Longitudinal normals for piezoelectric elastic media

A Duda¹, T Paszkiewicz², S Wolski²

¹Institute of Theoretical Physics, University of Wroclaw, pl. Maxa Borna 9, PL-50-204, Wroclaw, Poland
²Chair of Physics, Rzeszów University of Technology, ul. W. Pola 1, PL-35-959 Rzeszów, Poland

E-mail: ardud@ift.uni.wroc.pl

Abstract. We show that the problem of finding components of longitudinal normals for all piezoelectric classes is equivalent to the problem of solving two sets of two polynomial equations up to 6th degree. It is proved that the number of longitudinal normals for triclinic media cannot exceed 36. If the number of longitudinal normals contained in any plane is finite, then it cannot be larger than 6. Directions of longitudinal normals are found for quartz, LiGaO₂, and Ba₂NaNb₅O₁₅. For these compounds we numerically studied how piezoelectric terms of the propagation matrix influence the number and directions of the longitudinal normals.

1. Introduction
The goal of this paper is to study the problem of one of kinds of special directions of propagation of acoustic waves in piezoelectric elastic media. Special directions of propagation of sound could generally be divided into longitudinal normals, transverse normals, and degenerate directions. Longitudinal normals are directions along which a pure longitudinal wave could propagate. Transverse normals are directions along which a pure transverse wave could propagate. Degenerate directions, called also the acoustic axes [1]-[3], are directions for which phase velocity of at least two modes are equal.

The propagation matrices for acoustic waves propagating in a longitudinal or transverse direction have comparatively simple form, making it possible to use results of measurement of phase velocities of sound propagating in these directions to determine elastic constants of a medium. Moreover, Helbig [4] has shown that ratios of components of polarization vectors propagating in directions close to longitudinal normals are related in a simple way to ratios of appropriate combinations of elastic constants of a medium. This fact could be used to obtain information about elastic properties of media. For these reasons, it is important to know the maximal number as well as components of longitudinal normals for each acoustic symmetry class. This general problem has been the subject of research of many authors [1]-[9], who investigated properties of longitudinal normals for non-piezoelectric media. However, Bogdanov [10] considered longitudinal normals contained in coordinate planes of piezoelectric media belonging to the symmetry class mm2.

In our previous papers [11, 12], with the help of the method of eliminants, we studied general properties of longitudinal axes of non-piezoelectric elastic media, and calculated their directions for a number of media of different symmetries. In the present paper, we shall extend this method to piezoelectric elastic media belonging to all symmetry classes.
2. Longitudinal normals for triclinic media

For piezoelectric media, the polarization vectors of the elastic wave which propagates in the direction \( \mathbf{n} \) are eigenvectors of the propagation matrix \( \Gamma^{(p)}(\mathbf{n}) = [\Gamma^{(np)}(\mathbf{n}) + \mathbf{e} \otimes \mathbf{e} / \rho \varepsilon] \), with the elements \( \Gamma^{(p)}_{il}(n) \)

\[
\Gamma^{(p)}_{il}(n) = \rho^{-1} \sum_{j,m=1}^{3} \left[ C^{E}_{ijklm} + \frac{e_{ij}(\mathbf{n})e_{lm}(\mathbf{n})}{\varepsilon S(\mathbf{n})} \right] n_j n_m,
\]

where \( C_{ijklm} \) are elements of tensor of elastic stiffness constants, while \( \Gamma^{(np)}_{il}(n) = \rho^{-1} \sum_{j,m=1}^{3} C^{E}_{ijklm} n_j n_m \),

\[
e_{ij}(\mathbf{n}) = \sum_{k=1}^{3} e_{ij,k} n_k, \quad \varepsilon S(n) = \sum_{l,r=1}^{3} \varepsilon_{S_{lr}} n_l n_r,
\]

where \( \rho \) is the density, \( e_{lm,r} \) are elements of the tensor of electro-acoustical constants, and \( \varepsilon_{S_{lm}} \) \((l,m,r = 1,2,3)\) are elements of the tensor of dielectric permittivity constants characterizing elastic piezoelectric media. Squares of phase velocities are eigenvalues of matrices \( \Gamma^{(v)}(n) \), \( u = p, np \).

