Zero-order ray-theory Green tensor in a heterogeneous anisotropic elastic medium

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ABSTRACT

Although synthetic seismograms can, in many cases, be generated by direct numerical methods, approximate analytical ray–theory solutions are often very useful in forward and especially inverse problems of seismic wave propagation in complex 3–D media. In this paper, the frequency–domain zero–order ray–theory Green tensor in a heterogeneous anisotropic elastic medium is derived from the zero–order ray–theory approximation using the representation theorem applied in ray–centred coordinates.

Keywords: ray theory, Green tensor, travel time, amplitude, anisotropy, heterogeneous media, paraxial approximation, wave propagation

1. INTRODUCTION

This paper is devoted to the zero–order ray–theory approximation of the Green tensor in a heterogeneous anisotropic elastic medium, which is useful for forward and especially inverse problems of seismic wave propagation in complex 3–D media. Although synthetic seismograms can, in many cases, be generated by direct numerical methods, approximate analytical ray–theory solutions are very useful for various reasons, e.g.: (a) it is often advantageous to combine forward modelling by means of direct numerical methods with ray–based inverse iterations during inversion of seismic data; (b) direct numerical methods are still not applicable at highest frequencies; (c) the accuracy and validity of numerical solutions must be confirmed by comparison with analytical results; (d) analytical results often provide more insight into the physical processes involved than rote numerical solutions; (e) the ray theory often provides a powerful intuitive approach to many problems, which is computationally simpler and faster than rote application of direct numerical methods.

The high–frequency asymptotic approximation of the Green tensor for a homogeneous anisotropic elastic medium has been derived by many authors, for details refer to *Červený (2001, Sec. 2.5.5).* The normal method for finding the zero–order ray–theory Green tensor in a heterogeneous anisotropic elastic medium is to match a general zero–order ray–theory approximation for a heterogeneous anisotropic elastic medium to the high–frequency asymptotic approximation of the exact Green tensor for a homogeneous anisotropic elastic medium in the vicinity of a point source. However, this matching derivation is neither satisfactory, nor comfortable, because the medium may be heterogeneous at the source, and even the derivation of the Green tensor for a homogeneous anisotropic elastic medium is non–trivial.

In this paper, we thus provide an alternative method of deriving the zero–order ray–theory Green tensor by deriving it directly in a heterogeneous anisotropic elastic medium. The derivation is performed in the frequency domain. We start with the zero–order ray–theory approximation of the solution of the elastodynamic equation, and use the representation theorem in ray–centred coordinates to derive the amplitude coefficients of the Green tensor and the phase shift of the Green tensor. Although we could perform the derivation in other coordinates, ray–centred coordinates are most convenient, because we use *Červený's (2001)* expressions for the geometrical spreading in ray–centred coordinates.

The Einstein summation over the pairs of identical Roman indices (both subscripts and superscripts) $i, j, k, ... = 1, 2, 3$ or $I, J, K, ... = 1, 2$ is used throughout this paper.

2. ELASTODYNAMIC EQUATION AND THE GREEN TENSOR

The seismic wavefield in an anisotropic elastic medium specified in terms of elastic moduli $c_{ijkl} = c_{ijkl}(\mathbf{x})$ and density $\varrho = \varrho(\mathbf{x})$ satisfies the elastodynamic equation for displacement $u_i(\mathbf{x}, t)$ (*Červený, 2001, Eq. 2.1.17*). We denote the corresponding elastodynamic Green tensor (*Červený, 2001, Eq. 2.5.37*) by $G_{im}(\mathbf{x}, \mathbf{x}', t)$.

In this paper, we shall work in the frequency domain with the 1–D Fourier transform

$$G_{im}(\mathbf{x}, \mathbf{x}', \omega) = \int \mathrm{d}t \; G_{im}(\mathbf{x}, \mathbf{x}', t) \exp(\mathrm{i}\omega t) \tag{1}$$

of the elastodynamic Green tensor, and with the analogous Fourier transform of the displacement. We use the same symbols for a function of time and for its Fourier transform, and distinguish them by arguments t for time and ω for circular frequency.

Note that the phase shifts derived in this paper correspond to the factor $\exp(\mathrm{i}\omega t)$ in Fourier transform (1), and would be opposite for a factor $\exp(-\mathrm{i}\omega t)$.

The anisotropic elastodynamic equation for the displacement in the frequency domain reads (*Červený, 2001, Eq. 2.1.27*)

$$\left[c_{ijkl}(\mathbf{x})\, u_{k,l}(\mathbf{x}, \omega)\right]_{,j} + \omega^2 \varrho(\mathbf{x})\, u_i(\mathbf{x}, \omega) + f_i(\mathbf{x}, \omega) = 0 \quad , \tag{2}$$

where subscript $_{,j}$ following a comma stands for the partial derivative with respect to Cartesian spatial coordinate x^j. The force density $f_i(\mathbf{x}, \omega)$ represents the source of the wavefield.

