Ray series for electromagnetic waves in static heterogeneous bianisotropic dielectric media

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Summary
The paper is devoted to the ray–theory approximation of electromagnetic waves propagating in heterogeneous bianisotropic media. We consider the anisotropic ray theory in which the two electromagnetic waves differing by their polarizations are strictly decoupled and propagate with sufficiently different velocities. We develop the ray theory in terms of the magnetic vector potential with the Weyl gauge (zero electric potential).

Keywords
Electromagnetic waves, heterogeneous media, bianisotropic media, ray theory, ray series, travel time, amplitude, magnetic vector potential, Weyl gauge (zero electric potential).

1. Introduction

This paper is devoted to the ray–theory approximation of electromagnetic waves propagating in heterogeneous bianisotropic media. We study the anisotropic ray theory in which the two electromagnetic waves differing by their polarizations are strictly decoupled and propagate with sufficiently different velocities. We develop the ray theory in terms of the magnetic vector potential with the Weyl gauge (zero electric potential).

1.1. Brief overview of related methods

In computational electromagnetics, the most popular methods for electromagnetic wave propagation in complex media are the full–wave methods mostly based on the weak formulation or on the integral formulation. These methods are represented by the finite–difference techniques (e.g., Capoglu & Smith, 2008; Teixeira, 2008; Fang, Wu & Zhang, 2009), finite–element techniques (e.g., Teixeira, 2008), or multiscale methods (e.g., Chen & Liu, 2013). However, these approaches are limited just to short propagation distances measured in wavelengths, especially in 3–D wave propagation.

Electromagnetic scattering problems are most frequently solved by the method of moments (Harrington, 1993). Although its further developments, such as the multilevel fast multipole algorithm (e.g., Chew et al., 2001), make possible to solve scattering problems of still increasing complexity, its application to "electrically large" problems is still the issue (Fang, Wu & Zhang, 2010).

A way out of the difficulty with restriction to short propagation distances measured in wavelengths is to solve such problems using the ray methods.

The standard ray theory of electromagnetic wave radiation applies to an unbounded homogeneous isotropic medium (Hoop, 1995, chapter 26; Bladel, 2007, chapter 7). Extensions to the electromagnetic Green tensor in homogeneous bianisotropic media were summarized by Olyslager & Lindell (2002). Electromagnetic wave propagation in

Seismic Waves in Complex 3–D Structures, **26** (2016), 167–182 (ISSN 2336–3827, online at http://sw3d.cz)

homogeneous anisotropic (uniaxial, gyrotropic and bianisotropic) media were described by Kong (1986, chapter II), for example.

An overview of the ray methods for heterogeneous isotropic media was given by Bladel (2007, sec. 8.3), for example. For an extension to chiral media, refer to Lindell & Sihvola (1991). The asymptotic ray theory for transient diffusive electromagnetic fields in isotropic media was constructed by Hoop, Oristaglio & Habashy (1996). A more advanced treatment of the subject including the case of an heterogeneous anisotropic dielectric was given by Felsen & Marcuvitz (2003, sec. 1.7).

A concise introduction to electromagnetic beam techniques can be found in Bladel (2007, sec. 8.4). The pulsed–beam propagation method for non–dispersive heterogeneous isotropic media was introduced by Heyman (1994). The extension of the pulsed–beam propagation method that incorporates dispersion can be found in Melamed & Felsen (2000).

Electromagnetic field representations in horizontally layered media with piecewise constant properties for the time–harmonic case were studied by, e.g., Felsen & Marcuvitz (2003, sec. 5.2) or Tai (1994, chapter 11), relying largely on the standard theory of Sommerfeld (1949, chapter IV). The corresponding pulsed electromagnetic Green tensors were detailed by Štumpf, Hoop & Vandenbosch (2013).

It seems that a complete ray theory of electromagnetic waves in *heterogeneous bianisotropic media* is presently missing in the literature.

1.2. Anisotropic ray theory of electromagnetic waves in heterogeneous bianisotropic media

In this paper, we consider linear dielectric media which are generally bianisotropic. We consider the linear constitutive relations for bianisotropic media in the Boys–Post representation without spatial dispersion (Lakhtakia, 2000; Post, 2003; Weiglhofer, 2003; Strunc, 2007). The Boys–Post representation $\mathbf{D}=\mathbf{D}(\mathbf{E},\mathbf{B})$, $\mathbf{H}=\mathbf{H}(\mathbf{E},\mathbf{B})$ of the constitutive relations is more natural than the Tellegen representation $\mathbf{D}=\mathbf{D}(\mathbf{E},\mathbf{H})$, $\mathbf{B}=\mathbf{B}(\mathbf{E},\mathbf{H})$, and is best suited for the formulation in terms of the magnetic vector potential $\mathbf{A}$. For the sake of simplicity, we assume that the media are static (do not change with time). In this case we can work in frequency domain, apply 3–D spatial rays, and avoid 4–D space–time rays. We assume that the media are so smoothly heterogeneous that we can apply the high–frequency ray–theory approximation.

There are two electromagnetic waves propagating in bianisotropic media. They differ by their polarizations. The ray theory described in this paper is applicable if these two waves are strictly decoupled and propagate with sufficiently different velocities. Whenever it is reasonable to emphasize this property, we may refer to the ray theory described in this paper as the *anisotropic ray theory*. If the velocities of the waves are not sufficiently different, the two wave polarizations are coupled (Kravtsov, 1968), and we have to replace the anisotropic ray theory by the *coupling ray theory* which will be described in another paper. The zero–order coupling ray theory represents a generalization of the zero–order anisotropic ray theory and relies on most results of the standard anisotropic ray theory described in this paper.

Whereas the ray methods for electromagnetic waves have traditionally been expressed in terms of the electric field strength vector $\mathbf{E}$ and magnetic induction vector $\mathbf{B}$ or magnetic field strength vector $\mathbf{H}$ (Luneburg, 1944), we shall develop the ray methods in terms of the magnetic vector potential **A**, which is simpler and more advantageous while inducing no drawbacks. The few authors who already considered ray methods in terms of the magnetic vector potential usually assumed the Lorenz gauge, which is best suited for vacuum and well applicable to electromagnetic fields with electrostatic components. Instead of the Lorenz gauge or the Coulomb gauge, we shall assume the Weyl gauge (zero electric potential), which is best suited for electromagnetic wave fields without significant electrostatic components. The Weyl gauge reduces the electromagnetic field variables to just 3 components of the magnetic vector potential **A** which is then parallel with the electric field strength vector **E** in the frequency domain. This reduction of ray methods from 6 components of the electric field strength vector **E** and magnetic induction vector **B** to just 3 components of the magnetic vector potential **A** represents a great advantage for both theory and numerical methods while inducing no drawbacks for the study of electromagnetic wave propagation.