A pure longitudinal wave could propagate in the direction \( \mathbf{n}_u \), if, and only if, the following equation is fulfilled

\[
\Gamma^{(v)}(\mathbf{n}_u)\mathbf{n}_u = [c_u(\mathbf{n}_u)]^2 \mathbf{n}_u
\]

where \( c(\mathbf{n}) \) is the phase velocity and \( \Gamma_u \) is the propagation matrix for a given medium (piezoelectric or non-piezoelectric). We shall denote unit vectors fulfilling this condition by \( \mathbf{n}_{ul} \).

Eq. (4) implies that

\[
\begin{bmatrix} n_{ul}^{(1)} & n_{ul}^{(2)} & n_{ul}^{(3)} \end{bmatrix} = \begin{bmatrix} \Omega_{ul}^{(1)} & \Omega_{ul}^{(2)} & \Omega_{ul}^{(3)} \end{bmatrix},
\]

where

\[
\Omega_{ul}^{(i)} = \lambda_u^{-1} \sum_{v=1}^{3} \Gamma^{(u)}_{iv}(\mathbf{n}_u)n_{ul}^{(v)},
\]

and \( \lambda_u = c_u^2 \). Further, we shall omit the index \( u \).

2.1. Longitudinal normals lying out of OXY plane

The z-axis of the Cartesian coordinate system is directed in accord with general conventions (cf. ref. [13]). Therefore, one may consider longitudinal axes lying in plane perpendicular to z-axis as well as longitudinal axes lying out this plane.

Two vectors \( \mathbf{n} \) and \( \Omega \) are equal if

\[
\Omega_{l}^{(1)} / \Omega_{l}^{(3)} = n_{l}^{(1)} / n_{l}^{(3)}, \quad \Omega_{l}^{(2)} / \Omega_{l}^{(3)} = n_{l}^{(2)} / n_{l}^{(3)}, \quad (n_{l}^{3} \neq 0).
\]

By making substitutions

\[
x = n_{l}^{(1)} / n_{l}^{(3)}, \quad y = n_{l}^{(1)} / n_{l}^{(3)},
\]

the set of equations (7) is transformed into a set of two polynomial equations for \( x \) and \( y \). Unlike for non-piezoelectric media [11, 12], for piezoelectric media these equations are not of fourth but of sixth degree.
For each solution of the aforementioned set, one can find exactly one longitudinal normal, because for each pair \((x, y)\) one can find exactly one triple of numbers \([n_{i}^{(1)}, n_{i}^{(2)}, n_{i}^{(3)}]\) which fulfill the condition

\[
[n_{i}^{(1)}]^{2} + [n_{i}^{(2)}]^{2} + [n_{i}^{(3)}]^{2} = 1. \tag{9}
\]

Namely,

\[
\begin{pmatrix}
\pm x \\
\pm y \\
\pm 1
\end{pmatrix}
\frac{1}{\sqrt{1 + x^2 + y^2}}, \frac{1}{\sqrt{1 + x^2 + y^2}}, \frac{1}{\sqrt{1 + x^2 + y^2}}, \tag{10}
\]

On the other hand, each longitudinal normal crosses the sphere in two points.

According to the Bezout theorem [14], if the number of solutions of the set of polynomial equations is finite, then it cannot be larger then the product of degrees of equations which form this set. Because the degree of each equation belonging to this set is 6, the maximal number of longitudinal normals cannot be larger than 36. Of course, there can exist longitudinal axes lying in the chosen plane, but generally we can choose the z-axis in such a way that longitudinal axes lying in plane perpendicular to z-axis are absent. The choice of z-axis cannot influence the number of solutions of considered set of equations.

