Comparison of quasi–isotropic approximations of the coupling ray theory with the exact solution in the 1-D anisotropic "oblique twisted crystal" model

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Summary

Commonly used quasi–isotropic approximations of the coupling ray theory are discussed. The coupling ray theory and its quasi–isotropic approximations are then numerically compared with the exact analytical solution for the plane S wave, propagating along the axis of spirality in the 1-D anisotropic "oblique twisted crystal" model.

Keywords

Coupling ray theory, quasi–isotropic approximation, seismic anisotropy, travel time, amplitude, Green function.

1. Introduction

There are two different high–frequency asymptotic ray theories, the *isotropic ray theory* assuming equal velocities of both S–wave polarizations and the *anisotropic ray theory* assuming both S–wave polarizations strictly decoupled. In the isotropic ray theory, the S–wave polarization vectors do not rotate about the ray, whereas in the anisotropic ray theory they coincide with the eigenvectors of the Christoffel matrix which may rotate rapidly about the ray.

In "weakly anisotropic" models, at moderate frequencies, the S–wave polarization tends to remain unrotated round the ray but is partly attracted by the rotation of the eigenvectors of the Christoffel matrix. The intensity of the attraction increases with frequency. The isotropic and anisotropic ray theories are thus limiting cases and the gap between them has to be filled. A ray theory providing continuous transition between the isotropic and anisotropic ray theories was proposed by Coates & Chapman (1990) and is called the *coupling ray theory*. The numerical algorithm of calculation of the frequency–dependent complex–valued S–wave polarization vectors of the coupling ray theory has been proposed by Bulant & Klimeš (2002). For a brief summary of the method refer to Section 2.

There are many possible modifications and approximations of the coupling ray theory. For example, the reference ray may be calculated in different ways (Bakker 2002), the Christoffel matrix may be approximated by its quasi–isotropic projections onto the plane perpendicular to the reference ray and onto the line tangent to the reference ray (Pšenčík 1998), travel times corresponding to the anisotropic ray theory may be approximated in several ways, e.g., by linear quasi–isotropic perturbation with respect to the density–normalized elastic moduli (Pšenčík 1998), etc. Commonly used quasi–isotropic approximations of the coupling ray theory are discussed in Section 3.

The results of the isotropic ray theory, anisotropic ray theory and coupling ray theory have been compared with the exact solution in the "simplified twisted crystal" model analytically by Klimeš (1999) and numerically by Bulant, Klimeš & Pšenčík (1999; 2000).

The effects of the anisotropic common ray approximation by Bakker (2002) and the less accurate isotropic common ray approximation have been studied by Klimeš & Bulant (2002). The effect of the quasi–isotropic projection of the Green tensor has been numerically demonstrated by Bulant & Klimeš (2002) on the example of synthetic seismograms calculated by the coupling ray theory in a 1-D anisotropic model.

The effects of the quasi–isotropic approximation of the Christoffel matrix, the quasi–isotropic projection of the Green tensor and the quasi–isotropic approximation of travel times are numerically demonstrated in this paper. In Section 4, a simple 1-D anisotropic "oblique twisted crystal" model is introduced, and the exact solution for the one–wave plane–wave propagator matrix is briefly summarized. The numerical results of the coupling ray theory and its above–mentioned quasi–isotropic approximations are then compared with the exact solution in Section 5.

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.

2. Coupling ray theory for S waves

Assume a *reference ray* in the phase space, parametrized by reference travel time τ, with reference slowness vectors $p_i(\tau)$ known at all its points $x_j(\tau)$. The reference ray should be close to the ray of the wave under study. In particular, the reference ray is best represented by the anisotropic ray theory ray, with the initial condition for the vectorial amplitude given by the relevant eigenvector of the Christoffel matrix corresponding to the ray. Then the travel time of the selected polarization is exact, and only the travel–time difference between the S–wave polarizations is approximate. The coupling ray theory may then also be used at high frequencies because the approximate travel–time difference influences only the coupling due to low–frequency scattering.

Using the reference slowness vectors, we can calculate reference Christoffel matrix

$$\Gamma_{jk}(\tau) = p_i(\tau)\; a_{ijkl}(x_m(\tau))\; p_l(\tau) \tag{1}$$

and its eigenvectors $g_{i1}(\tau)$, $g_{i2}(\tau)$, $g_{i3}(\tau)$ along the reference ray. Assume that eigenvectors $g_{i1}(\tau)$ and $g_{i2}(\tau)$ correspond to S waves and that they vary continuously along the reference ray. Continuity is not required in regions where the corresponding two eigenvalues are equal. Let us denote $\tau_1(\tau)$ and $\tau_2(\tau)$ the travel times corresponding to polarizations $g_{i1}(\tau)$ and $g_{i2}(\tau)$, respectively. They may be approximated by quadratures along the unperturbed reference ray,

$$\frac{\mathrm{d}\tau_1}{\mathrm{d}\tau} = [\Gamma_{jk} g_{j1} g_{k1}]^{-\frac{1}{2}} \;, \quad \frac{\mathrm{d}\tau_2}{\mathrm{d}\tau} = [\Gamma_{jk} g_{j2} g_{k2}]^{-\frac{1}{2}} \;. \tag{2}$$