The lower–case Roman indices take values 1, 2 and 3. The lower–case Greek indices take values 1, 2, 3 and 4. The Einstein summation over repetitive indices is used throughout the paper.

2. Maxwell equations with constitutive relations

2.1. Time–domain Maxwell equations with constitutive relations

Maxwell equations

$$\varepsilon^{ijk} E_{k,j} + B^i_{,4} = 0 \tag{1}$$

and

$$B^k_{,k} = 0 \tag{2}$$

for *electric field strength* $E_j = E_j(x^m, x^4)$ and *magnetic induction* $B^j = B^j(x^m, x^4)$ are satisfied if we put

$$E_k = A_{4,k} - A_{k,4} \tag{3}$$

and

$$B^k = \varepsilon^{klm} A_{m,l} \quad , \tag{4}$$

where $A_i = A_i(x^m, x^4)$ is the *magnetic vector potential* and $A_4 = A_4(x^m, x^4)$ represents *minus electric potential* $\varphi = \varphi(x^m, x^4)$,

$$A_4 = -\varphi \quad . \tag{5}$$

The Maxwell equations for *electric displacement* $D^j = D^j(x^m, x^4)$ and *magnetic field strength* $H_j = H_j(x^m, x^4)$ read

$$\varepsilon^{ijk} H_{k,j} - D^i_{,4} = J^i \tag{6}$$

and

$$D^k_{,k} = J^4 \quad , \tag{7}$$

where $J^4 = J^4(x^m, x^4)$ represents *electric charge density* $\rho = \rho(x^m, x^4)$,

$$J^4 = \rho \quad , \tag{8}$$

and $J^i = J^i(x^m, x^4)$ is the *electric current density.*

We thus need the *constitutive relations* which express the mutual dependence between the above mentioned quantities E^k, B^k, D^j, H_j, J^j and J^4.

In this paper, we consider *dielectric media* in which the electric current density and electric charge density vanish outside the source region,

$$J^\gamma = 0 \quad , \tag{9}$$

and 4–vector J^γ represents just the source term.

We assume the constitutive relations in the *Boys–Post representation* which express the dependence of the electric displacement D^j and magnetic field strength H_j on electric field strength E_j and magnetic induction B^j. In this paper, we consider just the *linear* constitutive relations in the Boys–Post representation.

The point constitutive relations without any dispersion can be expressed as (Weiglhofer, 2000, eq. 1.12; 2003, eq. 57)

$$D^i = \varepsilon^{ij} E_j + \alpha^i{}_j B^j \quad , \tag{10}$$

and (Weiglhofer, 2000, eq. 1.13, 2003, eq. 58)

$$H_i = \beta_i{}^j E_j + \mu^{-1}_{ij} B^j \quad . \tag{11}$$

We insert constitutive relations (10) and (11) into Maxwell equations (6),

$$\varepsilon^{ijk} (\beta_k{}^l E_l + \mu^{-1}_{kl} B^l)_{,j} - (\varepsilon^{ij} E_j + \alpha^i{}_j B^j)_{,4} = J^i \quad , \tag{12}$$

and (7),

$$(\varepsilon^{ij} E_j + \alpha^i{}_j B^j)_{,i} = J^4 \quad . \tag{13}$$

We insert expressions (3) and (4) into Maxwell equations (12),

$$\varepsilon^{ijk} [\beta_k{}^l (A_{4,l} - A_{l,4}) + \mu^{-1}_{kl} \varepsilon^{lmn} A_{n,m}]_{,j} - [\varepsilon^{ij} (A_{4,j} - A_{j,4}) + \alpha^i{}_j \varepsilon^{jlm} A_{m,l}]_{,4} = J^i \quad , \tag{14}$$

and (13),

$$[\varepsilon^{ij} (A_{4,j} - A_{j,4}) + \alpha^i{}_j \varepsilon^{jlm} A_{m,l}]_{,i} = J^4 \quad . \tag{15}$$

We define *constitutive tensor* $\chi^{\alpha\beta\gamma\delta}$ by relations

$$\chi^{4i4j} = -\chi^{i44j} = -\chi^{4ij4} = \chi^{i4j4} = -\varepsilon^{ik} \quad , \tag{16}$$

$$\chi^{ij4k} = -\chi^{ijk4} = \varepsilon^{ijr} \beta_r{}^k \quad , \tag{17}$$

$$\chi^{4ikl} = -\chi^{i4kl} = -\alpha^i{}_s \varepsilon^{skl} \tag{18}$$

and

$$\chi^{ijkl} = \varepsilon^{ijr} \mu^{-1}_{rs} \varepsilon^{skl} \quad . \tag{19}$$

The constitutive tensor is skew with respect to its first pair of superscripts,

$$\chi^{\alpha\beta\gamma\delta} = -\chi^{\beta\alpha\gamma\delta} \quad , \tag{20}$$

and its last pair of superscripts,

$$\chi^{\alpha\beta\gamma\delta} = -\chi^{\alpha\beta\delta\gamma} \quad . \tag{21}$$

The 36 distinct components of the constitutive tensor read

$$\chi^{\alpha\beta\gamma\delta} = \begin{array}{c} \\ 41 \\ 42 \\ 43 \\ 23 \\ 31 \\ 12 \end{array} \begin{array}{c} \begin{array}{cccccc} 41 & 42 & 43 & 23 & 31 & 12 \end{array} \\ \begin{pmatrix} -\varepsilon^{11} & -\varepsilon^{12} & -\varepsilon^{13} & -\alpha^1{}_1 & -\alpha^1{}_2 & -\alpha^1{}_3 \\ -\varepsilon^{21} & -\varepsilon^{22} & -\varepsilon^{23} & -\alpha^2{}_1 & -\alpha^2{}_2 & -\alpha^2{}_3 \\ -\varepsilon^{31} & -\varepsilon^{32} & -\varepsilon^{33} & -\alpha^3{}_1 & -\alpha^3{}_2 & -\alpha^3{}_3 \\ \beta_1{}^1 & \beta_1{}^2 & \beta_1{}^3 & \mu^{-1}_{11} & \mu^{-1}_{12} & \mu^{-1}_{13} \\ \beta_2{}^1 & \beta_2{}^2 & \beta_2{}^3 & \mu^{-1}_{21} & \mu^{-1}_{22} & \mu^{-1}_{23} \\ \beta_3{}^1 & \beta_3{}^2 & \beta_3{}^3 & \mu^{-1}_{31} & \mu^{-1}_{32} & \mu^{-1}_{33} \end{pmatrix} \end{array} \quad . \tag{22}$$

