to Euler's theorem on homogeneous functions, the parameter along rays is then proportional to the travel time. Note that order $N = -1$ is best suited for travel–time perturbations.

The homogeneous Hamiltonian function of degree N for tracing the reference anisotropic–ray–theory rays reads

$$H_{(a)} = \tfrac{1}{N}(G_{(a)})^{\frac{N}{2}} \quad , \tag{23}$$

its first–order partial phase–space derivatives are

$$H'_{(a)} = \tfrac{1}{2} G'_{(a)} (G_{(a)})^{\frac{N}{2}-1} \quad , \tag{24}$$

and its second–order partial phase–space derivatives are

$$H'^{\star}_{(a)} = \tfrac{1}{2} G'^{\star}_{(a)} (G_{(a)})^{\frac{N}{2}-1} + \tfrac{N-2}{4} G'_{(a)} G^{\star}_{(a)} (G_{(a)})^{\frac{N}{2}-2} \quad . \tag{25}$$

The anisotropic–ray–theory S–wave rays are smoothly but very sharply bent in a vicinity of the S–wave singularity or when crossing the split intersection singularity, and cannot be used as the reference rays, which was demonstrated by Bulant & Klimeš (2018). In this case, we need the reference common S–wave rays.

3.3. Reference common S–wave rays

In the coupling ray theory, both S–wave polarizations are coupled. It is thus useful to have reference common rays equally suitable for both S–wave polarizations. For common–ray tracing, we shall thus consider the averaged Hamiltonian function of both S–wave polarizations,

$$H = \tfrac{1}{2N} \left[(G_{(1)})^{\frac{N}{2}} + (G_{(2)})^{\frac{N}{2}} \right] \quad . \tag{26}$$

Note that we obtain different anisotropic common rays and different reference travel–time fields for different N. The first–order partial phase–space derivatives read

$$H' = \tfrac{1}{4} \left[G'_{(1)} (G_{(1)})^{\frac{N}{2}-1} + G'_{(2)} (G_{(2)})^{\frac{N}{2}-1} \right] \quad , \tag{27}$$

and the second–order partial phase–space derivatives read (Klimeš, 2006, eq. 31)

$$\begin{aligned} H'^{\star} = \frac{1}{4} \left[\Gamma'^{\star}_{(11)} (G_{(1)})^{\frac{N}{2}-1} + \Gamma'^{\star}_{(22)} (G_{(2)})^{\frac{N}{2}-1} \right] + \frac{\Gamma'_{(13)} \Gamma^{\star}_{(13)} (G_{(1)})^{\frac{N}{2}-1}}{2\,(G_{(1)} - G_{(3)})} + \frac{\Gamma'_{(23)} \Gamma^{\star}_{(23)} (G_{(2)})^{\frac{N}{2}-1}}{2\,(G_{(2)} - G_{(3)})} \\ + \frac{C_0}{2} \Gamma'_{(12)} \Gamma^{\star}_{(12)} + \frac{N-2}{8} \left[\Gamma'_{(11)} \Gamma^{\star}_{(11)} (G_{(1)})^{\frac{N}{2}-2} + \Gamma'_{(22)} \Gamma^{\star}_{(22)} (G_{(2)})^{\frac{N}{2}-2} \right] , \end{aligned} \tag{28}$$

where

$$C_0 = \frac{(G_{(1)})^{\frac{N}{2}-1} - (G_{(2)})^{\frac{N}{2}-1}}{G_{(1)} - G_{(2)}} \quad . \tag{29}$$

The term with $G_{(1)} - G_{(2)}$ in the denominator is possibly singular. It is thus desirable to carry out the division by $G_{(1)} - G_{(2)}$ analytically. For $N=2$ (Klimeš, 2006, eq. 32),

$$C_0 = 0 \quad . \tag{30}$$

For $N=1$ (Klimeš, 2006, eq. 33),

$$C_0 = -\frac{1}{(G_{(1)})^{\frac{1}{2}} (G_{(2)})^{\frac{1}{2}} [(G_{(1)})^{\frac{1}{2}} + (G_{(2)})^{\frac{1}{2}}]} \quad . \tag{31}$$

For $N=-1$ (Klimeš, 2006, eq. 34),

$$C_0 = -\frac{G_{(1)} + (G_{(1)} G_{(2)})^{\frac{1}{2}} + G_{(2)}}{(G_{(1)})^{\frac{3}{2}} (G_{(2)})^{\frac{3}{2}} [(G_{(1)})^{\frac{1}{2}} + (G_{(2)})^{\frac{1}{2}}]} \quad . \tag{32}$$

For $N=-2$ (Klimeš, 2006, eq. 35),

$$C_0 = -\frac{G_{(1)} + G_{(2)}}{(G_{(1)})^2 (G_{(2)})^2} \quad . \tag{33}$$

The above equations can be used at an S–wave singularity and its vicinity if both the orthonormal S–wave eigenvectors $g_{i(1)}$ and $g_{i(2)}$ of the complex–valued Christoffel matrix are well defined.

4. Complex–valued Hamiltonian function expressed without the eigenvectors of the Christoffel matrix

4.1. Reference P–wave rays

Eigenvector $g_{i(3)}$ corresponding to the P wave is usually well defined for both symmetric real–valued and complex–valued Christoffel matrices. However, one of the S–wave eigenvectors $g_{i(1)}$ and $g_{i(2)}$ need not exist in a case of a complex–valued Christoffel matrix (Klimeš, 2020), which prevents us from using expression (21) to calculate the second–order phase space derivatives of the P–wave eigenvalue.

We thus define matrix

$$G_{ij} = g_{i(3)}\, g_{j(3)} \quad , \tag{34}$$

where $g_{i(3)}$ is the unit complex–valued eigenvector of the symmetric complex–valued Christoffel matrix corresponding to complex–valued P–wave eigenvalue $G_{(3)}$. Matrix (34) can be expressed in terms of the matrix

$$D_{ij} = \tfrac{1}{2}\, \varepsilon_{ikl}\, \varepsilon_{jmn}\, (G_{(3)}\delta_{km} - \Gamma_{km})\, (G_{(3)}\delta_{km} - \Gamma_{ln}) \tag{35}$$

of the cofactors of 3×3 matrix $G_{(3)}\delta_{ij} - \Gamma_{ij}$ (Červený, 1972) as

$$G_{ij} = D_{ij}[\mathrm{tr}(D_{mn})]^{-1} \quad . \tag{36}$$

Note that

$$\mathrm{tr}(D_{mn}) = (G_{(3)} - G_{(1)})(G_{(3)} - G_{(2)}) \quad . \tag{37}$$

We define symmetric projection matrix

$$E_{ij} = \delta_{ij} - G_{ij} \tag{38}$$

onto the plane perpendicular to eigenvector $g_{k(3)}$, and the projection

$$F_{ij} = \Gamma_{ij} - G_{(3)} G_{ij} \tag{39}$$

of the Christoffel matrix onto the plane perpendicular to eigenvector $g_{k(3)}$.