The coupling ray theory solution u_i of the elastodynamic equations may then be expressed, for S waves, as linear combination

$$u_i = \sum_{M=1}^{2} A\; g_{iM}\; a_M \exp(\mathrm{i}\omega\overline{\tau}) \tag{3}$$

of the anisotropic ray theory solutions, where

$$\overline{\tau}(\tau) = \tfrac{1}{2}[\tau_1(\tau) + \tau_2(\tau)] \tag{4}$$

is the average travel time, and $A = A(\tau)$ is the complex–valued scalar amplitude in the high–frequency approximation (Červený 1972), corresponding to the system of reference rays. The coupling ray theory equation for complex–valued amplitude factors $a_M = a_M(\tau)$ reads

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \left[\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\frac{\mathrm{d}\varphi}{\mathrm{d}\tau} - \begin{pmatrix} \mathrm{i} & 0 \\ 0 & -\mathrm{i} \end{pmatrix}\frac{\omega}{2}\frac{\mathrm{d}(\tau_2-\tau_1)}{\mathrm{d}\tau}\right]\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} \;, \tag{5}$$

where

$$\frac{\mathrm{d}\varphi}{\mathrm{d}\tau} = g_{k2}\frac{\mathrm{d}g_{k1}}{\mathrm{d}\tau} = -g_{k1}\frac{\mathrm{d}g_{k2}}{\mathrm{d}\tau} \tag{6}$$

is the angular velocity of the eigenvector rotation.

2.1. Coupling ray theory S–wave propagator matrix

Propagator matrix Π^g of equation (5), defined as

$$\Pi^g_{MN}(\tau,\tau_0) = \frac{\partial\, a_M(\tau)}{\partial\, a_N(\tau_0)} \quad , \tag{7}$$

is a complex–valued 2×2 matrix satisfying equation

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\Pi^g = \left[\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\frac{\mathrm{d}\varphi}{\mathrm{d}\tau} - \begin{pmatrix} \mathrm{i} & 0 \\ 0 & -\mathrm{i} \end{pmatrix}\frac{\mathrm{d}\varepsilon}{\mathrm{d}\tau}\right]\Pi^g \quad , \tag{8}$$

directly following from equation (5). Here

$$\varepsilon(\tau) = \tfrac{1}{2}\omega\;[\tau_2(\tau) - \tau_1(\tau)] \quad . \tag{9}$$

Note that propagator matrix Π^g is symplectic and unitary.

It is difficult to integrate equation (8) by the Runge–Kutta or another numerical method which requires derivative $\frac{\mathrm{d}\varphi}{\mathrm{d}\tau}$ along the reference ray to be calculated, because this derivative is undefined in the singular regions of the two equal eigenvalues of Christoffel matrix (1). The method of calculating propagator matrix Π^g, fit for equation (8), has been proposed by Červený (2001) and Bulant & Klimeš (2002), with emphasis on numerical implementation. The method does not require the calculation of the angular velocity $\frac{\mathrm{d}\varphi}{\mathrm{d}\tau}$ of the rotation of the eigenvectors of the Christoffel matrix along the reference ray and does not require $\frac{\mathrm{d}\varphi}{\mathrm{d}\tau}$ to be smooth or finite along the reference ray. This is an important property, because the angular velocity of the rotation is undefined in the singular regions of the two equal eigenvalues of the Christoffel matrix.

The proposed method of solving equation (8) takes advantage of the chain rule. Since Π^g is a propagator matrix satisfying the chain rule, it may be numerically calculated as the product of propagator matrices Π^g corresponding to reasonably small segments of the reference ray (Červený 2001). Frequency–dependent propagator matrices along individual small ray segments may be approximated by the method of mean coefficients (Červený 2001). The accuracy of the proposed algorithm of numerical integration of the coupling equation has been estimated by Bulant & Klimeš (2002) in order to control the integration step so that the relative error in the wavefield amplitudes due to the integration is kept below a given limit, which is of principal importance for numerical applications.

The calculation of P–wave travel–time perturbations from a reference isotropic model to an anisotropic model and the calculation of the S–wave coupling ray theory travel–time and amplitude corrections along isotropic reference rays have been coded and added to the Fortran 77 package CRT (Bucha, Bulant & Klimeš 2001; Bucha & Bulant 2002).

