Analytical one–way plane–wave solution in the 1-D anisotropic "twisted crystal" model

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Summary

The exact analytical expressions for the 2×2 one–way propagator matrices of plane S waves, propagating along the axis of spirality in the simple 1-D anisotropic "twisted crystal" model, are presented. The analytical equations may be useful to test and debug approximate and numerical methods, e.g., the coupling ray theory, the high–order anisotropic ray theory or the finite differences. The exact solution is compared with the analytical equations for the coupling ray theory and zero–order anisotropic and isotropic ray theories.

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 along the x_3 axis. It is one of the simplest models useful to demonstrate the limits of applicability of the zero–order isotropic and anisotropic ray theories and to test the coupling ray theory, which is the generalization of both the zero–order isotropic and anisotropic ray theories and provides the continuous transition between them.

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 general initial conditions expressed in terms of displacement and stress has been derived by Lakhtakia (1994), who also presented explicit analytical equations for the simplified model with vanishing 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 shall study just the simplified model. On the contrary to Lakhtakia's paper, we shall not seek the solution for initial displacement and stress, but concentrate to the 2×2 one–way propagator matrices suitable for the comparison with the coupling ray theory of Coates & Chapman (1990). Our study has been motivated especially by the following objectives: (a) to test the applicability and accuracy of the coupling ray theory, (b) to assist in debugging the computer codes for the coupling ray theory, (c) to find the source of discrepancies between the numerical results of Bulant & Klimeš (1998) and Pšenčík (1998), (d) to assess the differences between various implementations of the coupling ray theory, (e) to study the convergence of high–order anisotropic ray theory at various degrees of anisotropy (Vavryčuk 1999), (f) to check the accuracy of finite–difference code by Vavryčuk (1999).

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2 "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 parameters (stiffness tensor). Lower–case subscripts take values $i, j, k, ... = 1, 2, 3$, upper–case subscripts take values $I, J, K, ... = 1, 2$, the Einstein summation over the pairs of identical indices is used.

For plane wave $u_i = u_i(x_3)$ propagating along the x_3 axis in 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 simplified 1-D anisotropic "twisted crystal" model we take

$$a_{33K3} = 0 \quad . \tag{3}$$

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 the 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 "twisted crystal" model we choose parameters a_{I3K3} in the form of

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

with

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

Matrix $\mathbf{B}$ must be positive definite,

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

Let us assume also

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

to simplify the derivation. The solution for $K = 0$ is obvious. Due to the separation of plane waves, other parameters than a_{i3K3} may be arbitrarily dependent on x_3. Elastodynamic equation (7) for the plane S wave in the "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 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 is 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 the 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 than 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 explicitly describes the rotation along the x_3 axis.

We now apply transformation

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

into 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

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

We now perform the derivative at the left–hand side

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

multiply the Pauli matrices

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

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 is the second–order counterpart to Lakhtakia's (1994) first–order equations (11a,b) for 3 displacement and 3 stress tensor components.

3.2 One–way propagator matrix

Since the 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 can split the 4 linearly independent solutions of elastodynamic equation (26) 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 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 the 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 plain 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 2×2 matrix $\mathbf{F}$.

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

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

and seek individual coefficients F_0, F_1, F_2 and F_3. We have put somewhat illogical imaginary unit at F_1, because otherwise we could observe purely imaginary F_1 with real–valued F_0, F_2, F_3 in the solution, as will be seen later on.

Introducing auxiliary coefficient

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

at "normalized" matrix

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

satisfying relation

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

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 simple form

$$\widehat{\mathbf{U}} = \exp(\mathrm{i}F_0 x_3)\,[\mathbf{1}\cos(\varphi x_3) + \mathrm{i}\mathbf{\Phi}\sin(\varphi x_3)] \tag{36}$$

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

$$\begin{aligned}\widehat{\mathbf{U}} =& \exp(\mathrm{i}\mathrm{Re}F_0 x_3)\,[\mathbf{1}\cos(\mathrm{Re}\varphi x_3) + \mathrm{i}\mathbf{\Phi}\sin(\mathrm{Re}\varphi x_3)] \\ &\times \exp(-\mathrm{Im}F_0 x_3)\,[\mathbf{1}\cosh(\mathrm{Im}\varphi x_3) - \mathbf{\Phi}\sinh(\mathrm{Im}\varphi x_3)] \quad .\end{aligned} \tag{37}$$

For one–way propagation we need

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

and the sign of F_0 corresponding to the direction of propagation.

