ANALYTICAL ONE–WAY PLANE–WAVE SOLUTION IN THE 1-D ANISOTROPIC "SIMPLIFIED TWISTED CRYSTAL" MODEL

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ABSTRACT

Analytical expressions for the exact 2×2 one–way propagator matrix of a plane S wave, propagating along the axis of spirality in the simple 1-D anisotropic "simplified twisted crystal" model, are presented. The analytical equations are useful in testing the applicability and accuracy of various approximate wavefield modelling methods, especially of the coupling ray theory and of its various quasi–isotropic approximations and various numerical implementations.

In addition to the exact analytical solution of the elastodynamic equation in the "simplified twisted crystal" model, the analytical solutions of the equations of the four ray methods are given. The ray methods are (a) the coupling ray theory, (b) the coupling ray theory with the quasi–isotropic perturbation of travel times, (c) the anisotropic ray theory, (d) the isotropic ray theory. These four approximate solutions of the elastodynamic equation are roughly compared with the exact solution. Both the exact analytical solution and the analytical ray–theory solutions in the "simplified twisted crystal" model are also helpful in debugging computer codes for various approximate wavefield modelling methods, especially for the coupling ray theory.

Keywords: anisotropy, S–wave coupling, polarization, elastic waves, exact solution

1. INTRODUCTION

The *"twisted crystal"* model is created of a homogeneous anisotropic elastic material by uniformly helicoidally twisting the x_1x_2 coordinate plane about the x_3 axis. It is one of the simplest models suitable for demonstrating the limits of applicability of the zero–order isotropic and anisotropic ray theories and for testing the coupling ray theory (*Coates and Chapman, 1990*; *Červený, 2001*), which is the generalization of both the zero–order isotropic and anisotropic ray theories, providing a continuous transition between them. Note that by the *model* we understand the spatial distributions of the elastic moduli and density. The model thus mathematically represents the elastic properties of a geological structure or of another body.

The great advantage of this model is that the exact solution for the plane wave propagating along the axis of spirality can be examined analytically. The general plane–wave solution for the general initial conditions expressed in terms of displacement and stress was derived by *Lakhtakia (1994)*, who also presented explicit analytical equations for the *"simplified twisted crystal"* model with vanishing elastic moduli a_{1333} and a_{2333}, in which the u_1 and u_2 displacement components are strictly separated from the longitudinal u_3 component.

In this paper we study only the simplified twisted crystal model. Contrary to Lakhtakia's paper, we do not seek the solution for initial displacement and stress, but concentrate on the 2×2 one–way propagator matrices suitable for comparison with the coupling ray theory of *Coates and Chapman (1990)*. The exact analytical solution in the simplified twisted crystal model is derived in Section 3. It is useful in testing the applicability and accuracy of various approximate wavefield modelling methods, especially of the coupling ray theory and of its various quasi–isotropic approximations and various numerical implementations (*Bulant, Klimeš and Pšenčík, 1999; 2000*; *Bulant et al., 2004*; *Bulant and Klimeš, 2004*).

In Section 4, the analytical solutions of the equations of the four ray methods are given. The ray methods are (a) the coupling ray theory, (b) the coupling ray theory with the quasi–isotropic perturbation of travel times, (c) the anisotropic ray theory, (d) the isotropic ray theory. These four approximate solutions of the elastodynamic equations are roughly compared with the exact solution. For the list of quasi–isotropic approximations of the coupling ray theory refer to *Bulant and Klimeš (2002; 2004)*. Both the exact analytical solution and the analytical ray–theory solutions in the simplified twisted crystal model are also helpful in debugging computer codes for various approximate wavefield modelling methods, especially for the coupling ray theory (*Bulant et al., 1999; 2000; 2004*).

The simplified twisted crystal model is designed for testing purposes and has no direct relation to geological structures, but the rotation of the eigenvectors of the Christoffel matrix about the ray and the related wave–propagation phenomena are similar as in the models of geological structures. In the simplified twisted crystal model, the rotation of the eigenvectors of the Christoffel matrix corresponds to the rotation of the crystal axes. In the models of geological structures, the rotation of the eigenvectors of the Christoffel matrix is usually caused by heterogeneities bending rays rather than by the rotation of the crystal axes.

2. "SIMPLIFIED TWISTED CRYSTAL" MODEL

The elastodynamic equation in the frequency domain reads

$$[\varrho a_{ijkl} u_{k,l}]_{,j} = -\varrho\,\omega^2 u_i \quad , \tag{1}$$

where a_{ijkl} are the density–normalized elastic moduli (stiffness tensor). The lower–case subscripts take values $i, j, k, ... = 1, 2, 3$, the upper–case subscripts take values $I, J, K, ... = 1, 2$, the Einstein summation over the pairs of identical indices is applied.

For plane wave $u_i = u_i(x_3)$, propagating along the x_3 axis in the 1-D anisotropic model $a_{i3k3} = a_{i3k3}(x_3)$ with constant density ϱ, elastodynamic equation (1) simplifies to

$$(a_{i3k3} u_{k,3})_{,3} = -\omega^2 u_i \quad . \tag{2}$$

In the 1-D anisotropic *simplified twisted crystal* model we take

$$a_{K333} = 0 \quad . \tag{3}$$

Components u_K are then fully separated from u_3,

$$(a_{I3K3} u_{K,3})_{,3} = -\omega^2 u_I \quad . \tag{4}$$

Introducing 2×2 symmetric matrix

$$\mathbf{A} = \begin{pmatrix} a_{1313} & a_{1323} \\ a_{2313} & a_{2323} \end{pmatrix} \quad , \tag{5}$$

the equation for

$$\mathbf{u} = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \tag{6}$$

may be expressed in matrix form as

$$(\mathbf{A}\mathbf{u}')' = -\omega^2 \mathbf{u} \quad , \tag{7}$$

where the prime denotes the derivative with respect to x_3, $\mathbf{u}' = \mathbf{u}_{,3}$.

In the 1-D anisotropic simplified twisted crystal model we choose elastic moduli a_{I3K3} in the form of

$$\mathbf{A} = v_0^2 \mathbf{B} \tag{8}$$

with

$$\mathbf{B} = \begin{pmatrix} 1 + \varepsilon\cos(2Kx_3) & \varepsilon\sin(2Kx_3) \\ \varepsilon\sin(2Kx_3) & 1 - \varepsilon\cos(2Kx_3) \end{pmatrix} \quad . \tag{9}$$

Here Kx_3 is the rotational angle of the crystal axes at x_3. Matrix $\mathbf{B}$ must be positive definite, i.e.

$$-1 < \varepsilon < 1 \quad . \tag{10}$$

Let us also assume

$$K \neq 0 \tag{11}$$

to simplify the derivation. The solution for $K = 0$ is obvious. Due to the separation of plane waves, other elastic moduli than a_{i3K3} may arbitrarily depend on x_3. Elastodynamic equation (7) for the plane S wave in the simplified twisted crystal model then reads

$$(\mathbf{B}\mathbf{u}')' = -k_0^2 \mathbf{u} \quad , \tag{12}$$

where

$$k_0 = \frac{\omega}{v_0} \quad . \tag{13}$$

Note that *Lakhtakia (1994)* uses the notation

$$c_{44} = \varrho v_0^2 \, (1+\varepsilon) \ , \quad c_{66} = \varrho v_0^2 \, (1-\varepsilon) \ , \quad \frac{\pi}{\Omega} = K \tag{14}$$

and that the equivalent model was used by *Vavryčuk (1999)* with notation

$$\gamma \sin^2(\vartheta) = \frac{-\varepsilon}{1+\varepsilon} \ , \quad \varphi = K x_3 \ . \tag{15}$$

3. ANALYTICAL SOLUTION

3.1. Decomposition into Pauli matrices

We decompose matrix $\mathbf{B}$ into the 2×2 identity matrix $\mathbf{1}$ and the Pauli matrices

$$\boldsymbol{\sigma}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \ , \quad \boldsymbol{\sigma}_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \ , \quad \boldsymbol{\sigma}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \ , \tag{16}$$

which satisfy relations

$$\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2 = -\boldsymbol{\sigma}_2\boldsymbol{\sigma}_1 = \mathrm{i}\boldsymbol{\sigma}_3 \ , \quad \boldsymbol{\sigma}_2\boldsymbol{\sigma}_3 = -\boldsymbol{\sigma}_3\boldsymbol{\sigma}_2 = \mathrm{i}\boldsymbol{\sigma}_1 \ , \quad \boldsymbol{\sigma}_3\boldsymbol{\sigma}_1 = -\boldsymbol{\sigma}_1\boldsymbol{\sigma}_3 = \mathrm{i}\boldsymbol{\sigma}_2 \tag{17}$$

and

$$\boldsymbol{\sigma}_1\boldsymbol{\sigma}_1 = \boldsymbol{\sigma}_2\boldsymbol{\sigma}_2 = \boldsymbol{\sigma}_3\boldsymbol{\sigma}_3 = \mathbf{1} \ . \tag{18}$$