3. Quasi–isotropic approximations of the coupling ray theory

The coupling ray theory by Coates & Chapman (1990) is applicable at all degrees of anisotropy, but it is often modified by various *quasi–isotropic approximations.*

3.1. Selection of the reference ray

The isotropic ray theory is always the limiting case of the coupling ray theory for decreasing anisotropy at a fixed frequency. On the other hand, the high–frequency limit of the coupling ray theory at a fixed anisotropy depends on the choice of the reference ray, and even on the choice of the *system* of reference rays, because the amplitudes are determined by the paraxial reference rays.

If we choose the *anisotropic ray theory reference ray* and select the initial polarization corresponding to the reference ray, the coupling ray theory will correctly limit to the anisotropic ray theory for high–frequencies. For other choices of reference rays, the high–frequency limit of the coupling ray theory at a fixed anisotropy is incorrect, although the differences may be small at the finite frequencies under consideration.

In the *anisotropic common ray approximation*, the common reference ray is traced using the averaged Hamiltonian of both S–wave polarizations (Bakker 2002).

In the less accurate *isotropic common ray approximation*, the reference ray is traced in the reference isotropic model. Moreover, the reference isotropic model may be selected in different ways, yielding quasi–isotropic approximations of various accuracy.

The method of estimating the errors due to the isotropic common ray approximation and anisotropic common ray approximation has been proposed by Klimeš & Bulant (2002).

3.2. Quasi–isotropic projection of the Green tensor

The coupling ray theory solution (3) may be approximated by its projection

$$\tilde{u}_i = h_{iM} h_{mM} u_m \tag{10}$$

onto the reference S–wave polarization plane, given by two orthonormal reference polarization vectors h_{k1}, h_{k2}. This approximation may simplify the modification of existing isotropic ray tracing codes for the coupling ray theory. The error of this approximation is obvious and can be calculated simply.

3.3. Quasi–isotropic approximation of the Christoffel matrix

The Christoffel matrix may be approximated by its projections onto the reference S–wave polarization plane and onto the reference P–wave polarization line. Denote the polarization vectors of the isotropic ray theory, or the reference polarization vectors in general, by h_{k1}, h_{k2} and h_{k3}. If the Christoffel matrix is approximated by its projections onto plane h_{j1}, h_{k2} and onto vector h_{l3},

$$\begin{aligned}\tilde{\Gamma}_{jk} &= h_{jM} h_{mM} \Gamma_{mn} h_{nN} h_{kN} + h_{j3} h_{m3} \Gamma_{mn} h_{n3} h_{k3} \\ &= \Gamma_{jk} - (h_{jM} h_{k3} + h_{j3} h_{kM}) h_{mM} \Gamma_{mn} h_{n3} \quad ,\end{aligned} \tag{11}$$

eigenvectors g_{k1} and g_{k2} become situated in plane h_{j1}, h_{k2} as in the zero-order quasi–isotropic approximation of Pšenčík (1998). This approximation includes the quasi–isotropic projection of the Green tensor described in Section 3.2.

The quasi–isotropic approximation of the Christoffel matrix is probably the worst quasi–isotropic approximation. The alteration of the coupling ray theory synthetic seismograms due to the quasi–isotropic approximation of the Christoffel matrix has been demonstrated by Bulant & Klimeš (2002).

3.4. Quasi–isotropic perturbation of travel times

The anisotropic ray theory travel times used in the coupling ray theory should be calculated by the numerical quadrature of equations (2) along the reference ray. The quasi–isotropic perturbation of travel times just corrects the reference travel time by the linear perturbation with respect to the density–normalized elastic moduli,

$$\frac{\mathrm{d}\tau_1}{\mathrm{d}\tau} \approx (\Gamma^0_{jk} g_{j1} g_{k1})^{-\frac{1}{2}} - \frac{1}{2}(\Gamma_{jk} - \Gamma^0_{jk}) g_{j1} g_{k1} (\Gamma^0_{jk} g_{j1} g_{k1})^{-\frac{3}{2}} . \tag{12}$$

Assuming that

$$\Gamma^0_{jk} g_{j1} g_{k1} = 1 \quad , \tag{13}$$

see Section 3.3, equation (12) becomes

$$\frac{\mathrm{d}\tau_1}{\mathrm{d}\tau} \approx \frac{3}{2} - \frac{1}{2} \Gamma_{jk} g_{j1} g_{k1} \quad , \tag{14}$$

as in the quasi–isotropic approximation of Pšenčík (1998). Analogously for $\frac{\mathrm{d}\tau_2}{\mathrm{d}\tau}$. The quasi–isotropic perturbation of travel times leads to an erroneous time shift in synthetic seismograms but has a negligible impact on the amplitudes.

