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Group velocity along general direction in a general anisotropic medium

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Abstract

An attempt has been made to study the three-dimensional wave propagation in a general anisotropic medium. A procedure is presented to solve the inverse problem of finding the group velocity in a given direction of ray travel, without using numerical differentiation. The phase direction, derived from the given ray direction, is used to calculate phase velocity. Then, such a phase velocity and phase direction are used to calculate group velocity. Analytical expressions are derived for the directional derivatives of phase velocity which are used to calculate group velocity. Algebraic expressions are derived in a computation convenient manner. Newton's method (without numerical differentiation) for solving a system of two non-linear simultaneous equations is the only numerical method used. The ray directions along which a wave (or energy) can travel with more than one group velocity may be difficult to treat. Variations of phase velocity and group velocity with ray direction in three dimensions are plotted for a hypothetical model of general anisotropic medium. © 2002 Elsevier Science Ltd. All rights reserved.

Keywords: 3-D anisotropy; Ray direction; Group velocity; Phase velocity; Newton's method

1. Introduction

Elastic anisotropy is a widespread observation in the areas of economic and scientific interest (Crampin, 1987). The preferential alignments in the Earth ranging from mineral orientations, grains, or microcracks to regional fractures result in the seismic anisotropy. In exploration studies (McCollum and Snell, 1944; White and Sengush, 1953; Gretener, 1961; Van der Stoep, 1966; Helbig, 1984; Leary and Henyey, 1985; Kerner et al., 1989; Corrigan, 1989; and many others) velocity anisotropy measured from travel times have suggested the presence of significant anisotropy in sedimentary basins. Similar results for earth's crust and mantle have been obtained in earthquake studies (Gupta, 1973; Crampin, 1985; Thomsen, 1986; Rai and Hanson, 1988; and many others). Crampin (1994) reviewed various studies related to the observation of shear-wave splitting and confirmed that shear-wave splitting was present in almost all the rocks in the uppermost half of the crust.

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The study of anisotropic elasticity is also important for understanding the mechanical behaviour of composite materials (Barga, 1990; Fan and Hwu, 1998). The complex variable formulation derived by Stroh (1958) and Lekhnitskii (1968) for anisotropic elasticity has been proved to be a powerful mathematical tool to obtain exact closed form solutions. In the last two decades, the applications of acoustic microscopy and fibre-reinforced composites have initiated the interest in the wave propagation in layered anisotropic media (Barga, 1990). Physics of granular media (Mehta, 1991; Nagel, 1992; Norris and Johnson, 1997) represents an active area of current research activity. Sound speeds in such media depend upon the stress-induced anisotropy existing there. Surface wave propagation in anisotropic media has enormous applications in the non-destructive evaluation of materials (Buden and Datta, 1990; Chai and Wu, 1994; Wu and Wu, 2000).

Synge's (1957) was one of the early detailed study of elastic waves in anisotropic media. Musgrave (1970) presented a concise, elegant treatment of anisotropy with symmetry properties, based on algebraic solutions. Since then there have been a large number of studies discussing wave propagation in anisotropic media. Almost all of the analytical studies, among these, restricted the anisotropic propagation to a fixed (symmetry or arbitrary) plane and hence solved a 2-D problem. Energy propagation in anisotropic media is, in fact, a three-dimensional phenomenon. Study of propagation in one plane (particularly a symmetry plane) may give no indication of its behaviour in neighbouring directions, particularly near singularities (Crampin and Yedlin, 1981). Symmetry planes are a special case of general anisotropy and the intersection of a wave surface with a symmetry plane takes a particularly simple form. This provides a convenient escape from complex relations among phase velocity and group velocity, in three dimensions. It is usually impossible to extrapolate from such a special case of anisotropy to the general one. It may be the reason that the algebraic analysis of group velocity and, hence, polarisation are conveniently avoided for a general direction of anisotropic propagation (Crampin, 1981; Dellinger, 1991).

In an anisotropic medium energy travels with group velocity along a ray at an angle to the propagation direction. It is the group velocity that is measured in observations of arrival times rather than the phase velocity that appears in equation of motion and most other analytical expressions (Crampin, 1989). The group velocity is also required for the interpretation of both real and synthetic data. The present work suggests an analytical method to analyse the group velocity along a general ray direction in a general anisotropic medium.

2. Definition of the problem

Mathematically, the group velocity for a wave is derived (numerically or analytically) from its phase velocity. Phase velocities of all the possible waves, in a medium with a given set of elastic parameters, are calculated from an eigenvalue problem for a given direction of phase propagation. In an unbounded isotropic medium body-wave phase velocity and group velocity are same and equal in all directions. In an anisotropic medium, directions of phase and group velocity surfaces are same, only, along symmetry axes and planes. So, for spherical waves, from a point source, in a general anisotropic medium, these velocities are different both in magnitude and direction. The literature available for anisotropic propagation allows to calculate the phase velocities from the given elastic constants and density of the medium. Phase velocity of each wave varies with its direction of propagation. Group velocity components for each wave are derived from the differentiation of its phase velocity (Ben-Menahem and Sena, 1990). Ray direction of a wave is determined from the group velocity components. That means, ray direction is decided by the phase velocity and phase direction and cannot be controlled directly. Here, below, are mentioned the problems of two different kinds which are directly related to the above discussion.