Maxwell equations (14) and (15) with linear constitutive relations in the Boys–Post representation then read (Post, 2003, eq. 26)

$$(\chi^{\alpha\beta\gamma\delta} A_{\delta,\gamma})_{,\beta} = J^{\alpha} \quad . \tag{23}$$

Differentiating these Maxwell equations, we obtain the continuity equation

$$J^{\alpha}_{,\alpha} = 0 \quad . \tag{24}$$

If the initial conditions for the Maxwell equations satisfy the fourth Maxwell equation (23) and the continuity equation is satisfied, the fourth Maxwell equation (23) follows from the first three Maxwell equations (23). We can thus replace the fourth Maxwell equation (23) by its initial conditions and by the continuity equation for the source terms. For the electromagnetic wave propagation, we then need just the first three of four Maxwell equations (23),

$$(\chi^{i\beta\gamma\delta} A_{\delta,\gamma})_{,\beta} = J^{i} \quad . \tag{25}$$

In our coordinate system, we choose the Weyl gauge condition

$$A_4 = 0 \quad . \tag{26}$$

Maxwell equations (25) then simplify to

$$(\chi^{i\beta\gamma l} A_{l,\gamma})_{,\beta} = J^{i} \quad . \tag{27}$$

We separate the spatial and temporal derivatives in Maxwell equations (27),

$$(\chi^{ijkl} A_{l,k})_{,j} + (\chi^{ij4l} A_{l,4})_{,j} + (\chi^{i4kl} A_{l,k})_{,4} + (\chi^{i44l} A_{l,4})_{,4} = J^{i} \quad . \tag{28}$$

Within Weyl gauge condition (26), electric field strength $E_j = E_j(x^m, x^4)$ reads

$$E_k = -A_{k,4} \quad . \tag{29}$$

The magnetic induction is given by relation (4).

2.2. Fourier transform

For the sake of simplicity, we assume that the structure is time–independent (static) in our coordinate system,

$$\chi^{\alpha\beta\gamma\delta} = \chi^{\alpha\beta\gamma\delta}(x^m) \quad . \tag{30}$$

Our coordinate system and the Weyl gauge condition (26) are thus related to the static property of the medium.

In a static medium, we can efficiently work in the frequency domain. We define the Fourier transform

$$A_i(x^m, \omega) = (2\pi)^{-\frac{1}{2}} \int_{-\infty}^{+\infty} \mathrm{d}t \; A_i(x^m, x^4) \exp(\mathrm{i}\omega x^4) \tag{31}$$

of the magnetic vector potential. Note that coefficient $(2\pi)^{-\frac{1}{2}}$ can arbitrarily be modified.

2.3. Frequency–domain Maxwell equations with constitutive relations

In frequency domain, Maxwell equations (28) with linear constitutive relations in the Boys–Post representation for $A_i = A_i(x^m,\omega)$ read

$$(\chi^{ijkl}A_{l,k})_{,j} - \mathrm{i}\omega(\chi^{ij4l}A_l)_{,j} - \mathrm{i}\omega\chi^{i4kl}A_{l,k} - \omega^2\chi^{i44l}A_l = J^i \quad . \tag{32}$$

Here electric current density J^i represents the source term. Outside the source, the Maxwell equations in a dielectric medium read

$$(\chi^{ijkl}A_{l,k})_{,j} - \mathrm{i}\omega(\chi^{ij4l}A_l)_{,j} - \mathrm{i}\omega\chi^{i4kl}A_{l,k} - \omega^2\chi^{i44l}A_l = 0 \quad . \tag{33}$$

Within Weyl gauge condition (26), electric field strength $E_j = E_j(x^m,\omega)$ in the frequency domain is a simple multiple of the magnetic vector potential,

$$E_k = \mathrm{i}\omega\, A_k \quad . \tag{34}$$

3. Ray theory in the frequency domain

3.1. Standard ray series

We express the frequency–domain magnetic vector potential $A_j = A_j(x^m,\omega)$ in terms of its vectorial amplitude $a_i = a_i(x^m,\omega)$ and travel time $\tau = \tau(x^m)$ as

$$A_i = a_i \exp(\mathrm{i}\omega\tau) \quad . \tag{35}$$

We express the vectorial amplitude in the form of asymptotic series

$$a_i = \sum_{n=0}^{\infty}(\mathrm{i}\omega)^{-n}\, a_i^{[n]} \quad , \tag{36}$$

where $a_i^{[n]} = a_i^{[n]}(x^m,\omega)$ is the n–th order vectorial amplitude.

The electric field strength is given by relation (34). Magnetic induction $B^j = B^j(x^m,\omega)$ reads

$$B^i = \mathrm{i}\omega\varepsilon^{ijk}\tau_{,j}A_k + \varepsilon^{ijk}a_{k,j}\exp(\mathrm{i}\omega\tau) \quad , \tag{37}$$

see relation (4) with (35). If we neglect the term of order ω^{-1}, the magnetic induction may be approximated by

$$B^i \approx \varepsilon^{ijk}\tau_{,j}E_k \quad , \tag{38}$$

where electric field strength $E_k = E_k(x^m,\omega)$ is given by (34).