4. Twisted crystal models

The *twisted crystal* model is created of a homogeneous anisotropic elastic material by uniformly helicoidally twisting the $x_1 x_2$ coordinate plane along the x_3 axis. It is one of the simplest models useful for demonstrating the limits of applicability of the zero–order isotropic and anisotropic ray theories and for testing the coupling ray theory (Coates & Chapman 1990), which is the generalization of both the zero–order isotropic and anisotropic ray theories and provides continuous transition between them.

The great advantage of this model is that the exact analytical solution for the plane S wave propagating along the axis of spirality can be examined analytically (Lakhtakia 1994; Klimeš 1999). 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 a_{1333} and a_{2333}, in which the u_1 and u_2 displacement components are strictly separated from the longitudinal u_3 component. Klimeš (1999) derived the 2×2 one–way propagator matrices in the simplified twisted crystal model, suitable for comparison with the coupling ray theory.

In this paper, we shall modify the simplified twisted crystal model towards the *oblique twisted crystal model* in order to allow the quasi–isotropic approximations of the coupling ray theory to be studied.

The elastodynamic equation in the frequency domain reads

$$[\varrho a_{ijkl} u_{k,l}]_{,j} = -\varrho\,\omega^2 u_i \quad , \tag{15}$$

where a_{ijkl} are the density–normalized elastic moduli (stiffness tensor).

For the plane wave $u_i = u_i(x_3)$ propagating along the x_3 axis in the 1-D anisotropic model $a_{ijk3} = a_{ijk3}(x_3)$ with constant density ϱ, elastodynamic equation (15) simplifies to

$$[a_{i3k3} u_{k,3}]_{,3} = -\omega^2 u_i \quad . \tag{16}$$

Equation (16) contains only 6 elastic moduli $a_{i3k3} = a_{i3k3}(x_3)$. Due to the separation of plane waves, the 15 remaining elastic moduli a_{ijKL} may be arbitrarily dependent on x_3. Moreover, the 6 elastic moduli a_{IJKL} may be arbitrarily dependent on all three spatial coordinates x_i.

4.1. Simplified twisted crystal model

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

$$\overline{a}_{K333} = 0 \quad . \tag{17}$$

Components u_K are then fully separated from u_3. We choose moduli $\overline{a}_{I3K3}$ in the form of

$$\begin{pmatrix} \overline{a}_{1313} & \overline{a}_{1323} & \overline{a}_{1333} \\ \overline{a}_{2313} & \overline{a}_{2323} & \overline{a}_{2333} \\ \overline{a}_{3313} & \overline{a}_{3323} & \overline{a}_{3333} \end{pmatrix} = \begin{pmatrix} v_S^2 B_{11} & v_S^2 B_{12} & 0 \\ v_S^2 B_{21} & v_S^2 B_{22} & 0 \\ 0 & 0 & v_P^2 \end{pmatrix} \tag{18}$$

with symmetric 2×2 matrix $\mathbf{B}$ defined by

$$\begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} = \begin{pmatrix} 1+\varepsilon\cos(2Kx_3) & \varepsilon\sin(2Kx_3) \\ \varepsilon\sin(2Kx_3) & 1-\varepsilon\cos(2Kx_3) \end{pmatrix} . \tag{19}$$

Elastodynamic equation (16) for the plane S wave in the simplified twisted crystal model then reads

$$[\mathbf{B}\mathbf{u}']' = -k_S^2 \mathbf{u} \quad , \tag{20}$$

where the prime denotes the derivative with respect to x_3 and

$$\mathbf{u} = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \quad , \quad k_S = \frac{\omega}{v_S} \quad . \tag{21}$$

Elastodynamic equation (16) for the plane P wave in the simplified twisted crystal model reads

$$v_P^2 u_3'' = -\omega^2 u_3 \quad . \tag{22}$$

4.2. Exact analytical solution in the simplified twisted crystal model

The 3×3 one–way propagator matrix $\overline{U}_{ij}$ of elastodynamic equation (16) in the simplified twisted crystal model may be decomposed into its S–wave part U_{ij}^S and P–wave part U_{ij}^P,

$$\overline{U}_{ij} = U_{ij}^S + U_{ij}^P \quad . \tag{23}$$

The S–wave part of the 3×3 one–way propagator matrix reads

$$\begin{pmatrix} U_{11}^S & U_{12}^S & U_{13}^S \\ U_{21}^S & U_{22}^S & U_{23}^S \\ U_{31}^S & U_{32}^S & U_{33}^S \end{pmatrix} = \begin{pmatrix} U_{11}^S & U_{12}^S & 0 \\ U_{21}^S & U_{22}^S & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad , \tag{24}$$

where U_{IJ}^S are the components of the 2×2 one–way S–wave propagator matrix $\mathbf{U}^S$ of elastodynamic equation (20) for the plane S wave. The P–wave part of the 3×3 one–way propagator matrix reads

$$\begin{pmatrix} U_{11}^P & U_{12}^P & U_{13}^P \\ U_{21}^P & U_{22}^P & U_{23}^P \\ U_{31}^P & U_{32}^P & U_{33}^P \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & U_{33}^P \end{pmatrix} \quad , \tag{25}$$

where U_{33}^P is the one–way P–wave propagator of elastodynamic equation (22) for the plane P wave.