The frequency–domain Green tensor for an elastic medium is the solution of equation (*Červený, 2001, Eq. 2.5.38*)

$$\left[c_{ijkl}(\mathbf{x})\, G_{km,l}(\mathbf{x}, \mathbf{x}', \omega)\right]_{,j} + \omega^2 \varrho(\mathbf{x})\, G_{im}(\mathbf{x}, \mathbf{x}', \omega) + \delta_{im}\, \delta(\mathbf{x}-\mathbf{x}') = 0 \quad , \tag{3}$$

analytical with respect to the inverse Fourier transform. The spatial partial derivatives in elastodynamic equation (3) are related to coordinates x^i. Here $\delta(\mathbf{x})$ is the 3–D Dirac distribution.

We assume that the elastic moduli obey symmetry relation

$$c_{ijkl}(\mathbf{x}) = c_{klij}(\mathbf{x}) \tag{4}$$

important for the representation theorem.

3. REPRESENTATION THEOREM

Here we consider volume V which need not contain the support of force density $f_i(\mathbf{x},\omega)$ and assume symmetry relation (4). The representation theorem then reads (*Červený, 2001, Eq. 2.6.4*)

$$\begin{aligned} u_m(\mathbf{x}',\omega) = & \int_V \mathrm{d}^3\mathbf{x}\; G_{im}(\mathbf{x},\mathbf{x}',\omega)\, f_i(\mathbf{x},\omega) \\ & + \oint_{\partial V} \mathrm{d}S(\mathbf{x}) \left[G_{im}(\mathbf{x},\mathbf{x}',\omega)\, n_j(\mathbf{x})\, c_{ijkl}(\mathbf{x})\, u_{k,l}(\mathbf{x},\omega) \right. \\ & \qquad \left. - G_{im,j}(\mathbf{x},\mathbf{x}',\omega)\, c_{ijkl}(\mathbf{x})\, u_k(\mathbf{x},\omega)\, n_l(\mathbf{x}) \right] \;, \end{aligned} \tag{5}$$

where $n_i(\mathbf{x})$ is the unit normal to the surface ∂V of volume V pointing outside V.

The integral over volume V represents the wavefield corresponding to the sources situated inside V. The integral over the surface ∂V of V represents the wavefield corresponding to the sources situated outside V, and is zero if all sources are situated inside V.

For $f_i(\mathbf{x},\omega) = \delta_{in}\,\delta(\mathbf{x}–\mathbf{x}'')$, the above representation theorem (5) yields $u_m(\mathbf{x}',\omega) = G_{mn}(\mathbf{x}',\mathbf{x}'',\omega)$. Integrating over the whole space, the surface integral in representation theorem (5) vanishes and we obtain the reciprocity relation (*Červený, 2001, Eq. 2.6.5*)

$$G_{mn}(\mathbf{x}',\mathbf{x}'',\omega) = G_{nm}(\mathbf{x}'',\mathbf{x}',\omega) \;\; . \tag{6}$$

4. ZERO–ORDER RAY–THEORY APPROXIMATION

The zero–order ray–theory approximation of the solution of elastodynamic equation (2) may be composed of individual arrivals. Hereinafter, we shall consider just one of these arrivals. The zero–order ray–theory approximation of one arrival in a smooth heterogeneous anisotropic elastic medium without structural interfaces reads

$$u_i(\mathbf{x},\omega) \simeq \frac{g_i(\mathbf{x})}{\sqrt{\varrho(\mathbf{x})\, v(\mathbf{x})}\, L(\mathbf{x})}\, C\, \exp[\mathrm{i}\varphi(\mathbf{x})]\, \exp[\mathrm{i}\omega\, \tau(\mathbf{x})] \;\; , \tag{7}$$

where factor C is constant along the ray, $\varrho(\mathbf{x})$ is the density, $\tau(\mathbf{x})$ is the travel time, $v(\mathbf{x})$ is the corresponding phase velocity, $\varphi(\mathbf{x})$ is the phase shift due to caustics, and $L(\mathbf{x})$ is the geometrical spreading measured along wavefronts.

Hereinafter, notation $\simeq$ means that we have neglected the terms which can asymptotically be neglected for $\omega \to +\infty$.

Geometrical spreading $L(\mathbf{x})$ may be expressed in various forms. At each point $\mathbf{x}$ of the ray, we choose two linearly independent vectors $\mathbf{h}_1(\mathbf{x})$ and $\mathbf{h}_2(\mathbf{x})$ situated in the wavefront tangent plane. We may then parametrize points $\mathbf{x}'''$ of the wavefront tangent plane by parameters $q^1(\mathbf{x})$ and $q^2(\mathbf{x})$ called ray–centred coordinates:

$$\mathbf{x}''' = \mathbf{h}_1(\mathbf{x})\, q^1(\mathbf{x}) + \mathbf{h}_2(\mathbf{x})\, q^2(\mathbf{x}) \quad . \tag{8}$$

For a more detailed description of ray–centred coordinates refer to *Klimeš (2006)*.

For the geometrical spreading measured along wavefronts, we use expression (*Červený, 2001, Eq. 4.14.39c*)

$$L(\mathbf{x}) = \sqrt{|\mathbf{h}_1(\mathbf{x}) \times \mathbf{h}_2(\mathbf{x})|\,|\det[\mathbf{Q}(\mathbf{x})]|} \quad , \tag{9}$$

where $|\mathbf{h}_1 \times \mathbf{h}_2|$ is the norm of the cross product of the contravariant basis vectors $\mathbf{h}_1$ and $\mathbf{h}_2$ of the ray–centred coordinate system, and $\mathbf{Q}$ is the 2×2 matrix of geometrical spreading in ray–centred coordinates,

$$Q^{AB}(\mathbf{x}) = \frac{\partial q^A(\mathbf{x})}{\partial \gamma_B} \quad , \tag{10}$$

where γ_B are the ray parameters.