3.2. Ray–theory Maxwell equations

The spatial gradient of magnetic vector potential (35) reads

$$A_{l,k} = (\mathrm{i}\omega\tau_{,k}a_l + a_{l,k})\exp(\mathrm{i}\omega\tau) \quad . \tag{39}$$

We insert expressions (35) and (39) into Maxwell equations (33) and obtain ray–theory Maxwell equations

$$\begin{aligned} &-\omega^2\chi^{ijkl}\tau_{,j}\tau_{,k}a_l + \mathrm{i}\omega\big[\chi^{ijkl}\tau_{,j}a_{l,k} + (\chi^{ijkl}\tau_{,k}a_l)_{,j}\big] + (\chi^{ijkl}a_{l,k})_{,j} \\ &+\omega^2(\chi^{ij4l}+\chi^{i4jl})\tau_{,j}a_l - \mathrm{i}\omega\big[(\chi^{ij4l}a_l)_{,j} + \chi^{i4jl}a_{l,j}\big] - \omega^2\chi^{i44l}a_l = 0 \quad . \end{aligned} \tag{40}$$

We define 3×3 *Kelvin–Christoffel matrix*

$$\Gamma^{il}(x^m,p_n,p_4) = \chi^{i\beta\gamma l}(x^m)p_\beta p_\gamma \quad . \tag{41}$$

We can express the terms of order $(\mathrm{i}\omega)^2$ in ray–theory Maxwell equations (40) by means of linear operator

$$N^i(a_m, \tau_{,n}) = \Gamma^{il}(x^m, \tau_{,n}, -1)\, a_l \tag{42}$$

using definition (41). The terms of order $\mathrm{i}\omega$ can be expressed by means of linear operator

$$M^i(a_m, \tau_{,n}) = \chi^{ijkl}\tau_{,j}a_{l,k} + (\chi^{ijkl}\tau_{,k}a_l)_{,j} - \chi^{i4jl}a_{l,j} - (\chi^{ij4l}a_l)_{,j} \quad , \tag{43}$$

and the terms of order 1 can be expressed by means of linear operator

$$L^i(a_m) = (\chi^{ijkl}a_{l,k})_{,j} \quad . \tag{44}$$

Ray–theory Maxwell equations (40) then read

$$(\mathrm{i}\omega)^2 N^i(a_m, \tau_{,n}) + \mathrm{i}\omega M^i(a_m, \tau_{,n}) + L^i(a_m) = 0 \quad . \tag{45}$$

Inserting series (36) into ray–theory Maxwell equations (45), we obtain the Maxwell equations in the form

$$\sum_{n=0}^{\infty} \Big[(\mathrm{i}\omega)^{2-n}\, N^i\big(a_k^{[n]}, \tau_{,l}\big) + (\mathrm{i}\omega)^{1-n}\, M^i\big(a_k^{[n]}, \tau_{,l}\big) + (\mathrm{i}\omega)^{-n}\, L^i\big(a_k^{[n]}\big) \Big] = 0 \quad . \tag{46}$$

Sorting series (46) according to the order of $\mathrm{i}\omega$, we obtain the system of equations

$$N^i\big(a_k^{[n]}, \tau_{,l}\big) + M^i\big(a_k^{[n-1]}, \tau_{,l}\big) + L^i\big(a_k^{[n-2]}\big) = 0 \quad , \quad n = 0, 1, 2, \ldots \quad , \tag{47}$$

where $a_k^{[-1]} = 0$ and $a_k^{[-2]} = 0$, i.e., operator M^i is missing in equation (47) for $n = 0$ and operator L^i is missing in equation (47) for $n = 0, 1$.

3.3. Kelvin–Christoffel equation

Equation (47) for $n = 0$ constitutes the matrix Kelvin–Christoffel equation

$$\Gamma^{il}(x^m, \tau_{,n}, -1)\, a_l^{[0]} = 0 \quad . \tag{48}$$

In order to satisfy Kelvin–Christoffel equation (48), the 3×3 Kelvin–Christoffel matrix (41) must be singular,

$$\det\big[\Gamma^{ad}(x^\mu, \tau_{,n}, -1)\big] = 0 \quad , \tag{49}$$

which represents the first–order partial differential equations for several branches of travel time $\tau = \tau(x^m)$. We shall refer to each of these first–order partial differential equations as the *Eikonal equation*.

We select one of the branches of travel time $\tau = \tau(x^m)$ satisfying characteristic equation (49) and denote the corresponding zero eigenvalue by G, the corresponding right–hand unit eigenvector by g_i, and the corresponding left–hand unit eigenvector by $\vec{g}_i$. The zero–order vectorial amplitude then reads

$$a_i^{[0]} = a^{[0]}\, g_i \quad , \tag{50}$$

where the zero–order ray–theory amplitude $a^{[0]}$ will be determined by the *transport equation* in Section 3.7.

3.4. Eikonal equation and the Hamiltonian function

We define phase–space functions $p_4 = p_4(x^m, p_n)$ as the solutions of Characteristic equation

$$\det\left[\Gamma^{ad}(x^m, p_n, p_4)\right] = 0 \tag{51}$$

for given coordinates x^m and slowness vector p_n. Functions $p_4 = p_4(x^m, p_n)$ are homogeneous functions of the first degree with respect to slowness vector p_n.

The determinant of a 3×3 matrix reads

$$\det\left[\Gamma^{ad}(x^m, p_n, p_4)\right] = \tfrac{1}{6}\varepsilon_{abc}\varepsilon_{ijk}\Gamma^{ai}(x^m, p_n, p_4)\Gamma^{bj}(x^m, p_n, p_4)\Gamma^{ck}(x^m, p_n, p_4) \quad . \tag{52}$$

We introduce three 3×3 matrices

$$\Gamma_0^{ad}(x^m) = \chi^{a44d}(x^m) \quad , \tag{53}$$

$$\Gamma_1^{ad}(x^m, p_n) = \left[\chi^{a4cd}(x^m) + \chi^{ac4d}(x^m)\right] p_c \quad , \tag{54}$$

$$\Gamma_2^{ad}(x^m, p_n) = \chi^{abcd}(x^m)\, p_b\, p_c \quad , \tag{55}$$

and express the 3×3 Kelvin–Christoffel matrix as

$$\Gamma^{ad}(x^m, p_n, p_4) = (p_4)^2\Gamma_0^{ad}(x^m) + p_4\,\Gamma_1^{ad}(x^m, p_n) + \Gamma_2^{ad}(x^m, p_n) \quad . \tag{56}$$