Suppose, we are given a general anisotropic medium defined by a particular set of elastic parameters in a given (say, Cartesian) co-ordinate system. Then, for the study of wave travel (directly or after scattering

from inhomogeneities) from source to receiver, we can know or fix only the ray direction of a wave. To find the magnitude of the group velocity along this particular ray direction will be the main problem needed to be solved.

In an anisotropic medium, the observational seismology can, at the most, provide only the group velocity of different waves in different directions. To explain the elastic properties of such a medium, these directional group velocities are required to be linked with the elastic constants. Mathematically, the elastic constants of a medium are linked directly, only, to the phase velocities of different waves, varying with their propagation directions. Hence, to study the effects of group velocity changes on the elastic constants, it will be required to calculate the phase direction (and then phase velocity) from the ray direction and group velocity of each wave.

In the above mentioned problems, the common and main part is to calculate the phase direction of a wave for a given ray direction in three dimensions. To find phase velocity along, thus found, phase direction is a simple algebra. Relations are available to calculate the group velocity, when the phase velocity and phase direction are known.

In the present study, the procedure to find group velocity along a given ray direction is divided into four steps, which are as follows:

- (i) Solve the eigenvalue problem to calculate phase velocity as a function of phase direction, in a general anisotropic medium.
- (ii) Derive the group velocity from phase velocity in three dimensions.
- (iii) For a given (arbitrary) direction of ray in three dimensions, find the corresponding direction of phase propagation.
- (iv) Use the above found phase direction to calculate phase velocity and then group velocity.

3. Phase velocity

Consider a general anisotropic medium represented by the elastic constants in two-suffix notation, c_{ij} . Define a row matrix $N = (n_x, n_y, n_z)$, where n_j denotes the components of a unit vector normal to wave surface and, hence, representing the direction of phase propagation. In an anisotropic medium there are generally three body-waves propagating with velocities which vary with the direction of phase propagation. Their polarizations are orthogonal and fixed for the particular direction of phase propagation. The waves are called quasi-waves because polarizations may not be along the dynamic axes. Further, define (Fryer and Frazer, 1987):

$$\alpha = NAN', \quad \beta = NBN', \quad \gamma = NCN', \quad \delta = NDN', \quad \eta = NEN', \quad \zeta = NFN', \quad (1)$$

where N' denotes the transpose of row matrix N ; A, B, C, D, E and F are square matrices of order 3. For general anisotropy, these are defined as follows:

$$\begin{aligned} A &= \{a_{11}, a_{16}, a_{15}; a_{16}, a_{66}, a_{56}; a_{15}, a_{56}, a_{55}\}, \\ B &= \{a_{66}, a_{26}, a_{46}; a_{26}, a_{22}, a_{24}; a_{46}, a_{24}, a_{44}\}, \\ C &= \{a_{55}, a_{45}, a_{35}; a_{45}, a_{44}, a_{34}; a_{35}, a_{34}, a_{33}\}, \\ D &= \{a_{16}, a_{12}, a_{14}; a_{66}, a_{26}, a_{46}; a_{56}, a_{25}, a_{45}\}, \\ E &= \{a_{15}, a_{14}, a_{13}; a_{56}, a_{46}, a_{36}; a_{55}, a_{45}, a_{35}\}, \\ F &= \{a_{56}, a_{46}, a_{36}; a_{25}, a_{24}, a_{23}; a_{45}, a_{44}, a_{34}\}, \end{aligned} \quad (2)$$

where $a_{ij} = c_{ij}/\rho$. ρ is the density of the medium.

In an anisotropic medium, the eigenvalue problem is represented by the following cubic equation in V^2 :

$$V^6 + 3aV^4 + 3bV^2 + c = 0, \quad (3)$$

where

$$\begin{aligned} a &= -\frac{1}{3}(\alpha + \beta + \gamma), \\ b &= \frac{1}{3}(\alpha\beta + \alpha\gamma + \beta\gamma - \delta^2 - \eta^2 - \zeta^2), \\ c &= \alpha\zeta^2 + \gamma\delta^2 + \beta\eta^2 - \alpha\beta\gamma - 2\eta\delta\zeta. \end{aligned} \quad (4)$$

$\alpha, \beta, \gamma, \delta, \eta$ and ζ are as defined in relations (1) and (2).

The real roots of Eq. (3) are written as

$$V_m^2 = 2\sqrt{-H} \cos \left\{ \frac{\psi - 2\pi(m-1)}{3} \right\} - a \quad (m = 1, 2, 3), \quad (5)$$

where $\psi = \tan^{-1}(\Delta/G)$, $\Delta = \sqrt{-(G^2 + H^3)}$; $H = b - a^2$; and $G = (3ab - c - 2a^3)/2$. V_m ($m = 1, 2, 3$) defines the magnitudes of phase velocities of three quasi-waves in the direction of unit vector N . These waves, represented by $m = 1, 2$ and 3 , are called the qP, qS1 and qS2 waves respectively, where qS1 is the faster of the two split shear-waves (Crampin, 1981).