The expression

$$G'_{(3)} = \Gamma'_{ij} G_{ij} \tag{40}$$

for the first–order phase space derivatives of the P–wave eigenvalue follows from expression (20). The expression

$$G'^{\star}_{(3)} = \Gamma'^{\star}_{ij} G_{ij} + 2\Gamma'_{ij}\Gamma^{\star}_{kl} G_{ik} P_{jl} \quad , \tag{41}$$

where

$$P_{ij} = [(G_{(3)} - G_{(1)} - G_{(2)}) E_{ij} + F_{ij}][(G_{(3)} - G_{(1)})(G_{(3)} - G_{(2)})]^{-1} \quad , \tag{42}$$

for the second–order phase space derivatives of the P–wave eigenvalue follows from expression (21).

4.2. Reference common S–wave rays

The limit

$$\lim_{G_{(2)}\to G_{(1)}} C_0 = \left(\tfrac{N}{2}-1\right)\left(G_{(1)}\right)^{\frac{N}{2}-2} \quad . \tag{43}$$

of factor C_0 in expression (28) at an S–wave singularity can be obtained by l'Hospital's rule. Since factor C_0 is finite, the last but one term $\frac{C_0}{2}\,\Gamma'_{(12)}\Gamma^{\star}_{(12)}$ in expression (28) is undefined at an S–wave singularity because eigenvectors $g_{i(1)}$ and $g_{i(2)}$ have no limit there. The same applies to the last term. We thus rewrite expression (28) as

$$H'^{\star} = \frac{1}{4}\left[\Gamma'^{\star}_{(11)}\left(G_{(1)}\right)^{\frac{N}{2}-1} + \Gamma'^{\star}_{(22)}\left(G_{(2)}\right)^{\frac{N}{2}-1}\right] + \frac{\Gamma'_{(13)}\Gamma^{\star}_{(13)}\left(G_{(1)}\right)^{\frac{N}{2}-1}}{2\left(G_{(1)}-G_{(3)}\right)} + \frac{\Gamma'_{(23)}\Gamma^{\star}_{(23)}\left(G_{(2)}\right)^{\frac{N}{2}-1}}{2\left(G_{(2)}-G_{(3)}\right)}$$
$$+\tfrac{B}{2}\,\Gamma'_{(12)}\Gamma^{\star}_{(12)} + \tfrac{N-2}{8}\left[\Gamma'_{(11)}\Gamma^{\star}_{(11)}\left(G_{(1)}\right)^{\frac{N}{2}-2} + 2\,\Gamma'_{(12)}\Gamma^{\star}_{(12)}\left(G_{(1)}G_{(2)}\right)^{\frac{N}{4}-1} + \Gamma'_{(22)}\Gamma^{\star}_{(22)}\left(G_{(2)}\right)^{\frac{N}{2}-2}\right], \tag{44}$$

where

$$B = C_0 - \left(\tfrac{N}{2}-1\right)\left(G_{(1)}\right)^{\frac{N}{4}-1}\left(G_{(2)}\right)^{\frac{N}{4}-1} \quad . \tag{45}$$

The limit

$$\lim_{G_{(2)}\to G_{(1)}} B = 0 \quad . \tag{46}$$

of B at an S–wave singularity directly follows from limit (43).

We shall see below that all terms in expression (44) have defined limits when approaching an S–wave singularity.

To transform derivatives Γ'_i and $\Gamma'^{\star}_{ij}$ of the Christoffel matrix into matrices $\Gamma'_{(aa)}$ and $\Gamma'^{\star}_{(ab)}$ determined by definitions (17) and (18), we need matrices

$$g_{i(1)}\,g_{k(1)} = \left[F_{ij} - E_{ij}G_{(2)}\right]\left[G_{(1)} - G_{(2)}\right]^{-1} \tag{47}$$

and

$$g_{i(2)}\,g_{k(2)} = -\left[F_{ik} - E_{ik}G_{(1)}\right]\left[G_{(1)} - G_{(2)}\right]^{-1} \tag{48}$$

in addition to matrix (34). Unfortunately, matrices (47) and (48) are undefined at an S–wave singularity because eigenvectors $g_{i(1)}$ and $g_{i(2)}$ have no limit there. We thus construct linear combinations

$$C_{ik0} = g_{i(1)}\,g_{k(1)}\left(G_{(1)}\right)^{\frac{N}{2}-1} + g_{i(2)}\,g_{k(2)}\left(G_{(2)}\right)^{\frac{N}{2}-1} \quad , \tag{49}$$

$$C_{ik1} = g_{i(1)}\,g_{k(1)}\left(G_{(1)}\right)^{\frac{N}{2}-1}G_{(2)} + g_{i(2)}\,g_{k(2)}\left(G_{(2)}\right)^{\frac{N}{2}-1}G_{(1)} \tag{50}$$

and

$$C_{ik3} = g_{i(1)}\,g_{k(1)}\left(G_{(1)}\right)^{\frac{N}{4}-1} + g_{i(2)}\,g_{k(2)}\left(G_{(2)}\right)^{\frac{N}{4}-1} \tag{51}$$

of matrices (47) and (48) useful in calculating expression (44).

We insert relations (47) and (48) into definition (49) and obtain

$$C_{ik0} = C_0\,F_{ik} - C_1\,E_{ik} \quad , \tag{52}$$

where C_0 is given by definition (29) and

$$C_1 = \left[\left(G_{(1)}\right)^{\frac{N}{2}-1}G_{(2)} - \left(G_{(2)}\right)^{\frac{N}{2}-1}G_{(1)}\right]\left[G_{(1)} - G_{(2)}\right]^{-1} \quad . \tag{53}$$

We insert relations (47) and (48) into definition (50) and obtain

$$C_{ik1} = C_1\,F_{ik} - C_2\,E_{ik} \quad , \tag{54}$$

where

$$C_2 = \left[(G_{(1)})^{\frac{N}{2}-1}(G_{(2)})^2 - (G_{(2)})^{\frac{N}{2}-1}(G_{(1)})^2\right]\left[G_{(1)} - G_{(2)}\right]^{-1} \quad . \tag{55}$$

We insert relations (47) and (48) into definition (51) and obtain

$$C_{ik3} = C_3\, F_{ik} - C_4\, E_{ik} \quad , \tag{56}$$

where

$$C_3 = \left[(G_{(1)})^{\frac{N}{4}-1} - (G_{(2)})^{\frac{N}{4}-1}\right]\left[G_{(1)} - G_{(2)}\right]^{-1} \tag{57}$$

and

$$C_4 = \left[(G_{(1)})^{\frac{N}{4}-1}G_{(2)} - (G_{(2)})^{\frac{N}{4}-1}G_{(1)}\right]\left[G_{(1)} - G_{(2)}\right]^{-1} \quad . \tag{58}$$

