Elastic plane waves in solids

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1 Some results regarding eigenvalue problems

Consider a square matrix M_{ij} of size $n \times n$, with real or complex values. An eigenvalue problem, for eigenvalues λ and eigenvectors u_i is of the form

$$M_{ij} u_j = \lambda u_i \tag{1}$$

Eigenvalues are roots of the characteristics polynomial: $|M_{ij} - \lambda \delta_{ij}| = 0$.

There are exactly n eigenvalues $\lambda^{(k)}$ and at most n eigenvectors $u_i^{(k)}$ (a priori complex valued). Eigenvectors are non vanishing and can be normalized ($u_i^{(k)} u_i^{(k)} = 1$); they can be arranged in a matrix $X_{ik} = u_i^{(k)}$ such that (1) becomes

$$M_{ij} X_{jk} = X_{ij} \Lambda_{jk} \text{ with } \Lambda_{jk} = \lambda^{(k)} \delta_{jk} \tag{2}$$

If X is invertible, then $M = X \Lambda X^{-1}$.

If M is real and symmetric, eigenvalues are real and eigenvectors are orthogonal: $X^{-1} = X^T$.

In practice, there exist very efficient solvers to obtain eigenvalues and eigenvectors.

2 Non piezoelectric anisotropic solid

2.1 Christoffel equation

We neglect gravity in the elastodynamic equation, $\rho \frac{\partial^2 u_i}{\partial t^2} = \frac{\partial T_{ij}}{\partial x_j}$. Together with Hooke's law, $T_{ij} = c_{ijkl} \frac{\partial u_l}{\partial x_k}$, we have the anisotropic wave equation:

$$\rho \frac{\partial^2 u_i}{\partial t^2} = c_{ijkl} \frac{\partial^2 u_l}{\partial x_j \partial x_k} \tag{3}$$

For harmonic plane waves of the form $u_i(t, \boldsymbol{r}) = \hat{u}_i \exp(\mathrm{i}\omega(t - s\,\boldsymbol{n}\,.\,\boldsymbol{r}))$, the Christoffel equation is obtained

$$\rho\, \hat{u}_i = s^2\, c_{ijkl}\, n_j\, n_k\, \hat{u}_l \tag{4}$$

Slowness $s(\boldsymbol{n}) = k(\boldsymbol{n}) / \omega$ (in s/m) is a function of the propagation direction as measured by unit vector $\boldsymbol{n}$. A quantity of the type $\sqrt{c/\rho}$ is homogeneous to a velocity.
Introducing the symmetric Christoffel tensor, $\Gamma_{il} = c_{ijkl}\, n_j\, n_k$, an eigenvalue problem is obtained:

$$\rho\, \hat{u}_i = s^2\, \Gamma_{il}\, \hat{u}_l \tag{5}$$

Warning: Γ_{il} is a function of direction $\boldsymbol{n}$.

2.2 Isotropic case

In the isotropic case, wave properties are invariant with the propagation direction. Consider for instance x_1 as the propagation direction:

$$\Gamma = \begin{pmatrix} c_{11} & 0 & 0 \\ 0 & c_{44} & 0 \\ 0 & 0 & c_{44} \end{pmatrix} \text{ with } c_{44} = \frac{c_{11} - c_{12}}{2} \tag{6}$$

The matrix is diagonal; there is one simple eigenvalue and one double eigenvalue (so there are 3 eigenvalues in total).

- The wave with velocity $V_L = \sqrt{c_{11}/\rho}$ is a longitudinal wave, since the eigenvector is $\hat{u} = (1,0,0)^T$.
- Waves with velocity $V_S = \sqrt{c_{44}/\rho}$ are shear waves: two eigenvectors are $\hat{u} = (0,1,0)^T$ and $\hat{u} = (0,0,1)^T$.
- Since $c_{12} > 0$, $V_S < V_L / \sqrt{2}$. The longitudinal velocity is always larger than the shear velocity.
- Those properties remain true for any solution to the wave equation (this can be seen considering the plane wave spectrum).

2.3 Examples for a cubic crystal

Considering the shape of the elastic tensor for cubic crystals:

$$\Gamma = \begin{pmatrix} c_{11}\, n_1^2 + c_{44}(n_2^2 + n_3^2) & (c_{12} + c_{44})\, n_1\, n_2 & (c_{12} + c_{44})\, n_1\, n_3 \\ . & c_{11}\, n_2^2 + c_{44}(n_1^2 + n_3^2) & (c_{12} + c_{44})\, n_2\, n_3 \\ . & . & c_{11}\, n_3^2 + c_{44}(n_1^2 + n_2^2) \end{pmatrix}$$

Propagation along [1,0,0] – Γ is diagonal, with one simple eigenvalue, c_{11}, and one double eigenvalue, c_{44}. There are thus one longitudinal wave with velocity $\sqrt{c_{11}/\rho}$ and two shear waves with velocity $\sqrt{c_{44}/\rho}$.