4. Group velocity

In a spherical co-ordinate system (r, θ, ϕ) , let $V_m(\theta, \phi)$ define the phase velocity of wave m in the direction of $N\{ = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta) \}$ in Cartesian co-ordinate system. The group velocity of this wave, following Ben-Menahem and Sena (1990), is given by

$$\mathbf{w}^{(m)} = V_m \hat{\mathbf{e}}_r + \frac{\partial V_m}{\partial \theta} \hat{\mathbf{e}}_\theta + \frac{1}{\sin \theta} \frac{\partial V_m}{\partial \phi} \hat{\mathbf{e}}_\phi. \quad (6)$$

Ray direction or the direction of energy flux is determined from the components of group velocity, which are expressed as follows:

$$\begin{aligned} w_x/V_m &= \cos \phi \sin \theta + \cos \phi \cos \theta T_\theta - \frac{\sin \phi}{\sin \theta} T_\phi, \\ w_y/V_m &= \sin \phi \sin \theta + \sin \phi \cos \theta T_\theta + \frac{\cos \phi}{\sin \theta} T_\phi, \\ w_z/V_m &= \cos \theta - \sin \theta T_\theta. \end{aligned} \quad (7)$$

The magnitude of the group velocity is

$$w_m = V_m \sqrt{1 + T_\theta^2 + \frac{1}{\sin^2 \theta} T_\phi^2}, \quad (8)$$

and direction (θ_g, ϕ_g) , in spherical co-ordinates, is given by

$$\theta_g = \tan^{-1} \left(\frac{\sqrt{w_x^2 + w_y^2}}{w_z} \right), \quad \phi_g = \tan^{-1} \left(\frac{w_y}{w_x} \right). \quad (9)$$

T_θ and T_ϕ in (7) and (8) are defined by

$$T_j = \frac{1}{V_m} (V_m)_j = \frac{1}{2V_m^2} (V_m^2)_j \quad (j = \theta, \phi). \quad (10)$$

5. Phase direction from ray direction

In the forward problem, group velocity of a wave m ($= 1$ or 2 or 3) is calculated from its phase velocity V_m along a given phase direction (θ, ϕ) , using relations (7)–(9). In this study, we need to deal with an inverse problem. The purpose is to find phase direction, i.e. (θ, ϕ) for a given ray direction, in the co-ordinate system fixed by the choice of elastic constants of the anisotropic medium. This is possible only after reducing the relations (7) to a system of two non-linear simultaneous equations in θ and ϕ , for any given values of θ_g and ϕ_g . The equations are obtained from (7) by expressing the group velocity components w_j ($j = x, y, z$) in terms of θ_g and ϕ_g and then taking the ratios of these components to eliminate V_m and w_m . Such a system of equations is given by

$$\sin \phi_g f_1 - \cos \phi_g f_2 = 0 \quad \text{and} \quad \sin \theta_g f_3 - \cos \theta_g \sqrt{f_1^2 + f_2^2} = 0, \quad (11)$$

where

$$f_1 = \cos \phi \sin \theta + \cos \phi \cos \theta T_\theta - \frac{\sin \phi}{\sin \theta} T_\phi,$$

$$f_2 = \sin \phi \sin \theta + \sin \phi \cos \theta T_\theta + \frac{\cos \phi}{\sin \theta} T_\phi \quad \text{and}$$

$$f_3 = \cos \theta - \sin \theta T_\theta.$$

Newton's method for two variables is applied to solve this system numerically for θ and ϕ . This method will require the evaluation of partial derivatives of functions f_j , for $j = 1, 2, 3$, with respect to θ and ϕ . To avoid numerical differentiation, analytical expressions for partial derivatives are presented in Appendix A.

6. Discussion

The phase direction, phase velocity and group velocity can be calculated from a given ray direction but with following exceptions. Newton's method for a system of non-linear simultaneous equations may fail to deliver when a local minimum occurs in the root search region. This can be avoided by the slight shift of initial root. Singularities are the phase directions along which the phase velocities of qS1 wave and qS2 wave approach each other. Mathematically, it is the value of (θ, ϕ) for which the Δ (as defined in Section 3) vanishes. Near a singularity the directional derivatives of phase velocity change rapidly and the direction of local extremum represents the singularity. Therefore, existence of local extremum at the singularity fails the Newton's method. Singularities can be numerically inspected from $\Delta = 0$, for a given model of anisotropic medium.