Matrix $\mathbf{B}$ may then be expressed as

$$\begin{aligned} \mathbf{B} &= \mathbf{1} + \varepsilon\boldsymbol{\sigma}_3 \cos(2Kx_3) + \varepsilon\boldsymbol{\sigma}_1 \sin(2Kx_3) \\ &= \mathbf{1} + \varepsilon\boldsymbol{\sigma}_3 \left[\mathbf{1}\cos(2Kx_3) + \mathrm{i}\boldsymbol{\sigma}_2 \sin(2Kx_3)\right] \\ &= \mathbf{1} + \varepsilon\boldsymbol{\sigma}_3 \exp(2\mathrm{i}\boldsymbol{\sigma}_2 K x_3) \quad , \end{aligned} \tag{19}$$

or in the form of

$$\begin{aligned} \mathbf{B} &= \mathbf{1} + \varepsilon\boldsymbol{\sigma}_3 \left[\cos(Kx_3) + \mathrm{i}\boldsymbol{\sigma}_2 \sin(Kx_3)\right] \exp(\mathrm{i}\boldsymbol{\sigma}_2 K x_3) \\ &= \mathbf{1} + \varepsilon \left[\cos(Kx_3) - \mathrm{i}\boldsymbol{\sigma}_2 \sin(Kx_3)\right] \boldsymbol{\sigma}_3 \exp(\mathrm{i}\boldsymbol{\sigma}_2 K x_3) \\ &= \exp(-\mathrm{i}\boldsymbol{\sigma}_2 K x_3)[\mathbf{1} + \varepsilon\boldsymbol{\sigma}_3] \exp(\mathrm{i}\boldsymbol{\sigma}_2 K x_3) \quad , \end{aligned} \tag{20}$$

which is much more suitable for our purposes, because it explicitly describes the rotation about the x_3 axis.

We now apply transformation

$$\mathbf{u} = \exp(-\mathrm{i}\boldsymbol{\sigma}_2 K x_3)\widehat{\mathbf{u}} \tag{21}$$

to the coordinate system rotating with the crystal axes. Inserting the transformation equation, together with its first derivative

$$\mathbf{u}' = \exp(-\mathrm{i}\boldsymbol{\sigma}_2 K x_3) \left[\widehat{\mathbf{u}}' - K\mathrm{i}\boldsymbol{\sigma}_2\widehat{\mathbf{u}}\right] \tag{22}$$

and expression (20) for matrix $\mathbf{B}$, into elastodynamic equation (12), we arrive at

$$[\exp(-\mathrm{i}\boldsymbol{\sigma}_2 K x_3)\,(\mathbf{1}+\varepsilon\boldsymbol{\sigma}_3)\,(\widehat{\mathbf{u}}'-K\mathrm{i}\boldsymbol{\sigma}_2\widehat{\mathbf{u}})]' = -k_0^2\exp(-\mathrm{i}\boldsymbol{\sigma}_2 K x_3)\widehat{\mathbf{u}} \quad . \tag{23}$$

We now perform the derivative on the left–hand side

$$(\mathbf{1}+\varepsilon\boldsymbol{\sigma}_3)\,(\widehat{\mathbf{u}}''-K\mathrm{i}\boldsymbol{\sigma}_2\widehat{\mathbf{u}}') - K\mathrm{i}\boldsymbol{\sigma}_2\,(\mathbf{1}+\varepsilon\boldsymbol{\sigma}_3)\,(\widehat{\mathbf{u}}'-K\mathrm{i}\boldsymbol{\sigma}_2\widehat{\mathbf{u}}) = -k_0^2\widehat{\mathbf{u}} \quad , \tag{24}$$

multiply the Pauli matrices

$$(\mathbf{1}+\varepsilon\boldsymbol{\sigma}_3)\,\widehat{\mathbf{u}}'' - 2K\mathrm{i}\boldsymbol{\sigma}_2\widehat{\mathbf{u}}' - K^2\boldsymbol{\sigma}_2\,(\mathbf{1}+\varepsilon\boldsymbol{\sigma}_3)\,\boldsymbol{\sigma}_2\widehat{\mathbf{u}} = -k_0^2\widehat{\mathbf{u}} \tag{25}$$

and finally arrive at the elastodynamic equation

$$(\mathbf{1}+\varepsilon\boldsymbol{\sigma}_3)\,\widehat{\mathbf{u}}'' - 2K\mathrm{i}\boldsymbol{\sigma}_2\widehat{\mathbf{u}}' = -\left[(k_0^2-K^2)\mathbf{1}+\varepsilon K^2\boldsymbol{\sigma}_3\right]\widehat{\mathbf{u}} \tag{26}$$

expressed in the coordinate system rotating with the crystal axes. This equation has constant coefficients and represents the second–order counterpart to *Lakhtakia*'s *(1994,* eqs. 11a,b*)* first–order equations for 3 displacement and 3 stress tensor components.

3.2. One–way propagator matrix

Since elastodynamic equation (26) has constant coefficients, we may seek its 2×2 one–way propagator matrix in the form of

$$\widehat{\mathbf{U}} = \exp(\mathrm{i}\mathbf{F}x_3) \tag{27}$$

with unknown 2×2 matrix $\mathbf{F}$. This assumption enables the 4 linearly independent solutions of elastodynamic equation (26) to be split into 2 one–way propagator matrices corresponding to the propagation in two opposite directions. However, there are also 2 mixed propagator matrices of the above form combining the propagation in opposite directions within a single propagator matrix, and 2 propagator matrices corresponding to the stationary solutions. We may thus expect 6 solutions of the above form, but wish to determine just two one–way propagator matrices, each corresponding to propagation in a single direction.

The derivatives of the propagator matrix are

$$\widehat{\mathbf{U}}' = \mathrm{i}\mathbf{F}\exp(\mathrm{i}\mathbf{F}x_3) \tag{28}$$

and

$$\widehat{\mathbf{U}}'' = -\mathbf{F}^2\exp(\mathrm{i}\mathbf{F}x_3) \quad . \tag{29}$$

Elastodynamic equation (26) reduces, after insertion of these expressions, into algebraic matrix equation

$$(\mathbf{1}+\varepsilon\boldsymbol{\sigma}_3)\,\mathbf{F}^2 - 2K\boldsymbol{\sigma}_2\mathbf{F} = \left(k_0^2-K^2\right)\mathbf{1}+\varepsilon K^2\boldsymbol{\sigma}_3 \tag{30}$$

for the 2×2 matrix $\mathbf{F}$.

We decompose the unknown matrix $\mathbf{F}$ into the identity and Pauli matrices,

$$\mathbf{F} = F_0\mathbf{1} + \mathrm{i}F_1\boldsymbol{\sigma}_1 + F_2\boldsymbol{\sigma}_2 + F_3\boldsymbol{\sigma}_3 \quad , \tag{31}$$

and seek the individual coefficients F_0, F_1, F_2 and F_3. We have put the somewhat illogical imaginary unit in front of the F_1 term, because otherwise we would observe purely imaginary F_1 with real–valued F_0, F_2, F_3 in the solution, as will be seen later on. The decomposition (31) of matrix $\mathbf{F}$ is just a formal parametrization designed to convert matrix equation (30) into four scalar equations, although analogous coefficients describing the coupling ray theory in Section 4.2 have a simple meaning.

Introducing auxiliary coefficient

$$\varphi = \sqrt{F_3^2 + F_2^2 - F_1^2} \tag{32}$$

and "normalized" matrix

$$\mathbf{\Phi} = [F_1 \mathrm{i}\boldsymbol{\sigma}_1 + F_2\boldsymbol{\sigma}_2 + F_3\boldsymbol{\sigma}_3]\,\varphi^{-1} \tag{33}$$

satisfying relation

$$\mathbf{\Phi}\mathbf{\Phi} = \mathbf{1} \quad , \tag{34}$$

matrix $\mathbf{F}$ may be expressed in the form of

$$\mathbf{F} = F_0\mathbf{1} + \varphi\mathbf{\Phi} \quad . \tag{35}$$

For real–valued F_0 and φ, the one–way propagator matrix (27) of elastodynamic equation (26) in crystal axes takes the simple form

$$\widehat{\mathbf{U}} = \exp(\mathrm{i}F_0x_3)\,[\mathbf{1}\cos(\varphi x_3) + \mathrm{i}\mathbf{\Phi}\sin(\varphi x_3)] \tag{36}$$

convenient for calculations. If F_0 and φ are complex–valued, this expression has to be slightly generalized,

$$\begin{aligned}\widehat{\mathbf{U}} =& \exp(\mathrm{iRe}F_0x_3)\,[\mathbf{1}\cos(\mathrm{Re}\varphi x_3) + \mathrm{i}\mathbf{\Phi}\sin(\mathrm{Re}\varphi x_3)] \\ &\times \exp(-\mathrm{Im}F_0x_3)\,[\mathbf{1}\cosh(\mathrm{Im}\varphi x_3) - \mathbf{\Phi}\sinh(\mathrm{Im}\varphi x_3)] \ .\end{aligned} \tag{37}$$

For one–way propagation we require

$$|\mathrm{Im}F_0| \geq |\mathrm{Im}\varphi| \tag{38}$$

and the sign of F_0 corresponding to the direction of propagation. If inequality (38) fails to hold, matrix (37) would exponentially increase in both directions.