Propagation along [1,1,0] – There are 3 distinct eigenvalues: c_{44}, $\frac{1}{2}(c_{11} - c_{12})$ and $\frac{1}{2}(c_{11} + c_{12}) + c_{44}$. There are thus one pure shear wave polarized along x_3, with velocity $\sqrt{c_{44}/\rho}$; one quasi-shear wave with velocity $\sqrt{(c_{11} - c_{12})/2\rho}$; one quasi-longitudinal wave with velocity $\sqrt{(2c_{44} + c_{11} + c_{12})/2\rho}$.

2.4 Slowness, phase velocity and energy (group) velocity

For harmonic plane waves:

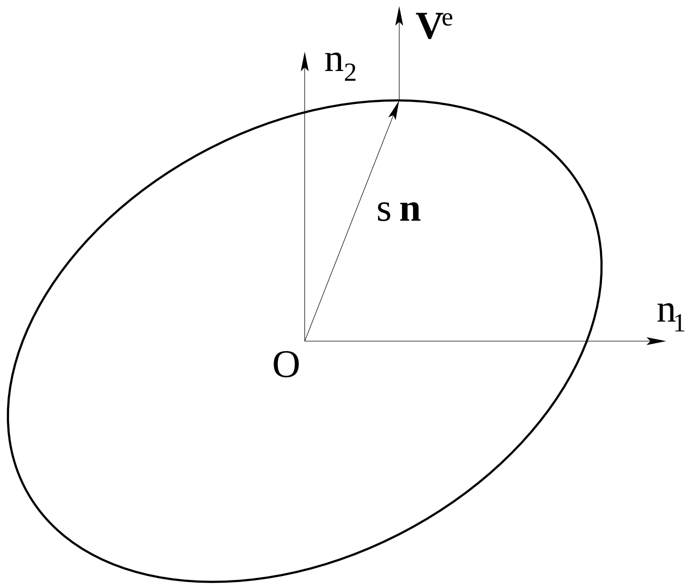
- Kinetic energy density: $e_c = \frac{1}{2}\rho\omega^2\,\hat{u}_i\,\hat{u}_i$.
- Potential energy density: $e_p = \frac{1}{2}\,c_{ijkl}\,S_{ij}\,S_{kl} = \frac{1}{2}\,\omega^2\,s^2\,\Gamma_{il}\,\hat{u}_i\,\hat{u}_l$. From Cristoffel's equation, it follows that $e_p = e_c$: kinetic and potential energies are equal for harmonic plane waves.
- Total energy density: $e = e_c + e_p = \rho\omega^2\,\hat{u}_i\,\hat{u}_i$.
- Poynting's vector
  $P_i = -T_{ij}\,\frac{\partial u_j}{\partial t} = -c_{ijkl}\,\frac{\partial u_k}{\partial x_l}\,\frac{\partial u_j}{\partial t} = s\,\omega^2\,c_{ijkl}\,\hat{u}_j\,\hat{u}_k\,n_l$
- Energy velocity is by definition $V_i^e = P_i\,/\,e$
  An important relation linking phase velocity and energy velocity: $V_i^e\,n_i = v$.
- Furthermore, the equality of energy velocity and spatial group velocity can be demonstrated.

3 Characteristic surfaces

3.1 Slowness surface

By definition, the slowness surface is the locus of vector $\boldsymbol{s} = s\,\boldsymbol{n}$ as a function of $\boldsymbol{n}$ (it is a spatial representation of the dispersion relation $\boldsymbol{k}(\omega,\ \boldsymbol{n})\ /\omega$). The energy velocity (or spatial group velocity is orthogonal to the slowness surface.

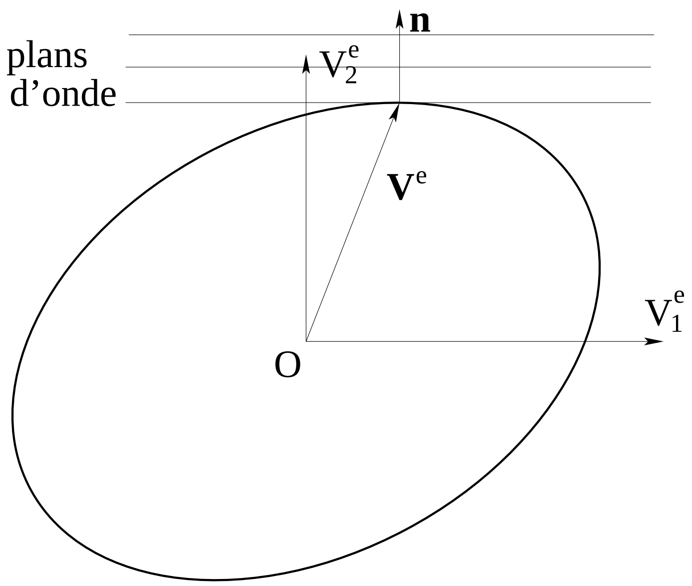
There always exist 3 slowness surfaces: one quasi-L and 2 quasi-S. They are symmetric with respect to the origin (they are revolution surfaces).