The finite limits

$$\lim_{G_{(2)}\to G_{(1)}} C_1 = \left(\tfrac{N}{2} - 2\right)(G_{(1)})^{\frac{N}{2}-1} \quad , \tag{59}$$

$$\lim_{G_{(2)}\to G_{(1)}} C_2 = \left(\tfrac{N}{2} - 3\right)(G_{(1)})^{\frac{N}{2}} \quad , \tag{60}$$

$$\lim_{G_{(2)}\to G_{(1)}} C_3 = \left(\tfrac{N}{4} - 1\right)(G_{(1)})^{\frac{N}{4}-2} \tag{61}$$

and

$$\lim_{G_{(2)}\to G_{(1)}} C_4 = \left(\tfrac{N}{4} - 2\right)(G_{(1)})^{\frac{N}{4}-1} \tag{62}$$

at an S–wave singularity can be obtained by l'Hospital's rule.

Inserting definitions (17)–(18) into expression (27) and considering relations (47)–(49), we arrive at expression

$$H' = \frac{1}{4}\Gamma'_{ij}C_{ij0} \quad . \tag{63}$$

Inserting definitions (17)–(18) into expression (44) and considering relations (47)–(51), we arrive at expression

$$\begin{aligned} H'^{\star} = {} & \frac{1}{4}\Gamma'^{\star}_{ij}C_{ij0} + \frac{\Gamma'_{ij}\Gamma^{\star}_{kl}\left(C_{ik1} - G_{(3)}C_{ik0}\right)G_{jl}}{2\,(G_{(1)} - G_{(3)})(G_{(2)} - G_{(3)})} \\ & + \tfrac{C}{2}\,\Gamma'_{ij}\Gamma^{\star}_{kl}\left(F_{ik} - E_{ik}G_{(1)}\right)\left(F_{jl} - E_{jl}G_{(2)}\right) + \tfrac{N-2}{8}\,\Gamma'_{ij}\Gamma^{\star}_{kl}C_{ik3}C_{jl3} \quad , \end{aligned} \tag{64}$$

where

$$C = -B\left[G_{(1)} - G_{(2)}\right]^{-2} \quad . \tag{65}$$

Considering (46), we apply l'Hospital's rule twice to calculate

$$\lim_{G_{(2)}\to G_{(1)}} B\left[G_{(1)} - G_{(2)}\right]^{-1} = 0 \quad . \tag{66}$$

Considering (66), we then apply l'Hospital's rule three times to calculate

$$\lim_{G_{(2)}\to G_{(1)}} C = -\left(\tfrac{N}{2} - 1\right)\left(\tfrac{N}{2} - 2\right)\tfrac{N}{48}(G_{(1)})^{\frac{N}{2}-4} \quad . \tag{67}$$

Definitions (29), (53), (55), (57), (58) and (65) of coefficients C_0, C_1, C_2, C_3, C_4 and C are applicable outside S–wave singularities. They are not applicable in a vicinity of S–wave singularities due to rounding errors. Limits (43), (59)–(62) and (67) of coefficients C_0, C_1, C_2, C_3, C_4 and C are applicable at S–wave singularities but are inaccurate in a vicinity of S–wave singularities.

We thus need the expressions for coefficients C_0, C_1, C_2, C_3, C_4 and C applicable both outside S–wave singularities and at S–wave singularities in order to use expressions (63) and (64). We now derive such expressions for cases $N=2$, $N=1$, $N=-1$ and $N=-2$. Note that order $N=-1$ is best suited for perturbation expansion of complex–valued travel time along real–valued reference rays.

4.2.1. Common S–wave Hamiltonian function of the second order

For $N=2$, factor C_0 is given by expression (30), and factors

$$C_1 = -1 \tag{68}$$

and

$$C_2 = -\big(G_{(1)} + G_{(2)}\big) \tag{69}$$

simply follow from definitions (53) and (55). Factor

$$C = 0 \quad , \tag{70}$$

is a simple special case of definitions (45) and (65) with factor (30). Factors C_3 and C_4 are irrelevant because

$$N-2 = 0 \quad . \tag{71}$$

4.2.2. Common S–wave Hamiltonian function of the first order

For $N=1$, factor C_0 is given by expression (31). Factor (53) reads

$$C_1 = -\frac{(G_{(1)})^{\frac{3}{2}} - (G_{(2)})^{\frac{3}{2}}}{(G_{(1)})^{\frac{1}{2}}(G_{(2)})^{\frac{1}{2}}\big(G_{(1)} - G_{(2)}\big)} \quad . \tag{72}$$

We reduce the fraction in expression (72) by factor $(G_{(1)})^{\frac{1}{2}} - (G_{(2)})^{\frac{1}{2}}$ and obtain

$$C_1 = -\frac{G_{(1)} + (G_{(1)})^{\frac{1}{2}}(G_{(2)})^{\frac{1}{2}} + G_{(2)}}{(G_{(1)})^{\frac{1}{2}}(G_{(2)})^{\frac{1}{2}}\big[(G_{(1)})^{\frac{1}{2}} + (G_{(2)})^{\frac{1}{2}}\big]} \quad . \tag{73}$$

Factor (55) reads

$$C_2 = -\frac{(G_{(1)})^{\frac{5}{2}} - (G_{(2)})^{\frac{5}{2}}}{(G_{(1)})^{\frac{1}{2}}(G_{(2)})^{\frac{1}{2}}\big(G_{(1)} - G_{(2)}\big)} \quad . \tag{74}$$

We reduce the fraction in expression (74) by factor $(G_{(1)})^{\frac{1}{2}} - (G_{(2)})^{\frac{1}{2}}$ and arrive at

$$C_2 = -\frac{(G_{(1)})^2 + (G_{(1)})^{\frac{3}{2}}(G_{(2)})^{\frac{1}{2}} + G_{(1)}G_{(2)} + (G_{(1)})^{\frac{1}{2}}(G_{(2)})^{\frac{3}{2}} + (G_{(2)})^2}{(G_{(1)})^{\frac{1}{2}}(G_{(2)})^{\frac{1}{2}}\big[(G_{(1)})^{\frac{1}{2}} + (G_{(2)})^{\frac{1}{2}}\big]} \quad . \tag{75}$$

Note that factor (75) may also be expressed as

$$C_2 = -\frac{[(G_{(1)})^{\frac{1}{2}} + (G_{(2)})^{\frac{1}{2}}][(G_{(1)})^{\frac{3}{2}} + (G_{(2)})^{\frac{3}{2}}] + G_{(1)}G_{(2)}}{(G_{(1)})^{\frac{1}{2}}(G_{(2)})^{\frac{1}{2}}\big[(G_{(1)})^{\frac{1}{2}} + (G_{(2)})^{\frac{1}{2}}\big]} \quad . \tag{76}$$