The 2×2 one–way propagator matrix of elastodynamic equation (12) in Cartesian coordinates is then

$$\begin{aligned}\mathbf{U} =& \exp(\mathrm{iRe}F_0x_3)\,[\mathbf{1}\cos(Kx_3) - \mathrm{i}\boldsymbol{\sigma}_2\sin(Kx_3)]\,[\mathbf{1}\cos(\mathrm{Re}\varphi x_3) + \mathrm{i}\mathbf{\Phi}\sin(\mathrm{Re}\varphi x_3)] \\ &\times \exp(-\mathrm{Im}F_0x_3)\,[\mathbf{1}\cosh(\mathrm{Im}\varphi x_3) - \mathbf{\Phi}\sinh(\mathrm{Im}\varphi x_3)] \quad .\end{aligned} \tag{39}$$

We now determine the frequency–dependent coefficients F_0, F_1, F_2 and F_3.

3.3. Determination of the frequency–dependent coefficients

The matrix products of $\mathbf{F}$ appearing in matrix equation (30) are

$$\mathbf{F}^2 = (F_0^2 - F_1^2 + F_2^2 + F_3^2)\mathbf{1} + 2F_0(F_1 \mathrm{i}\boldsymbol{\sigma}_1 + F_2\boldsymbol{\sigma}_2 + F_3\boldsymbol{\sigma}_3) \quad , \tag{40}$$

$$\boldsymbol{\sigma}_3\mathbf{F}^2 = (F_0^2 - F_1^2 + F_2^2 + F_3^2)\boldsymbol{\sigma}_3 + 2F_0(-F_1\boldsymbol{\sigma}_2 - F_2\mathrm{i}\boldsymbol{\sigma}_1 + F_3\mathbf{1}) \tag{41}$$

and

$$\boldsymbol{\sigma}_2\mathbf{F} = F_0\boldsymbol{\sigma}_2 + F_1\boldsymbol{\sigma}_3 + F_2\mathbf{1} + F_3\mathrm{i}\boldsymbol{\sigma}_1 \quad . \tag{42}$$

After the insertion of the products into matrix equation (30), the comparison of the coefficients of matrices $\mathbf{1}$, $\boldsymbol{\sigma}_1$, $\boldsymbol{\sigma}_2$ and $\boldsymbol{\sigma}_3$ yields a system of four equations for unknown F_0, F_1, F_2 and F_3,

$$(F_0^2 - F_1^2 + F_2^2 + F_3^2) + 2\varepsilon F_0 F_3 - 2KF_2 = k_0^2 - K^2 \quad , \tag{43}$$

$$2F_0F_1 - 2\varepsilon F_0 F_2 - 2KF_3 = 0 \quad , \tag{44}$$

$$2F_0F_2 - 2\varepsilon F_0 F_1 - 2KF_0 = 0 \tag{45}$$

and

$$2F_0F_3 + \varepsilon(F_0^2 - F_1^2 + F_2^2 + F_3^2) - 2KF_1 = \varepsilon K^2 \quad . \tag{46}$$

In solving this system of equations for F_0, F_1, F_2 and F_3, we first express F_0, F_2 and F_3 in terms of F_1, and then find the expression for F_1.

The two solutions of equations (43) to (46) with $F_0 = 0$ correspond to the stationary solutions of the elastodynamic equation. Since we are not interested in the stationary solutions, we assume $F_0 \neq 0$ and equation (45) then yields

$$\boxed{F_2 = K + \varepsilon F_1} \quad . \tag{47}$$

After inserting (47), equation (44) reads

$$2F_0F_1 - 2\varepsilon F_0(K + \varepsilon F_1) - 2KF_3 = 0 \quad , \tag{48}$$

which yields

$$\boxed{F_3 = F_0\left[-\varepsilon + \frac{F_1(1-\varepsilon^2)}{K}\right]} \quad . \tag{49}$$

Equation (43), with expression (47) for F_2 inserted, reads

$$F_0^2 - F_1^2 + K^2 + 2K\varepsilon F_1 + \varepsilon^2 F_1^2 - \varepsilon^2 F_0^2 + [\varepsilon F_0 + F_3]^2 - 2K^2 - 2K\varepsilon F_1 = k_0^2 - K^2 \tag{50}$$

and, after inserting relation (49) for F_3, may be simplified to

$$\left[F_0^2 - F_1^2\right]\left[1-\varepsilon^2\right] + \left[\frac{F_0F_1(1-\varepsilon^2)}{K}\right]^2 = k_0^2 \quad . \tag{51}$$

The unknown F_0 may thus be expressed in terms of F_1,

$$\boxed{F_0^2 = \left[\frac{k_0^2}{1-\varepsilon^2} + F_1^2\right]\left[1 + \frac{F_1^2(1-\varepsilon^2)}{K^2}\right]^{-1}} \quad . \tag{52}$$

The sign of F_0 has to be determined according to the desired direction of the one–way plane–wave propagation. Two possible signs of F_0 correspond to the two one–way propagator matrices in opposite directions. For example, if the time factor is $\exp(-\mathrm{i}\omega t)$ for positive circular frequencies ω, positive $\mathrm{Re}F_0$ corresponds to the propagation in the direction of the positive half–axis x_3 and negative $\mathrm{Re}F_0$ to the propagation in the direction of the negative half–axis x_3. If the time factor is $\exp(\mathrm{i}\omega t)$, the relation between the signs and the directions of propagation is opposite.

The term on the right–hand side of equation (46) is cancelled by inserting relation (47) for F_2,

$$2F_0F_3 + \varepsilon(F_0^2 - F_1^2 + 2K\varepsilon F_1 + \varepsilon^2 F_1^2 + F_3^2) - 2KF_1 = 0 \quad . \tag{53}$$

Collecting the terms with F_1 on the right–hand side and inserting expression (49) for F_3, we arrive at

$$F_0^2 \left[2\left(-\varepsilon + \frac{F_1(1-\varepsilon^2)}{K} \right) + \varepsilon + \varepsilon \left(-\varepsilon + \frac{F_1(1-\varepsilon^2)}{K} \right)^2 \right] = F_1 \left[2K + \varepsilon F_1 \right] (1-\varepsilon^2) \ , \tag{54}$$

which may be simplified to

$$F_0^2 \left[2\frac{F_1(1-\varepsilon^2)}{K} - \varepsilon + \varepsilon \frac{F_1^2(1-\varepsilon^2)}{K^2} \right] = F_1 \left[2K + \varepsilon F_1 \right] \quad . \tag{55}$$

After inserting expression (52) for F_0^2, this equation reads

$$\left[\frac{k_0^2}{1-\varepsilon^2} + F_1^2 \right] \left[2KF_1(1-\varepsilon^2) + \varepsilon F_1^2(1-\varepsilon^2) - \varepsilon K^2 \right] = F_1 \left[2K + \varepsilon F_1 \right] \left[K^2 + F_1^2(1-\varepsilon^2) \right] \tag{56}$$

and may be simplified to

$$k_0^2 \left[2KF_1 + \varepsilon F_1^2 - \frac{\varepsilon K^2}{1-\varepsilon^2} \right] = 2K^2 \left[K + \varepsilon F_1 \right] F_1 \quad . \tag{57}$$

The quadratic equation for F_1 is thus

$$\varepsilon(k_0^2 - 2K^2)F_1^2 + 2K(k_0^2 - K^2)F_1 - \frac{\varepsilon k_0^2 K^2}{1-\varepsilon^2} = 0 \quad . \tag{58}$$

Equation (58) has imaginary roots for

$$(1-|\varepsilon|)\, K^2 \le k_0^2 \le (1+|\varepsilon|)\, K^2 \tag{59}$$

(*Lakhtakia and Meredith, 1999*, eq. 22). In frequency band (59), the one–way propagating wave is exponentially attenuating due to back scattering.

Equation (58) has real–valued roots either for

$$k_0^2 \le (1-|\varepsilon|)\, K^2 \quad \text{or} \quad k_0^2 \ge (1+|\varepsilon|)\, K^2 \quad . \tag{60}$$

In frequency band (60), there is no attenuation due to back scattering. The larger root (in absolute value)

$$\widetilde{F}_1 = -\frac{K(k_0^2 - K^2)}{\varepsilon(k_0^2 - 2K^2)} \left[1 + \sqrt{1 + \frac{\varepsilon^2 k_0^2 (k_0^2 - 2K^2)}{(1-\varepsilon^2)(k_0^2 - K^2)^2}} \right] \tag{61}$$

of quadratic equation (58) leads to the propagator matrices with mixed directions of propagation. We thus select the smaller root

$$F_1 = -\frac{k_0^2 K^2}{(1-\varepsilon^2)(k_0^2 - 2K^2)} \frac{1}{\widetilde{F}_1} \quad , \tag{62}$$

i.e.

$$\boxed{F_1 = \frac{\varepsilon K k_0^2}{(k_0^2 - K^2)\sqrt{1-\varepsilon^2}\left[\sqrt{1-\varepsilon^2} + \sqrt{1-\varepsilon^2\left(\frac{K^2}{k_0^2 - K^2}\right)^2}\,\right]} \quad ,} \tag{63}$$

leading to the one–way propagator matrices.

3.4. Resonant frequencies

For resonant frequencies within the domain (59), where F_0, F_1, F_2 and F_3 are complex–valued, we may again determine F_1 from equation (63), arbitrarily selecting one of the complex–conjugate roots. After inserting into (52) and determining F_0 with its real part corresponding to the desired direction of propagation, we check for the proper sign of the imaginary part of F_0. The imaginary part of F_0 has to compensate the exponential increment of cosh in equation (39). That is why $\mathrm{Im}F_0$ should be positive for the propagation in the direction of the positive half–axis x_3 and negative for the propagation in the direction of the negative half–axis x_3, independently of time factor $\exp(\pm i\omega t)$. If the imaginary part does not correspond to the direction of propagation, we replace F_0 and F_1 by their complex conjugates. Equations (49), (47) and finally (39) are then used as they are.