Note that factor C in Eq. (7) depends on the initial conditions and on the choice of ray parameters γ_B. Term $|\mathbf{h}_1 \times \mathbf{h}_2|$ is required if the contravariant basis vectors $\mathbf{h}_1$ and $\mathbf{h}_2$ of the ray–centred coordinate system are not orthonormal. We may choose vectors $\mathbf{h}_1$ and $\mathbf{h}_2$ orthonormal and remove $|\mathbf{h}_1 \times \mathbf{h}_2|$ from all equations without loss of generality.

Green tensor $G_{im}(\mathbf{x}, \mathbf{x}', \omega)$ is the solution of the elastodynamic equation corresponding to a point source at point $\mathbf{x}'$. The rays from a point source can be parametrized by two components $p^{(q)}_K = \partial\tau/\partial q^K$ of the slowness vector in ray–centred coordinates. The special case of matrix (10) of geometrical spreading for $\gamma_B = p^{(q)}_B(\mathbf{x}')$ reads

$$Q_2^{AB}(\mathbf{x}, \mathbf{x}') = \frac{\partial q^A(\mathbf{x})}{\partial p^{(q)}_B(\mathbf{x}')} \quad . \tag{11}$$

The zero–order ray–theory approximation (7) specified to the Green tensor reads

$$G_{im}(\mathbf{x}, \mathbf{x}', \omega) \simeq \frac{g_i(\mathbf{x})}{\sqrt{\varrho(\mathbf{x})\, v(\mathbf{x})}\, L(\mathbf{x}, \mathbf{x}')}\, C_m(\mathbf{x}, \mathbf{x}')\, \exp[\mathrm{i}\varphi(\mathbf{x}, \mathbf{x}')]\, \exp[\mathrm{i}\omega\,\tau(\mathbf{x}, \mathbf{x}')] \quad , \tag{12}$$

where

$$L(\mathbf{x}, \mathbf{x}') = \sqrt{|\mathbf{h}_1(\mathbf{x}) \times \mathbf{h}_2(\mathbf{x})|\,|\det[\mathbf{Q}_2(\mathbf{x}, \mathbf{x}')]|\,|\mathbf{h}_1(\mathbf{x}') \times \mathbf{h}_2(\mathbf{x}')|} \tag{13}$$

is the relative geometrical spreading. We have included factor $\sqrt{|\mathbf{h}_1(\mathbf{x}') \times \mathbf{h}_2(\mathbf{x}')|}$ in definition (13) in order to render the relative geometrical spreading independent of the choice of ray–centred coordinates and equivalent to the definition of *Červený (2001, Eq. 4.14.45)*.

Quantities $\varrho(\mathbf{x})$, $v(\mathbf{x})$, $g_i(\mathbf{x})$, $\tau(\mathbf{x}, \mathbf{x}')$ and $L(\mathbf{x}, \mathbf{x}')$ correspond to the ray from point $\mathbf{x}'$ to point $\mathbf{x}$ and have already been defined. We just need to determine factors $C_m(\mathbf{x}, \mathbf{x}')$ and phase shift $\varphi(\mathbf{x}, \mathbf{x}')$ corresponding to the ray from $\mathbf{x}'$ to $\mathbf{x}$.

5. APPLICATION OF THE RECIPROCITY RELATION

We know that the two–point travel time is reciprocal:

$$\tau(\mathbf{x},\mathbf{x}') = \tau(\mathbf{x}',\mathbf{x}) \quad . \tag{14}$$

We insert the zero–order ray–theory approximation (12) of Green tensor into the reciprocity relation (6), and obtain equations

$$\frac{g_i(\mathbf{x})\, C_m(\mathbf{x},\mathbf{x}')}{\sqrt{\varrho(\mathbf{x})\, v(\mathbf{x})}\, L(\mathbf{x},\mathbf{x}')} = \frac{g_m(\mathbf{x}')\, C_i(\mathbf{x}',\mathbf{x})}{\sqrt{\varrho(\mathbf{x}')\, v(\mathbf{x}')}\, L(\mathbf{x}',\mathbf{x})} \quad , \tag{15}$$

and

$$\varphi(\mathbf{x},\mathbf{x}') = \varphi(\mathbf{x}',\mathbf{x}) \qquad (\mathrm{mod}\ 2\pi) \quad . \tag{16}$$

The decomposition of vector $C_m(\mathbf{x},\mathbf{x}')$ into its norm and a unit vector then must read

$$C_m(\mathbf{x},\mathbf{x}') = C(\mathbf{x},\mathbf{x}')\, g_m(\mathbf{x}') \quad . \tag{17}$$

We now need to determine factor $C(\mathbf{x},\mathbf{x}')$ and phase shift $\varphi(\mathbf{x},\mathbf{x}')$ corresponding to the ray from $\mathbf{x}'$ to $\mathbf{x}$. These quantities can be determined using the representation theorem.