Factor (57) reads

$$C_3 = -\frac{(G_{(1)})^{\frac{3}{4}} - (G_{(2)})^{\frac{3}{4}}}{(G_{(1)})^{\frac{3}{4}}(G_{(2)})^{\frac{3}{4}}\big[G_{(1)} - G_{(2)}\big]} \quad . \tag{77}$$

We reduce the fraction in expression (77) by factor $(G_{(1)})^{\frac{1}{4}} - (G_{(2)})^{\frac{1}{4}}$ obtain

$$C_3 = -\frac{(G_{(1)})^{\frac{1}{2}} + (G_{(1)})^{\frac{1}{4}}(G_{(2)})^{\frac{1}{4}} + (G_{(2)})^{\frac{1}{2}}}{(G_{(1)})^{\frac{3}{4}}(G_{(2)})^{\frac{3}{4}}\big[(G_{(1)})^{\frac{1}{4}} + (G_{(2)})^{\frac{1}{4}}\big]\big[(G_{(1)})^{\frac{1}{2}} + (G_{(2)})^{\frac{1}{2}}\big]} \quad . \tag{78}$$

Factor (58) reads

$$C_4 = -\frac{(G_{(1)})^{\frac{7}{4}} - (G_{(2)})^{\frac{7}{4}}}{(G_{(1)})^{\frac{3}{4}}(G_{(2)})^{\frac{3}{4}}\left[G_{(1)} - G_{(2)}\right]} \quad . \tag{79}$$

We reduce the fraction in expression (79) by factor $(G_{(1)})^{\frac{1}{4}} - (G_{(2)})^{\frac{1}{4}}$ and arrive at

$$C_4 = -\frac{(G_{(1)})^{\frac{6}{4}} + (G_{(1)})^{\frac{5}{4}}(G_{(2)})^{\frac{1}{4}} + G_{(1)}(G_{(2)})^{\frac{2}{4}} + (G_{(1)})^{\frac{3}{4}}(G_{(2)})^{\frac{3}{4}} + (G_{(1)})^{\frac{2}{4}}G_{(2)} + (G_{(1)})^{\frac{1}{4}}(G_{(2)})^{\frac{5}{4}} + (G_{(2)})^{\frac{6}{4}}}{(G_{(1)})^{\frac{3}{4}}(G_{(2)})^{\frac{3}{4}}\left[(G_{(1)})^{\frac{1}{4}} + (G_{(2)})^{\frac{1}{4}}\right]\left[(G_{(1)})^{\frac{1}{2}} + (G_{(2)})^{\frac{1}{2}}\right]} \quad . \tag{80}$$

Note that factor (80) may also be expressed as

$$C_4 = -\frac{\left[(G_{(1)})^{\frac{1}{2}} + (G_{(1)})^{\frac{1}{4}}(G_{(2)})^{\frac{1}{4}} + (G_{(2)})^{\frac{1}{2}}\right]\left[G_{(1)} + G_{(2)}\right] + (G_{(1)})^{\frac{3}{4}}(G_{(2)})^{\frac{3}{4}}}{(G_{(1)})^{\frac{3}{4}}(G_{(2)})^{\frac{3}{4}}\left[(G_{(1)})^{\frac{1}{4}} + (G_{(2)})^{\frac{1}{4}}\right]\left[(G_{(1)})^{\frac{1}{2}} + (G_{(2)})^{\frac{1}{2}}\right]} \quad . \tag{81}$$

Definitions (45) and (65) with factor (31) yield

$$C = \frac{1}{2}\frac{2 - (G_{(1)})^{-\frac{1}{4}}(G_{(2)})^{-\frac{1}{4}}\left[(G_{(1)})^{\frac{1}{2}} + (G_{(2)})^{\frac{1}{2}}\right]}{(G_{(1)})^{\frac{1}{2}}(G_{(2)})^{\frac{1}{2}}\left[(G_{(1)})^{\frac{1}{2}} + (G_{(2)})^{\frac{1}{2}}\right]\left[G_{(1)} - G_{(2)}\right]^2} \quad , \tag{82}$$

which reads

$$C = -\frac{1}{2}\frac{(G_{(1)})^{\frac{1}{2}} + (G_{(2)})^{\frac{1}{2}} - 2(G_{(1)})^{\frac{1}{4}}(G_{(2)})^{\frac{1}{4}}}{(G_{(1)})^{\frac{3}{4}}(G_{(2)})^{\frac{3}{4}}\left[(G_{(1)})^{\frac{1}{2}} + (G_{(2)})^{\frac{1}{2}}\right]\left[G_{(1)} - G_{(2)}\right]^2} \quad . \tag{83}$$

We reduce the fraction in expression (83) by factor $[(G_{(1)})^{\frac{1}{4}} - (G_{(2)})^{\frac{1}{4}}]^2$ and arrive at

$$C = -\frac{1}{2}\frac{1}{(G_{(1)})^{\frac{3}{4}}(G_{(2)})^{\frac{3}{4}}\left[(G_{(1)})^{\frac{1}{4}} + (G_{(2)})^{\frac{1}{4}}\right]^2\left[(G_{(1)})^{\frac{1}{2}} + (G_{(2)})^{\frac{1}{2}}\right]^3} \quad . \tag{84}$$

4.2.3. Common S–wave Hamiltonian function of the minus first order

For $N = -1$, factor C_0 is given by expression (32). Factor (53) reads

$$C_1 = -\frac{(G_{(1)})^{\frac{5}{2}} - (G_{(2)})^{\frac{5}{2}}}{(G_{(1)})^{\frac{3}{2}}(G_{(2)})^{\frac{3}{2}}\left(G_{(1)} - G_{(2)}\right)} \quad . \tag{85}$$

We reduce the fraction in expression (85) by factor $(G_{(1)})^{\frac{1}{2}} - (G_{(2)})^{\frac{1}{2}}$ and arrive at

$$C_1 = -\frac{(G_{(1)})^2 + (G_{(1)})^{\frac{3}{2}}(G_{(2)})^{\frac{1}{2}} + G_{(1)}G_{(2)} + (G_{(1)})^{\frac{1}{2}}(G_{(2)})^{\frac{3}{2}} + (G_{(2)})^2}{(G_{(1)})^{\frac{3}{2}}(G_{(2)})^{\frac{3}{2}}\left[(G_{(1)})^{\frac{1}{2}} + (G_{(2)})^{\frac{1}{2}}\right]} \quad . \tag{86}$$