From relations (7), it is clear that the group velocity for a wave can be the same for more than one phase directions. Even there may be different group velocities of a wave in the same ray direction. In other words, it is possible for energy (representing a particular quasi-wave) to travel with more than one group velocity in a given ray direction, that is, triplications or cusps in the wavefronts of quasi-shear waves are possible (Dellinger, 1991). This indicates that correspondence between phase direction and group direction is not one to one. So, for an assumed ray direction, there may be more than one phase direction possible and these

may be quite near to each other. While solving numerically, using Newton's method, it will be difficult to find the number and values of all such different phase directions which lead to the same ray direction. However, solving the forward problem to calculate the phase velocity, group velocity and ray direction for a given phase direction, the ray directions (and their number) of triplications can be checked by inspection.

7. Numerical computation

Analysis of phase velocity, group velocity and their difference for a real crystal is possible even by solving forward problem. Hence, the purpose of the numerical computation is restricted to check the suggested process of finding the phase direction from a given ray direction. Thus obtained phase direction is, then, used to compute the group velocity of each quasi-wave (qP , $qS1$, $qS2$) along the given direction of its ray

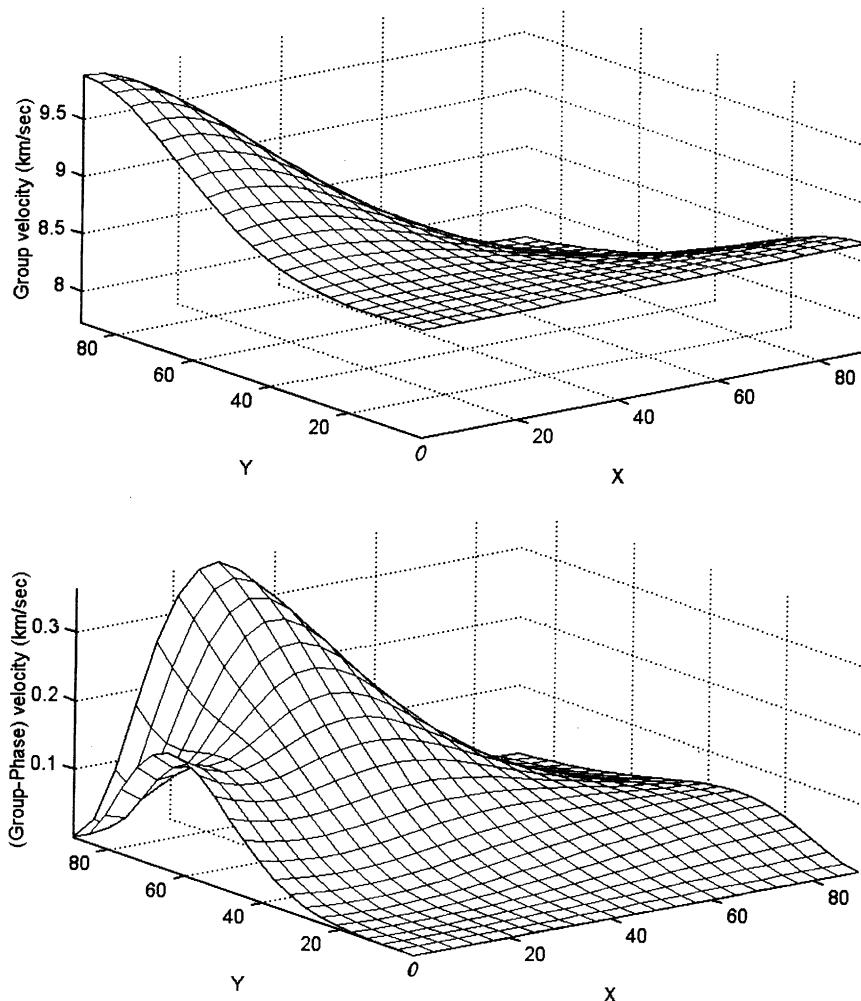


Fig. 1. qP wave: variations of the group and phase velocities with ray direction ($=(X, Y)$ deg.).

travel in three dimensions. So a hypothetical model of an anisotropic elastic medium is considered by altering the elastic constants, given by Verma (1960), for the olivine. These are as follows:

$$c_{11} = 324.0 \times 10^9 \text{ Nm}^{-2}, \quad c_{12} = 59.0 \times 10^9 \text{ Nm}^{-2}, \quad c_{13} = 79.0 \times 10^9 \text{ Nm}^{-2},$$

$$c_{22} = 198.0 \times 10^9 \text{ Nm}^{-2}, \quad c_{23} = 78.0 \times 10^9 \text{ Nm}^{-2}, \quad c_{33} = 198.0 \times 10^9 \text{ Nm}^{-2},$$

$$c_{44} = 66.7 \times 10^9 \text{ Nm}^{-2}, \quad c_{55} = 81.0 \times 10^9 \text{ Nm}^{-2}, \quad c_{66} = 79.3 \times 10^9 \text{ Nm}^{-2}.$$

Density ρ is 3.324 gcm^{-3} . The symbolic values assumed for some other elastic constants are $\{c_{14}, c_{15}, c_{16}, c_{24}, c_{25}, c_{26}\} = \{1, 2, 3, 4, 5, 6\} \times 10^9 \text{ Nm}^{-2}$.