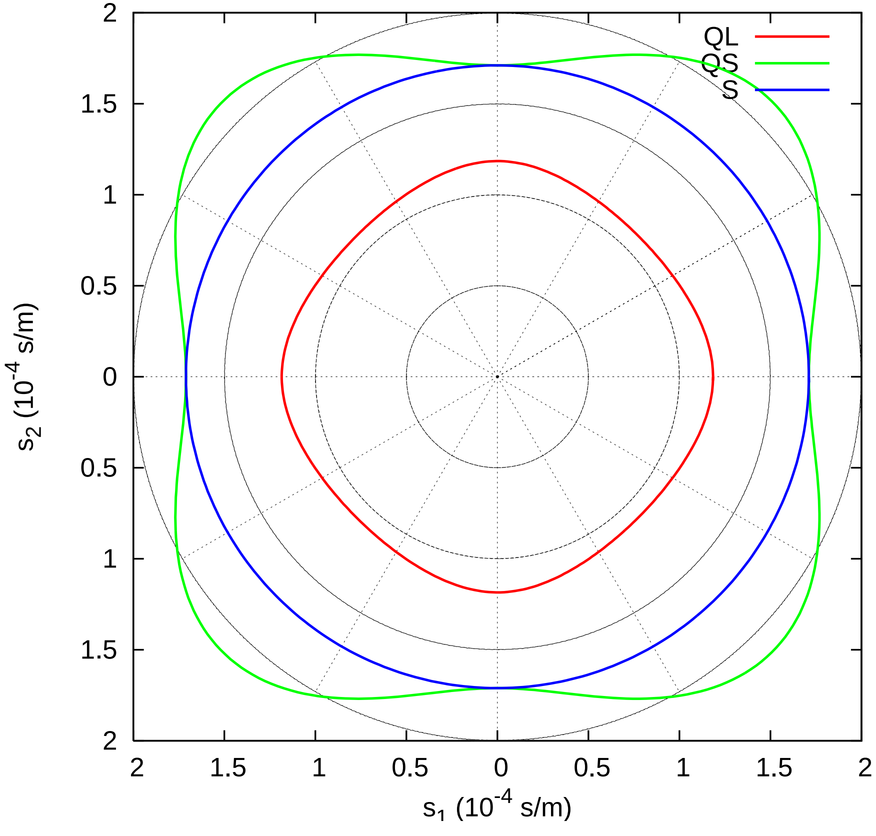
3.2 Wave surface

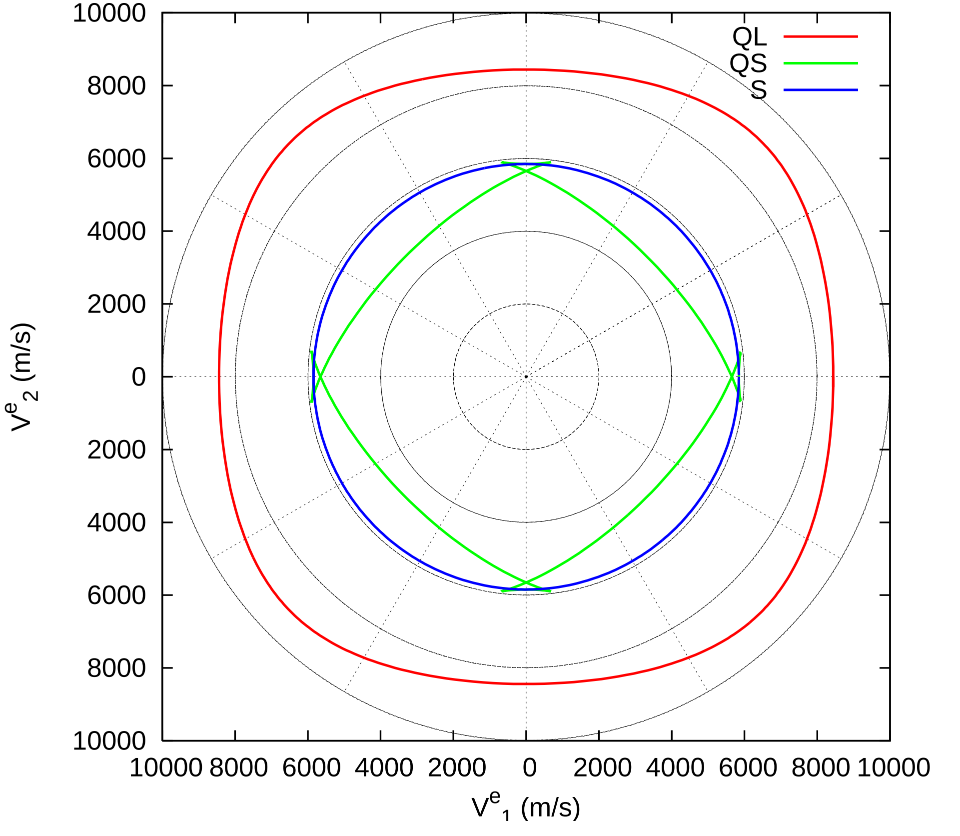
By definition, the wave surface is the locus of the energy vector $\boldsymbol{V}^e$ as a function of $\boldsymbol{n}$. Physically, it is the surface reached after a unit time by the wave emitted from a point source at frequency ω.