In this paper, we omit any discussion of the resonant frequencies and of the circular Bragg phenomenon, because the resonant frequencies with strong back scattering are far outside the validity regions of the ray methods. Refer, e.g., to *Venugopal and Lakhtakia (1998)* or to *Lakhtakia and Meredith (1999)*.

In the rest of this subsection, we only check whether inequality (38) is satisfied. The reader not interested in this proof may proceed to Section 4.

Equations (43) and (46) yield

$$(1-\varepsilon^2)(F_0^2 - F_1^2 + F_2^2 + F_3^2) = 2K(F_2 - \varepsilon F_1) + k_0^2 - K^2 - \varepsilon^2 K^2 \quad . \tag{64}$$

Inserting (47), we arrive at

$$F_0^2 - F_1^2 + F_2^2 + F_3^2 = \frac{k_0^2}{1-\varepsilon^2} + K^2 \quad , \tag{65}$$

i.e.

$$F_0^2 + \varphi^2 = \frac{k_0^2}{1-\varepsilon^2} + K^2 \quad . \tag{66}$$

Since the right–hand side of equation (66) is real–valued,

$$|\mathrm{Re}F_0||\mathrm{Im}F_0| = |\mathrm{Re}\varphi||\mathrm{Im}\varphi| \quad . \tag{67}$$

Under this condition, inequality (38) is equivalent to other inequalities,

$$|\mathrm{Im}F_0| \geq |\mathrm{Im}\varphi| \Longleftrightarrow |\mathrm{Re}\varphi| \geq |\mathrm{Re}F_0| \Longleftrightarrow \mathrm{Re}\varphi^2 \geq \mathrm{Re}F_0^2 \quad . \tag{68}$$

We now check the last inequality.

Let us parametrize k_0 by dimensionless parameter δ,

$$k_0^2 = (1+\delta)K^2 \quad , \tag{69}$$

to make the derivation more concise. With this notation, the resonant domain (59), in which F_1 is imaginary, is determined by inequality

$$|\delta| \leq |\varepsilon| \quad . \tag{70}$$

Equation (63) then reads

$$F_1 = K\frac{\varepsilon(1+\delta)}{\delta\sqrt{1-\varepsilon^2}\left(\sqrt{1-\varepsilon^2}+\sqrt{1-\varepsilon^2\delta^{-2}}\right)} \quad , \tag{71}$$

and may be inserted into (52) to yield

$$\frac{F_0^2}{K^2} = \frac{1+\delta}{1-\varepsilon^2}\;\frac{\delta^2\left(\sqrt{1-\varepsilon^2}+\sqrt{1-\varepsilon^2\delta^{-2}}\right)^2+\varepsilon^2(1+\delta)}{\delta^2\left(\sqrt{1-\varepsilon^2}+\sqrt{1-\varepsilon^2\delta^{-2}}\right)^2+\varepsilon^2(1+\delta)^2} \quad , \tag{72}$$

which may be rearranged to read

$$\frac{F_0^2}{K^2} = \frac{1+\delta}{1-\varepsilon^2}\;\frac{2\delta+\varepsilon^2(1-\delta)+2\delta\sqrt{1-\varepsilon^2}\sqrt{1-\varepsilon^2\delta^{-2}}}{2\delta+2\varepsilon^2+2\delta\sqrt{1-\varepsilon^2}\sqrt{1-\varepsilon^2\delta^{-2}}} \quad . \tag{73}$$

Difference $\varphi^2 - F_0^2$, useful to test the inequality, may now be expressed using (66) in terms of F_0^2,

$$\frac{\varphi^2-F_0^2}{K^2} = 1+\frac{1+\delta}{1-\varepsilon^2}-2\frac{F_0^2}{K^2} = -\frac{\varepsilon^2+\delta}{1-\varepsilon^2}+2\left[\frac{1+\delta}{1-\varepsilon^2}-\frac{F_0^2}{K^2}\right] \quad . \tag{74}$$

Inserting (73), we arrive at

$$\frac{\varphi^2-F_0^2}{K^2} = -\frac{\varepsilon^2+\delta}{1-\varepsilon^2}+2\frac{1+\delta}{1-\varepsilon^2}\;\frac{\varepsilon^2(1+\delta)}{2\delta+2\varepsilon^2+2\delta\sqrt{1-\varepsilon^2}\sqrt{1-\varepsilon^2\delta^{-2}}} \quad . \tag{75}$$

The possibly imaginary square root may be removed from the denominator,

$$\frac{\varphi^2-F_0^2}{K^2} = -\frac{\varepsilon^2+\delta}{1-\varepsilon^2}+\frac{\varepsilon^2(1+\delta)^2\left(\delta+\varepsilon^2-\delta\sqrt{1-\varepsilon^2}\sqrt{1-\varepsilon^2\delta^{-2}}\right)}{(1-\varepsilon^2)\left[(\delta+\varepsilon^2)^2-(1-\varepsilon^2)(\delta^2-\varepsilon^2)\right]} \quad , \tag{76}$$

the denominator may be expanded,

$$\frac{\varphi^2-F_0^2}{K^2} = -\frac{\varepsilon^2+\delta}{1-\varepsilon^2}+\frac{\varepsilon^2(1+\delta)^2\left(\delta+\varepsilon^2-\delta\sqrt{1-\varepsilon^2}\sqrt{1-\varepsilon^2\delta^{-2}}\right)}{(1-\varepsilon^2)(\delta^2+2\varepsilon^2\delta+\varepsilon^4+\varepsilon^2-\delta^2+\delta^2\varepsilon^2-\varepsilon^4)} \quad , \tag{77}$$

and rearranged to read

$$\frac{\varphi^2-F_0^2}{K^2} = -\frac{\varepsilon^2+\delta}{1-\varepsilon^2}+\frac{\varepsilon^2(1+\delta)^2\left(\delta+\varepsilon^2-\delta\sqrt{1-\varepsilon^2}\sqrt{1-\varepsilon^2\delta^{-2}}\right)}{(1-\varepsilon^2)\varepsilon^2(1+\delta)^2} \quad . \tag{78}$$

We now see that

$$\frac{\varphi^2 - F_0^2}{K^2} = -\delta\sqrt{\frac{1-\varepsilon^2\delta^{-2}}{1-\varepsilon^2}} \quad , \tag{79}$$

i.e.

$$F_0^2 - \varphi^2 = \frac{k_0^2 - K^2}{\sqrt{1-\varepsilon^2}}\sqrt{1-\left(\frac{\varepsilon K^2}{k_0^2 - K^2}\right)^2} \quad . \tag{80}$$

Note that all the above equations, but not inequality (70), hold for all frequencies, and not for the resonant frequencies only.

For resonant frequencies given by inequality (70), the right–hand side of equation (79) is purely imaginary, and $\mathrm{Re}\varphi^2 = \mathrm{Re}F_0^2$. Equations (67) and (79) then imply equalities

$$|\mathrm{Re}F_0| = |\mathrm{Re}\,\varphi| \quad , \qquad |\mathrm{Im}F_0| = |\mathrm{Im}\varphi| \quad . \tag{81}$$

In consequence of (81), the amplitudes in propagator matrix (39) decrease exponentially to one half for the resonant frequencies, because the energy is gradually split equally into both propagation directions by multiple scattering.

3.5. Relation to Lakhtakia's eigenvalues

Equations (66) and (80) yield

$$(2F_0\varphi)^2 = \frac{k_0^4}{(1-\varepsilon^2)^2} + \frac{2k_0^2K^2}{1-\varepsilon^2} + K^4 - \frac{k_0^4}{1-\varepsilon^2} + \frac{2k_0^2K^2}{1-\varepsilon^2} - K^4 = \frac{4k_0^2K^2}{1-\varepsilon^2} + \frac{\varepsilon^2k_0^4}{(1-\varepsilon^2)^2} \; . \tag{82}$$

Comparing equations (66) and (82) with *Lakhtakia*'s *(1994,* eqs. 22a,b*)* equations, we see that Lakhtakia's eigenvalues g_2, g_3, g_5 and g_6, corresponding to S waves, are

$$g_n = \pm F_0 \pm \varphi \quad . \tag{83}$$

Among these eigenvalues, $g_n = F_0 \pm \varphi$ are simultaneously the eigenvalues of matrix (35), while $g_n = -F_0 \mp \varphi$ are the eigenvalues of the analogous matrix corresponding to the opposite direction of propagation. Eigenvectors $\widehat{\mathbf{f}}_n$ corresponding to eigenvalues $g_n = F_0 \pm \varphi$ are collinear with the columns of the respective singular matrices $\mathbf{1} \pm \mathbf{\Phi}$. Multiplying equation (27) from the right by eigenvector $\widehat{\mathbf{f}}_n$, we obtain the solution $\widehat{\mathbf{U}}(x_3)\,\widehat{\mathbf{f}}_n = \widehat{\mathbf{f}}_n \exp(\mathrm{i}g_nx_3)$ of equation (26), elliptically polarized in the coordinate system rotating with the crystal axes. Eigenvalues g_n thus represent the wavenumbers of the eigenmodes $\widehat{\mathbf{U}}(x_3)\,\widehat{\mathbf{f}}_n$. For resonant frequencies, one eigenvalue of matrix (35) is real–valued, whereas the other is purely imaginary, see (81).