The P–wave part of the one–way plane–wave propagator matrix is very simple,

$$U_{33}^P = \exp\left(\pm\frac{\mathrm{i}\omega}{v_S}x_3\right) \quad . \tag{26}$$

The anisotropic ray theory yields this exact solution.

In this paper, we shall study only the S–wave part of the one–way plane–wave propagator matrix. The 2×2 one–way propagator matrix $\mathbf{U}^S$ of elastodynamic equation (20) may be described by four frequency–dependent coefficients F_0, F_1, F_2 and F_3 (Klimeš 1999),

$$\begin{aligned} \mathbf{U}^S = {} & \exp(\mathrm{i}\,\mathrm{Re}(F_0)x_3)[\mathbf{1}\cos(Kx_3) - \mathrm{i}\boldsymbol{\sigma}_2\sin(Kx_3)] \\ & \times[\mathbf{1}\cos(\mathrm{Re}(\varphi)x_3) + \mathrm{i}\boldsymbol{\Phi}\sin(\mathrm{Re}(\varphi)x_3)] \\ & \times\exp(-\mathrm{Im}(F_0)x_3) \\ & \times[\mathbf{1}\cosh(\mathrm{Im}(\varphi)x_3) - \boldsymbol{\Phi}\sinh(\mathrm{Im}(\varphi)x_3)] \quad , \end{aligned} \tag{27}$$

where $\mathbf{1}$ is the 2×2 identity matrix,

$$\boldsymbol{\Phi} = [F_1 \mathrm{i}\boldsymbol{\sigma}_1 + F_2\boldsymbol{\sigma}_2 + F_3\boldsymbol{\sigma}_3]\varphi^{-1} \quad , \tag{28}$$

$$\varphi = \sqrt{F_3^2 + F_2^2 - F_1^2} \tag{29}$$

and

$$\boldsymbol{\sigma}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \boldsymbol{\sigma}_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad \boldsymbol{\sigma}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{30}$$

are the Pauli matrices. The exact one–way propagator matrix has coefficients

$$F_1 = \frac{\varepsilon K k_{\mathrm{S}}^2}{(k_{\mathrm{S}}^2 - K^2)\sqrt{1-\varepsilon^2}\left[\sqrt{1-\varepsilon^2} + \sqrt{1-\varepsilon^2\left(\frac{K^2}{k_{\mathrm{S}}^2-K^2}\right)^2}\,\right]}, \tag{31}$$

$$F_2 = K + \varepsilon F_1 \quad , \tag{32}$$

$$F_3 = F_0\left[-\varepsilon + \frac{F_1(1-\varepsilon^2)}{K}\right] \quad , \tag{33}$$

$$F_0^2 = \left[\frac{k_{\mathrm{S}}^2}{1-\varepsilon^2} + F_1^2\right]\left[1 + \frac{F_1^2(1-\varepsilon^2)}{K^2}\right]^{-1} \quad . \tag{34}$$

The sign of F_0 has to be determined according to the desired direction of the one–way plane–wave propagation and corresponds to the sign of the exponent in equation (26). 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. For resonant frequencies within domain

$$(1-|\varepsilon|)\,K^2 \le k_{\mathrm{S}}^2 \le (1+|\varepsilon|)\,K^2 \quad , \tag{35}$$

where F_0, F_1, F_2 and F_3 are complex–valued, we may determine F_1 from equation (31), arbitrarily selecting one of the complex–conjugate roots. After inserting into (31) 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 increase of cosh in equation (27). That is why $\mathrm{Im}(F_0)$ should be positive for propagation in the direction of the positive half–axis x_3 and negative for propagation in the direction of the negative half–axis x_3, independently of 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 (32), (33) and (27) are then used as they are.

4.3. Oblique twisted crystal model

In the simplified twisted crystal model, S–wave polarization vectors g_{iM} of the anisotropic ray theory are situated in the same plane as the reference S–wave polarization vectors, see equations (10) and (11). Then neither the quasi–isotropic projection of the Green tensor, nor the quasi–isotropic approximation of the Christoffel matrix have any impact on the results of the coupling ray theory. We thus modify the model in order to demonstrate these quasi–isotropic approximations.