We define the matrices

$$\overline{\Gamma}_{\bullet\, ai} = \tfrac{1}{2}\,\varepsilon_{abc}\,\varepsilon_{ijk}\,\Gamma_\bullet^{bj}\,\Gamma_\bullet^{ck} \tag{57}$$

of cofactors of given 3×3 matrices $\Gamma_\bullet^{ij}$, where $\bullet = 0, 1, 2$. The determinant of 3×3 Kelvin–Christoffel matrix (56) then reads

$$\begin{aligned}\det\left[\Gamma^{ad}(x^m, p_n, p_4)\right] &= (p_4)^6\Gamma_0(x^m) + (p_4)^5\Gamma_1(x^m, p_n) + (p_4)^4\Gamma_2(x^m, p_n) \\ &+(p_4)^3\Gamma_3(x^m, p_n) + (p_4)^2\Gamma_4(x^m, p_n) + p_4\,\Gamma_5(x^m, p_n) + \Gamma_6(x^m, p_n)\end{aligned} \tag{58}$$

with coefficients

$$\Gamma_0(x^m, p_n) = \det\left[\Gamma_0^{ad}(x^m)\right] \quad , \tag{59}$$

$$\Gamma_1(x^m, p_n) = \overline{\Gamma}_{0\,rs}(x^m)\Gamma_1^{rs}(x^m, p_n) \quad , \tag{60}$$

$$\Gamma_2(x^m, p_n) = \Gamma_0^{rs}(x^m)\overline{\Gamma}_{1\,rs}(x^m, p_n) + \overline{\Gamma}_{0\,rs}(x^m)\Gamma_2^{rs}(x^m, p_n) \quad , \tag{61}$$

$$\Gamma_3(x^m, p_n) = \varepsilon_{abc}\varepsilon_{ijk}\Gamma_0^{ai}(x^m)\Gamma_1^{bj}(x^m, p_n)\Gamma_2^{ck}(x^m, p_n) + \det\left[\Gamma_1^{ad}(x^m, p_n)\right] \quad , \tag{62}$$

$$\Gamma_4(x^m, p_n) = \Gamma_0^{rs}(x^m, p_n)\overline{\Gamma}_{2\,rs}(x^m, p_n) + \overline{\Gamma}_{1\,rs}(x^m, p_n)\Gamma_2^{rs}(x^m, p_n) \quad , \tag{63}$$

$$\Gamma_5(x^m, p_n) = \Gamma_1^{rs}(x^m, p_n)\overline{\Gamma}_{2\,rs}(x^m, p_n) \tag{64}$$

and

$$\Gamma_6(x^m, p_n) = \det\left[\Gamma_2^{ad}(x^m)\right] \quad . \tag{65}$$

Since $\Gamma_2^{ij}(x^m, p_n)$ is a singular matrix obeying identities

$$\Gamma_2^{ij}(x^m, p_n)\, p_j = 0 \tag{66}$$

and

$$p_i\,\Gamma_2^{ij}(x^m, p_n) = 0 \quad , \tag{67}$$

matrix $\Gamma_2^{ad}(x^m, p_n)$ is singular,

$$\det\left[\Gamma_2^{ad}(x^m, p_n)\right] = 0 \quad , \tag{68}$$

and the matrix $\overline{\Gamma}_{2\,ij}(x^m, p_n)$ of its cofactors is a multiple of dyadic p_ip_j. Then

$$\Gamma_5(x^m, p_n) = 0 \tag{69}$$

and

$$\Gamma_6(x^m, p_n) = 0 \quad . \tag{70}$$

The sixth–order Characteristic equation (51) thus has two zero solutions $p_4 = 0$. The other four solutions $p_4 = p_4(x^m, p_n)$ are the solutions of fourth–order polynomial equation

$$(p_4)^4\Gamma_0(x^m) + (p_4)^3\Gamma_1(x^m, p_n) + (p_4)^2\Gamma_2(x^m, p_n) + p_4\,\Gamma_3(x^m, p_n) + \Gamma_4(x^m, p_n) = 0 \quad . \tag{71}$$

This fourth–order polynomial equation for p_4 has two solutions with negative real parts and two solutions with positive real parts. All solutions $p_4 = p_4(x^m, p_n)$ are homogeneous functions of the first degree with respect to p_n.

In order to identify parameter ω with circular frequency, we need $p_4 = -1$. We thus consider two solutions with negative real parts only. We choose one of them, and rescale the slowness vector

$$p_n \longrightarrow p_n/(-p_4) \tag{72}$$

in order to obtain

$$p_4 \longrightarrow -1 \quad . \tag{73}$$

The Hamilton–Jacobi equation for travel time τ then reads

$$p_4(x^m, \tau_{,n}) = -1 \quad , \tag{74}$$

where $p_4(x^m, p_n)$ is the homogeneous Hamiltonian function of the first degree with respect to slowness vector p_n. Since the perturbation expansions of travel time are most accurate for homogeneous Hamiltonian functions of the minus first degree with respect to slowness vector p_n, we shall consider Hamiltonian function

$$H(x^m, p_n) = [p_4(x^m, p_n)]^{-1} \tag{75}$$

which is a homogeneous function of the minus first degree with respect to slowness vector p_n, and express the Hamilton–Jacobi equation for travel time τ as

$$H(x^m, \tau_{,n}) = -1 \quad . \tag{76}$$

The methods for solving the Hamilton–Jacobi equation are already mostly developed (Hamilton, 1837; Červený, 1972; Klimeš, 2002; 2010).

3.5. Hamiltonian equations of rays

The corresponding rays satisfy Hamilton equations

$$\frac{\mathrm{d}x^i}{\mathrm{d}\gamma} = \frac{\partial H}{\partial p_i}(x^m, p_n) \quad , \tag{77}$$

$$\frac{\mathrm{d}p_i}{\mathrm{d}\gamma} = -\frac{\partial H}{\partial x^i}(x^m, p_n) \quad , \tag{78}$$

where $\frac{\partial H}{\partial x^i}$ and $\frac{\partial H}{\partial p_i}$ denote the partial derivatives of Hamiltonian function $H(x^m, p_n)$ of six phase–space coordinates x^m, p_n.

For our homogeneous Hamiltonian function with respect to p_n, independent parameter γ along rays coincides with travel time τ, and

$$V^i(x^m) = \frac{\partial H}{\partial p_i}\big(x^m, \tau_{,n}(x^r)\big) \tag{79}$$

represents the ray–velocity vector.