The $2{\times}2$ one–way propagator matrix of elastodynamic equation (12) in the Cartesian coordinates is then

$$\boxed{\begin{aligned}\mathbf{U} =& \exp(\mathrm{i}\mathrm{Re}F_0 x_3)\,[\mathbf{1}\cos(K x_3) - \mathrm{i}\boldsymbol{\sigma}_2\sin(K x_3)]\,[\mathbf{1}\cos(\mathrm{Re}\varphi x_3) + \mathrm{i}\mathbf{\Phi}\sin(\mathrm{Re}\varphi x_3)] \\ &\times \exp(-\mathrm{Im}F_0 x_3)\,[\mathbf{1}\cosh(\mathrm{Im}\varphi x_3) - \mathbf{\Phi}\sinh(\mathrm{Im}\varphi x_3)] \quad , \qquad (39)\end{aligned}}$$

We shall 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 at matrices $\mathbf{1}$, $\boldsymbol{\sigma}_1$, $\boldsymbol{\sigma}_2$ and $\boldsymbol{\sigma}_3$ yields the 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

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

The two solutions of this system of equations 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) yields

$$\boxed{F_2 = K + \varepsilon F_1 \quad . \qquad (47)}$$

After insertion of (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 insertion of relation (49) for F_3, may be simplified to

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

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 the 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 signs are opposite.

The term at 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 at 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 insertion of 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

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

when the one–way propagating wave is exponentially attenuating due to back scattering.

Equation (58) has real–valued roots either for

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

when there is no attenuation due to back scattering. The larger root (in absolute value)

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

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 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 insertion into (52) and determination of 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 increase 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 the time factor $\exp(\pm \mathrm{i}\omega t)$. 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 the rest of this subsection, we only check whether inequality (38) is satisfied. 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 ones,

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

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 into

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

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,

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

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.,

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

For resonant frequencies given by inequality (70), equations (67) and (79) 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) are exponentially decreasing to one half for the resonant frequencies, because the energy is gradually split half by half 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) equations (22a,b), we see that Lakhtakia's eigenvalues g_2, g_3, g_4 and g_5 corresponding to S waves are

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

4 Comparison with the ray methods

The ray theories, like the isotropic ray theory, anisotropic ray theory or coupling ray theory (Coates & Chapman 1990), are high–frequency asymptotic methods and should thus be applied at sufficiently high frequencies, for $k_0 \gg K$. We will thus assume that the order of K/k_0 is comparable with the order of ε and 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) up to the second order in ε and K/k_0 are

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

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

$$F_2 \approx K \quad , \tag{85c}$$

$$F_3 \approx -\frac{\varepsilon}{2}k_0 \quad . \tag{85d}$$

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 (106a–d), (111a–d), (116a–d) or (121a–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

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

We now estimate the relative error

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

with

$$\Delta\mathbf{U} = \mathbf{U} - \mathbf{U}^{\rm ray} \quad , \tag{88}$$

of the one-way propagator matrix in terms of differences (86). Symbol $\mathbf{A}^{+}$ denotes the Hermitian adjoint matrix to $\mathbf{A}$.

Under assumption (84), coefficients F_0, F_1, F_2 and F_3 are real–valued and equation (36) yields

$$\begin{aligned}\Delta\widehat{\mathbf{U}} \simeq \exp({\rm i}F_0x_3)\,\{&[\mathbf{1}\cos(\varphi x_3) + {\rm i}\boldsymbol{\Phi}\sin(\varphi x_3)]\,{\rm i}\Delta F_0 x_3 \\ &+ [-\mathbf{1}\sin(\varphi x_3) + {\rm i}\boldsymbol{\Phi}\cos(\varphi x_3)]\,\Delta\varphi x_3 + {\rm i}\Delta\boldsymbol{\Phi}\sin(\varphi x_3)\} \; ,\end{aligned} \tag{89}$$