6. APPLICATION OF THE REPRESENTATION THEOREM

We assume that point $\mathbf{x}$ is situated inside volume V and point $\mathbf{x}'$ outside volume V. The representation theorem (5) applied to the Green tensor than reads

$$\begin{aligned} G_{mn}(\mathbf{x},\mathbf{x}',\omega) = \oint_{\partial V} \mathrm{d}S(\mathbf{x}''')\, \big[& G_{im}(\mathbf{x}''',\mathbf{x},\omega)\, n_j(\mathbf{x}''')\, c_{ijkl}(\mathbf{x}''')\, G_{kn,l}(\mathbf{x}''',\mathbf{x}',\omega) \\ & - G_{im,j}(\mathbf{x}''',\mathbf{x},\omega)\, c_{ijkl}(\mathbf{x}''')\, G_{kn}(\mathbf{x}''',\mathbf{x}',\omega)\, n_l(\mathbf{x}''') \big] \quad . \end{aligned} \tag{18}$$

We apply the high–frequency approximations

$$G_{kn,l}(\mathbf{x}''',\mathbf{x}',\omega) \simeq \mathrm{i}\omega\, G_{kn}(\mathbf{x}''',\mathbf{x}',\omega)\, p_l(\mathbf{x}''',\mathbf{x}') \tag{19}$$

and

$$G_{kn,l}(\mathbf{x}''',\mathbf{x},\omega) \simeq \mathrm{i}\omega\, G_{kn}(\mathbf{x}''',\mathbf{x},\omega)\, p_l(\mathbf{x}''',\mathbf{x}) \tag{20}$$

of the spatial derivatives of the Green tensors to the representation theorem (18), and arrive at approximation

$$\begin{aligned} G_{mn}(\mathbf{x},\mathbf{x}',\omega) \simeq \mathrm{i}\omega \oint_{\partial V} & \mathrm{d}S(\mathbf{x}''')\, G_{im}(\mathbf{x}''',\mathbf{x},\omega)\, c_{ijkl}(\mathbf{x}''')\, G_{kn}(\mathbf{x}''',\mathbf{x}',\omega) \\ & \times \big[n_j(\mathbf{x}''')\, p_l(\mathbf{x}''',\mathbf{x}') - p_j(\mathbf{x}''',\mathbf{x})\, n_l(\mathbf{x}''') \big] \quad . \end{aligned} \tag{21}$$

We separate points $\mathbf{x}$ and $\mathbf{x}'$ by a surface coinciding with the wavefront tangent plane in the vicinity of the ray in which the contributions to integral (21) are not negligible. We parametrize the wavefront tangent plane by ray–centred coordinates q^1 and q^2, see Eq. (8). Then

$$\mathrm{d}S(\mathbf{x}''') = |\mathbf{h}_1(\mathbf{x}'') \times \mathbf{h}_2(\mathbf{x}'')|\, \mathrm{d}q^1\, \mathrm{d}q^2 \tag{22}$$

and

$$n_i(\mathbf{x}''') = -v(\mathbf{x}'')\,p_i(\mathbf{x}'',\mathbf{x}') \quad . \tag{23}$$

We simultaneously apply approximations

$$p_i(\mathbf{x}''',\mathbf{x}') \simeq p_i(\mathbf{x}'',\mathbf{x}') \quad , \tag{24}$$

$$p_i(\mathbf{x}''',\mathbf{x}) \simeq p_i(\mathbf{x}'',\mathbf{x}) = -p_i(\mathbf{x}'',\mathbf{x}') \quad , \tag{25}$$

and

$$c_{ijkl}(\mathbf{x}''') \simeq c_{ijkl}(\mathbf{x}'') \tag{26}$$

to Eq. (21), which then reads

$$\begin{aligned} G_{mn}(\mathbf{x},\mathbf{x}',\omega) \simeq -2\mathrm{i}\omega \iint &\mathrm{d}q^1\mathrm{d}q^2\, G_{im}(\mathbf{x}''',\mathbf{x},\omega)\, c_{ijkl}(\mathbf{x}'')\, G_{kn}(\mathbf{x}''',\mathbf{x}',\omega) \\ &\times p_j(\mathbf{x}'',\mathbf{x}')\, p_l(\mathbf{x}'',\mathbf{x}')\, v(\mathbf{x}'')\, |\mathbf{h}_1(\mathbf{x}'') \times \mathbf{h}_2(\mathbf{x}'')| \quad , \end{aligned} \tag{27}$$

where $\mathbf{x}''' = \mathbf{x}'''(q^1,q^2)$. We insert the paraxial approximation

$$G_{im}(\mathbf{x}''',\mathbf{x}',\omega) \simeq \frac{g_i(\mathbf{x}'')\, g_m(\mathbf{x}')\, C(\mathbf{x}'',\mathbf{x}')}{\sqrt{\varrho(\mathbf{x}'')\, v(\mathbf{x}'')}\, L(\mathbf{x}'',\mathbf{x}')} \exp[\mathrm{i}\varphi(\mathbf{x}'',\mathbf{x}')] \exp[\mathrm{i}\omega\,\tau(\mathbf{x}''',\mathbf{x}')] \tag{28}$$

with

$$\tau(\mathbf{x}''',\mathbf{x}') \simeq \tau(\mathbf{x}'',\mathbf{x}') + \tfrac{1}{2} q^K M_{KL}(\mathbf{x}'',\mathbf{x}') q^L \tag{29}$$

of the Green tensor (12) with vector (17) into the integrand of Eq. (27). In paraxial expansion (29), we have denoted

$$M_{KL} = \frac{\partial \tau(\mathbf{x}'',\mathbf{x}')}{\partial q^A \partial q^B} \quad . \tag{30}$$