Note that factor (86) may also be expressed as

$$C_1 = -\frac{[(G_{(1)})^{\frac{1}{2}} + (G_{(2)})^{\frac{1}{2}}][(G_{(1)})^{\frac{3}{2}} + (G_{(2)})^{\frac{3}{2}}] + G_{(1)}G_{(2)}}{(G_{(1)})^{\frac{3}{2}}(G_{(2)})^{\frac{3}{2}}\left[(G_{(1)})^{\frac{1}{2}} + (G_{(2)})^{\frac{1}{2}}\right]} \quad . \tag{87}$$

Factor (55) reads

$$C_2 = -\frac{(G_{(1)})^{\frac{7}{2}} - (G_{(2)})^{\frac{7}{2}}}{(G_{(1)})^{\frac{3}{2}}(G_{(2)})^{\frac{3}{2}}\left(G_{(1)} - G_{(2)}\right)} \quad . \tag{88}$$

We reduce the fraction in expression (88) by factor $(G_{(1)})^{\frac{1}{2}} - (G_{(2)})^{\frac{1}{2}}$ and arrive at

$$C_2 = -\frac{(G_{(1)})^3 + (G_{(1)})^{\frac{5}{2}}(G_{(2)})^{\frac{1}{2}} + (G_{(1)})^2 G_{(2)} + (G_{(1)})^{\frac{3}{2}}(G_{(2)})^{\frac{3}{2}} + G_{(1)}(G_{(2)})^2 + (G_{(1)})^{\frac{1}{2}}(G_{(2)})^{\frac{5}{2}} + (G_{(2)})^3}{(G_{(1)})^{\frac{3}{2}}(G_{(2)})^{\frac{3}{2}}\left[(G_{(1)})^{\frac{1}{2}} + (G_{(2)})^{\frac{1}{2}}\right]} \quad . \tag{89}$$

Note that factor (89) may also be expressed as

$$C_2 = -\frac{\left[G_{(1)} + (G_{(1)})^{\frac{1}{2}}(G_{(2)})^{\frac{1}{2}} + G_{(2)}\right]\left[(G_{(1)})^2 + (G_{(2)})^2\right] + (G_{(1)})^{\frac{3}{2}}(G_{(2)})^{\frac{3}{2}}}{(G_{(1)})^{\frac{3}{2}}(G_{(2)})^{\frac{3}{2}}\left[(G_{(1)})^{\frac{1}{2}} + (G_{(2)})^{\frac{1}{2}}\right]} \quad . \tag{90}$$

Factor (57) reads

$$C_3 = -\frac{(G_{(1)})^{\frac{5}{4}} - (G_{(2)})^{\frac{5}{4}}}{(G_{(1)})^{\frac{5}{4}}(G_{(2)})^{\frac{5}{4}}\left[G_{(1)} - G_{(2)}\right]} \quad . \tag{91}$$

We reduce the fraction in expression (91) by factor $(G_{(1)})^{\frac{1}{4}} - (G_{(2)})^{\frac{1}{4}}$ and arrive at

$$C_3 = -\frac{G_{(1)} + (G_{(1)})^{\frac{3}{4}}(G_{(2)})^{\frac{1}{4}} + (G_{(1)})^{\frac{1}{2}}(G_{(2)})^{\frac{1}{2}} + (G_{(1)})^{\frac{1}{4}}(G_{(2)})^{\frac{3}{4}} + G_{(2)}}{(G_{(1)})^{\frac{5}{4}}(G_{(2)})^{\frac{5}{4}}\left[(G_{(1)})^{\frac{1}{4}} + (G_{(2)})^{\frac{1}{4}}\right]\left[(G_{(1)})^{\frac{1}{2}} + (G_{(2)})^{\frac{1}{2}}\right]} \quad . \tag{92}$$

Note that factor (92) may also be expressed as

$$C_3 = -\frac{\left[(G_{(1)})^{\frac{1}{4}} + (G_{(2)})^{\frac{1}{4}}\right]\left[(G_{(1)})^{\frac{3}{4}} + (G_{(2)})^{\frac{3}{4}}\right] + (G_{(1)})^{\frac{1}{2}}(G_{(2)})^{\frac{1}{2}}}{(G_{(1)})^{\frac{5}{4}}(G_{(2)})^{\frac{5}{4}}\left[(G_{(1)})^{\frac{1}{4}} + (G_{(2)})^{\frac{1}{4}}\right]\left[(G_{(1)})^{\frac{1}{2}} + (G_{(2)})^{\frac{1}{2}}\right]} \quad . \tag{93}$$

Factor (58) reads

$$C_4 = -\frac{(G_{(1)})^{\frac{9}{4}} - (G_{(2)})^{\frac{9}{4}}}{(G_{(1)})^{\frac{5}{4}}(G_{(2)})^{\frac{5}{4}}\left[G_{(1)} - G_{(2)}\right]} \quad . \tag{94}$$

We reduce the fraction in expression (94) by factor $(G_{(1)})^{\frac{1}{4}} - (G_{(2)})^{\frac{1}{4}}$ and arrive at

$$C_4 = -\frac{\begin{array}{c}(G_{(1)})^2 + (G_{(1)})^{\frac{7}{4}}(G_{(2)})^{\frac{1}{4}} + (G_{(1)})^{\frac{6}{4}}(G_{(2)})^{\frac{2}{4}} + (G_{(1)})^{\frac{5}{4}}(G_{(2)})^{\frac{3}{4}} + (G_{(1)})^{\frac{4}{4}}(G_{(2)})^{\frac{4}{4}} \\ + (G_{(1)})^{\frac{3}{4}}(G_{(2)})^{\frac{5}{4}} + (G_{(1)})^{\frac{2}{4}}(G_{(2)})^{\frac{6}{4}} + (G_{(1)})^{\frac{1}{4}}(G_{(2)})^{\frac{7}{4}} + (G_{(2)})^2\end{array}}{(G_{(1)})^{\frac{5}{4}}(G_{(2)})^{\frac{5}{4}}\left[(G_{(1)})^{\frac{1}{4}} + (G_{(2)})^{\frac{1}{4}}\right]\left[(G_{(1)})^{\frac{1}{2}} + (G_{(2)})^{\frac{1}{2}}\right]} \quad . \tag{95}$$

Note that factor (95) may also be expressed as

$$C_4 = -\frac{(G_{(1)})^{\frac{5}{4}} + (G_{(2)})^{\frac{5}{4}}}{(G_{(1)})^{\frac{5}{4}}(G_{(2)})^{\frac{5}{4}}} - \frac{1}{(G_{(1)})^{\frac{1}{4}}(G_{(2)})^{\frac{1}{4}}\left[(G_{(1)})^{\frac{1}{4}} + (G_{(2)})^{\frac{1}{4}}\right]\left[(G_{(1)})^{\frac{1}{2}} + (G_{(2)})^{\frac{1}{2}}\right]} \quad . \tag{96}$$