Using the above numerical values, the variations of group velocity, and its difference from phase velocity, with ray direction are presented in Figs. 1–3. Both the polar angle and azimuth for the ray direction

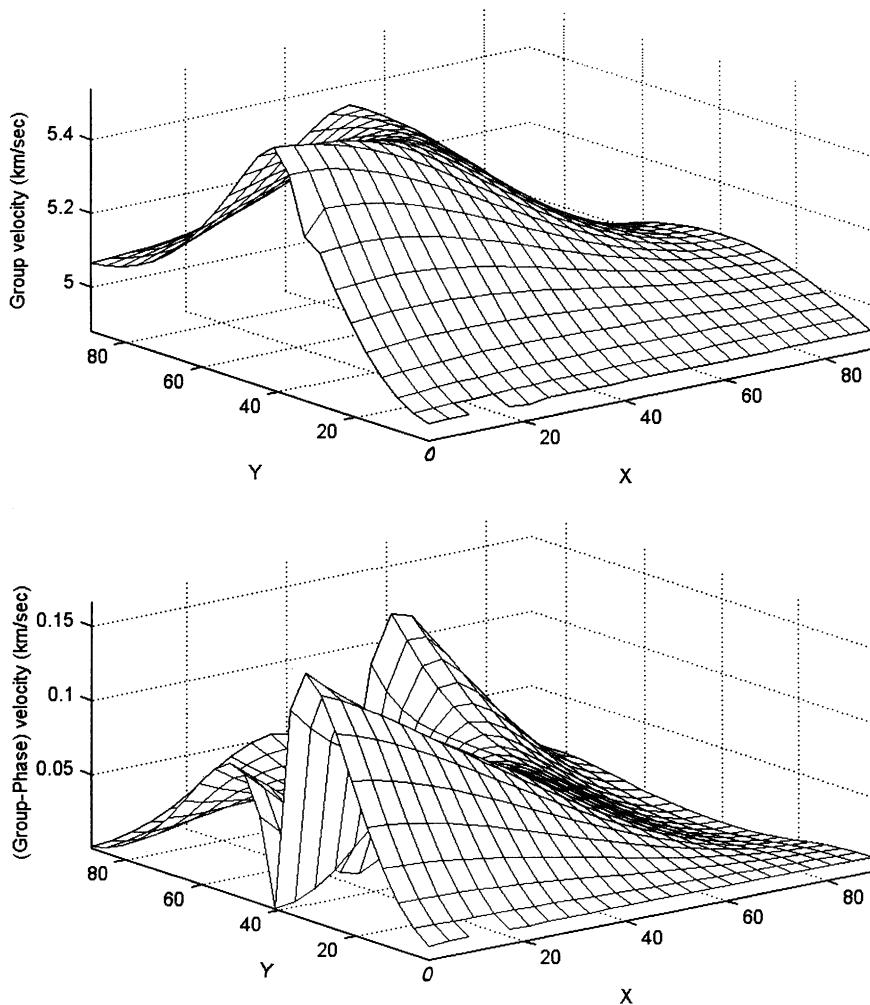


Fig. 2. qS1 wave: variations of the group and phase velocities with ray direction ($= (X, Y)$ deg.).