Considering identity

$$c_{ijkl}(\mathbf{x}'') g_i(\mathbf{x}'') p_j(\mathbf{x}'',\mathbf{x}') g_k(\mathbf{x}'') p_l(\mathbf{x}'',\mathbf{x}') = \varrho(\mathbf{x}'') \tag{31}$$

following from the Christoffel equation, relation (27) reads

$$\begin{aligned} G_{mn}(\mathbf{x},\mathbf{x}',\omega) \simeq{}& \frac{g_m(\mathbf{x})\, g_n(\mathbf{x}')\, C(\mathbf{x}'',\mathbf{x}')\, C(\mathbf{x}'',\mathbf{x})}{L(\mathbf{x}'',\mathbf{x})\, L(\mathbf{x}'',\mathbf{x}')} |\mathbf{h}_1(\mathbf{x}'') \times \mathbf{h}_2(\mathbf{x}'')|\; I(\mathbf{x},\mathbf{x}'',\mathbf{x}') \\ &\times \exp\{\mathrm{i}\,[\varphi(\mathbf{x}'',\mathbf{x}) + \varphi(\mathbf{x}'',\mathbf{x}')]\} \exp\{\mathrm{i}\omega\,[\tau(\mathbf{x}'',\mathbf{x}) + \tau(\mathbf{x}'',\mathbf{x}')]\} \quad , \end{aligned} \tag{32}$$

where

$$I(\mathbf{x},\mathbf{x}'',\mathbf{x}') = -2\mathrm{i}\omega \iint \mathrm{d}q^1\mathrm{d}q^2 \exp\big\{\mathrm{i}\omega\,\tfrac{1}{2} q^K [M_{KL}(\mathbf{x}'',\mathbf{x}) + M_{KL}(\mathbf{x}'',\mathbf{x}')] q^L\big\} \quad . \tag{33}$$

We replace Green tensor $G_{mn}(\mathbf{x},\mathbf{x}',\omega)$ in Eq. (32) by expression (12) with vector (17) and obtain equation

$$\begin{aligned} \frac{C(\mathbf{x},\mathbf{x}')\, \exp[\mathrm{i}\varphi(\mathbf{x},\mathbf{x}')]}{\sqrt{\varrho(\mathbf{x})\, v(\mathbf{x})}\, L(\mathbf{x},\mathbf{x}')} = {}& \frac{C(\mathbf{x}'',\mathbf{x}')\, C(\mathbf{x}'',\mathbf{x})}{L(\mathbf{x}'',\mathbf{x})\, L(\mathbf{x}'',\mathbf{x}')} |\mathbf{h}_1(\mathbf{x}'') \times \mathbf{h}_2(\mathbf{x}'')|\; I(\mathbf{x},\mathbf{x}'',\mathbf{x}') \\ &\times \exp\{\mathrm{i}\,[\varphi(\mathbf{x}'',\mathbf{x}) + \varphi(\mathbf{x}'',\mathbf{x}')]\} \quad . \end{aligned} \tag{34}$$

We calculate integral (33) analogously as *Coates and Chapman (1990)* or *Ursin and Tygel (1997)*, and obtain

$$I(\mathbf{x},\mathbf{x}'',\mathbf{x}') = -2\mathrm{i}\,\frac{2\pi\,\exp\left\{\mathrm{i}\frac{\pi}{4}\mathrm{sgn}[M_{KL}(\mathbf{x}'',\mathbf{x})+M_{KL}(\mathbf{x}'',\mathbf{x}')]\right\}}{\sqrt{|\det[M_{KL}(\mathbf{x}'',\mathbf{x})+M_{KL}(\mathbf{x}'',\mathbf{x}')]|}} \quad . \tag{35}$$

We now insert this expression into relation (34). The complex modulus of the resulting relation reads

$$\frac{C(\mathbf{x},\mathbf{x}')}{\sqrt{\varrho(\mathbf{x})\,v(\mathbf{x})}\,L(\mathbf{x},\mathbf{x}')} = 4\pi\,\frac{|\mathbf{h}_1(\mathbf{x}'')\times\mathbf{h}_2(\mathbf{x}'')|\;C(\mathbf{x}'',\mathbf{x}')\,C(\mathbf{x}'',\mathbf{x})}{L(\mathbf{x}'',\mathbf{x})\,L(\mathbf{x}'',\mathbf{x}')\sqrt{|\det[M_{KL}(\mathbf{x}'',\mathbf{x})+M_{KL}(\mathbf{x}'',\mathbf{x}')]|}} \quad , \tag{36}$$

and the complex argument reads

$$\varphi(\mathbf{x},\mathbf{x}') = \varphi(\mathbf{x}'',\mathbf{x}) + \varphi(\mathbf{x}'',\mathbf{x}') + \tfrac{\pi}{4}\left\{\mathrm{sgn}[M_{KL}(\mathbf{x}'',\mathbf{x})+M_{KL}(\mathbf{x}'',\mathbf{x}')] - 2\right\} \quad (\mathrm{mod}\ 2\pi) \quad . \tag{37}$$