By solving the set of Eqs. (7), one can determine all longitudinal normals for a given medium. This set could be written in the following form

\[
A_{0}(y) + A_{1}(y)x + A_{2}(y)x^2 + A_{3}(y)x^3 + A_{4}(y)x^4 + A_{5}(y)x^5 + A_{6}(y)x^6 = 0, \tag{11}
\]

\[
B_{0}(y) + B_{1}(y)x + B_{2}(y)x^2 + B_{3}(y)x^3 + B_{4}(y)x^4 + B_{5}(y)x^5 + B_{6}(y)x^6 = 0, \tag{12}
\]

where

\[
A_{\sigma}(y), B_{\sigma}(y) \quad (\sigma = 0, 1, 2, 3) \tag{13}
\]

are univariate polynomials in the variable \(y\). They depend on characteristics of electro-elastic properties of piezoelectric media, namely, on components \(C_{i,j,k,l}, \epsilon_{ij}\) and \(\epsilon_{ijk} \ (i, j, k, l = 1, \ldots, 3)\).

With the use of MAPLE system we obtained the explicit form of Eqs. (11), (12) for each symmetry class. Generally, the explicit form of Eqs. (11), (12) for piezoelectric media different than cubic, are too involved to be displayed here. Let us note that in the case of cubic nonpiezoelectric media these equations are very simple and their solutions are vectors defining the symmetry axes [11, 12]. For cubic piezoelectric media belonging to the 43m symmetry class, these equations read

\[
2C_{44}\epsilon n_{1}^{2}n_{2}n_{3}^{2} + 12e_{14}^{4}n_{1}^{2}n_{2}n_{3}^{2} + C_{11}\epsilon n_{1}^{2}n_{2}^{3}n_{3}^{2} + 2C_{44}\epsilon n_{2}n_{3}^{2} + C_{11}\epsilon n_{2}n_{2}^{3}n_{3}^{2} + C_{12}\epsilon n_{2}n_{2}^{3}n_{3}^{2} + C_{12}\epsilon n_{2}n_{2}^{3}n_{3}^{2} + C_{12}\epsilon n_{2}^{3}n_{3} = 0, \tag{14}
\]

\[
C_{12}\epsilon n_{1}n_{2}n_{3}^{2} + 2C_{44}\epsilon n_{1}n_{3}n_{2}^{2} - 2C_{44}\epsilon n_{2}n_{2}^{3}n_{3}^{2} + C_{11}\epsilon n_{1}n_{2}n_{2}^{3}n_{3} + C_{12}\epsilon n_{1}n_{2}n_{2}^{3}n_{3} + C_{12}\epsilon n_{1}n_{2}n_{2}^{3}n_{3} + C_{12}\epsilon n_{1}n_{2}n_{2}^{3}n_{3}
\]

\[
+2C_{44}\epsilon n_{1}n_{3}n_{2}^{2} + C_{11}\epsilon n_{1}n_{3}n_{2}^{2} + 12e_{14}^{4}n_{1}n_{3}n_{2}^{2} + C_{12}\epsilon n_{1}n_{3}n_{2}^{2} + C_{12}\epsilon n_{1}n_{3}n_{2}^{2} + C_{12}\epsilon n_{1}n_{3}n_{2}^{2} + C_{12}\epsilon n_{1}n_{3}n_{2}^{2} + C_{12}\epsilon n_{1}n_{3}n_{2}^{2} = 0. \tag{15}
\]

The set of Eqs. (11), (12) is solved by the method of eliminants [11, 12]. In Sect. 3, we show their solutions for several piezoelectric elastic media of low and middle symmetry. We also
considered also two piezoelectric cubic media, namely, CuCl belonging to the symmetry class 43m and Bi$_{12}$GeO$_{20}$ (belonging to the class 23). For these media, results of calculations show that all their longitudinal axes are directed along the fourfold, threefold, and twofold symmetry axes.