It is also an equiphase surface: the phase of the wave is a constant at the surface. $\boldsymbol{n}$ is orthogonal to the wave surface; phasefronts are tangent to the wave surface.

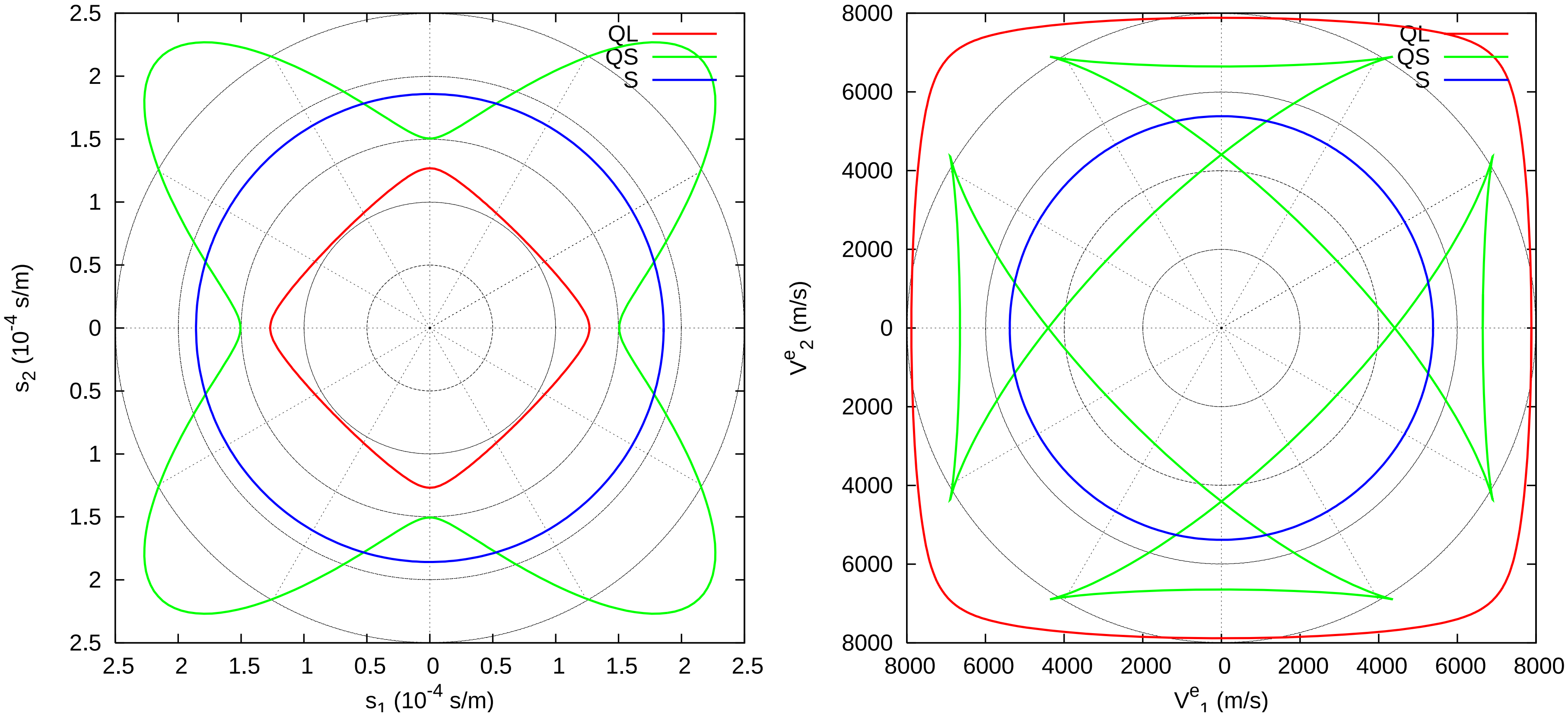


3.3 Example: silicon (Si, cubic m3m)

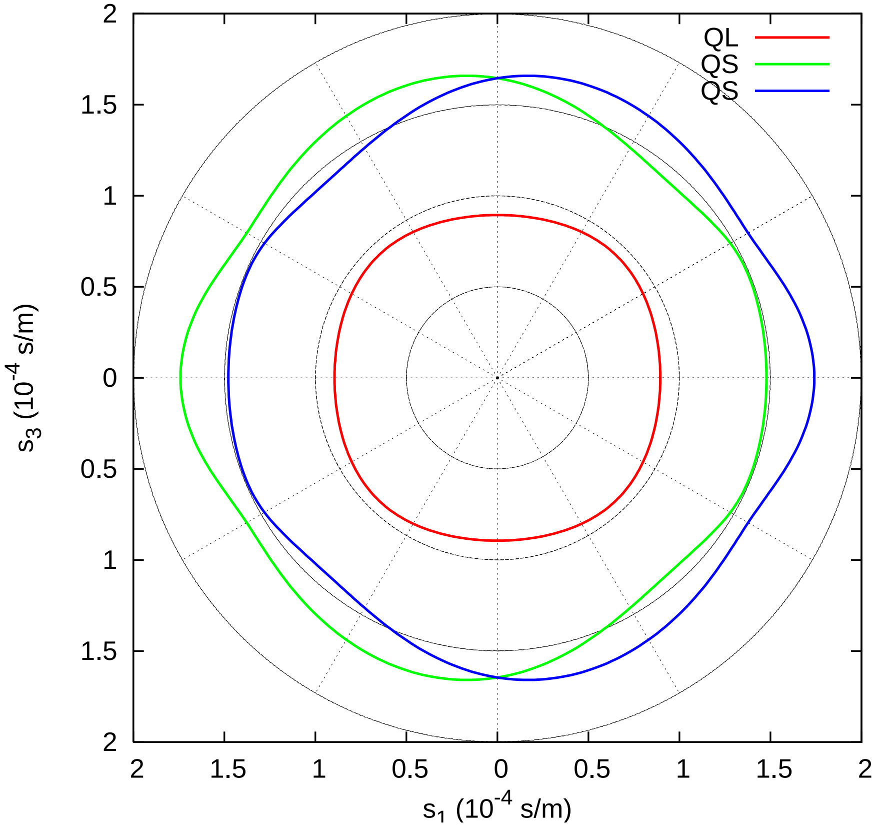


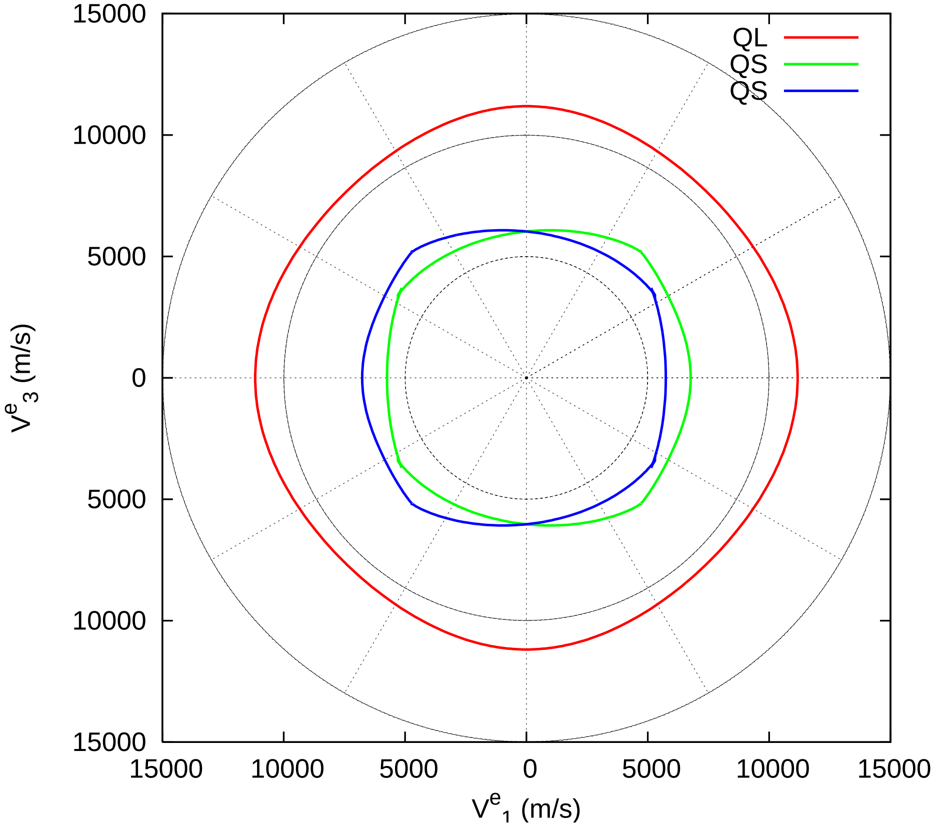


3.4 Example: rutile (TiO_2, tetragonal 4/mmm)



3.5 Example: sapphire (Al_2O_3, trigonal $\bar{3}$m)

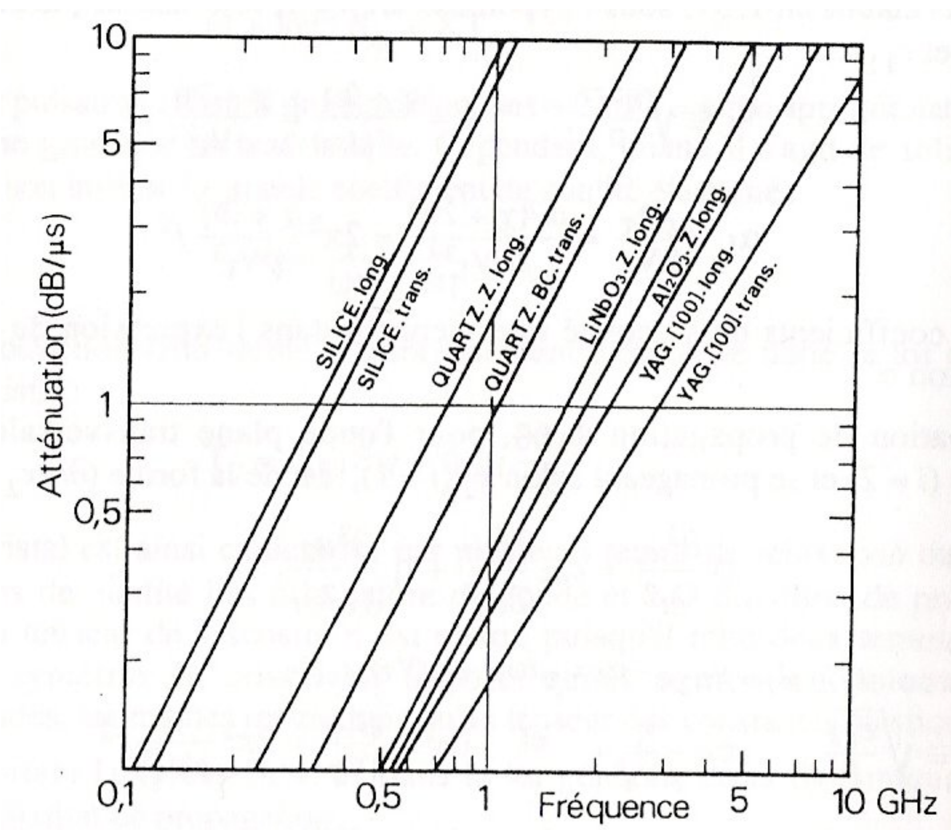




3.6 Attenuation

- Elastic wave losses in solids are due to thermal conduction, to interaction with phonons (thermal fluctuations of the lattice), to diffusion on defects of the crystal, and so on. They are approximately proportional to ω^2.