where

$$\Delta\varphi \simeq [F_3\Delta F_3 + F_2\Delta F_2 - F_1\Delta F_1]\varphi^{-1} \quad , \tag{90}$$

see (32), and

$$\Delta\boldsymbol{\Phi} \simeq [\Delta F_1{\rm i}\boldsymbol{\sigma}_1 + \Delta F_2\boldsymbol{\sigma}_2 + \Delta F_3\boldsymbol{\sigma}_3]\,\varphi^{-1} - \boldsymbol{\Phi}\Delta\varphi\,\varphi^{-1} \quad , \tag{91}$$

see (33). Multiplying (89) by

$$\widehat{\mathbf{U}}^{-1} = \exp(-{\rm i}F_0x_3)\,[\mathbf{1}\cos(\varphi x_3) - {\rm i}\boldsymbol{\Phi}\sin(\varphi x_3)] \quad , \tag{92}$$

we arrive at

$$\widehat{\mathbf{U}}^{-1}\Delta\widehat{\mathbf{U}} \simeq \mathbf{1}{\rm i}\Delta F_0x_3 + {\rm i}\boldsymbol{\Phi}\Delta\varphi x_3 + [\mathbf{1}\cos(\varphi x_3) - {\rm i}\boldsymbol{\Phi}\sin(\varphi x_3)]\,{\rm i}\Delta\boldsymbol{\Phi}\sin(\varphi x_3) \; . \tag{93}$$

Since F_1 is small with respect to F_2 or F_3, we may use approximations

$$\varphi \approx \sqrt{F_2^2 + F_3^2} \approx k_0\sqrt{\left(\frac{\varepsilon}{2}\right)^2 + \left(\frac{K}{k_0}\right)^2} \quad , \tag{94}$$

$$\boldsymbol{\Phi} \approx [F_2\boldsymbol{\sigma}_2 + F_3\boldsymbol{\sigma}_3]\,\varphi^{-1} \tag{95}$$

and

$$\Delta\varphi \approx [F_3\Delta F_3 + F_2\Delta F_2]\varphi^{-1} \tag{96}$$

to equations (32), (33) and (90), respectively. Since ${\rm Tr}\boldsymbol{\Phi} = 0$, ${\rm Tr}\Delta\boldsymbol{\Phi} = 0$ and

$$\boldsymbol{\Phi}^{+} \approx \boldsymbol{\Phi} \quad , \tag{97}$$

equation (87) with (93) yields

$$\Delta^{\rm ray} \approx \sqrt{\begin{array}{c}[\Delta F_0x_3]^2 + [\Delta\varphi x_3]^2 + \frac{1}{2}{\rm Tr}(\Delta\boldsymbol{\Phi}^{+}\Delta\boldsymbol{\Phi})[\sin(\varphi x_3)]^2 \\ +\frac{1}{2}{\rm Tr}(\boldsymbol{\Phi}{\rm i}(\Delta\boldsymbol{\Phi}^{+} - \Delta\boldsymbol{\Phi}))\Delta F_0x_3[\sin^2(\varphi x_3)]^2 \\ +\frac{1}{2}{\rm Tr}(\boldsymbol{\Phi}(\Delta\boldsymbol{\Phi}^{+} + \Delta\boldsymbol{\Phi}))\Delta\varphi x_3\cos(\varphi x_3)\sin(\varphi x_3)\end{array}} \quad , \tag{98}$$

see (34). Since the Pauli matrices are Hermitian symmetric, equations (91), (95) (96) and (97) yield

$$\tfrac{1}{2}\mathrm{Tr}(\mathbf{\Phi}\mathrm{i}(\Delta\mathbf{\Phi}^{+} - \Delta\mathbf{\Phi})) \approx 0 \tag{99}$$

and

$$\tfrac{1}{2}\mathrm{Tr}(\mathbf{\Phi}(\Delta\mathbf{\Phi}^{+} + \Delta\mathbf{\Phi})) \approx 0 \quad . \tag{100}$$