Definitions (45) and (65) with factor (32) yield

$$C = \frac{G_{(1)} + (G_{(1)}G_{(2)})^{\frac{1}{2}} + G_{(2)} - \frac{3}{2}(G_{(1)})^{\frac{1}{4}}(G_{(2)})^{\frac{1}{4}}\left[(G_{(1)})^{\frac{1}{2}} + (G_{(2)})^{\frac{1}{2}}\right]}{(G_{(1)})^{\frac{3}{2}}(G_{(2)})^{\frac{3}{2}}\left[(G_{(1)})^{\frac{1}{2}} + (G_{(2)})^{\frac{1}{2}}\right]\left[G_{(1)} - G_{(2)}\right]^2} \quad . \tag{97}$$

The numerator in expression (97) may be converted into a product,

$$C = \frac{\left[(G_{(1)})^{\frac{1}{2}} + \frac{1}{2}(G_{(1)})^{\frac{1}{4}}(G_{(2)})^{\frac{1}{4}} + (G_{(2)})^{\frac{1}{2}}\right]\left[(G_{(1)})^{\frac{1}{2}} - 2(G_{(1)})^{\frac{1}{4}}(G_{(2)})^{\frac{1}{4}} + (G_{(2)})^{\frac{1}{2}}\right]}{(G_{(1)})^{\frac{3}{2}}(G_{(2)})^{\frac{3}{2}}\left[(G_{(1)})^{\frac{1}{2}} + (G_{(2)})^{\frac{1}{2}}\right]\left[G_{(1)} - G_{(2)}\right]^2} \quad . \tag{98}$$

We reduce the fraction in expression (98) by factor $[(G_{(1)})^{\frac{1}{4}} - (G_{(2)})^{\frac{1}{4}}]^2$ and arrive at

$$C = \frac{(G_{(1)})^{\frac{1}{2}} + \frac{1}{2}(G_{(1)})^{\frac{1}{4}}(G_{(2)})^{\frac{1}{4}} + (G_{(2)})^{\frac{1}{2}}}{(G_{(1)})^{\frac{3}{2}}(G_{(2)})^{\frac{3}{2}}\left[(G_{(1)})^{\frac{1}{4}} + (G_{(2)})^{\frac{1}{4}}\right]^2\left[(G_{(1)})^{\frac{1}{2}} + (G_{(2)})^{\frac{1}{2}}\right]^3} \quad . \tag{99}$$

4.2.4. Common S–wave Hamiltonian function of the minus second order

For $N=-2$, factor C_0 is given by expression (33). Factor (53) reads

$$C_1 = -\frac{(G_{(1)})^3 - (G_{(2)})^3}{(G_{(1)})^2(G_{(2)})^2\left(G_{(1)} - G_{(2)}\right)} \quad . \tag{100}$$

We reduce the fraction in (100) by factor $G_{(1)} - G_{(2)}$ and obtain

$$C_1 = -\frac{(G_{(1)})^2 + G_{(1)}G_{(2)} + (G_{(2)})^2}{(G_{(1)})^2(G_{(2)})^2} \quad . \tag{101}$$

Factor (55) reads

$$C_2 = -\frac{(G_{(1)})^4 - (G_{(2)})^4}{(G_{(1)})^2(G_{(2)})^2\left(G_{(1)} - G_{(2)}\right)} \quad . \tag{102}$$

We reduce the fraction in (102) by factor $G_{(1)} - G_{(2)}$ and obtain

$$C_2 = -\frac{\left[G_{(1)} + G_{(2)}\right]\left[(G_{(1)})^2 + (G_{(1)})^2\right]}{(G_{(1)})^2(G_{(2)})^2} \quad . \tag{103}$$

Factor (57) reads

$$C_3 = -\frac{(G_{(1)})^{\frac{3}{2}} - (G_{(2)})^{\frac{3}{2}}}{(G_{(1)})^{\frac{3}{2}}(G_{(2)})^{\frac{3}{2}}\left[G_{(1)} - G_{(2)}\right]} \quad . \tag{104}$$

We reduce the fraction in (104) by factor $(G_{(1)})^{\frac{1}{2}} - (G_{(2)})^{\frac{1}{2}}$ and obtain

$$C_3 = -\frac{G_{(1)} + (G_{(1)})^{\frac{1}{2}}(G_{(2)})^{\frac{1}{2}} + G_{(2)}}{(G_{(1)})^{\frac{3}{2}}(G_{(2)})^{\frac{3}{2}}\left[(G_{(1)})^{\frac{1}{2}} + (G_{(2)})^{\frac{1}{2}}\right]} \quad . \tag{105}$$

Factor (58) reads

$$C_4 = -\frac{(G_{(1)})^{\frac{5}{2}} - (G_{(2)})^{\frac{5}{2}}}{(G_{(1)})^{\frac{3}{2}}(G_{(2)})^{\frac{3}{2}}\left[G_{(1)} - G_{(2)}\right]} \quad . \tag{106}$$

We reduce the fraction in (99) by factor $(G_{(1)})^{\frac{1}{2}} - (G_{(2)})^{\frac{1}{2}}$ and arrive at

$$C_4 = -\frac{(G_{(1)})^2 + (G_{(1)})^{\frac{3}{2}}(G_{(2)})^{\frac{1}{2}} + G_{(1)}G_{(2)} + (G_{(1)})^{\frac{1}{2}}(G_{(2)})^{\frac{3}{2}} + (G_{(2)})^2}{(G_{(1)})^{\frac{3}{2}}(G_{(2)})^{\frac{3}{2}}\left[(G_{(1)})^{\frac{1}{2}} + (G_{(2)})^{\frac{1}{2}}\right]} \quad . \tag{107}$$

Note that factor (107) may also be expressed as

$$C_4 = -\frac{\left[(G_{(1)})^{\frac{1}{2}} + (G_{(2)})^{\frac{1}{2}}\right]\left[(G_{(1)})^{\frac{3}{2}} + (G_{(2)})^{\frac{3}{2}}\right] + G_{(1)}G_{(2)}}{(G_{(1)})^{\frac{3}{2}}(G_{(2)})^{\frac{3}{2}}\left[(G_{(1)})^{\frac{1}{2}} + (G_{(2)})^{\frac{1}{2}}\right]} \quad . \tag{108}$$

Definitions (45) and (65) with factor (33) yield

$$C = \frac{G_{(1)} + G_{(2)} - 2(G_{(1)})^{\frac{1}{2}}(G_{(2)})^{\frac{1}{2}}}{(G_{(1)})^2 (G_{(2)})^2 [G_{(1)} - G_{(2)}]^2} \quad . \tag{109}$$

We reduce the fraction in (109) by factor $[(G_{(1)})^{\frac{1}{2}} - (G_{(2)})^{\frac{1}{2}}]^2$ and obtain

$$C = \frac{1}{(G_{(1)})^2 (G_{(2)})^2 \left[(G_{(1)})^{\frac{1}{2}} + (G_{(2)})^{\frac{1}{2}}\right]^2} \quad . \tag{110}$$

5. Reference real–valued Hamiltonian function

The reference Hamiltonian function

$$\widetilde{H}(x^m, p_n) = \sum_{\Omega=0}^{+\infty} \frac{\mathrm{i}^\Omega}{\Omega!} \, \mathrm{Re}[H^{,k_1 k_2 \ldots k_\Omega}(x^m, \mathrm{Re}\, p_n)] \, \mathrm{Im}(p_{k_1}) \, \mathrm{Im}(p_{k_2}) \ldots \mathrm{Im}(p_{k_\Omega}) \quad , \tag{111}$$

which is real–valued for real–valued slowness vectors p_k and thus yields real–valued reference rays, was derived by Klimeš & Klimeš (2011, eq. 7).