4. COMPARISON WITH THE RAY METHODS

The ray methods, such as the isotropic ray theory, anisotropic ray theory or coupling ray theory (*Coates and Chapman, 1990*), are high–frequency asymptotic methods and should thus be applied at sufficiently high frequencies, for $k_0 \gg K$. We thus assume that the order of K/k_0 is comparable with the order of ε, and that both quantities are small,

$$\frac{K}{k_0} \ll 1 \quad , \qquad |\varepsilon| \ll 1 \quad . \tag{84}$$

The Taylor expansions of coefficients (47), (49), (52) and (63) with fixed k_0 up to the third order in ε and K/k_0 are

$$F_0 \approx k_0 + \frac{3\varepsilon^2}{8} k_0 \quad , \tag{85a}$$

$$F_1 \approx \frac{\varepsilon}{2} K \quad , \tag{85b}$$

$$F_2 \approx K + \frac{\varepsilon^2}{2} K \quad , \tag{85c}$$

$$F_3 \approx -\frac{\varepsilon}{2} k_0 - \frac{5\varepsilon^3}{16} k_0 + \frac{\varepsilon}{2} \frac{K^2}{k_0} \quad . \tag{85d}$$

Before proceeding to the individual ray methods in Sections 4.2 to 4.5, we shall derive the approximate relations for estimating the relative error of an approximate one–way propagator matrix in Section 4.1. The relations are then used in Sections 4.2 to 4.5.

4.1. Relative difference between the exact and approximate one–way propagator matrices

Assume that the approximate solution has the form of (39), with coefficients F_0, F_1, F_2 and F_3 replaced by coefficients $F_0^{\rm ray}$, $F_1^{\rm ray}$, $F_2^{\rm ray}$ and $F_3^{\rm ray}$ describing the approximate solution. These coefficients may represent, e.g., coefficients (108a–d), (113a–d), (119a–d) or (124a–d) given later in this paper. The relative difference between the exact solution and the approximate solution may then be expressed in terms of differences

$$\Delta F_0^{\rm ray} = F_0 - F_0^{\rm ray} \; , \;\; \Delta F_1^{\rm ray} = F_1 - F_1^{\rm ray} \; , \;\; \Delta F_2^{\rm ray} = F_2 - F_2^{\rm ray} \; , \;\; \Delta F_3^{\rm ray} = F_3 - F_3^{\rm ray} \; . \tag{86}$$

In Sections 4.2 to 4.5, superscript $^{\rm ray}$ takes values $^{\rm crt}$, $^{\rm qi}$, $^{\rm ani}$, $^{\rm iso}$, respectively. In the rest of this subsection, we omit superscript $^{\rm ray}$ with $\Delta F_0^{\rm ray}$, $\Delta F_1^{\rm ray}$, $\Delta F_2^{\rm ray}$ and $\Delta F_3^{\rm ray}$, and use ΔF_0, ΔF_1, ΔF_2 and ΔF_3 instead.

We now estimate the relative error

$$\Delta^{\rm ray} = \frac{\|\mathbf{U}^{-1}\Delta\mathbf{U}\|}{\|\mathbf{1}\|} = \frac{\|\widehat{\mathbf{U}}^{-1}\Delta\widehat{\mathbf{U}}\|}{\|\mathbf{1}\|} = \sqrt{\tfrac{1}{2}{\rm Tr}\left([\widehat{\mathbf{U}}^{-1}\Delta\widehat{\mathbf{U}}]^{+}\,\widehat{\mathbf{U}}^{-1}\Delta\widehat{\mathbf{U}}\right)} \quad , \tag{87}$$

of the one-way propagator matrix in terms of differences (86). Here

$$\Delta\mathbf{U} = \mathbf{U} - \mathbf{U}^{\mathrm{ray}} \quad . \tag{88}$$

Symbol $\mathbf{A}^{+}$ denotes the matrix Hermitian adjoined to $\mathbf{A}$.

We approximate difference (88) by linear Taylor expansion with respect to differences (86). To preserve the accuracy, the linear Taylor expansion should be considered midway between F_α^{ray} and F_α, at

$$\overline{F}_\alpha = \tfrac{1}{2}(F_\alpha + F_\alpha^{\mathrm{ray}}) \quad . \tag{89}$$

For $|\Delta F_\alpha| \ll |F_\alpha|$, we use approximation $\overline{F}_\alpha \approx F_\alpha$, but if $F_\alpha^{\mathrm{ray}} = 0$, we have $\overline{F}_\alpha = \frac{1}{2}F_\alpha$. We may thus put

$$\overline{F}_\alpha \approx W_\alpha F_\alpha \tag{90}$$

(no summation over α), where $W_\alpha = 1$ for $|\Delta F_\alpha| \ll |F_\alpha|$ and $W_\alpha = \frac{1}{2}$ for $F_\alpha^{\mathrm{ray}} = 0$.

Under assumption (84), coefficients $\overline{F}_0$, $\overline{F}_1$, $\overline{F}_2$ and $\overline{F}_3$ are real–valued and equation (36) yields

$$\begin{aligned}\Delta\widehat{\mathbf{U}} \simeq \exp(\mathrm{i}\overline{F}_0 x_3)\,\{&[\mathbf{1}\cos(\overline{\varphi}x_3) + \mathrm{i}\boldsymbol{\Phi}\sin(\overline{\varphi}x_3)]\,\mathrm{i}\Delta F_0 x_3 \\ &+ [-\mathbf{1}\sin(\overline{\varphi}x_3) + \mathrm{i}\boldsymbol{\Phi}\cos(\overline{\varphi}x_3)]\,\Delta\varphi x_3 + \mathrm{i}\Delta\boldsymbol{\Phi}\sin(\overline{\varphi}x_3)\} \ ,\end{aligned} \tag{91}$$

where

$$\Delta\varphi \simeq [\overline{F}_3\Delta F_3 + \overline{F}_2\Delta F_2 - \overline{F}_1\Delta F_1]\overline{\varphi}^{-1} \quad , \tag{92}$$

see (32) with $\varphi = \overline{\varphi}$ and $F_\alpha = \overline{F}_\alpha$, and

$$\Delta\boldsymbol{\Phi} \simeq [\Delta F_1 \mathrm{i}\boldsymbol{\sigma}_1 + \Delta F_2\boldsymbol{\sigma}_2 + \Delta F_3\boldsymbol{\sigma}_3]\,\overline{\varphi}^{-1} - \boldsymbol{\Phi}\Delta\varphi\,\overline{\varphi}^{-1} \quad , \tag{93}$$

see (33) with $\varphi = \overline{\varphi}$ and $F_\alpha = \overline{F}_\alpha$. Multiplying (91) by

$$\widehat{\mathbf{U}}^{-1} = \exp(-\mathrm{i}\overline{F}_0 x_3)\,[\mathbf{1}\cos(\overline{\varphi}x_3) - \mathrm{i}\boldsymbol{\Phi}\sin(\overline{\varphi}x_3)] \quad , \tag{94}$$

we arrive at

$$\widehat{\mathbf{U}}^{-1}\Delta\widehat{\mathbf{U}} \simeq \mathbf{1}\mathrm{i}\Delta F_0 x_3 + \mathrm{i}\boldsymbol{\Phi}\Delta\varphi x_3 + [\mathbf{1}\cos(\overline{\varphi}x_3) - \mathrm{i}\boldsymbol{\Phi}\sin(\overline{\varphi}x_3)]\,\mathrm{i}\Delta\boldsymbol{\Phi}\sin(\overline{\varphi}x_3) \ . \tag{95}$$

Since $\overline{F}_1$ is small with respect to $\overline{F}_2$ or $\overline{F}_3$, we may use approximations

$$\overline{\varphi} \approx \sqrt{\overline{F}_2^2 + \overline{F}_3^2} \approx k_0\sqrt{\left(W_3\frac{\varepsilon}{2}\right)^2 + \left(W_2\frac{K}{k_0}\right)^2} \quad , \tag{96}$$

$$\boldsymbol{\Phi} \approx \left[\overline{F}_2\boldsymbol{\sigma}_2 + \overline{F}_3\boldsymbol{\sigma}_3\right]\overline{\varphi}^{-1} \tag{97}$$

and

$$\Delta\varphi \approx [\overline{F}_3\Delta F_3 + \overline{F}_2\Delta F_2]\overline{\varphi}^{-1} \tag{98}$$

of equations (32), (33) and (92), respectively. Since $\mathrm{Tr}\boldsymbol{\Phi} = 0$, $\mathrm{Tr}\Delta\boldsymbol{\Phi} = 0$ and

$$\boldsymbol{\Phi}^{+} \approx \boldsymbol{\Phi} \quad , \tag{99}$$

equation (87) with (95) yields

$$\Delta^{\mathrm{ray}} \approx \sqrt{\begin{array}{c}[\Delta F_0 x_3]^2 + [\Delta\varphi x_3]^2 + \frac{1}{2}\mathrm{Tr}(\Delta\boldsymbol{\Phi}^{+}\Delta\boldsymbol{\Phi})[\sin(\overline{\varphi}x_3)]^2 \\ +\frac{1}{2}\mathrm{Tr}(\boldsymbol{\Phi}\mathrm{i}(\Delta\boldsymbol{\Phi}^{+} - \Delta\boldsymbol{\Phi}))\Delta F_0 x_3[\sin(\overline{\varphi}x_3)]^2 \\ +\frac{1}{2}\mathrm{Tr}(\boldsymbol{\Phi}(\Delta\boldsymbol{\Phi}^{+} + \Delta\boldsymbol{\Phi}))\Delta\varphi x_3\cos(\overline{\varphi}x_3)\sin(\overline{\varphi}x_3)\end{array}} \quad , \tag{100}$$

see (34). Since the Pauli matrices are Hermitian symmetrical, equations (93), (97), (98) and (99) yield

$$\tfrac{1}{2}\mathrm{Tr}(\mathbf{\Phi}\mathrm{i}(\Delta\mathbf{\Phi}^{+}-\Delta\mathbf{\Phi}))\approx 0 \tag{101}$$

and

$$\tfrac{1}{2}\mathrm{Tr}(\mathbf{\Phi}(\Delta\mathbf{\Phi}^{+}+\Delta\mathbf{\Phi}))\approx 0 \quad . \tag{102}$$