In the *oblique twisted crystal model*, we select elastic moduli

$$a_{i3k3} = E_{im}E_{kn}\overline{a}_{m3n3} \quad , \tag{36}$$

where E_{im} are the components of a constant 3×3 unitary matrix. Elastic moduli $\overline{a}_{i3k3}$, corresponding to the simplified twisted crystal model, are given by (18).

Constant 3×3 unitary matrix E_{im}, describing rotation in 3-D space, has three independent components and may be expressed in terms of vector E_k. The direction of vector E_k specifies the axis of rotation, while the length

$$E = \sqrt{E_k E_k} \tag{37}$$

of vector E_k specifies the angle of rotation about the half–axis given by vector E_k. The generating matrix of the rotation is

$$I_{ij} = \varepsilon_{ijk}E_kE^{-1} \quad , \tag{38}$$

and the projection matrix onto the plane of rotation is

$$P_{ij} = \delta_{ij} - E_iE_jE^{-2} \quad . \tag{39}$$

The generating and projection matrices satisfy relation

$$I_{ij}I_{jk} = -P_{ik} \quad , \tag{40}$$

analogous to relation $\mathrm{ii}=-1$ for the imaginary unit. Unitary matrix E_{ij} is then the exponential function of $I_{ij}E$,

$$E_{ij} = P_{ij}\cos(E) + I_{ij}\sin(E) + \delta_{ij} - P_{ij} \quad , \tag{41}$$

i.e.

$$E_{ij} = \delta_{ij}\cos(E) + E_iE_jE^{-2}[1-\cos(E)] + \varepsilon_{ijk}E_kE^{-1}\sin(E) \quad . \tag{42}$$

4.4. Exact analytical solution in the oblique twisted crystal model

The exact 3×3 one–way propagator matrix U_{ij} of elastodynamic equation (16) in the oblique twisted crystal model is

$$U_{ij} = E_{im}E_{jn}\overline{U}_{mn} \quad , \tag{43}$$

where $\overline{U}_{mn}$ are the components of the 3×3 one–way propagator matrix (23) in the simplified twisted crystal model. Indeed, elastodynamic equation (16) with elastic moduli (36) and one–way propagator matrix (43) is equivalent to the same equation with elastic moduli $\overline{a}_{i3k3}$ and one–way propagator matrix $\overline{U}_{ij}$.

5. Numerical comparison with the exact solution

For the numerical comparison, we define the relative (with respect to the initial conditions) difference between one–way propagator matrices $\mathbf{U}^{\mathrm{S}}$ and $\mathbf{U}^{\mathrm{S}}_0$ as

$$\Delta = \sqrt{\tfrac{1}{2}\mathrm{tr}\Big([\mathbf{U}^{\mathrm{S}}_0 - \mathbf{U}^{\mathrm{S}}]^{+}[\mathbf{U}^{\mathrm{S}}_0 - \mathbf{U}^{\mathrm{S}}]\Big)} \quad , \qquad (44)$$

where $\mathbf{U}^{+}$ denotes the matrix Hermitian adjoint to $\mathbf{U}$.

5.1. Model for the numerical comparison

We use the simplified twisted crystal model designed by Vavryčuk (1999). The relation to Vavryčuk's (1999) notation is

$$\varepsilon = \frac{-\gamma\sin^2(\theta)}{1+\gamma\sin^2(\theta)} \ , \quad v_{\mathrm{S}}^2 = a_{44}[1+\gamma\sin^2(\theta)] \ , \quad \varphi = Kx_3 \ . \qquad (45)$$

The selected numerical values in (45) are

$$\gamma\sin^2(\theta) = 0.15\times 0.75 = 0.1125 \quad , \qquad (46)$$

$$v_{\mathrm{S}}^2 = 6.0\,\mathrm{km}^2\mathrm{s}^{-2}\times[1{+}0.15{\times}0.75] = 6.675\,\mathrm{km}^2\mathrm{s}^{-2} \ . \quad (47)$$

The relative difference between the faster and slower S–wave velocities is thus about 10%. Parameter K describing the rotation of the crystal axes along the x_3 axis has the value

$$K = 0.032\,\mathrm{km}^{-1} \quad . \qquad (48)$$

The source–receiver distance corresponds to the crystal axes rotated by π radians,

$$x_3 = \frac{\pi}{K} \doteq 98.17477\,\mathrm{km} \quad . \qquad (49)$$

The *resonant frequency*, see (35), is

$$F = \left|\frac{v_{\mathrm{S}}K}{2\pi}\right| \doteq 0.0132\ \mathrm{Hz} \qquad (50)$$

and the *coupling frequency* (Klimeš 1999, section 4.1) is

$$\left|\frac{2}{\varepsilon}\right| F \doteq 0.260\,\mathrm{Hz} \quad . \qquad (51)$$

The squared P wave velocity in (18) is

$$v_{\mathrm{P}}^2 = 3v_{\mathrm{S}}^2 \quad . \qquad (52)$$

The rotation vector for the oblique twisted crystal model is

$$E_1 = 0.10 \quad , \qquad E_2 = 0 \quad , \qquad E_3 = 0 \quad . \qquad (53)$$

The rotation angle (0.10 radians) thus roughly corresponds to the strength of the anisotropy (10% difference between the S–wave velocities).