- Losses are larger in metals compared to insulators; in polycristals compared to single crystals.



4 Piezoelectric anisotropic solids

4.1 Stiffened elastic constants for harmonic plane waves

The elastodynamic equation and the Poisson equation

$$-\mathrm{i}\omega s\,\hat{T}_{ij}\,n_j = -\,\rho\omega^2\,\hat{u}_i \text{ and } \hat{D}_j\,n_j = 0 \tag{7}$$

with the constitutive equations

$$\hat{T}_{ij} = -\mathrm{i}\omega s\,(c_{ijkl}\,n_k\,\hat{u}_l + e_{kij}\,n_k\,\hat{\phi}) \text{ and } \hat{D}_j = -\mathrm{i}\omega s\,(e_{jkl}\,n_k\,\hat{u}_l - \varepsilon_{jk}\,n_k\,\hat{\phi}) \tag{8}$$

lead to

$$\rho\,\hat{u}_i = s^2\,(\Gamma_{il}\,\hat{u}_l + \gamma_i\,\hat{\phi}) \text{ and } \gamma_l\,\hat{u}_l = \varepsilon\,\hat{\phi} \text{ with } \gamma_i = e_{kij}\,n_j\,n_k \text{ and } \varepsilon = \varepsilon_{jk}\,n_j\,n_k \tag{9}$$

Eliminating the electric potential leads to Christoffel's equation with stiffened constants

$$\rho\,\hat{u}_i = s^2\,\bar{\Gamma}_{il}\,\hat{u}_l \text{ with } \bar{\Gamma}_{il} = \Gamma_{il} + \frac{\gamma_i\,\gamma_l}{\varepsilon} \tag{10}$$

This equation is a useful means to obtain the acoustic part of harmonic plane waves in piezoelectric media.