Note that matrix $M_{KL}(\mathbf{x}'',\mathbf{x})$ in relations (35)–(37) corresponds to the direction of propagation from point $\mathbf{x}$ to point $\mathbf{x}''$, whereas *Coates and Chapman (1990)* assumed the opposite direction of propagation. We thus derive, in the next section, the identity analogous to the identity of *Coates and Chapman (1990, Eq. 66)* but corresponding to the directions of propagation considered here.

7. PROPAGATOR MATRIX OF GEODESIC DEVIATION IN RAY–CENTRED COORDINATES

We assume that the basis vectors $\mathbf{h}_K(\mathbf{x}'')$ of the ray–centred coordinate system along the ray from $\mathbf{x}$ to $\mathbf{x}'$ and along the ray from $\mathbf{x}'$ to $\mathbf{x}$ are equal.

We decompose the 4×4 propagator matrix of geodesic deviation in ray–centred coordinates into four 2×2 submatrices:

$$\mathbf{\Pi}(\mathbf{x},\mathbf{x}') = \begin{pmatrix} \mathbf{Q}_1(\mathbf{x},\mathbf{x}') & \mathbf{Q}_2(\mathbf{x},\mathbf{x}') \\ \mathbf{P}_1(\mathbf{x},\mathbf{x}') & \mathbf{P}_2(\mathbf{x},\mathbf{x}') \end{pmatrix} \quad . \tag{38}$$

The definitions of the individual 2×2 submatrices read

$$Q_1^{AB}(\mathbf{x},\mathbf{x}') = \frac{\partial q^A(\mathbf{x})}{\partial q^B(\mathbf{x}')} \quad , \qquad Q_2^{AB}(\mathbf{x},\mathbf{x}') = \frac{\partial q^A(\mathbf{x})}{\partial p_B^{(q)}(\mathbf{x}')} \quad ,$$
$$P_1^{AB}(\mathbf{x},\mathbf{x}') = \frac{\partial p_A^{(q)}(\mathbf{x})}{\partial q^B(\mathbf{x}')} \quad , \qquad P_2^{AB}(\mathbf{x},\mathbf{x}') = \frac{\partial p_A^{(q)}(\mathbf{x})}{\partial p_B^{(q)}(\mathbf{x}')} \quad . \tag{39}$$

Note that submatrix $\mathbf{Q}_2(\mathbf{x},\mathbf{x}')$ has already been defined by Eq. (11). In definitions (38)–(39), the direction of propagation is assumed from point $\mathbf{x}'$ to point $\mathbf{x}$. We analogously decompose and define propagator matrices $\mathbf{\Pi}(\mathbf{x}'',\mathbf{x}')$ and $\mathbf{\Pi}(\mathbf{x},\mathbf{x}'')$.

Since the propagator matrices are symplectic, the inverse matrix to $\mathbf{\Pi}(\mathbf{x},\mathbf{x}'')$ reads

$$[\mathbf{\Pi}(\mathbf{x},\mathbf{x}'')]^{-1} = \begin{pmatrix} \mathbf{P}_2^{\mathrm{T}}(\mathbf{x},\mathbf{x}'') & -\mathbf{Q}_2^{\mathrm{T}}(\mathbf{x},\mathbf{x}'') \\ -\mathbf{P}_1^{\mathrm{T}}(\mathbf{x},\mathbf{x}'') & \mathbf{Q}_1^{\mathrm{T}}(\mathbf{x},\mathbf{x}'') \end{pmatrix} \quad . \tag{40}$$

Propagator matrix $\mathbf{\Pi}(\mathbf{x}'', \mathbf{x})$ differs from matrix (40) just by the direction of propagation along the same ray segment, and can be expressed as

$$\mathbf{\Pi}(\mathbf{x}'', \mathbf{x}) = \begin{pmatrix} \mathbf{P}_2^{\mathrm{T}}(\mathbf{x}, \mathbf{x}'') & \mathbf{Q}_2^{\mathrm{T}}(\mathbf{x}, \mathbf{x}'') \\ \mathbf{P}_1^{\mathrm{T}}(\mathbf{x}, \mathbf{x}'') & \mathbf{Q}_1^{\mathrm{T}}(\mathbf{x}, \mathbf{x}'') \end{pmatrix} \quad . \tag{41}$$

The 2×2 matrices (30) of the second–order derivatives of travel time in ray–centred coordinates read

$$\mathbf{M}(\mathbf{x}'', \mathbf{x}') = \mathbf{P}_2(\mathbf{x}'', \mathbf{x}') \, [\mathbf{Q}_2(\mathbf{x}'', \mathbf{x}')]^{-1} \tag{42}$$

and

$$\mathbf{M}(\mathbf{x}'', \mathbf{x}) = \mathbf{Q}_1^{\mathrm{T}}(\mathbf{x}, \mathbf{x}'') \, [\mathbf{Q}_2^{\mathrm{T}}(\mathbf{x}, \mathbf{x}'')]^{-1} = [\mathbf{Q}_2(\mathbf{x}, \mathbf{x}'')]^{-1} \mathbf{Q}_1(\mathbf{x}, \mathbf{x}'') \quad . \tag{43}$$