Similarly,

$$\tfrac{1}{2}\mathrm{Tr}(\Delta\mathbf{\Phi}^{+}\Delta\mathbf{\Phi}) \approx [\Delta F_1^2+\Delta F_2^2+\Delta F_3^2]\varphi^{-2}-2[F_2\Delta F_2+F_3\Delta F_3]\Delta\varphi\varphi^{-2}+\Delta\varphi^2\varphi^{-2} \; . \tag{101}$$

Inserting (96), we arrive at

$$\tfrac{1}{2}\mathrm{Tr}(\Delta\mathbf{\Phi}^{+}\Delta\mathbf{\Phi}) \approx [\Delta F_1^2]\varphi^{-2} + [F_2\Delta F_3 - F_3\Delta F_2]^2\varphi^{-4} \quad . \tag{102}$$

Finally we obtain relative error

$$\Delta^{\mathrm{ray}} \approx \sqrt{\Delta_0^2 + \Delta_1^2 + \Delta_2^2 + \Delta_3^2} \tag{103}$$

approximately composed of four parts

$$\Delta_0 = \Delta F_0 \, x_3 \quad , \tag{104a}$$

$$\Delta_1 = \Delta F_1 \, \varphi^{-1} \, \sin(\varphi x_3) \quad , \tag{104b}$$

$$\Delta_2 = [F_2\Delta F_3 - F_3\Delta F_2] \, \varphi^{-2} \, \sin(\varphi x_3) \quad , \tag{104c}$$

$$\Delta_3 = \Delta\varphi \, x_3 \quad , \tag{104d}$$

where we may insert (85c, d), (94) and (96),

$$\Delta_0 = \frac{\Delta F_0}{k_0}\frac{k_0}{K}\, K x_3 \quad , \tag{105a}$$

$$\Delta_1 = \frac{\Delta F_1}{k_0}\left[\left(\frac{\varepsilon}{2}\right)^2 + \left(\frac{K}{k_0}\right)^2\right]^{-\frac{1}{2}} \sin(\varphi x_3) \quad , \tag{105b}$$

$$\Delta_2 = \left[\frac{\varepsilon}{2}\frac{\Delta F_2}{k_0} + \frac{K}{k_0}\frac{\Delta F_3}{k_0}\right]\left[\left(\frac{\varepsilon}{2}\right)^2 + \left(\frac{K}{k_0}\right)^2\right]^{-1} \sin(\varphi x_3) \quad , \tag{105c}$$

$$\Delta_3 = \left[\frac{K}{k_0}\frac{\Delta F_2}{k_0} - \frac{\varepsilon}{2}\frac{\Delta F_3}{k_0}\right]\left[\left(\frac{\varepsilon}{2}\right)^2 + \left(\frac{K}{k_0}\right)^2\right]^{-\frac{1}{2}} \frac{k_0}{K}\, K x_3 \quad . \tag{105d}$$

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 $K x_3$ 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, the rotational angle $K x_3$ usually does not exceed few radians.

4.1 Coupling ray theory

The coupling ray theory implemented by Bulant & Klimeš (1998) according to the equations of Coates & Chapman (1990) gives in the "twisted crystal" model approximate solution in the form of (39) with F_0, F_1, F_2 and F_3 replaced by

$$F_0^{\mathrm{crt}} = k_0 \, \frac{\sqrt{1+\varepsilon}+\sqrt{1-\varepsilon}}{2\sqrt{1-\varepsilon^2}} \quad , \tag{106a}$$

$$F_1^{\mathrm{crt}} = 0 \quad , \tag{106b}$$

$$F_2^{\mathrm{crt}} = K \quad , \tag{106c}$$

$$F_3^{\mathrm{crt}} = -k_0 \, \frac{\sqrt{1+\varepsilon}-\sqrt{1-\varepsilon}}{2\sqrt{1-\varepsilon^2}} \quad . \tag{106d}$$

Coefficient F_0 is the arithmetic average of the travel times of the two S wave polarizations along the reference ray in the phase–space. Coefficient F_2 attempts to prevent the rotation of polarization vectors about the ray. Coefficient F_3 is responsible to account for the difference between the travel times of the two S wave polarizations. Non–zero coefficients F_2 and F_3 mutually interfere in such a way that the larger one partly cancels the action of the smaller one. We may call the frequency at which $|F_2| = |F_3|$ the *coupling frequency* in this model. In this way, F_2 is dominant at low frequencies (considerably lower than the coupling frequency) and F_3 is dominant at high frequencies (considerably higher than the coupling frequency).