4.2 Electromechanical coupling

Consider for instance propagation along [010] (axis x_2) in lithium niobate ($LiNbO_3$, trigonal 3m)

$$\Gamma = \begin{pmatrix} c_{66} & 0 & 0 \\ . & c_{11} & -c_{14} \\ . & . & c_{44} \end{pmatrix} \text{ with } c_{66} = \frac{c_{11} - c_{12}}{2}$$

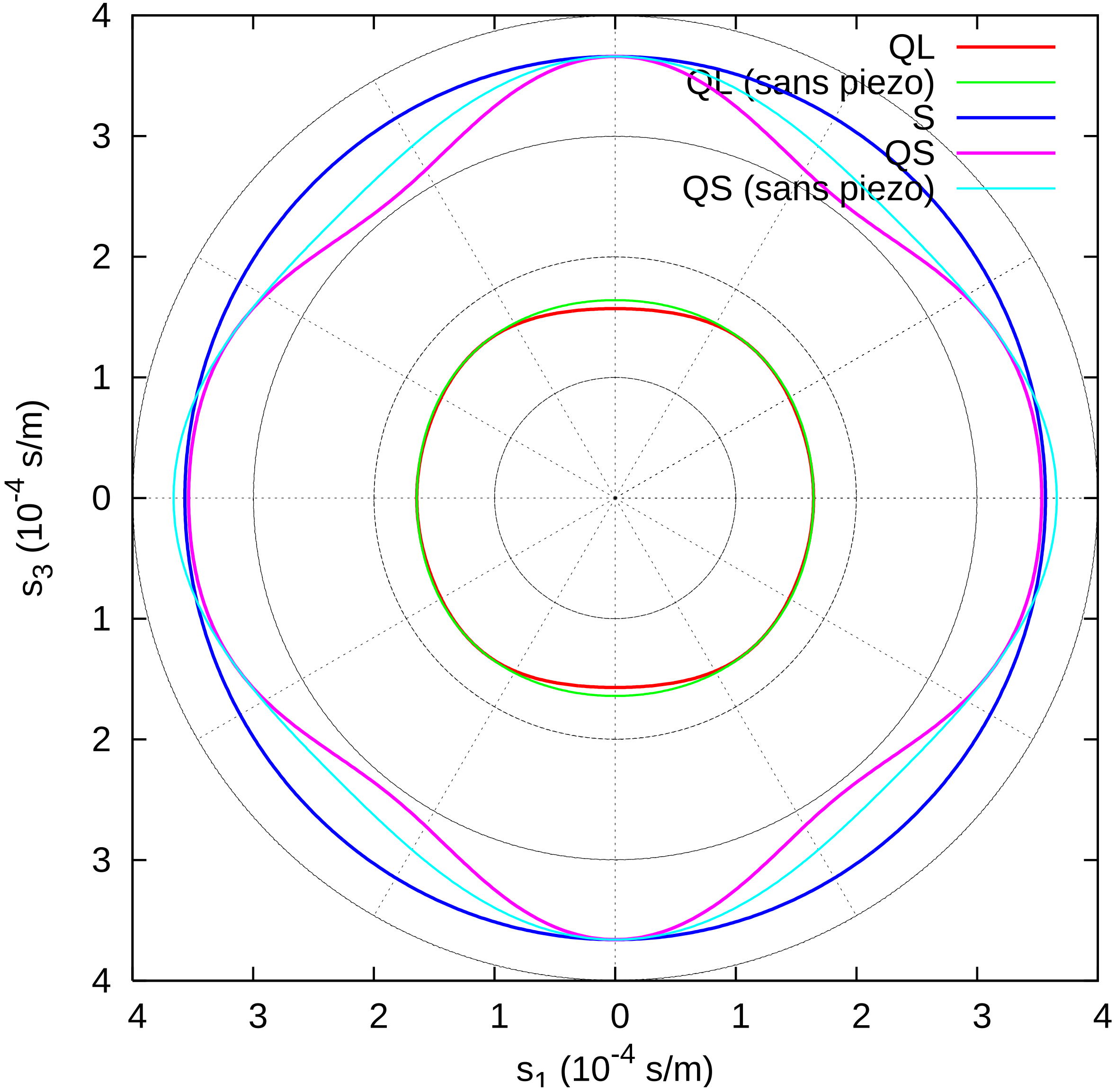
There is a shear wave with velocity $\sqrt{c_{66} / \rho}$ and a QS wave and a QL wave with velocities $2\rho v^2 = \Gamma_{22} + \Gamma_{33} \pm \sqrt{(\Gamma_{22} - \Gamma_{33})^2 + 4\Gamma_{23}^2}$.
Moreover, we find

$$\gamma_1 = 0; \gamma_2 = e_{22}; \gamma_3 = e_{15}; \varepsilon = \varepsilon_{11}$$