For real–valued reference slowness vectors p_k, reference Hamiltonian function (111) and its phase–space derivatives

$$\widetilde{H}^{,k_1 k_2 \ldots k_\Omega}_{,j_1 j_2 \ldots j_\Phi}(x^m, p_n) = \frac{\partial}{\partial x^{j_1}} \frac{\partial}{\partial x^{j_2}} \cdots \frac{\partial}{\partial x^{j_\Phi}} \frac{\partial}{\partial p_{k_1}} \frac{\partial}{\partial p_{k_2}} \cdots \frac{\partial}{\partial p_{k_\Omega}} \widetilde{H}(x^m, p_n) \tag{112}$$

read (Klimeš & Klimeš, 2011, eq. 11)

$$\widetilde{H}^{,k_1 k_2 \ldots k_\Omega}_{,j_1 j_2 \ldots j_\Phi}(x^m, p_n) = \mathrm{Re}[H^{,k_1 k_2 \ldots k_\Omega}_{,j_1 j_2 \ldots j_\Phi}(x^m, p_n)] \quad . \tag{113}$$

The first–order phase–space derivatives (113) are required for tracing the real–valued reference rays, and the second–order phase–space derivatives (113) are required for solving the equations of geodesic deviation of the real–valued reference rays.

In order to obtain the independent variable along a ray equal to reference travel time τ^0, we normalize reference slowness vector p_i so that the value of complex–valued Hamiltonian function $H(x^m, p_n)$ satisfies relation (Klimeš & Klimeš, 2011, eq. 55)

$$\mathrm{Re}[H(x^m, p_n)] = \tfrac{1}{N} \quad , \tag{114}$$

where N is the degree of Hamiltonian function $H(x^m, p_n)$ homogeneous with respect to slowness vector p_i.

6. Transformation of reference real–valued rays at structural interfaces

Real–valued reference Hamiltonian function (113) with its phase–space derivatives can be used for transforming the real–valued reference rays and the corresponding propagator matrix of geodesic deviation at structural interfaces using the equations by Klimeš (2010).

7. Perturbation expansion of complex–valued travel time

For a convenient perturbation from reference Hamiltonian function $\widetilde{H}(x^m, p_n)$ to complex–valued Hamiltonian function $H(x^m, p_n)$, we define the one–parametric perturbation Hamiltonian function (Klimeš & Klimeš, 2011, eq. 8)

$$H(x^m, p_n, \alpha) = \widetilde{H}(x^m, p_n) + [H(x^m, p_n) - \widetilde{H}(x^m, p_n)]\,\alpha \quad , \tag{115}$$

linear with respect to perturbation parameter α. We denote the phase–space and perturbation derivatives of the perturbation Hamiltonian function as

$$H^{,k_1k_2\ldots k_\Omega}_{,j_1j_2\ldots j_\Phi\alpha\ldots\alpha}(x^m, p_n, \alpha) = \frac{\partial}{\partial x^{j_1}}\frac{\partial}{\partial x^{j_2}}\cdots\frac{\partial}{\partial x^{j_\Phi}}\,\frac{\partial}{\partial p_{k_1}}\frac{\partial}{\partial p_{k_2}}\cdots\frac{\partial}{\partial p_{k_\Omega}}\,\frac{\partial}{\partial \alpha}\cdots\frac{\partial}{\partial \alpha}H(x^m, p_n, \alpha)\ . \tag{116}$$

For each value of α, the corresponding Hamilton–Jacobi equation defines the complex–valued travel time $\tau = \tau(x^k, \alpha)$. For $\alpha = 0$, we obtain the real–valued reference travel time $\tau^0 = \tau^0(x^m)$ corresponding to the real–valued reference rays. For $\alpha = 1$, we obtain the complex–valued travel time which we approximate by the perturbation expansion along the real–valued reference rays.

For real–valued reference slowness vectors p_k, the first–order perturbation derivative of perturbation Hamiltonian function (115) and of its phase–space derivatives reads (Klimeš & Klimeš, 2011, eq. 13)

$$H^{,k_1k_2\ldots k_\Omega}_{,j_1j_2\ldots j_\Phi\alpha}(x^m, p_n, 0) = \mathrm{i}\ \mathrm{Im}\big[H^{,k_1k_2\ldots k_\Omega}_{,j_1j_2\ldots j_\Phi}(x^m, p_n)\big] \quad . \tag{117}$$

The second–order and higher–order perturbation derivatives of perturbation Hamiltonian function (115) and of its phase–space derivatives vanish (Klimeš & Klimeš, 2011, eq. 15),

$$H^{,k_1k_2\ldots k_\Omega}_{,j_1j_2\ldots j_\Phi\alpha\alpha}(x^m, p_n, 0) = H^{,k_1k_2\ldots k_\Omega}_{,j_1j_2\ldots j_\Phi\alpha\alpha\alpha}(x^m, p_n, 0) = \ldots = 0 \quad . \tag{118}$$

These perturbation derivatives of the Hamiltonian function can be used to calculate the perturbation derivatives of travel time and of its spatial derivatives according to Klimeš (2002; 2016).

The perturbation expansion of complex–valued travel time $\tau = \tau(x^k, \alpha)$ is its Taylor expansion (Klimeš & Klimeš, 2011, eq. 31),

$$\tau(x^m, \alpha) \approx \tau(x^m, 0) + \tau_{,\alpha}(x^m, 0)\,\alpha + \tfrac{1}{2}\tau_{,\alpha\alpha}(x^m, 0)\,\alpha^2 + \tfrac{1}{6}\tau_{,\alpha\alpha\alpha}(x^m, 0)\,\alpha^3 + \ldots \tag{119}$$

with respect to perturbation parameter α. The Greek subscripts following a comma denote partial derivatives with respect to perturbation parameter α, here referred to as perturbation derivatives.

The first–order perturbation derivative $\tau_{,\alpha}$ in the perturbation expansion (119) of travel time is determined by equation (Klimeš & Klimeš, 2011, eq. 34),

$$\frac{\mathrm{d}\tau_{,\alpha}}{\mathrm{d}\tau^0} = -\mathrm{i}\ \mathrm{Im}[H(x^m, p_n)] \quad . \tag{120}$$

The first–order term in the perturbation expansion (119) of travel time is purely imaginary.