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

$$F_0^{\mathrm{crt}} \approx k_0 + \frac{3\varepsilon^2}{8} k_0 \quad , \tag{107a}$$

$$F_1^{\mathrm{crt}} = 0 \quad , \tag{107b}$$

$$F_2^{\mathrm{crt}} = K \quad , \tag{107c}$$

$$F_3^{\mathrm{crt}} \approx -\frac{\varepsilon}{2} k_0 \quad . \tag{107d}$$

We see that

$$\left|\frac{K}{k_0}\right| \approx \left|\frac{\varepsilon}{2}\right| \quad . \tag{108}$$

for the coupling frequency. The differences of the coefficients are

$$\Delta F_0^{\mathrm{crt}} \approx 0 \quad , \tag{109a}$$

$$\Delta F_1^{\mathrm{crt}} \approx \frac{\varepsilon}{2} K \quad , \tag{109b}$$

$$\Delta F_2^{\mathrm{crt}} \approx 0 \quad , \tag{109c}$$

$$\Delta F_3^{\mathrm{crt}} \approx 0 \quad . \tag{109d}$$

The relative error

$$\Delta^{\mathrm{crt}} \approx \left|\frac{\varepsilon}{2}\right| \left|\frac{K}{k_0}\right| \left[\left(\frac{\varepsilon}{2}\right)^2 + \left(\frac{K}{k_0}\right)^2 \right]^{-\frac{1}{2}} |\sin(\varphi x_3)| \tag{110}$$

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

4.2 Quasi–isotropic approach

The coupling ray theory implemented according to Pšenčík (1998) gives in the "twisted crystal" model with reference velocity v_R approximate solution in the form of (39) with F_0, F_1, F_2 and F_3 replaced by

$$F_0^{\rm qi} = k_0 \frac{v_0}{v_R} \left[\frac{3}{2} - \frac{1}{2} \left(\frac{v_0}{v_R} \right)^2 \right] \quad , \tag{111a}$$

$$F_1^{\rm qi} = 0 \quad , \tag{111b}$$

$$F_2^{\rm qi} = K \quad , \tag{111c}$$

$$F_3^{\rm qi} = -\frac{k_0}{2} \varepsilon \left(\frac{v_0}{v_R} \right)^3 \quad . \tag{111d}$$

We assume that

$$\left| \frac{\Delta v}{v_R} \right| = \left| \frac{v_0 - v_R}{v_R} \right| \ll 1 \quad . \tag{112}$$

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

$$F_0^{\rm qi} \approx k_0 - \frac{3}{2} \left(\frac{\Delta v}{v_R} \right)^2 k_0 \quad , \tag{113a}$$

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

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

$$F_3^{\rm qi} \approx -\frac{\varepsilon}{2} k_0 - \frac{3\varepsilon}{2} \frac{\Delta v}{v_R} k_0 \quad . \tag{113d}$$

The differences of the coefficients are

$$\Delta F_0^{\rm qi} \approx \frac{3}{2} \left[\left(\frac{\varepsilon}{2} \right)^2 + \left(\frac{\Delta v}{v_R} \right)^2 \right] k_0 \quad , \tag{114a}$$

$$\Delta F_1^{\rm qi} \approx \frac{\varepsilon}{2} K \quad , \tag{114b}$$

$$\Delta F_2^{\rm qi} \approx 0 \quad , \tag{114c}$$

$$\Delta F_3^{\rm qi} \approx 3 \frac{\varepsilon}{2} \frac{\Delta v}{v_R} k_0 \quad . \tag{114d}$$