Differentiating the Kelvin–Christoffel matrix (56) with respect to phase–space coordinates x^m, p_n, and putting $p_4 = -1$, we obtain equations

$$\frac{\partial \Gamma^{ad}}{\partial x^i} = -2\frac{\partial p_4}{\partial x^i}\chi^{a44d} + \frac{\partial p_4}{\partial x^i}\big(\chi^{ab4d}+\chi^{a4bd}\big)p_b + \chi^{a44d}_{,i} - \big(\chi^{ab4d}+\chi^{a4bd}\big)_{,i}p_b + \chi^{abcd}_{,i}p_b p_c \quad (80)$$

and

$$\frac{\partial \Gamma^{ad}}{\partial p_i} = -2\frac{\partial p_4}{\partial p_i}\chi^{a44d} + \frac{\partial p_4}{\partial p_i}\big(\chi^{ab4d}+\chi^{a4bd}\big)p_b - \big(\chi^{ai4d}+\chi^{a4id}\big) + \big(\chi^{aicd}+\chi^{acid}\big)p_c \ . \quad (81)$$

Multiplying expressions (80) and (81) by eigenvectors $\vec{g}_a$ and g_d and putting the products zero, we obtain relations

$$\frac{\partial H}{\partial x^i} = -\frac{1}{2\,\varrho}\,\vec{g}_a \chi^{a\beta\gamma d}_{,i} p_\beta p_\gamma g_d \quad (82)$$

and

$$\frac{\partial H}{\partial p_i} = -\frac{1}{2\,\varrho}\,\vec{g}_a \big(\chi^{ai\gamma d}+\chi^{a\gamma id}\big)p_\gamma g_d \quad (83)$$

with

$$\varrho = -\tfrac{1}{2}\,\vec{g}_a \big(\chi^{a4\gamma d}+\chi^{a\gamma 4d}\big)p_\gamma g_d \quad (84)$$

for the phase–space derivatives of Hamiltonian function (75). In above relations (82)–(84), we assume that $p_4 = -1$. Looking at constitutive tensor (22), we see that quantity ϱ is dominated by term $\vec{g}_a\chi^{a44d}g_d = \vec{g}_a\varepsilon^{ad}g_d$ and should be positive.

3.6. Principal and additional amplitude components

Analogously to the zero–order vectorial amplitude (50), we define the amplitude components with respect to the three right–hand eigenvectors of the Kelvin–Christoffel matrix: eigenvector g_i corresponding to the selected eigenvalue $G = 0$ and other two eigenvectors $g_i^\perp$ corresponding to other two eigenvalues $G^\perp$. We decompose each vectorial amplitude $a_i^{[n]}$ into principal component $a^{[n]}$ and two additional components $a^{\perp\,[n]}$,

$$a_i^{[n]} = a_i^{[n]} g_i + \sum_\perp a^{\perp\,[n]}\, g_i^\perp \quad , \quad (85)$$

where the summation is performed over two superscripts $^\perp$. Considering expression (50), we assume that both $a^{\perp\,[0]} = 0$.

We multiply equation (47) for $n > 0$ by two left–hand eigenvectors $\vec{g}_i^\perp$. Since

$$N^i\big(a_m^{[n]}, \tau_{,n}\big) = \sum_\perp a^{\perp\,[n]}\, G^\perp\, g_i^\perp \quad , \quad (86)$$

we immediately obtain two additional components

$$\boxed{a^{\perp\,[n]} = -\big[\vec{g}_i^\perp M^i(a_k^{[n-1]}, \tau_{,n}) + \vec{g}_i^\perp L^i(a_k^{[n-2]})\big]\,\big(G^\perp\big)^{-1}} \quad (87)$$

in terms of the lower–order vectorial amplitudes.

3.7. Transport equation for principal amplitude components

To obtain the transport equation, we multiply ray–theory Maxwell equations (47) by left–hand eigenvector $\vec{g}_i$, consider relation (86), and obtain transport equation

$$\vec{g}_i M^i(a_k^{[n]}, \tau_{,n}) + \vec{g}_i L^i(a_k^{[n-1]}) = 0 \tag{88}$$

for principal amplitude components. We decompose the amplitude argument of linear operator M^i according to decomposition (85) and arrive at equation

$$\vec{g}_i M^i(a^{[n]} g_k, \tau_{,n}) = -\sum_{\perp} \vec{g}_i M^i(a^{\perp[n]} g_k^{\perp}, \tau_{,n}) - \vec{g}_i L^i(a_k^{[n-1]}) \quad . \tag{89}$$

We multiply operator (43) by left–hand eigenvector $\vec{g}_i$, and obtain relation

$$\begin{aligned}\vec{g}_i M^i(a^{[n]} g_m, \tau_{,n}) = {} & \vec{g}_i \chi^{ikjl} \tau_{,k} (a^{[n]} g_l)_{,j} + \vec{g}_i (\chi^{ijkl} \tau_{,k} a^{[n]} g_l)_{,j} \\ & - \vec{g}_i \chi^{i4jl} (a^{[n]} g_l)_{,j} - \vec{g}_i (\chi^{ij4l} a^{[n]} g_l)_{,j} \quad ,\end{aligned} \tag{90}$$

which we express in terms of ray velocity vector (79) given by (83) as

$$\vec{g}_i M^i(a^{[n]} g_m, \tau_{,n}) = -2\varrho V^j a_{,j}^{[n]} - (\varrho V^j)_{,j} a^{[n]} + 2\varrho\, S\, a^{[n]} \quad . \tag{91}$$

The first two terms on the right–hand side of relation (91) are well known from the ray series with a constitutive tensor symmetric with respect to the first and second pairs of indices (Červený, 2001, eq. 5.7.23). We see that quantity ϱ specified by definition (84) plays here an analogous role to the density in propagation of elastic waves.

Quantity S in the rightmost term of transport equation (91) can be determined using relation (90) as

$$S = \tfrac{1}{2\,\varrho} \left[(\varrho V^j)_{,j} + \vec{g}_i \chi^{ikjl} \tau_{,k} g_{l,j} + \vec{g}_i (\chi^{ijkl} \tau_{,k} g_l)_{,j} - \vec{g}_i \chi^{i4jl} g_{l,j} - \vec{g}_i (\chi^{ij4l} g_l)_{,j} \right] \quad , \tag{92}$$

and vanishes for constitutive tensor $\chi^{\alpha\beta\gamma\delta}(x^m) = \chi^{\gamma\delta\alpha\beta}(x^m)$ symmetric with respect to the first and second pairs of indices. We shall study this quantity (92) in more detail in the next subsection.

For each $n > 0$, we define quantity

$$Z^{[n-1]} = \frac{1}{2\sqrt{\varrho}} \left[\sum_{\perp} \vec{g}_i M^i \big(a^{\perp[n]} g_k^{\perp}, \tau_{,n} \big) + \vec{g}_i L^i \big(a_k^{[n-1]} \big) \right] \quad , \tag{93}$$

where additional amplitude components $a^{\perp[n]}$ are given by expression (87). Quantity (93) is thus determined by the amplitudes up to the $(n-1)^{\text{th}}$ order.