2.2. Longitudinal normals inside OXY plane

For directions inside OXY plane, \( n_i^{(3)} = 0 \). Therefore, Eqs. (5) are equivalent to

\[
\sum_{j=1}^{3} \Gamma_{3j} n_i^{(j)} = 0, \quad \left( \sum_{j=1}^{3} \Gamma_{2j} n_i^{(j)} \right) n_i^{(1)} = \left( \sum_{j=1}^{3} \Gamma_{1j} n_i^{(j)} \right) n_i^{(2)}.
\] (16)

Table 1. Components of the direction vectors of longitudinal normals for three piezoelectric compounds. Their symmetry classes are indicated in brackets. The corresponding phase velocities (m/s) are also indicated.

| No. | SiO$_2$ (32) | LiGaO$_2$ (mm2) | BaNaNb$_5$O$_{15}$ (mm2) |
|-----|--------------|-----------------|--------------------------|
| (1) | [1,0,0]      | [1,0,0]         | [1,0,0]                  |
|     | 3245         | 5120            | 5746                     |
|     | 3381         | 4060            | 5782                     |
|     | 3531         | 3787            | 6715                     |
| (2) | [0,0,1]      | [0,1,0]         | [0,0,1]                  |
|     | 4727         | 4727            | 6360                     |
|     | 3751         | 4060            | 5354                     |
|     | 3503         | 3787            | 6827                     |
| (3) | [0.5,0.886,0]| [0, 0, 1]       | [0,0,1]                  |
|     | 3245         | 5120            | 5746                     |
|     | 3365         | 3693            | 6005                     |
|     | 3502         | 3787            | 5763                     |
| (4) | [0.5, -0.866, 0] | [0.458, 0.610, 0.646] | [0.588, -0.809, 0] |
|     | 3245         | 5120            | 5746                     |
|     | 3531         | 3788            | 5737                     |
|     | 3513         | 3637            | 6870                     |
| (5) | [0.0, 0.755, 0.656] | [-0.458, 0.610, 0.646] | [0.588, -0.809, 0] |
|     | 3362         | 3904            | 7061                     |
|     | 3531         | 3788            | 5737                     |
|     | 3513         | 3637            | 6870                     |
| (6) | [0.654, -0.377, 0.656] | [0.458, -0.610, 0.646] | [0.588, -0.809, 0] |
|     | 3362         | 3904            | 7061                     |
|     | 3531         | 3788            | 5737                     |
| (7) | [-0.654, -0.377, 0.656] | [-0.458, -0.610, 0.646] | [0.588, -0.809, 0] |
|     | 3362         | 3904            | 7061                     |
|     | 3531         | 3788            | 5737                     |
| (8) | [0.0, 0.164, 0.945] | [0.853, 0.522, 0] | [0.853, 0.522, 0] |
|     | 4080         | 5067            | 6144                     |
|     | 3482         | 3794            | 5850                     |
| (9) | [-0.0, -0.328, 0.945] | [0.717, 0.0, 0.697] | [0.853, 0.522, 0] |
|     | 4080         | 5067            | 6144                     |
|     | 3482         | 3794            | 5850                     |
| (10) | [0.0, 0.328, 0.945] | [0.717, 0.0, 0.697] | [0.853, 0.522, 0] |
|     | 4080         | 5067            | 6144                     |
|     | 3765         | 3886            | 5603                     |
| (11) | [0.827, 0.478, 0.295] | [0.5, -0.866, 0] | [0.853, 0.522, 0] |
|     | 4367         | 4847            | 5334                     |
|     | 3765         | 3886            | 5603                     |
| (12) | [-0.827, 0.478, 0.295] | [0.5, -0.866, 0] | [0.853, 0.522, 0] |
|     | 4367         | 4847            | 5334                     |
|     | 3483         | 4222            | 6572                     |
| (13) | [-0.955, 0.295] | [0.5, 0.866, 0] | [0.853, 0.522, 0] |
|     | 4367         | 4847            | 5334                     |
|     | 3483         | 4222            | 6572                     |