Then

$$\begin{aligned} &\mathbf{M}(\mathbf{x}'', \mathbf{x}) + \mathbf{M}(\mathbf{x}'', \mathbf{x}') \\ &= [\mathbf{Q}_2(\mathbf{x}, \mathbf{x}'')]^{-1} [\mathbf{Q}_1(\mathbf{x}, \mathbf{x}'') \mathbf{Q}_2(\mathbf{x}'', \mathbf{x}') + \mathbf{Q}_2(\mathbf{x}, \mathbf{x}'') \mathbf{P}_2(\mathbf{x}'', \mathbf{x}')] \, [\mathbf{Q}_2(\mathbf{x}'', \mathbf{x}')]^{-1} \; . \end{aligned} \tag{44}$$

Chain rule

$$\mathbf{\Pi}(\mathbf{x}, \mathbf{x}') = \mathbf{\Pi}(\mathbf{x}, \mathbf{x}'') \, \mathbf{\Pi}(\mathbf{x}'', \mathbf{x}') \tag{45}$$

for propagator matrices (38) implies relation

$$\mathbf{Q}_2(\mathbf{x}, \mathbf{x}') = \mathbf{Q}_1(\mathbf{x}, \mathbf{x}'') \mathbf{Q}_2(\mathbf{x}'', \mathbf{x}') + \mathbf{Q}_2(\mathbf{x}, \mathbf{x}'') \mathbf{P}_2(\mathbf{x}'', \mathbf{x}') \quad . \tag{46}$$

Relation (44) with Eq. (46) reads

$$\mathbf{M}(\mathbf{x}'', \mathbf{x}) + \mathbf{M}(\mathbf{x}'', \mathbf{x}') = [\mathbf{Q}_2(\mathbf{x}, \mathbf{x}'')]^{-1} \mathbf{Q}_2(\mathbf{x}, \mathbf{x}') \, [\mathbf{Q}_2(\mathbf{x}'', \mathbf{x}')]^{-1} \quad , \tag{47}$$

and we see that

$$\begin{aligned} &\left| \det[\mathbf{M}(\mathbf{x}'', \mathbf{x}) + \mathbf{M}(\mathbf{x}'', \mathbf{x}')] \right| \\ &\qquad = \left| \det[\mathbf{Q}_2(\mathbf{x}, \mathbf{x}'')] \right|^{-1} \left| \det[\mathbf{Q}_2(\mathbf{x}, \mathbf{x}')] \right| \left| \det[\mathbf{Q}_2(\mathbf{x}'', \mathbf{x}')] \right|^{-1} \quad . \end{aligned} \tag{48}$$

8. COMPLETING THE DERIVATION

We now apply the results of previous Sections 5, 6 and 7 to determining factors $C_m(\mathbf{x}, \mathbf{x}')$ and phase shift $\varphi(\mathbf{x}, \mathbf{x}')$ in approximation (12).

8.1. Amplitude Coefficient of the Green Tensor

We insert relations (13) and (48) into Eq. (36) and arrive at relation

$$\frac{C(\mathbf{x}, \mathbf{x}')}{\sqrt{\varrho(\mathbf{x}) \, v(\mathbf{x})}} = 4\pi \, C(\mathbf{x}'', \mathbf{x}') \, C(\mathbf{x}'', \mathbf{x}) \quad . \tag{49}$$

We put $\mathbf{x}'' = \mathbf{x}$ in Eq. (49) and obtain

$$C(\mathbf{x}, \mathbf{x}) = \frac{1}{4\pi} \frac{1}{\sqrt{\varrho(\mathbf{x}) \, v(\mathbf{x})}} \quad . \tag{50}$$

Since $C(\mathbf{x}', \mathbf{x}) = C(\mathbf{x}, \mathbf{x})$ and $C(\mathbf{x}, \mathbf{x}') = C(\mathbf{x}', \mathbf{x}')$, we analogously obtain

$$C(\mathbf{x}, \mathbf{x}') = \frac{1}{4\pi} \frac{1}{\sqrt{\varrho(\mathbf{x}') \, v(\mathbf{x}')}} \quad . \tag{51}$$