The relative error of the propagator matrix is

$$\Delta^{\rm qi} \approx \sqrt{ \begin{array}{c} \left[\tfrac{3}{2}\right]^2 \left[\left(\tfrac{\varepsilon}{2}\right)^2 + \left(\tfrac{\Delta v}{v_R}\right)^2 \right]^2 [k_0 x_3]^2 + 3^2 \left[\tfrac{\varepsilon}{2}\right]^4 \left[\tfrac{\Delta v}{v_R}\right]^2 \left[\left(\tfrac{\varepsilon}{2}\right)^2 + \left(\tfrac{K}{k_0}\right)^2 \right]^{-1} [k_0 x_3]^2 \\ + \left[\tfrac{\varepsilon}{2}\right]^2 \left[\tfrac{K}{k_0}\right]^2 \left[\left(\tfrac{\varepsilon}{2}\right)^2 + \left(\tfrac{K}{k_0}\right)^2 + \left(3\tfrac{\Delta v}{v_R}\right)^2 \right] \left[\left(\tfrac{\varepsilon}{2}\right)^2 + \left(\tfrac{K}{k_0}\right)^2 \right]^{-2} [\sin(\varphi x_3)]^2 \end{array} } \quad . \tag{115}$$

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 are increasing with the frequency. The quasi–isotropic approach is nearly as good as the coupling ray theory at low frequencies but has considerably greater error than the coupling ray theory at the coupling frequency, roughly by the multiplicative factor of $\sqrt{\left[1 + \left(\frac{8\Delta v}{\varepsilon v_R}\right)^2\right] \left[1 + \left(\frac{3}{2} K x_3\right)^2\right]}$. At high frequencies, $\left|\frac{K}{k_0}\right| \ll \left|\frac{\varepsilon}{2}\right|$, the error increases as $\frac{3}{2}\left|\frac{k_0}{K}\right|\left|\frac{\varepsilon}{2}\right|\sqrt{\left(\frac{\varepsilon}{2}\right)^2+2\left(\frac{\Delta v}{v_R}\right)^2+4\left(\frac{\varepsilon}{2}\frac{k_0}{K}\frac{\Delta v}{v_R}\right)^2}\,|Kx_3|$ and 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 is bad, too, see (120) below. The quasi–isotropic approach to the coupling ray theory thus cannot bridge the whole gap between the isotropic and anisotropic ray theories.

4.3 Anisotropic ray theory

The zero–order anisotropic ray theory gives in the "twisted crystal" model approximate solution in the form of (39) with F_0, F_1, F_2 and F_3 replaced by

$$F_0^{\mathrm{ani}}=k_0\,\frac{\sqrt{1+\varepsilon}+\sqrt{1-\varepsilon}}{2\sqrt{1-\varepsilon^2}}\quad, \tag{116a}$$

$$F_1^{\mathrm{ani}}=0\quad, \tag{116b}$$

$$F_2^{\mathrm{ani}}=0\quad, \tag{116c}$$

$$F_3^{\mathrm{ani}}=-k_0\,\frac{\sqrt{1+\varepsilon}-\sqrt{1-\varepsilon}}{2\sqrt{1-\varepsilon^2}}\quad, \tag{116d}$$

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

$$F_0^{\mathrm{ani}}\approx k_0+\frac{3\varepsilon^2}{8}k_0\quad, \tag{117a}$$

$$F_1^{\mathrm{ani}}=0\quad, \tag{117b}$$

$$F_2^{\mathrm{ani}}=0\quad, \tag{117c}$$

$$F_3^{\mathrm{ani}}\approx-\frac{\varepsilon}{2}k_0\quad. \tag{117d}$$

The differences of the coefficients are

$$\Delta F_0^{\mathrm{ani}}\approx 0\quad, \tag{118a}$$

$$\Delta F_1^{\mathrm{ani}}\approx\frac{\varepsilon}{2}K\quad, \tag{118b}$$

$$\Delta F_2^{\mathrm{ani}}\approx K\quad, \tag{118c}$$

$$\Delta F_3^{\mathrm{ani}}\approx 0\quad. \tag{118d}$$

The zero–order anisotropic ray theory differs from the exact solution even by the first–order term in $\frac{K}{k_0}$. We thus neglect the second–order difference $\Delta F_1^{\mathrm{ani}}$ and the relative error of the propagator matrix is approximately

$$\Delta^{\mathrm{ani}}\approx\left|\frac{K}{k_0}\right|\sqrt{\left(\frac{\varepsilon}{2}\right)^2\left[\left(\frac{\varepsilon}{2}\right)^2+\left(\frac{K}{k_0}\right)^2\right]^{-2}[\sin(\varphi x_3)]^2+\left[\left(\frac{\varepsilon}{2}\right)^2+\left(\frac{K}{k_0}\right)^2\right]^{-1}[Kx_3]^2}\;. \tag{119}$$