The first–order perturbation derivative $\tau_{,i\alpha}$ of the spatial travel–time gradient is determined by equation (Klimeš & Klimeš, 2011, eq. 35)

$$\tau_{,i\alpha}(x^m, 0) = T_{a\alpha}\,Q^{-1}_{ai} \quad , \tag{121}$$

where Q^{-1}_{ai} are the elements of the matrix inverse to matrix

$$Q^i{}_a = \frac{\partial x^i}{\partial \gamma_a} \tag{122}$$

of geometrical spreading. The covariant derivatives $T_{a\alpha}$ of $\tau_{,\alpha}$ with respect to ray coordinates γ_a can be calculated using equation (Klimeš & Klimeš, 2011, eq. 36),

$$\frac{\mathrm{d}T_{,a\alpha}}{\mathrm{d}\tau^0} = -\mathrm{i}\,\mathrm{Im}[H_{,j}(x^m,p_n)]\;Q^j{}_a - \mathrm{i}\,\mathrm{Im}[H^{,j}(x^m,p_n)]\;P_{ja} \quad , \tag{123}$$

where

$$P_{ja} = \frac{\partial p_j}{\partial \gamma_a} \quad . \tag{124}$$

Since (Klimeš & Klimeš, 2011, eq. 37)

$$T_{,3\alpha} = -\mathrm{i}\,\mathrm{Im}[H(x^m,p_n)] \quad , \tag{125}$$

the quadrature of equation (123) is unnecessary for $a=3$.

The second–order perturbation derivative $\tau_{,\alpha\alpha}$ in the perturbation expansion (119) of travel time is determined by equation (Klimeš & Klimeš, 2011, eq. 41),

$$\frac{\mathrm{d}\tau_{,\alpha\alpha}}{\mathrm{d}\tau^0} = -2\,\mathrm{i}\,\mathrm{Im}[H^{,j}(x^m,p_n)]\,\tau_{,j\alpha}(x^m,0) - \mathrm{Re}[H^{,jk}(x^m,p_n)]\,\tau_{,j\alpha}(x^m,0)\,\tau_{,k\alpha}(x^m,0)\ . \tag{126}$$

The second–order term in the perturbation expansion (119) of travel time is real–valued.

If the Hamiltonian function is discontinuous at a smooth interface, all spatial and perturbation derivatives of travel time may be transformed at the interface using the equations by Klimeš (2016).

8. Conclusions

The complex–valued eigenvalues of complex–valued Christoffel matrix (5) are the solutions of cubic characteristic equation (6).

To trace the reference P–wave rays, we calculate the first–order and second–order phase–space derivatives of P–wave eigenvalue $G_{(3)}$ from expressions (40) and (41). We then convert the P–wave eigenvalue with its derivatives into the complex–valued homogeneous Hamiltonian function and its phase–space derivatives using relations (23)–(25).

To trace the reference common S–wave rays, we calculate the complex–valued homogeneous Hamiltonian function and its first–order and second–order phase–space derivatives using expressions (26), (63) and (64) with matrices (52), (54) and (56). Coefficients C_0, C_1, C_2, C_3, C_4 and C can be calculated according to the corresponding one of Sections 4.2.1–4.2.4.

We then rescale the reference slowness vector together with the complex–valued homogeneous Hamiltonian function and its first–order and second–order phase–space derivatives according to condition (114).

The real–valued reference rays can be traced using the real–valued reference Hamiltonian function and its phase–space derivatives obtained from the complex–valued Hamiltonian function by means of relation (113). The same real–valued reference Hamiltonian function with its phase–space derivatives can be used for transforming the real–valued reference rays at structural interfaces using the equations by Klimeš (2010).

The perturbation expansion of complex–valued travel time along the real–valued reference rays is described in Section 7.

Acknowledgements

The research has been supported by the Czech science foundation under contract 20-06887S, and by the members of the consortium "Seismic Waves in Complex 3–D Structures" (see "http://sw3d.cz").

References

Bulant, P. & Klimeš, L. (2008): Numerical comparison of the isotropic–common–ray and anisotropic–common–ray approximations of the coupling ray theory. *Geophys. J. int.*, **175**, 357–374, online at "http://sw3d.cz".

Bulant, P. & Klimeš, L. (2018): Comparison of the anisotropic–ray–theory rays and anisotropic common S–wave rays with the SH and SV reference rays in a velocity model with a split intersection singularity. *Stud. geophys. geod.*, **62**, 57–79, online at "http://sw3d.cz".

Červený, V. (1972): Seismic rays and ray intensities in inhomogeneous anisotropic media. *Geophys. J. R. astr. Soc.*, **29**, 1–13, online at "http://sw3d.cz".

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

Hamilton, W.R. (1837): Third supplement to an essay on the theory of systems of rays. *Trans. Roy. Irish Acad.*, **17**, 1–144, read January 23, 1832, and October 22, 1832.

Klimeš, L. (2002): Second–order and higher–order perturbations of travel time in isotropic and anisotropic media. *Stud. geophys. geod.*, **46**, 213–248, online at "http://sw3d.cz".

Klimeš, L. (2006): Common–ray tracing and dynamic ray tracing for S waves in a smooth elastic anisotropic medium. *Stud. geophys. geod.*, **50**, 449–461, online at "http://sw3d.cz".

Klimeš, L. (2010): Transformation of paraxial matrices at a general interface between two general media. *Seismic Waves in Complex 3–D Structures*, **20**, 115–126, online at "http://sw3d.cz".

Klimeš, L. (2016): Transformation of spatial and perturbation derivatives of travel time at a curved interface between two arbitrary media. *Stud. geophys. geod.*, **60**, 451–470, online at "http://sw3d.cz".

Klimeš, L. (2020): Two S–wave eigenvectors of the Christoffel matrix need not exist in anisotropic viscoelastic media. *Seismic Waves in Complex 3–D Structures*, **30**, 73–76, online at "http://sw3d.cz".

Klimeš, M. & Klimeš, L. (2011): Perturbation expansions of complex–valued traveltime along real–valued reference rays. *Geophys. J. int.*, **186**, 751–759, online at "http://sw3d.cz".

Vavryčuk, V. (2008): Real ray tracing in anisotropic viscoelastic media. *Geophys. J. int.*, **175**, 617–626.

Vavryčuk, V. (2010): Behaviour of rays at interfaces in anisotropic viscoelastic media. *Geophys. J. int.*, **181**, 1665–1677.

Vavryčuk, V. (2012): On numerically solving the complex eikonal equation using real ray–tracing methods: A comparison with the exact analytical solution. *Geophysics*, **77**, T109–T116.