Again, for a general case, the set of polynomial equations obtained from Eqs. (5) is too complicated to be displayed. The degrees of the corresponding polynomials equal 6, and they depend on the components \( n_i^{(1)}, n_i^{(2)} \). Therefore, they cannot have more than six solutions. For cubic media belonging to the symmetry class 43m, the considered equations are simple and identical with the suitable equation for non-piezoelectric media. One of them is a trivial identity \( 0 = 0 \), and the second one reads

\[
n_i^{(1)} (n_i^{(2)})^5 = (n_i^{(1)})^5 n_i^{(2)}.
\] (17)

We see that, similarly as in the case of non-piezoelectric media, in the case of piezoelectric media belonging to both 43m and 23 symmetry classes, the only longitudinal axes lying in the planes perpendicular to the four-fold symmetry axes are the symmetry axes.
3. Numerical results
3.1. Numerical results — longitudinal axes for selected compounds

We solved Eqs. (11) and (12) for three of compounds considered by Koos and Wolfe [15] and McCurdy and Every [16], namely, one trigonal – quartz SiO$_2$, belonging to the 32 symmetry class, and for two orthorhombic compounds – LiGaO$_2$ and BaNaNb$_5$O$_{15}$ belonging to the mm2 symmetry class. The results are shown in Table 1. Even in the case of two compounds belonging to the same class of the orthorhombic symmetry, the number of longitudinal normals is quite different. This indicates the strong dependence of the number and directions of the longitudinal axes on numerical values of their elasto-electric characteristics. The number of longitudinal normals of media of different crystalline symmetries, e.g. trigonal and orthorhombic considered by us, could be the same and much smaller than their maximal number.

The obtained vectors $n_l$ were used for numerical calculation of corresponding phase velocities. Results of calculations are collected in Table 1.

| SiO$_2$ | LiGaO$_2$ | BaNaNb$_5$O$_{15}$ |
|---------|------------|---------------------|
| p=3     | p=15       | p=15               |

![Graphs showing phase velocities](image)

**Figure 1.** The plots of the surfaces $\Sigma(r)$, defined in the text, for three considered compounds and for propagation matrices with and without piezoelectric terms. The power $p$ and direction vectors of longitudinal axes (cf. Table 1) are indicated.

3.2. Influence of piezoelectric term on longitudinal axes

In this section we shall study the influence of the term of $\Gamma^{(p)}(n)$ matrix related to piezoelectricity on the number of longitudinal normals and their directions. The numerical solutions of Eqs. (11) and (12) with the use of matrix elements of complete $\Gamma^{(p)}$ are presented in Table 1 for the chosen compounds.
To verify our numerical results and study the influence of the piezoelectric term of the propagation matrix, for each of chosen compounds we draw the surface $\Sigma(\mathbf{r})$ being the geometrical locus of points $\mathbf{r} = \mathcal{P}(\mathbf{n})\mathbf{n}$, where $\mathcal{P}(\mathbf{n}) = [F(\mathbf{n})]^p$. The function $F(\mathbf{n}) = \frac{2}{\pi} \arccos[n \cdot \mathbf{e}_{ql}(\mathbf{n})]$ is normalized to the unity. For each propagation direction $\mathbf{n}$, and for both $\Gamma_u$ ($u = p, np$) matrices the polarization vector $\mathbf{e}_{ql}(\mathbf{n})$ of the quasi-longitudinal mode is numerically calculated. Then, the arcos of the angle between $\mathbf{n}$ and the polarization vector $\mathbf{e}_{ql}(\mathbf{n})$ is calculated. The surface $\Sigma(\mathbf{r})$ has maxima for pure longitudinal modes. To make them more pronounced, we plot the $p$-th power ($p = 3$ or $15$) of $F(\mathbf{n})$.

Checking Fig 1, we conclude that the piezoelectric term of the propagation matrix generally influences the directions of longitudinal axes and changes their number. For example, “non-piezoelectric” LiGaO$_2$ crystal has two longitudinal axes more than “piezoelectric” one. In the case of quartz and BaNaNb$_5$O$_{15}$ crystals, the piezoelectric term does not change either number or directions of longitudinal axes. Numerical calculations performed with the use of MAPLE system confirm these results.

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