Considering definitions (91) and (93), the n^{th}–order transport equation (89) reads

$$\sqrt{\varrho}\, V^j a_{,j}^{[n]} + \tfrac{1}{2\sqrt{\varrho}} (\varrho V^j)_{,j} a^{[n]} = \sqrt{\varrho}\, S\, a^{[n]} + Z^{[n-1]} \quad . \tag{94}$$

The solution of transport equation (94) for $n = 0$ reads

$$\boxed{a^{[0]} = a_0^{[0]} \, (\varrho_0\, J_0)^{\frac{1}{2}} \, (\varrho\, J)^{-\frac{1}{2}} \, \exp\!\Big(\int_{\tau_0}^{\tau} \mathrm{d}\gamma\, S \Big) \quad ,} \tag{95}$$

where subscript $_0$ denotes the initial conditions.

Squared geometrical spreading

$$J = \det \left(\frac{\partial x^i}{\partial \gamma^a} \right) \tag{96}$$

(Babich, 1961, eq. 3.7; Červený, 2001, eq. 3.10.9) represents the Jacobian of transformation from ray coordinates $\gamma^1, \gamma^2, \gamma^3$ to spatial coordinates x^i. The ray coordinates are composed of ray parameters γ^1 and γ^2, and of independent parameter $\gamma^3 = \gamma$ along rays.

Factor $\exp\big(\int_{\tau_0}^{\tau} \mathrm{d}\gamma\, S\big)$ in (95) is present due to the skew part $\chi^{\alpha\beta\gamma\delta}(x^m) - \chi^{\gamma\delta\alpha\beta}(x^m)$ of the constitutive tensor, see the next subsection.

The solution of the transport equation for $n > 0$ reads (Červený, 2001, eq. 5.7.30)

$$a^{[n]} = a^{[0]} \left[\frac{a_0^{[n]}}{a_0^{[0]}} + \int_{\tau_0}^{\tau} \mathrm{d}\gamma\, \frac{Z^{[n-1]}}{a^{[0]}\sqrt{\varrho}} \right] \quad . \tag{97}$$

3.8. Quantity S responsible for amplitude correction

Exponential term $\exp\big(\int_{\tau_0}^{\tau} \mathrm{d}\gamma\, S\big)$ in expression (95) for the zero–order principal amplitude represents the main difference from the analogous standard expression derived for constitutive tensor (22) symmetric with respect to the first and second pairs of indices. We shall now derive various relations for quantity $S = S(x^m)$.

We insert ray velocity vector (79) given by (83) into definition (92) and obtain relation

$$S = \frac{1}{2\,\varrho} \Big\{ -\frac{1}{2} \Big[\vec{g}_i \big(\chi^{ijkl} + \chi^{ikjl}\big) \tau_{,k} g_l \Big]_{,j} + \vec{g}_i \chi^{ikjl} \tau_{,k} g_{l,j} + \vec{g}_i (\chi^{ijkl} \tau_{,k} g_l)_{,j}$$
$$+ \frac{1}{2} \Big[\vec{g}_i \big(\chi^{ij4l} + \chi^{i4jl}\big) g_l \Big]_{,j} - \vec{g}_i \chi^{i4jl} g_{l,j} - \vec{g}_i (\chi^{ij4l} g_l)_{,j} \Big\} \quad . \tag{98}$$

We express relation (98) as

$$S = \frac{1}{2\,\varrho} \Big\{ -\frac{1}{2} \Big[\vec{g}_i \big(\chi^{ijkl} + \chi^{ikjl}\big) \tau_{,k} g_l \Big]_{,j} + (\vec{g}_i \chi^{ijkl} \tau_{,k} g_l)_{,j} - \vec{g}_{i,j} \chi^{ijkl} \tau_{,k} g_l + \vec{g}_i \chi^{ikjl} \tau_{,k} g_{l,j}$$
$$+ \frac{1}{2} \Big[\vec{g}_i \big(\chi^{ij4l} + \chi^{i4jl}\big) g_l \Big]_{,j} - (\vec{g}_i \chi^{ij4l} g_l)_{,j} + \vec{g}_{i,j} \chi^{ij4l} g_l - \vec{g}_i \chi^{i4jl} g_{l,j} \Big\} \quad . \tag{99}$$

After summation, we obtain expression

$$S = \frac{1}{2\,\varrho} \Big\{ \frac{1}{2} \Big[\vec{g}_i \big(\chi^{ijkl} - \chi^{ikjl}\big) \tau_{,k} g_l \Big]_{,j} - \vec{g}_{i,j} \chi^{ijkl} \tau_{,k} g_l + \vec{g}_i \chi^{ikjl} \tau_{,k} g_{l,j}$$
$$- \frac{1}{2} \Big[\vec{g}_i \big(\chi^{ij4l} - \chi^{i4jl}\big) g_l \Big]_{,j} + \vec{g}_{i,j} \chi^{ij4l} g_l - \vec{g}_i \chi^{i4jl} g_{l,j} \Big\} \quad . \tag{100}$$

We differentiate the products in expression (100) and obtain new expression

$$S = \frac{1}{4\,\varrho} \Big\{ \vec{g}_i \big(\chi^{ijkl} - \chi^{ikjl}\big)_{,j} \tau_{,k} g_l - \vec{g}_{i,j} \big(\chi^{ijkl} + \chi^{ikjl}\big) \tau_{,k} g_l + \vec{g}_i \big(\chi^{ijkl} + \chi^{ikjl}\big) \tau_{,k} g_{l,j}$$
$$- \vec{g}_i \big(\chi^{ij4l} - \chi^{i4jl}\big)_{,j} g_l + \vec{g}_{i,j} \big(\chi^{ij4l} + \chi^{i4jl}\big) g_l - \vec{g}_i \big(\chi^{ij4l} + \chi^{i4jl}\big) g_{l,j} \Big\} \tag{101}$$