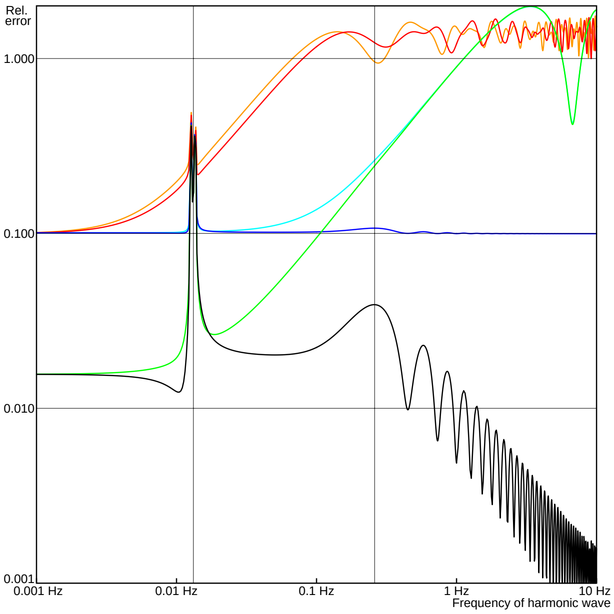

Figure 1: The relative differences of various approximations of the coupling ray theory (Coates & Chapman 1990) from the exact solution in the oblique twisted crystal model. **Black**: No quasi–isotropic approximation. **Blue**: quasi–isotropic projection of the Green tensor. **Red**: quasi–isotropic approximation of the Christoffel matrix. It includes the quasi–isotropic projection of the Green tensor. **Green**: quasi–isotropic approximation of travel times. **Cyan**: quasi–isotropic projection of the Green tensor combined with the quasi–isotropic approximation of travel times. **Yellow**: quasi–isotropic approximation of the Christoffel matrix combined with the quasi–isotropic approximation of travel times. The two vertical lines denote the resonant and coupling frequencies (50), (51). The relative error of 200% occurs, e.g., for an opposite polarization or an opposite phase.

5.2. Numerical results

The approximate 3×3 one–way propagator matrices of the plane S wave, corresponding to the coupling ray theory and its quasi–isotropic approximations, have been numerically calculated by means of the Fortran 77 package CRT (Bucha, Bulant & Klimeš 2001; Bucha & Bulant 2002). The relative differences of the coupling ray theory, its quasi–isotropic approximations and their combinations from the exact analytical solution are plotted on a log–log scale in Figure 1.

The coupling ray theory of Coates & Chapman (1990) yields excellent results in this model, except for the resonant frequencies, which are far outside the validity regions of the ray theories. On the other hand, the quasi–isotropic approximations applied here generate unnecessary additional errors and should be avoided when using the coupling ray theory.

