Tracing real-valued reference rays in anisotropic viscoelastic media

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ABSTRACT

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 the 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 the 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

1. INTRODUCTION

Attenuation is a very important phenomenon in wave propagation, and is essential whenever the intensity of waves matters. In ray methods, wave attenuation is described primarily by the imaginary part of the complex–valued travel time. The real part of the complex–valued travel time describes the energy propagation analogously as in elastic media, and can analogously be observed and picked in seismograms.

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 the 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. Therefore, we 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 the 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 the 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 and 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 the 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 $(n-1)$–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 the 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 and 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 the real–valued reference common S–wave rays instead of the 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, 2021*). 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 the 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 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 and 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 the complex–valued travel time along the 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 and Klimeš (2008)* in the examples of perturbations from the reference isotropic rays and the common reference anisotropic rays in an anisotropic elastic medium, and also numerically demonstrated by *Vavryčuk (2012)* in the examples of perturbations from the real–valued reference rays to the complex–valued travel time in two isotropic attenuating media.

We use the component 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 the 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

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

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 3×3×3×3 frequency–domain density–normalized stiffness tensor

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

where ϱ is a real–valued density. Density–normalized 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, $a_{ijkl}(x^m)$ are the density–normalized elastic moduli, and p_i are 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 is 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

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

where

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

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 the 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 the machine precision even in this case, independently of the kind of averaging. The numerical error of P–wave eigenvalue $G_{(3)}$ corresponds to the machine precision.

In this paper, we assume 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 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 complex–valued eigenvectors are mutually pseudo–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 pseudo–orthogonal S–wave eigenvectors $g_{i(1)}$ and $g_{i(2)}$ can be selected arbitrarily in the plane pseudo–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, 2021*). In the case of just a single S–wave eigenvector at a singularity, both S–wave eigenvectors diverge and approach the same infinite eigenvector corresponding to a circular polarization when approaching the S–wave singularity (*Klimeš, 2022*).

In this section, we summarize the equations for the Hamiltonian function. 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 eigenvectors.

In 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 can 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 if all three eigenvectors of the Christoffel matrix are well defined.

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 the anisotropic–ray–theory S–wave ray.

We consider here the homogeneous Hamiltonian functions 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 and 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 the 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*)

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

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 may be singular. It is thus desirable to perform 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*),

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

For $N\!=\!-1$ (*Klimeš, 2006, Eq. 34*),

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

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 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, as well as at least one S–wave eigenvector. However, one of the S–wave eigenvectors $g_{i(1)}$ and $g_{i(2)}$ need not exist in the case of a complex–valued Christoffel matrix (*Klimeš, 2021*), 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

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

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

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

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

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

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 taking into account 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

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

where

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

Taking into account relation (46), we apply l'Hospital's rule twice to calculate

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

Taking into account relation (66), we then apply l'Hospital's rule three times to calculate

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

The 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. The 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 apply 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 the complex–valued travel time along the 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) can also be expressed as

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

Factor (57) reads

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

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

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

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

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

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) can 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 obtain

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

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) can 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 obtain

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

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) can 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 expression (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 expression (102) by factor $G_{(1)} - G_{(2)}$ and arrive at

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

Factor (57) reads

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

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

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

Factor (58) reads

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

We reduce the fraction in expression (106) by factor $\left(G_{(1)}\right)^{\frac{1}{2}} - \left(G_{(2)}\right)^{\frac{1}{2}}$ and arrive at

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

Note that factor (107) can also be expressed as

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

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

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

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

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

5. REFERENCE REAL–VALUED HAMILTONIAN FUNCTION

The reference Hamiltonian function

$$\widetilde{H}(x^m,p_n) = \sum_{\Omega=0}^{+\infty} \frac{\mathrm{i}^\Omega}{\Omega!} \,\mathrm{Re}[H^{,k_1k_2\ldots k_\Omega}(x^m,\mathrm{Re}\,p_n)]\,\mathrm{Im}(p_{k_1})\,\mathrm{Im}(p_{k_2})\ldots\mathrm{Im}(p_{k_\Omega}) \quad , \tag{111}$$

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

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

$$\widetilde{H}^{,k_1k_2\ldots k_\Omega}_{,j_1j_2\ldots j_\Phi}(x^m,p_n) = \frac{\partial}{\partial x^{j_1}}\frac{\partial}{\partial x^{j_2}}\cdots\frac{\partial}{\partial x^{j_\Phi}}\,\frac{\partial}{\partial p_{k_1}}\frac{\partial}{\partial p_{k_2}}\cdots\frac{\partial}{\partial p_{k_\Omega}}\,\widetilde{H}(x^m,p_n) \tag{112}$$

read (*Klimeš and Klimeš, 2011, Eq. 11*)

$$\widetilde{H}^{,k_1k_2\ldots k_\Omega}_{,j_1j_2\ldots j_\Phi}(x^m,p_n) = \mathrm{Re}[H^{,k_1k_2\ldots k_\Omega}_{,j_1j_2\ldots j_\Phi}(x^m,p_n)] \quad . \tag{113}$$

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 and Klimeš, 2011, Eq. 55*)

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

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

6. TRANSFORMATION OF THE 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 *Farra and Le Bégat (1995)* or *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 and 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

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

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 and Klimeš, 2011, Eq. 13*)

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

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

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

The 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 and Klimeš, 2011, Eq. 31*)

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

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 and 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 and 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 the 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 and 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 and 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 and Klimeš, 2011, Eq. 41*)

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

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 can be transformed at the interface using the equations by *Klimeš (2016)*.

8. CONCLUSIONS

Together with the previous papers, this paper completes the algorithm of tracing the real–valued reference P–wave rays and the real–valued reference common S–wave rays in viscoelastic media, and of solving the corresponding equations of geodesic deviation. The algorithm is ready to be applied by anybody, and will extend the existing 3–D ray tracing code (*Bucha and Bulant, 2022*) from elastic media to viscoelastic media. The algorithm consists of the following steps.

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. The phase–space derivatives of the reference Hamiltonian function can be 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 to transform the real–valued reference rays and the corresponding propagator matrix of geodesic deviation at structural interfaces using the equations by *Farra and Le Bégat (1995)* or *Klimeš (2010)*.

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

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