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

$$\Delta^{\mathrm{ani}}\approx\left|\frac{2}{\varepsilon}\right|\left|\frac{K}{k_0}\right|\sqrt{[\sin(\varphi x_3)]^2+[Kx_3]^2}\quad, \tag{120}$$

which is greater than the error of the coupling ray theory, at the least, by the multiplicative factor of $\left|\frac{2}{\varepsilon}\right|$ at all high frequencies.

4.4 Isotropic ray theory

The zero–order isotropic ray theory is applied to the isotropic material which is in some sense close to the anisotropic material. The most accurate approach is to select the velocity in the vicinity of each isotropic ray such as it gives the travel time equal to the arithmetic average of anisotropic travel times of both S wave polarizations along the same phase–space curve in the anisotropic material.

Such an application of the zero–order isotropic ray theory gives in the "twisted crystal" model approximate solution in the form of (39) with F_0, F_1, F_2 and F_3 replaced by

$$F_0^{\rm iso} = k_0 \, \frac{\sqrt{1+\varepsilon}+\sqrt{1-\varepsilon}}{2\sqrt{1-\varepsilon^2}} \quad , \tag{121a}$$

$$F_1^{\rm iso} = 0 \quad , \tag{121b}$$

$$F_2^{\rm iso} = K \quad , \tag{121c}$$

$$F_3^{\rm iso} = 0 \quad , \tag{121d}$$

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

$$F_0^{\rm iso} \approx k_0 + \frac{3\varepsilon^2}{8} k_0 \quad , \tag{122a}$$

$$F_1^{\rm iso} = 0 \quad , \tag{122b}$$

$$F_2^{\rm iso} = K \quad , \tag{122c}$$

$$F_3^{\rm iso} = 0 \quad . \tag{122d}$$

The differences of the coefficients are

$$\Delta F_0^{\rm iso} \approx 0 \quad , \tag{123a}$$

$$\Delta F_1^{\rm iso} \approx \frac{\varepsilon}{2} K \quad , \tag{123b}$$

$$\Delta F_2^{\rm iso} \approx 0 \quad , \tag{123c}$$

$$\Delta F_3^{\rm iso} \approx -\frac{\varepsilon}{2} k_0 \tag{123d}$$

for the isotropic ray theory.

The zero–order isotropic ray theory differs from the exact solution even by the first–order term in $\frac{\varepsilon}{2}$. We thus neglect the second–order difference $\Delta F_1^{\rm iso}$ and the relative error of the propagator matrix is approximately

$$\Delta^{\rm crt} \approx \left|\frac{\varepsilon}{2}\right| \sqrt{\left(\frac{K}{k_0}\right)^2 [\sin(\varphi x_3)]^2 \left[\left(\frac{\varepsilon}{2}\right)^2 + \left(\frac{K}{k_0}\right)^2\right]^{-2} + \left(\frac{\varepsilon}{2}\right)^2 \left[\left(\frac{\varepsilon}{2}\right)^2 + \left(\frac{K}{k_0}\right)^2\right]^{-1} [k_0 x_3]^2} \ . \tag{124}$$

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

$$\Delta^{\rm iso} \approx \left|\frac{\varepsilon}{2}\right| \left|\frac{k_0}{k}\right| |\sin(\varphi x_3)| \quad , \tag{125}$$

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

5 Conluding remark

The equations of this paper has been coded and used by Bulant, Klimeš & Pšenčík (1999) to test the Fortran 77 code of packages ANRAY and CRT and to numerically demonstrate the applicability and accuracy of the coupling ray theory and zero–order anisotropic and isotropic ray theories, as outlined in the Introduction.

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