Similarly,

$$\tfrac{1}{2}\mathrm{Tr}(\Delta\mathbf{\Phi}^{+}\Delta\mathbf{\Phi})\approx[(\Delta F_1)^2+(\Delta F_2)^2+(\Delta F_3)^2]\overline{\varphi}^{-2}-2[\overline{F}_2\Delta F_2+\overline{F}_3\Delta F_3]\Delta\varphi\overline{\varphi}^{-3}+(\Delta\varphi)^2\overline{\varphi}^{-2} \ . \tag{103}$$

Inserting (98), we arrive at

$$\tfrac{1}{2}\mathrm{Tr}(\Delta\mathbf{\Phi}^{+}\Delta\mathbf{\Phi})\approx(\Delta F_1)^2\overline{\varphi}^{-2}+[\overline{F}_2\Delta F_3-\overline{F}_3\Delta F_2]^2\overline{\varphi}^{-4} \quad . \tag{104}$$

Finally we obtain relative error

$$\Delta^{\mathrm{ray}}\approx\sqrt{\Delta_0^2+\Delta_1^2+\Delta_2^2+\Delta_3^2} \tag{105}$$

approximately composed of four parts

$$\Delta_0=\Delta F_0\,x_3 \quad , \tag{106a}$$
$$\Delta_1=\Delta F_1\,\overline{\varphi}^{-1}\,\sin(\overline{\varphi}x_3) \quad , \tag{106b}$$
$$\Delta_2=[\overline{F}_2\Delta F_3-\overline{F}_3\Delta F_2]\,\overline{\varphi}^{-2}\,\sin(\overline{\varphi}x_3) \quad , \tag{106c}$$
$$\Delta_3=\Delta\varphi\,x_3 \quad , \tag{106d}$$

where we may insert (85c, d), (90), (96) and (98),

$$\Delta_0=\frac{\Delta F_0}{k_0}\frac{k_0}{K}\,Kx_3 \quad , \tag{107a}$$

$$\Delta_1\approx\frac{\Delta F_1}{k_0}\left[\left(W_3\frac{\varepsilon}{2}\right)^2+\left(W_2\frac{K}{k_0}\right)^2\right]^{-\frac{1}{2}}\sin(\overline{\varphi}x_3) \quad , \tag{107b}$$

$$\Delta_2\approx\left[W_3\frac{\varepsilon}{2}\frac{\Delta F_2}{k_0}+W_2\frac{K}{k_0}\frac{\Delta F_3}{k_0}\right]\left[\left(W_3\frac{\varepsilon}{2}\right)^2+\left(W_2\frac{K}{k_0}\right)^2\right]^{-1}\sin(\overline{\varphi}x_3) \ , \tag{107c}$$

$$\Delta_3\approx\left[W_2\frac{K}{k_0}\frac{\Delta F_2}{k_0}-W_3\frac{\varepsilon}{2}\frac{\Delta F_3}{k_0}\right]\left[\left(W_3\frac{\varepsilon}{2}\right)^2+\left(W_2\frac{K}{k_0}\right)^2\right]^{-\frac{1}{2}}\frac{k_0}{K}\,Kx_3 \ . \tag{107d}$$

The order of Δ_0, Δ_1, Δ_2 and Δ_0, in $\frac{\varepsilon}{2}$ and $\frac{K}{k_0}$ is smaller by 1 than the order of ΔF_0, ΔF_1, ΔF_2 and ΔF_3, because we consider the rotational angle Kx_3 of the crystal axes to be of order 0 in the powers of $\frac{\varepsilon}{2}$ and $\frac{K}{k_0}$. For example, in geophysical applications, rotational angle Kx_3 is usually caused by the heterogeneities bending rays rather than by the rotation of the crystal axes, and does not usually exceed a few radians.

4.2. Coupling ray theory

In the simplified twisted crystal model, the coupling ray theory implemented by *Bulant and Klimeš (2002)* according to the equations of *Coates and Chapman (1990)* yields the approximate solution in the form of (39) with F_0, F_1, F_2 and F_3 replaced by

$$F_0^{\mathrm{crt}} = k_0 \frac{\sqrt{1+\varepsilon}+\sqrt{1-\varepsilon}}{2\sqrt{1-\varepsilon^2}} \quad , \tag{108a}$$

$$F_1^{\mathrm{crt}} = 0 \quad , \tag{108b}$$

$$F_2^{\mathrm{crt}} = K \quad , \tag{108c}$$

$$F_3^{\mathrm{crt}} = -k_0 \frac{\sqrt{1+\varepsilon}-\sqrt{1-\varepsilon}}{2\sqrt{1-\varepsilon^2}} \quad . \tag{108d}$$

Coefficient F_0^{crt} is the arithmetic average of the travel times of the two S–wave polarizations along the reference ray in phase space. Coefficient F_2^{crt} attempts to prevent the rotation of the polarization vectors about the ray. Coefficient F_3^{crt} accounts for the difference between the travel times of the two S–wave polarizations. Non–zero coefficients F_2^{crt} and F_3^{crt} mutually interfere so that the larger partly cancels the action of the smaller. We may refer to the frequency at which $|F_2^{\mathrm{crt}}| = |F_3^{\mathrm{crt}}|$ as the *coupling frequency* in this model. Thus, F_2^{crt} is dominant at low frequencies (considerably lower than the coupling frequency) and F_3^{crt} is dominant at high frequencies (considerably higher than the coupling frequency).

The Taylor expansions of these coefficients up to the third order in ε and K/k_0 are

$$F_0^{\mathrm{crt}} \approx k_0 + \frac{3\varepsilon^2}{8} k_0 \quad , \tag{109a}$$

$$F_1^{\mathrm{crt}} = 0 \quad , \tag{109b}$$

$$F_2^{\mathrm{crt}} = K \quad , \tag{109c}$$

$$F_3^{\mathrm{crt}} \approx -\frac{\varepsilon}{2} k_0 - \frac{5\varepsilon^3}{16} k_0 \quad . \tag{109d}$$

We see that

$$\left|\frac{K}{k_0}\right| \approx \left|\frac{\varepsilon}{2}\right| \tag{110}$$

for the coupling frequency. The differences (86) of coefficients F_α from F_α^{crt} are

$$\Delta F_0^{\mathrm{crt}} \approx 0 \quad , \tag{111a}$$

$$\Delta F_1^{\mathrm{crt}} \approx \frac{\varepsilon}{2} K \quad , \tag{111b}$$

$$\Delta F_2^{\mathrm{crt}} \approx \frac{\varepsilon^2}{2} K \quad , \tag{111c}$$

$$\Delta F_3^{\mathrm{crt}} \approx \frac{\varepsilon}{2} \frac{K^2}{k_0} \quad . \tag{111d}$$

The contributions of $\Delta F_2^{\rm crt}$ and $\Delta F_3^{\rm crt}$ to the partial relative error (107d) cancel, while their contributions to the partial relative error (107c) are small compared with the contribution of $\Delta F_1^{\rm crt}$ to to the partial relative error (107b).

The relative error of the coupling ray theory is thus composed of the partial relative error (107b) only, with (111b), $W_2 = 1$ and $W_3 = 1$,

$$\Delta^{\rm crt} \approx \left|\frac{\varepsilon}{2}\right| \left|\frac{K}{k_0}\right| \left[\left(\frac{\varepsilon}{2}\right)^2 + \left(\frac{K}{k_0}\right)^2 \right]^{-\frac{1}{2}} |\sin(\overline{\varphi} x_3)| \quad . \tag{112}$$

The relative error of the propagator matrix is $\Delta^{\rm crt} \lesssim \left|\frac{\varepsilon}{2}\right|$ above the resonant frequencies, slowly decreasing to $\Delta^{\rm crt} \approx \left|\frac{\varepsilon}{2\sqrt{2}}\right|$ at the coupling frequency, $\left|\frac{K}{k_0}\right| = \left|\frac{\varepsilon}{2}\right|$, and further decreasing as $\Delta^{\rm crt} \approx \left|\frac{K}{k_0}\right|$ for high frequencies.