We differentiate characteristic equation

$$\Gamma^{il}\, g_l = G\, g_i \tag{102}$$

for the right–hand eigenvector with respect to spatial coordinates,

$$\Gamma^{il}_{,j}\, g_l + \Gamma^{il}\, g_{l,j} = G_{,j}\, g_i + G\, g_{i,j} \quad , \tag{103}$$

consider $G=0$ and birthonormality of the left–hand and right–hand eigenvectors, and obtain relation

$$g_{i,j} = -\sum_{\perp} g_i^{\perp}\vec{g}_k^{\perp}\Gamma^{kl}_{,j}g_l\left(G^{\perp}\right)^{-1} + g_i\vec{g}_k g_{k,j} \tag{104}$$

for the spatial gradient of the right–hand eigenvector. The rightmost term in relation (104) accounts for the undefined changes of the length of the right–hand eigenvector g_i. We differentiate characteristic equation

$$\vec{g}_i\Gamma^{il} = G\,\vec{g}_l \tag{105}$$

for the left–hand eigenvector with respect to spatial coordinates,

$$\vec{g}_i\Gamma^{il}_{,j} + \vec{g}_{i,j}\,\Gamma^{il} = G_{,j}\vec{g}_l + G\,\vec{g}_{l,j} \quad , \tag{106}$$

and obtain analogous relation

$$\vec{g}_{i,j} = -\sum_{\perp} \vec{g}_k\Gamma^{kl}_{,j}g_l^{\perp}\vec{g}_i^{\perp}\left(G^{\perp}\right)^{-1} + \vec{g}_i g_k\vec{g}_{k,j} \tag{107}$$

for the spatial gradient of the left–hand eigenvector. The rightmost term in relation (107) accounts for the undefined changes of the length of the left–hand eigenvector $\vec{g}_i$, and satisfies identity

$$g_k\vec{g}_{k,j} = -\vec{g}_k g_{k,j} \tag{108}$$

obtained by differentiating normalization condition

$$\vec{g}_k g_k = 1 \quad . \tag{109}$$

We insert the gradients (104) and (107) of the eigenvectors of the Christoffel matrix into expression (101), consider identity (108), and arrive at expression

$$\begin{aligned} S = {} & \frac{1}{4\,\varrho}\sum_{\perp}\left(\vec{g}_k\Gamma^{kl}_{,j}g_l^{\perp}\vec{g}_r^{\perp}\frac{\partial\Gamma^{rs}}{\partial p_j}g_s - \vec{g}_r\frac{\partial\Gamma^{rs}}{\partial p_j}g_s^{\perp}\vec{g}_k^{\perp}\Gamma^{kl}_{,j}g_l\right)\left(G^{\perp}\right)^{-1} \\ & + \frac{1}{4\,\varrho}\vec{g}_i\left(\chi^{ijkl}-\chi^{ikjl}\right)_{,j}\tau_{,k}g_l - \frac{1}{4\,\varrho}\vec{g}_i\left(\chi^{ij4l}-\chi^{i4jl}\right)_{,j}g_l - \vec{g}_k g_{k,j}V^j \quad , \end{aligned} \tag{110}$$

where ray–velocity vector V^j is given by definition (79) with derivative (83).

We now express the spatial derivatives $\Gamma^{kl}_{,j}$ of the Christoffel matrix in terms of its phase–space derivatives as

$$\Gamma^{kl}_{,j} = \frac{\partial\Gamma^{kl}}{\partial x^j} + \frac{\partial\Gamma^{kl}}{\partial p_s}\tau_{,sj} \quad . \tag{111}$$

For $p_4=-1$, Kelvin–Christoffel matrix (41) reads

$$\Gamma^{il}(x^m,p_n,-1) = \chi^{ijkl}(x^m)p_jp_k - \chi^{ij4l}(x^m)p_j - \chi^{i4jl}(x^m)p_j + \chi^{i44l}(x^m) \quad . \tag{112}$$

The partial derivatives of Kelvin–Christoffel matrix (112) with respect phase–space coordinates x^m and p_n read

$$\frac{\partial\Gamma^{kl}}{\partial x^j}(x^m,\tau_{,n},-1) = \chi^{krsl}_{,j}\tau_{,r}\tau_{,r} - \left(\chi^{kr4l}+\chi^{k4rl}\right)_{,j}\tau_{,r} + \chi^{k44l}_{,j} \tag{113}$$

and

$$\frac{\partial\Gamma^{kl}}{\partial p_j}(x^m,\tau_{,n},-1) = \left(\chi^{kjrl}+\chi^{krjl}\right)\tau_{,r} - \left(\chi^{kj4l}+\chi^{k4jl}\right) \quad . \tag{114}$$

Quantity (110) with identity (111) finally reads

$$S = \frac{1}{4\,\varrho} \sum_{\perp} \left(\vec{g}_k \frac{\partial \Gamma^{kl}}{\partial x^j} g_l^{\perp} \vec{g}_r^{\perp} \frac{\partial \Gamma^{rs}}{\partial p_j} g_s - \vec{g}_k \frac{\partial \Gamma^{kl}}{\partial p_j} g_l^{\perp} \vec{g}_r^{\perp} \frac{\partial \Gamma^{rs}}{\partial x^j} g_s \right) \left(G^{\perp} \right)^{-1}$$
$$+ \frac{1}{4\,\varrho} \vec{g}_i \left(\chi^{ijkl} - \chi^{ikjl} \right)_{,j} \tau_{,k} g_l - \frac{1}{4\,\varrho} \vec{g}_i \left(\chi^{ij4l} - \chi^{i4jl} \right)_{,j} g_l - \vec{g}_i \frac{\mathrm{d}g_i}{\mathrm{d}\gamma} \quad . \tag{115}$$

The last term $\vec{g}_i \frac{\mathrm{d}g_i}{\mathrm{d}\gamma}$ in expression (115) represents just the correction of principal amplitude $U^{[n]}$ in decomposition (85) due to the undefined length of right–hand eigenvector g_i, and vanish if we put

$$\vec{g}_i \frac{\mathrm{d}g_i}{\mathrm{d}\gamma} = 0 \tag{116}$$

along each ray.

Expression (115) for quantity S may be singular at slowness–surface singularities, but is regular at spatial caustics.

Quantity S vanishes for a constitutive tensor symmetric with respect to the first and second pairs of indices. For a non–symmetric constitutive tensor, quantity S vanishes in a homogeneous medium.

Acknowledgements

I am grateful to Martin Štumpf who provided me with useful information on various methods for calculating electromagnetic waves propagating in complex media.

The research has been supported by the Grant Agency of the Czech Republic under contract 16-01312S, and by the members of the consortium “Seismic Waves in Complex 3–D Structures” (see “http://sw3d.cz”).

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