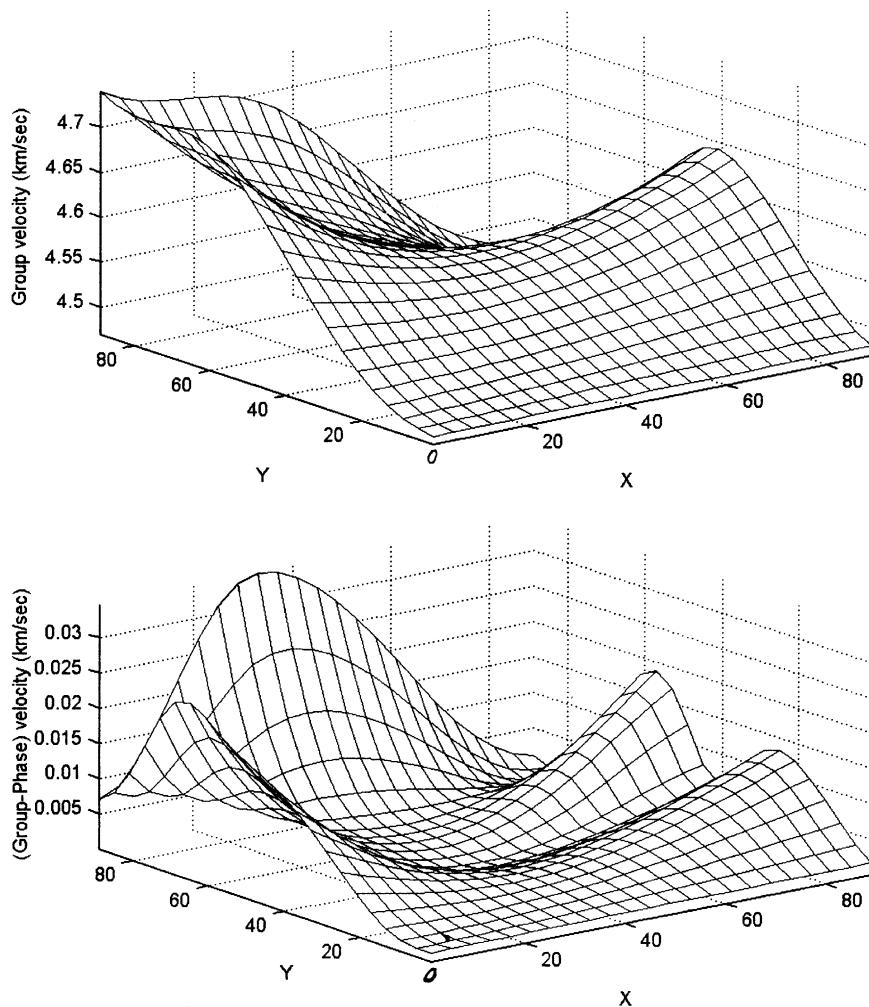


Fig. 3. qS2 wave: variations of the group and phase velocities with ray direction ($=(X, Y)$ deg.).

vary from 0° to 90° . To check the accuracy of various expressions used, the phase velocity and group velocity were calculated for the various symmetry planes of orthorhombic orthopyroxine (elastic constants from Kumazawa, 1969) and were verified with those obtained in Crampin (1981).

This work can, further, be used to study the polarisation and 3-D scattering in a general anisotropic medium. The researchers in this field would prefer to use the analytical derivatives presented in Appendix A.

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The author is grateful to Prof. Stuart Crampin, Department of Geology & Geophysics, University of Edinburgh (UK) for his encouraging cooperation.

Appendix A

For a given ray direction (θ_g, ϕ_g) , we define

$$f(\theta, \phi) = \sin \phi_g f_1 - \cos \phi_g f_2 \quad \text{and} \quad g(\theta, \phi) = \sin \theta_g f_3 - \cos \theta_g \sqrt{f_1^2 + f_2^2},$$

so that the system of two non-linear simultaneous equations is written as

$$f(\theta, \phi) = 0 \quad \text{and} \quad g(\theta, \phi) = 0.$$

Partial derivatives of functions $f(\theta, \phi)$ and $g(\theta, \phi)$ are expressed as

$$f_j = \sin \phi_g f_{1,j} - \cos \phi_g f_{2,j} \quad (j = \theta, \phi) \quad \text{and}$$

$$g_{,j} = \sin \theta_g f_{3,j} - \cos \theta_g (f_1 f_{1,j} + f_2 f_{2,j}) / \sqrt{f_1^2 + f_2^2} \quad (j = \theta, \phi),$$

where

$$f_{1,\theta} = \cos \phi \cos \theta (1 + T_{\theta,\theta}) - \cos \phi \sin \theta T_\theta - \sin \phi (T_{\phi,\theta} - \cos \theta T_\phi / \sin \theta) / \sin \theta,$$

$$f_{1,\phi} = -\sin \phi \sin \theta + \cos \phi \cos \theta T_{\theta,\phi} - \sin \phi \cos \theta T_\theta - (\sin \phi T_{\phi,\phi} + \cos \phi T_\phi) / \sin \theta,$$

$$f_{2,\theta} = \sin \phi \cos \theta (1 + T_{\theta,\theta}) - \sin \phi \sin \theta T_\theta + \cos \phi (T_{\phi,\theta} - \cos \theta T_\phi / \sin \theta) / \sin \theta,$$

$$f_{2,\phi} = \cos \phi \sin \theta + \sin \phi \cos \theta T_{\theta,\phi} + \cos \phi \cos \theta T_\theta + (\cos \phi T_{\phi,\phi} - \sin \phi T_\phi) / \sin \theta,$$

$$f_{3,\theta} = -\sin \theta (1 + T_{\theta,\theta}) - \cos \theta T_\theta \quad \text{and} \quad f_{3,\phi} = -\sin \theta T_{\theta,\phi}.$$

Derivatives of T_j are defined as

$$T_{j,k} = \frac{1}{2V_m^2} (V_m^2)_{jk} - 2T_j T_k \quad (j, k = \theta, \phi).$$

To calculate T_j and $T_{j,k}$ for each wave (for $m = 1, 2, 3$), the following relations will be required:

If we replace

$$h = \sqrt{-H}, \quad C_\psi = \cos \left\{ \frac{\psi - 2\pi(m-1)}{3} \right\} \quad \text{and} \quad S_\psi = \sin \left\{ \frac{\psi - 2\pi(m-1)}{3} \right\}$$

in (5), then for $j, k = \theta$ and ϕ

$$V_m^2 = 2hC_\psi - a,$$

$$(V_m^2)_{,j} = 2h_{,j}C_\psi - \frac{2}{3}h\psi_{,j}S_\psi - a_{,j},$$

$$(V_m^2)_{,jk} = (2h_{,jk} - \frac{2}{3}h\psi_{,j}\psi_{,k})C_\psi - \frac{2}{3}\{h\psi_{,jk} + (h_{,j}\psi_{,k} + \psi_{,j}h_{,k})\}S_\psi - a_{,jk},$$

where

$$h_{,j} = \frac{h}{2} \frac{H_j}{H}, \quad \psi_{,j} = -\frac{G}{A} \left(\frac{G_j}{G} - \frac{3}{2} \frac{H_j}{H} \right), \quad h_{,jk} = \frac{h}{2} \left(\frac{H_{jk}}{H} - \frac{1}{2} \frac{H_j}{H} \frac{H_{,k}}{H} \right),$$

$$\psi_{,jk} = \frac{G}{A} \left\{ -\frac{G_{jk}}{G} + \frac{3}{2} \frac{H_{jk}}{H} - \frac{G_j}{A} \frac{G_{,k}}{A} - \frac{3}{2} \frac{H^3}{A^2} \left(\frac{G_j}{G} \frac{H_{,k}}{H} + \frac{H_j}{H} \frac{G_{,k}}{G} \right) + \frac{3}{2} \frac{H_j H_{,k}}{H^2} \left(-1 + \frac{3}{2} \frac{H^3}{A^2} \right) \right\}$$

$$\begin{aligned}
H_j &= b_{,j} - 2aa_{,j}, & G_j &= 1.5(ab_{,j} + ba_{,j}) - .5c_{,j} - 3a^2a_{,j}, \\
H_{jk} &= b_{,jk} - 2(aa_{,jk} + a_{,j}a_{,k}) \quad (j, k = \theta, \phi), \\
G_{jk} &= 1.5(ab_{,jk} + ba_{,jk} + a_{,j}b_{,k} + b_{,j}a_{,k}) - .5c_{,jk} - 3a^2a_{,jk} - 6aa_{,j}a_{,k}, \\
a_{,j} &= -(\alpha_{,j} + \beta_{,j} + \gamma_{,j})/3, \\
a_{,jk} &= -(\alpha_{,jk} + \beta_{,jk} + \gamma_{,jk})/3, \\
b_{,j} &= \{\alpha(\beta_{,j} + \gamma_{,j}) + \alpha_{,j}(\beta + \gamma) + \beta_{,j}\gamma + \beta\gamma_{,j} - 2(\delta\delta_{,j} + \eta\eta_{,j} + \zeta\zeta_{,j})\}/3, \\
b_{,jk} &= \{\alpha(\beta_{,jk} + \gamma_{,jk}) + \alpha_{,jk}(\beta + \gamma) + \alpha_{,j}(\beta_{,k} + \gamma_{,k}) + \alpha_{,k}(\beta_{,j} + \gamma_{,j}) + \beta_{,jk}\gamma + \beta\gamma_{,jk} + \beta_{,j}\gamma_{,k} + \beta_{,k}\gamma_{,j} \\
&\quad - 2(\delta\delta_{,jk} + \eta\eta_{,jk} + \zeta\zeta_{,jk} + \delta_{,j}\delta_{,k} + \eta_{,j}\eta_{,k} + \zeta_{,j}\zeta_{,k})\}/3, \\
c_{,j} &= \zeta(\zeta\alpha_{,j} + 2\alpha\zeta_{,j}) + \eta(\eta\beta_{,j} + 2\beta\eta_{,j}) + \delta(\delta\gamma_{,j} + 2\gamma\delta_{,j}) - \alpha(\beta\gamma_{,j} + \gamma\beta_{,j}) - \beta\gamma\alpha_{,j} - 2\delta(\eta\zeta_{,j} + \zeta\eta_{,j}) - 2\eta\zeta\delta_{,j}, \\
c_{,jk} &= 2\alpha(\zeta\zeta_{,jk} + \zeta_{,j}\zeta_{,k}) + 2\zeta(\alpha_{,j}\zeta_{,k} + \alpha_{,k}\zeta_{,j}) + \zeta^2\alpha_{,jk} + 2\beta(\eta\eta_{,jk} + \eta_{,j}\eta_{,k}) + 2\eta(\beta_{,j}\eta_{,k} + \beta_{,k}\eta_{,j}) + \eta^2\beta_{,jk} \\
&\quad + 2\gamma(\delta\delta_{,jk} + \delta_{,j}\delta_{,k}) + 2\delta(\gamma_{,j}\delta_{,k} + \gamma_{,k}\delta_{,j}) + \delta^2\gamma_{,jk} - \{\alpha\beta\gamma_{,jk} + \alpha\beta_{,jk}\gamma + \alpha_{,jk}\beta\gamma + \alpha(\beta_{,j}\gamma_{,k} + \beta_{,k}\gamma_{,j}) \\
&\quad + \beta(\alpha_{,j}\gamma_{,k} + \alpha_{,k}\gamma_{,j}) + \gamma(\beta_{,j}\alpha_{,k} + \beta_{,k}\alpha_{,j})\} - 2\{\delta\eta\zeta_{,jk} + \delta\eta_{,jk}\zeta + \delta_{,jk}\eta\zeta + \delta(\eta_{,j}\zeta_{,k} + \eta_{,k}\zeta_{,j}) \\
&\quad + \eta(\delta_{,j}\zeta_{,k} + \delta_{,k}\zeta_{,j}) + \zeta(\eta_{,j}\delta_{,k} + \eta_{,k}\delta_{,j})\}, \\
\alpha_{,j} &= 2N_{,j}AN', \quad \beta_{,j} = 2N_{,j}BN', \quad \gamma_{,j} = 2N_{,j}CN', \\
\delta_{,j} &= N_{,j}(D + D')N', \quad \eta_{,j} = N_{,j}(E + E')N', \quad \zeta_{,j} = N_{,j}(F + F')N', \\
\alpha_{,jk} &= 2(N_{,jk}AN' + N_{,j}AN'_{,k}), \quad \beta_{,jk} = 2(N_{,jk}BN' + N_{,j}BN'_{,k}), \\
\gamma_{,jk} &= 2(N_{,jk}CN' + N_{,j}CN'_{,k}), \quad \delta_{,jk} = N_{,jk}(D + D')N' + N_{,j}(D + D')N'_{,k}, \\
\eta_{,jk} &= N_{,jk}(E + E')N' + N_{,j}(E + E')N'_{,k}, \quad \zeta_{,jk} = N_{,jk}(F + F')N' + N_{,j}(F + F')N'_{,k}.
\end{aligned}$$