Comparison of quasi–isotropic approximations

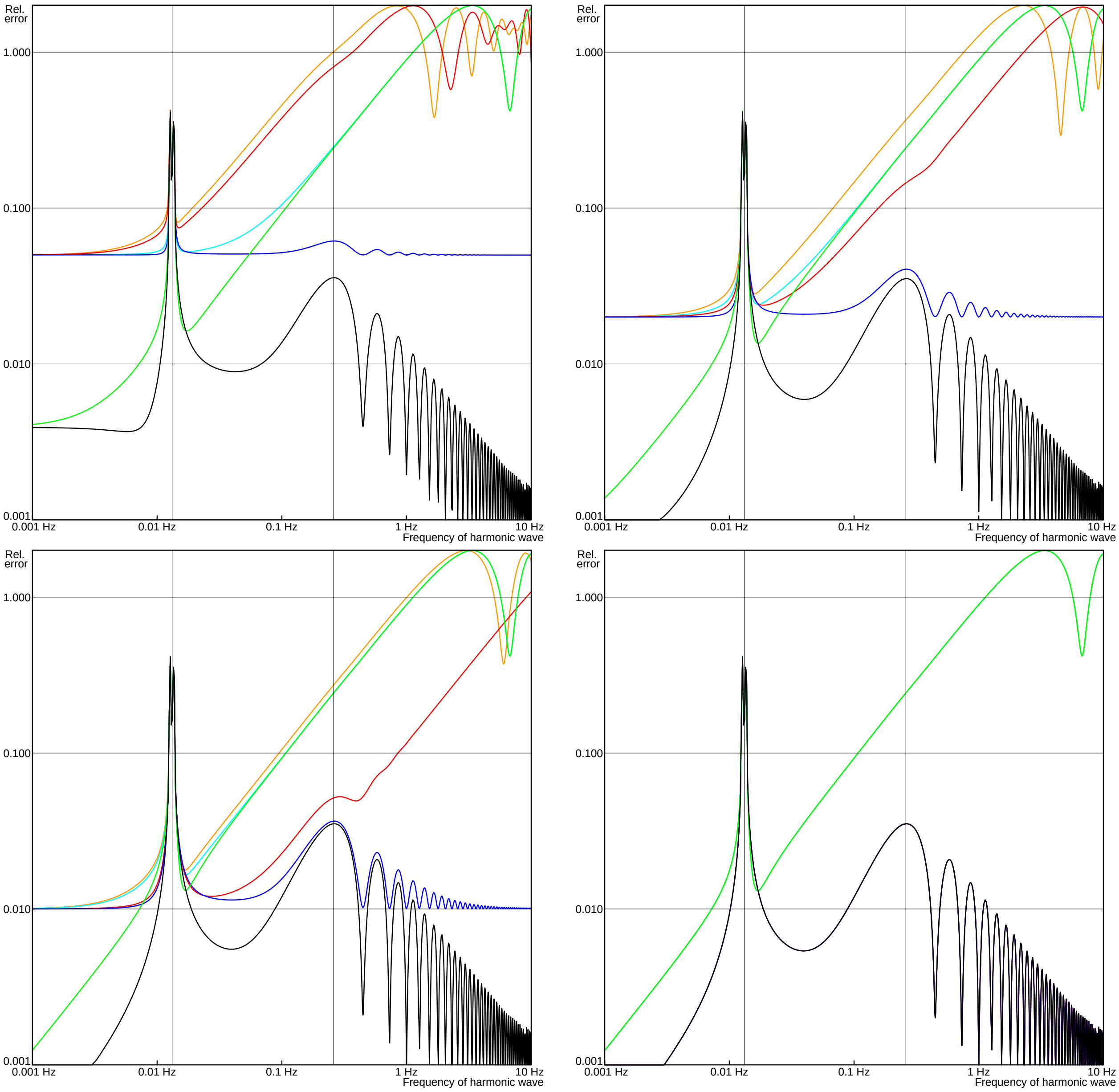

Figure 2: Analogous to Figure 1, but for different oblique twisted crystal models obtained by modifying rotation angle E_1 in data (53). Whereas the model for Figure 1 is given by $E_1 = 0.10$, the differences plotted here correspond to $E_1 = 0.05$ (top left), $E_1 = 0.02$ (top right), $E_1 = 0.01$ (bottom left) and $E_1 = 0.00$ (bottom right). Only the quasi–isotropic approximation of travel times can be demonstrated in the simplified twisted crystal model ($E_1 = 0.00$).

The error of the *quasi–isotropic projection of the Green tensor* (Section 3.2) can be estimated simply, is frequency–independent, and corresponds to the rotation angle in this model, see (53). This frequency–independent error may be expected to be proportional to the degree of anisotropy in generally anisotropic models on average.

The *quasi–isotropic approximation of the Christoffel matrix* (Section 3.3) generates the travel–time error. The wavefield error is then proportional to the frequency. The error is proportional to the square of the angle between the correct S–wave polarization plane and the reference S–wave polarization plane, in this case to the square of the rotation angle. The wavefield error, proportional to the frequency, may thus be expected to be proportional to the square of the degree of anisotropy in generally anisotropic models on average. The quasi–isotropic approximation of the Christoffel matrix seems to be the worst quasi–isotropic approximation.

The *quasi–isotropic perturbation of travel times* (Section 3.4) generates the travel–time error. The wavefield error is then proportional to the frequency. The error is proportional to the square of the difference between the anisotropic model and the reference isotropic model. The quasi–isotropic approximation of travel time thus depends on the reference velocity. The wavefield error, proportional to the frequency, may be expected to be proportional to the square of the degree of anisotropy in generally anisotropic models on average.

The *common ray approximations* (Section 3.1) have no impact on the coupling ray theory in this model. The inaccuracy due to the common ray approximations have been studied by (Klimeš & Bulant 2002).

The behaviour of the errors due to the quasi–isotropic approximations of the coupling ray theory when decreasing rotation angle E_1 in (53) towards the simplified twisted crystal model, used for comparison with the isotropic ray theory and anisotropic ray theory by Bulant, Klimeš & Pšenčík (1999; 2000), is demonstrated in Figure 2.

6. Conclusions

When using the coupling ray theory, the quasi–isotropic projection of the Green tensor, the quasi–isotropic approximation of the Christoffel matrix, and the quasi–isotropic approximation of travel times should be avoided.

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