8.2. Phase Shift due to Caustics

It is obvious from relation (47) that, for fixed $\mathbf{x}$ and $\mathbf{x}'$, $\mathrm{sgn}[M_{KL}(\mathbf{x}'',\mathbf{x}) + M_{KL}(\mathbf{x}'',\mathbf{x}')]$ is constant outside the caustics indicated by matrix $\mathbf{Q}_2(\mathbf{x},\mathbf{x}'') = \mathbf{Q}_2^{\mathrm{T}}(\mathbf{x}'',\mathbf{x})$ or by matrix $\mathbf{Q}_2(\mathbf{x}'',\mathbf{x}')$. We know that phase shift $\varphi(\mathbf{x}'',\mathbf{x}')$ changes at the caustic indicated by matrix $\mathbf{Q}_2(\mathbf{x}'',\mathbf{x}')$, where matrix $M_{KL}(\mathbf{x}'',\mathbf{x}')$ changes its signature through infinity, and that phase shift $\varphi(\mathbf{x}'',\mathbf{x})$ changes at the caustic indicated by matrix $\mathbf{Q}_2^{\mathrm{T}}(\mathbf{x}'',\mathbf{x})$, where matrix $M_{KL}(\mathbf{x}'',\mathbf{x})$ changes its signature through infinity. If one eigenvalue of matrix $M_{KL}(\mathbf{x}'',\mathbf{x}')$ changes its sign from negative to positive through infinity, we define $\Delta\mathrm{sgn}[M_{KL}(\mathbf{x}'',\mathbf{x}')] = +2$, and analogously for other changes of its signature due to the caustics indicated by matrix $\mathbf{Q}_2(\mathbf{x}'',\mathbf{x}')$. Phase shift $\varphi(\mathbf{x}'',\mathbf{x}')$ changes at the caustics indicated by matrix $\mathbf{Q}_2(\mathbf{x}'',\mathbf{x}')$, where $\mathrm{sgn}[M_{KL}(\mathbf{x}'',\mathbf{x})+M_{KL}(\mathbf{x}'',\mathbf{x}')]$ changes by $\Delta\mathrm{sgn}[M_{KL}(\mathbf{x}'',\mathbf{x}')]$, and analogously for phase shift $\varphi(\mathbf{x}'',\mathbf{x})$. The increment of phase shift $\varphi(\mathbf{x}'',\mathbf{x}')$ at caustic $\mathbf{x}''$ is thus

$$\Delta\varphi(\mathbf{x}'',\mathbf{x}') = -\tfrac{\pi}{4}\,\Delta\mathrm{sgn}[M_{KL}(\mathbf{x}'',\mathbf{x}')] \quad . \tag{52}$$

This phase–shift rule is identical to the phase–shift rule of *Lewis (1965, Eq. F.19)*, and is equivalent to the phase–shift rules of *Bakker (1998)* and *Klimeš (2010)*.

8.3. Initial Phase Shift

We assume that point $\mathbf{x}$ is not situated at a caustic corresponding to a point source at $\mathbf{x}'$. If point $\mathbf{x}''$ is approaching point $\mathbf{x}'$ against the direction of propagation, matrix $M_{KL}(\mathbf{x}'',\mathbf{x}')$ increases to infinity, and we may neglect finite matrix $M_{KL}(\mathbf{x}'',\mathbf{x})$. The limit of relation (37) for $\mathbf{x}'' \to \mathbf{x}'$ thus yields

$$\varphi(\mathbf{x},\mathbf{x}') = \varphi(\mathbf{x}',\mathbf{x}) + \varphi(\mathbf{x}',\mathbf{x}') + \tfrac{\pi}{4}\Big\{\lim_{\mathbf{x}''\to\mathbf{x}'} \mathrm{sgn}[M_{KL}(\mathbf{x}'',\mathbf{x}')] - 2\Big\} \qquad (\mathrm{mod}\ 2\pi)\ . \tag{53}$$

Because of the reciprocity (16) of the phase shift, Eq. (53) yields

$$\varphi(\mathbf{x}',\mathbf{x}') = \tfrac{\pi}{4}\Big\{2 - \lim_{\mathbf{x}''\to\mathbf{x}'} \mathrm{sgn}[M_{KL}(\mathbf{x}'',\mathbf{x}')]\Big\} \qquad (\mathrm{mod}\ 2\pi) \quad . \tag{54}$$

Note that point $\mathbf{x}''$ is approaching initial point $\mathbf{x}'$ along the ray against the direction of propagation.

9. CONCLUSIONS

We insert relation (17) with factor (51) into approximation (12). The zero–order ray–theory approximation of the Green tensor in heterogeneous anisotropic elastic media then reads

$$G_{im}(\mathbf{x},\mathbf{x}',\omega) \simeq \frac{1}{4\pi}\,\frac{g_i(\mathbf{x})\,g_m(\mathbf{x}')}{\sqrt{\varrho(\mathbf{x})\,v(\mathbf{x})\,\varrho(\mathbf{x}')\,v(\mathbf{x}')}\,L(\mathbf{x},\mathbf{x}')}\ \exp[\mathrm{i}\,\varphi(\mathbf{x},\mathbf{x}')]\ \exp[\mathrm{i}\omega\,\tau(\mathbf{x},\mathbf{x}')]\ . \tag{55}$$

The initial phase shift $\varphi(\mathbf{x}',\mathbf{x}')$ is given by relation (54), and its increment due to caustics by relation (52). The sign of the phase shift, as well as the amplitude of the Green tensor correspond to Fourier transform (1). If the right–hand side of the Fourier transform included a multiplicative factor of $(2\pi)^{-\frac{1}{2}}$ or $(2\pi)^{-1}$, the right–hand side of expression (55) should be multiplied by the same factor.

The generalization of the Green tensor to velocity models with structural interfaces is straightforward (*Červený, 2001, Eq. 5.4.17*).

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