For $N = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$, we have

$$N_{,\theta} = (\cos \theta \cos \phi, \cos \theta \sin \phi, -\sin \theta),$$

$$N_{,\phi} = (-\sin \theta \sin \phi, \sin \theta \cos \phi, 0),$$

$$N_{,\theta\theta} = -N,$$

$$N_{,\phi\phi} = (-\sin \theta \cos \phi, -\sin \theta \sin \phi, 0),$$

$$N_{,\theta\phi} = (-\cos \theta \sin \phi, \cos \theta \cos \phi, 0).$$

From the expressions derived above, the numerical computation of the functions $f(\theta, \phi)$ and $g(\theta, \phi)$ may appear a little cumbersome. A *Mathematica* code written below will help the implementation of these derivations:

```

vn[t_,p_] := {Sin[t] * Cos[p], Sin[t] * Sin[p], Cos[t]};
tn[t_,p_] := Transpose[vn[t,p]];
af[t_,p_] := vn[t,p].ma.tn[t,p];
bt[t_,p_] := vn[t,p].mb.tn[t,p];
gm[t_,p_] := vn[t,p].mc.tn[t,p];
dt[t_,p_] := vn[t,p].md.tn[t,p];
et[t_,p_] := vn[t,p].me.tn[t,p];
zt[t_,p_] := vn[t,p].mf.tn[t,p];
a[t_,p_] := -(af[t,p] + bt[t,p] + gm[t,p])/3;
b[t_,p_] := (af[t,p] * (bt[t,p] + gm[t,p]) + bt[t,p] * gm[t,p] - dt[t,p]^2 - et[t,p]^2 - zt[t,p]^2)/3;
c[t_,p_] := af[t,p] * zt[t,p]^2 + bt[t,p] * et[t,p]^2 + gm[t,p] * dt[t,p]^2 - af[t,p] * bt[t,p] * gm[t,p]
- 2dt[t,p] * et[t,p] * zt[t,p];
ch[t_,p_] := b[t,p] - a[t,p]^2;
cg[t_,p_] := 1.5 * a[t,p] * b[t,p] - .5 * c[t,p] - a[t,p]^3;
dlt[t_,p_] := Sqrt[-(cg[t,p]^2 + ch[t,p]^3)];
psi[t_,p_] := ArcTan[dlt[t,p]/cg[t,p]];
csi[t_,p_] := Cos[(psi[t,p] - 2(m - 1) * Pi)/3];
vms[t_,p_] := 2Sqrt[-ch[t,p]] * csi[t,p] - a[t,p];
tt[t_,p_] := .5 * D[vms[t,p], t]/vms[t,p];
tp[t_,p_] := .5 * D[vms[t,p], p]/vms[t,p];
f1[t_,p_] := Cos[p] * Sin[t] + Cos[p] * Cos[t] * tt[t,p] - Sin[p] * tp[t,p]/Sin[t];
f2[t_,p_] := Sin[p] * Sin[t] + Sin[p] * Cos[t] * tt[t,p] + Cos[p] * tp[t,p]/Sin[t];
f3[t_,p_] := Cos[t] - Sin[t] * tt[t,p];
f[t_,p_] := Sin[phg] * f1[t,p] - Cos[phg] * f2[t,p];
g[t_,p_] := Sin[thg] * f3[t,p] - Cos[thg] * Sqrt[f1[t,p]^2 + f2[t,p]^2];

```

In this code t, p, thg, phg represent the angles $\theta, \phi, \theta_g, \phi_g$ of the text, respectively. The matrices A, B, C, D, E, F , defined by Eqs. (2) in the main text, are represented by ma, mb, mc, md, me, mf , respectively.

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