4.3. Quasi–isotropic perturbation of travel times

The coupling ray theory implemented according to *Pšenčík (1998)* and *Pšenčík and Dellinger (2001)* includes the isotropic common ray approximation, the quasi–isotropic approximation of the Christoffel matrix, and the quasi–isotropic perturbation of travel times. For the list of quasi–isotropic approximations of the coupling ray theory refer to *Bulant and Klimeš (2002; 2004)*. Of these quasi–isotropic approximations, only the quasi–isotropic perturbation of travel times affects the coupling–ray–theory solution in the simplified twisted crystal model. In the simplified twisted crystal model with reference velocity v_R, the quasi–isotropic perturbation of travel times yields the approximate solution in the form of (39) with F_0, F_1, F_2 and F_3 replaced by

$$F_0^{\rm qi} = k_0 \frac{v_0}{v_R} \left[\frac{3}{2} - \frac{1}{2} \left(\frac{v_0}{v_R}\right)^2 \right] \quad , \tag{113a}$$

$$F_1^{\rm qi} = 0 \quad , \tag{113b}$$

$$F_2^{\rm qi} = K \quad , \tag{113c}$$

$$F_3^{\rm qi} = -\frac{k_0}{2} \varepsilon \left(\frac{v_0}{v_R}\right)^3 \quad . \tag{113d}$$

We assume that

$$\left|\frac{\Delta v}{v_R}\right| = \left|\frac{v_0 - v_R}{v_R}\right| \ll 1 \quad . \tag{114}$$

The Taylor expansions of these coefficients up to the third order in ε, K/k_0 and $\Delta v/v_R$ are

$$F_0^{\rm qi} \approx k_0 - \frac{3}{2}\left(\frac{\Delta v}{v_R}\right)^2 k_0 - \frac{1}{2}\left(\frac{\Delta v}{v_R}\right)^3 k_0 \quad , \tag{115a}$$

$$F_1^{\rm qi} = 0 \quad , \tag{115b}$$

$$F_2^{\rm qi} = K \quad , \tag{115c}$$

$$F_3^{\rm qi} \approx -\frac{\varepsilon}{2}k_0 - \frac{3\varepsilon}{2}\frac{\Delta v}{v_R}k_0 - \frac{3\varepsilon}{2}\left(\frac{\Delta v}{v_R}\right)^2 k_0 \quad . \tag{115d}$$

The differences (86) of coefficients F_α from $F_\alpha^{\rm qi}$ are

$$\Delta F_0^{\rm qi} \approx \frac{3}{2}\left[\left(\frac{\varepsilon}{2}\right)^2 + \left(\frac{\Delta v}{v_R}\right)^2\right] k_0 + \frac{1}{2}\left(\frac{\Delta v}{v_R}\right)^3 k_0 \quad , \tag{116a}$$

$$\Delta F_1^{\rm qi} \approx \frac{\varepsilon}{2}K \quad , \tag{116b}$$

$$\Delta F_2^{\rm qi} \approx \frac{\varepsilon^2}{2}K \quad , \tag{116c}$$

$$\Delta F_3^{\rm qi} \approx 3\frac{\varepsilon}{2}\frac{\Delta v}{v_R}k_0 + 3\frac{\varepsilon}{2}\left(\frac{\Delta v}{v_R}\right)^2 k_0 - \frac{5\varepsilon^3}{16}k_0 + \frac{\varepsilon}{2}\frac{K^2}{k_0} \quad . \tag{116d}$$

Analogously as in Section 4.2, the contributions of $\Delta F_2^{\rm crt}$, of the second term of $\Delta F_1^{\rm crt}$ and of the last three terms of $\Delta F_3^{\rm crt}$ to the relative error are small compared with the contributions of $\Delta F_1^{\rm crt}$, of the first term of $\Delta F_0^{\rm crt}$ and of the first term of $\Delta F_3^{\rm crt}$.

The relative error of the coupling ray theory with the quasi–isotropic perturbation of travel times is thus composed of all partial relative errors (107a)–(107d), with

$$\Delta F_0^{\rm qi} \approx \frac{3}{2}\left[\left(\frac{\varepsilon}{2}\right)^2 + \left(\frac{\Delta v}{v_R}\right)^2\right] k_0 \quad , \tag{117a}$$

$$\Delta F_1^{\rm qi} \approx \frac{\varepsilon}{2}K \quad , \tag{117b}$$

$$\Delta F_2^{\rm qi} \approx 0 \quad , \tag{117c}$$

$$\Delta F_3^{\rm qi} \approx 3\frac{\varepsilon}{2}\frac{\Delta v}{v_R}k_0 \quad , \tag{117d}$$

$W_2 = 1$ and $W_3 = 1$. At high frequencies, $\left|\frac{K}{k_0}\right| \ll \left|\frac{\varepsilon}{2}\right|$, the dominant partial relative errors are $\Delta F_0^{\rm qi}$ and $\Delta F_3^{\rm qi}$, causing relative time shifts $-\frac{3}{2}\left(\left|\frac{\varepsilon}{2}\right| \pm \frac{\Delta v}{v_R}\right)^2$ of the first (+) and second (−) S–wave polarizations. The relative error of the propagator matrix is

$$\Delta^{\rm qi} \approx \sqrt{\begin{array}{c}\left[\frac{3}{2}\right]^2\left[\left(\frac{\varepsilon}{2}\right)^2+\left(\frac{\Delta v}{v_R}\right)^2\right]^2[k_0x_3]^2 + 3^2\left[\frac{\varepsilon}{2}\right]^4\left[\frac{\Delta v}{v_R}\right]^2\left[\left(\frac{\varepsilon}{2}\right)^2+\left(\frac{K}{k_0}\right)^2\right]^{-1}[k_0x_3]^2\\ +\left[\frac{\varepsilon}{2}\right]^2\left[\frac{K}{k_0}\right]^2\left[\left(\frac{\varepsilon}{2}\right)^2+\left(\frac{K}{k_0}\right)^2+\left(3\frac{\Delta v}{v_R}\right)^2\right]\left[\left(\frac{\varepsilon}{2}\right)^2+\left(\frac{K}{k_0}\right)^2\right]^{-2}[\sin(\overline{\varphi}x_3)]^2\end{array}} \ . \tag{118}$$

At low frequencies, the bottom addend in the square root is dominant. The upper two addends in the square root become dominant at the coupling frequency, $\left|\frac{K}{k_0}\right| = \left|\frac{\varepsilon}{2}\right|$, and increase with frequency. The quasi–isotropic perturbation of travel times is nearly as good as the coupling ray theory at low frequencies, but is subject to a considerably larger error than the coupling ray theory at the coupling frequency, roughly by factor $\sqrt{\left[1+4\left(\frac{2\Delta v}{\varepsilon v_R}\right)^2\right]\left[1+2\left(\frac{3}{2}Kx_3\right)^2\right]}$. At high frequencies,

$\left|\frac{K}{k_0}\right| \ll \left|\frac{\varepsilon}{2}\right|$, the error increases as $\frac{3}{2}\left|\frac{k_0}{K}\right|\left|\frac{\varepsilon}{2}\right|\sqrt{\left(\frac{\varepsilon}{2}\right)^2+6\left(\frac{\Delta v}{v_R}\right)^2+\left(\frac{2}{\varepsilon}\right)^2\left(\frac{\Delta v}{v_R}\right)^4}\,|Kx_3|$. At high frequencies, $\left|\frac{K}{k_0}\right| \ll \left|\frac{\varepsilon}{2}\right|$, and with a good reference velocity, $\left|\frac{\Delta v}{v_R}\right| \ll \left|\frac{\varepsilon}{2}\right|$, the error increases as $\frac{3}{2}\left|\frac{k_0}{K}\right|\left(\frac{\varepsilon}{2}\right)^2|Kx_3|$. The error becomes worse than the error of the anisotropic ray theory at $\left|\frac{K}{k_0}\right| = \left|\frac{\varepsilon}{2}\right|^{\frac{3}{2}}$, where the anisotropic ray theory also fails, see (123) below. The coupling ray theory with the quasi–isotropic perturbation of travel times thus often cannot bridge the whole gap between the isotropic and anisotropic ray theories (*Bulant et al., 1999, 2000, 2004*, figures 1).

4.4. Anisotropic ray theory

In the simplified twisted crystal model, the zero–order anisotropic ray theory (*Červený, 1972*) yields the approximate solution in the form of (39) with F_0, F_1, F_2 and F_3 replaced by

$$F_0^{\rm ani} = k_0\,\frac{\sqrt{1+\varepsilon}+\sqrt{1-\varepsilon}}{2\sqrt{1-\varepsilon^2}} \quad , \tag{119a}$$

$$F_1^{\rm ani} = 0 \quad , \tag{119b}$$

$$F_2^{\rm ani} = 0 \quad , \tag{119c}$$

$$F_3^{\rm ani} = -k_0\,\frac{\sqrt{1+\varepsilon}-\sqrt{1-\varepsilon}}{2\sqrt{1-\varepsilon^2}} \quad , \tag{119d}$$

which differs from the coupling ray theory by zero coefficient $F_2^{\rm ani}$. The Taylor expansions of these coefficients up to the third order in ε and K/k_0 are

$$F_0^{\rm ani} \approx k_0 + \frac{3\varepsilon^2}{8}k_0 \quad , \tag{120a}$$

$$F_1^{\rm ani} = 0 \quad , \tag{120b}$$

$$F_2^{\rm ani} = 0 \quad , \tag{120c}$$

$$F_3^{\rm ani} \approx -\frac{\varepsilon}{2}k_0 - \frac{5\varepsilon^3}{16}k_0 \quad . \tag{120d}$$

The differences (86) of coefficients F_α from $F_\alpha^{\rm ani}$ are

$$\Delta F_0^{\rm ani} \approx 0 \quad , \tag{121a}$$

$$\Delta F_1^{\rm ani} \approx \frac{\varepsilon}{2}K \quad , \tag{121b}$$

$$\Delta F_2^{\rm ani} \approx K + \frac{\varepsilon^2}{2}K \quad , \tag{121c}$$

$$\Delta F_3^{\rm ani} \approx \frac{\varepsilon}{2}\frac{K^2}{k_0} \quad . \tag{121d}$$

The zero–order anisotropic ray theory differs from the exact solution even in the first–order term with respect to $\frac{K}{k_0}$ (the first term in $\Delta F_2^{\rm ani}$). We thus neglect the second–order difference $\Delta F_1^{\rm ani}$ and the third–order differences in $\Delta F_2^{\rm ani}$ and $\Delta F_3^{\rm ani}$.

The relative error of the anisotropic ray theory is thus composed of the partial relative errors (107c) and (107d), with $\Delta F_2^{\rm ani} \approx K$, $\Delta F_3^{\rm ani} \approx 0$, $W_2 = \frac{1}{2}$ and $W_3 = 1$. The relative error of the propagator matrix is approximately

$$\Delta^{\rm ani} \approx \left|\frac{K}{k_0}\right| \sqrt{\left(\frac{\varepsilon}{2}\right)^2 \left[\left(\frac{\varepsilon}{2}\right)^2 + \left(\frac{K}{2k_0}\right)^2\right]^{-2} [\sin(\overline{\varphi} x_3)]^2 + \left[\left(\frac{\varepsilon}{2}\right)^2 + \left(\frac{K}{2k_0}\right)^2\right]^{-1} \left[\frac{Kx_3}{2}\right]^2} \ . \tag{122}$$

The error is huge below and in the vicinity of the coupling frequency. At high frequencies, $\left|\frac{K}{k_0}\right| \ll \left|\frac{\varepsilon}{2}\right|$,

$$\Delta^{\rm ani} \approx \left|\frac{2}{\varepsilon}\right| \left|\frac{K}{k_0}\right| \sqrt{[\sin(\overline{\varphi} x_3)]^2 + \left[\frac{Kx_3}{2}\right]^2} \quad , \tag{123}$$

which is larger than the error of the coupling ray theory, at least, by factor $\left|\frac{2}{\varepsilon}\right|\sqrt{1+\left(\frac{Kx_3}{2}\right)^2}$ at all high frequencies.

4.5. Isotropic ray theory

The zero–order isotropic ray theory is applied to isotropic material which is, in a way, close to the anisotropic material under consideration. The most accurate approach is to select the velocity in the vicinity of each isotropic ray to yield a travel time equal to the arithmetic average of the anisotropic travel times of both S–wave polarizations along the same phase–space curve in the anisotropic material.

In the simplified twisted crystal model, this application of the zero–order isotropic ray theory yields the approximate solution in the form of (39) with F_0, F_1, F_2 and F_3 replaced by

$$F_0^{\rm iso} = k_0 \, \frac{\sqrt{1+\varepsilon} + \sqrt{1-\varepsilon}}{2\sqrt{1-\varepsilon^2}} \quad , \tag{124a}$$

$$F_1^{\rm iso} = 0 \quad , \tag{124b}$$

$$F_2^{\rm iso} = K \quad , \tag{124c}$$

$$F_3^{\rm iso} = 0 \quad , \tag{124d}$$

which differs from the coupling ray theory by zero coefficient $F_3^{\rm iso}$. The Taylor expansions of these coefficients up to the third order in ε, K/k_0 and $\Delta v/v_R$ are

$$F_0^{\rm iso} \approx k_0 + \frac{3\varepsilon^2}{8} k_0 \quad , \tag{125a}$$

$$F_1^{\rm iso} = 0 \quad , \tag{125b}$$

$$F_2^{\rm iso} = K \quad , \tag{125c}$$

$$F_3^{\rm iso} = 0 \quad . \tag{125d}$$

The differences (86) of coefficients F_α from $F_\alpha^{\rm iso}$ are

$$\Delta F_0^{\rm iso} \approx 0 \quad , \tag{126a}$$

$$\Delta F_1^{\rm iso} \approx \frac{\varepsilon}{2} K \quad , \tag{126b}$$

$$\Delta F_2^{\rm iso} \approx \frac{\varepsilon^2}{2} K \quad , \tag{126c}$$

$$\Delta F_3^{\rm iso} \approx -\frac{\varepsilon}{2} k_0 - \frac{5\varepsilon^3}{16} k_0 + \frac{\varepsilon}{2} \frac{K^2}{k_0} \quad . \tag{126d}$$

The zero–order isotropic ray theory differs from the exact solution even in the first–order term with respect to $\frac{\varepsilon}{2}$ (the first term in $\Delta F_3^{\rm iso}$). We thus neglect the second–order difference $\Delta F_1^{\rm iso}$ and the third–order differences in $\Delta F_2^{\rm iso}$ and $\Delta F_3^{\rm iso}$.

The relative error of the isotropic ray theory is thus composed of the partial relative errors (107c) and (107d), with $\Delta F_2^{\rm iso} \approx 0$, $\Delta F_3^{\rm iso} \approx -\frac{\varepsilon}{2} k_0$, $W_2 = 1$ and $W_3 = \frac{1}{2}$. The relative error of the propagator matrix is approximately

$$\Delta^{\rm crt} \approx \left|\frac{\varepsilon}{2}\right| \sqrt{\left(\frac{K}{k_0}\right)^2 [\sin(\overline{\varphi} x_3)]^2 \left[\left(\frac{\varepsilon}{4}\right)^2 + \left(\frac{K}{k_0}\right)^2\right]^{-2} + \left(\frac{\varepsilon}{4}\right)^2 \left[\left(\frac{\varepsilon}{4}\right)^2 + \left(\frac{K}{k_0}\right)^2\right]^{-1} [k_0 x_3]^2} \; . \tag{127}$$

The error is huge in the vicinity and above the coupling frequency. At low frequencies, $\left|\frac{\varepsilon}{2}\right| \ll \left|\frac{K}{k_0}\right| \ll 1$,

$$\Delta^{\rm iso} \approx \left|\frac{\varepsilon}{2}\right| \left|\frac{k_0}{K}\right| |\sin(\overline{\varphi} x_3)| \quad , \tag{128}$$

which is larger than the error of the coupling ray theory by factor $\left|\frac{k_0}{K}\right|$.

5. CONCLUDING REMARKS

The exact 2×2 one–way propagator matrix of a plane S wave, propagating along the axis of spirality in the simplified twisted crystal model, is given by equation (39) with equations (32), (33), (47), (49), (52) and (63). The exact analytical solution of the elastodynamic equation has been checked by comparison with *Vavryčuk*'s *(1999)* finite–difference code (*Bulant et al., 2004*).

The exact analytical solution of the elastodynamic equation in the simplified twisted crystal model is useful in testing the applicability and accuracy of various approximate wavefield modelling methods, especially of the coupling ray theory and of its various quasi–isotropic approximations and various numerical implementations (*Bulant et al., 1999; 2000; 2004*). Moreover, transformations of the simplified twisted crystal model and of the exact analytical solution enable new models with corresponding exact analytical solutions to be generated, in order to study wave–propagation phenomena not present in the simplified twisted crystal model (*Bulant and Klimeš, 2004*).

In addition to the exact analytical solution of the elastodynamic equation in the simplified twisted crystal model, the analytical solutions of the equations of the four ray methods are given in Section 4. The ray methods are (a) the coupling ray theory, (b) the coupling ray theory with the quasi–isotropic perturbation of travel times, (c) the anisotropic ray theory, (d) the isotropic ray theory. These four approximate solutions of the elastodynamic equation are useful for comparison with the exact solution (*Bulant et al., 1999; 2000; 2004*). Both the exact analytical solution and the analytical ray–theory solutions in the simplified twisted crystal model are also helpful in debugging computer codes for various approximate wavefield modelling methods, especially for the coupling ray theory (*Bulant et al., 1999; 2000; 2004*).

In the simplified twisted crystal model, the coupling ray theory is considerably more accurate than the isotropic and anisotropic ray theories. The error of the anisotropic ray theory is larger than the error of the coupling ray theory by factor $\left|\frac{2}{\varepsilon}\right| \sqrt{1 + \left(\frac{Kx_3}{2}\right)^2}$, i.e. more than by factor $\left|\frac{2}{\varepsilon}\right|$, at all high frequencies. Here ε specifies the degree of anisotropy of the simplified twisted crystal model through equation (9). In the simplified twisted crystal model, the quasi–isotropic perturbation of travel times makes the accuracy of the coupling ray theory considerably worse at the frequencies higher than the coupling frequency. The quasi–isotropic perturbation of travel times thus should be avoided.

For additional information, including electronic reprints, computer codes and data, refer to the consortium research project "Seismic Waves in Complex 3-D Structures" ("http://sw3d.mff.cuni.cz").

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