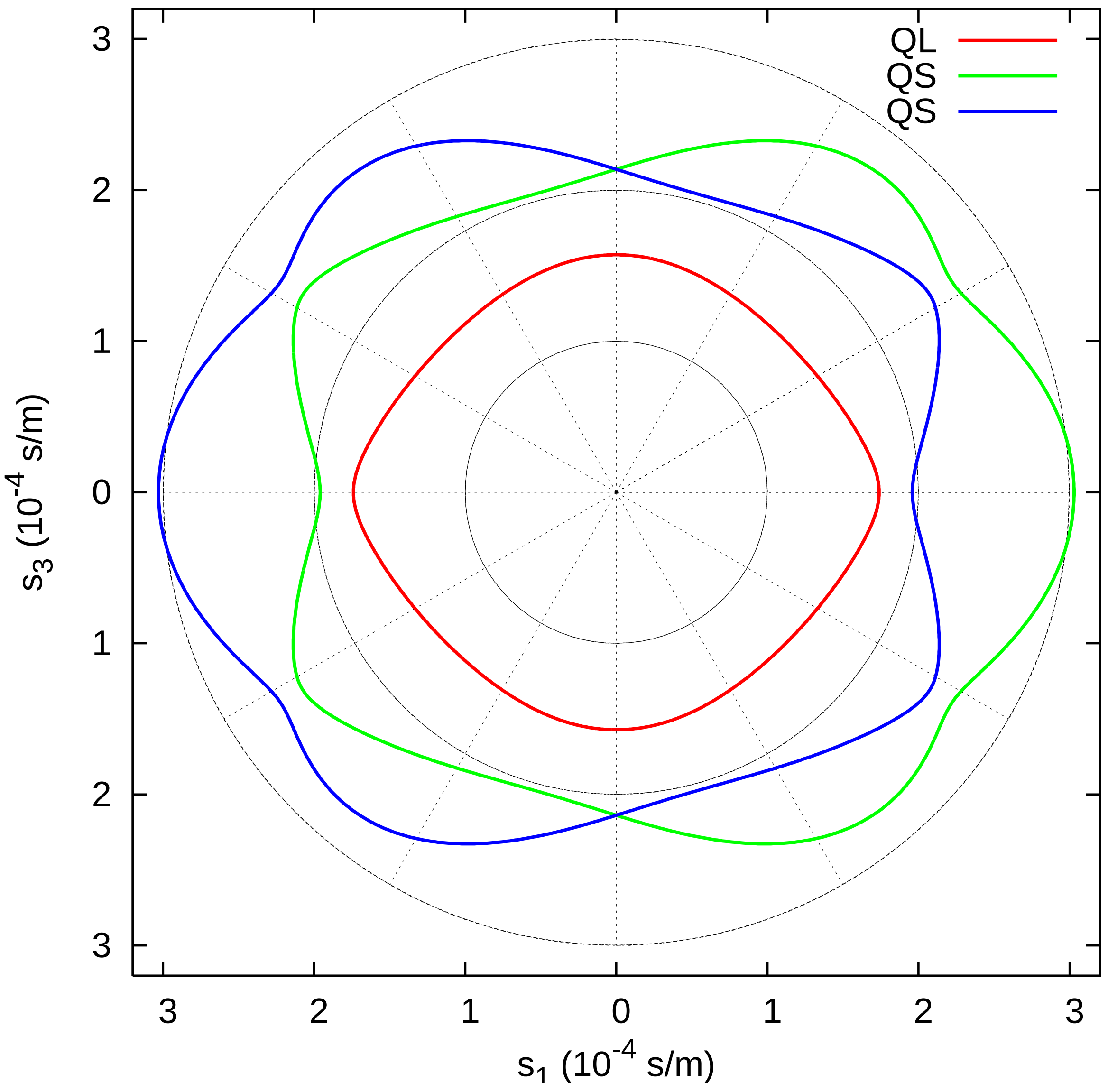
with $\bar{\Gamma}_{11} = \Gamma_{11}; \bar{\Gamma}_{22} = \Gamma_{22} + \gamma_2^2 / \varepsilon; \bar{\Gamma}_{23} = \Gamma_{23} + \gamma_2 \gamma_3 / \varepsilon; \bar{\Gamma}_{33} = \Gamma_{33} + \gamma_3^2 / \varepsilon$.
Piezoelectricity leads to a variation of the QS and QL velocities only. By definition, the electromechanical coupling is defined by the dimensionless quotient

$$K^2 = 2 \frac{\Delta v}{v} \tag{11}$$

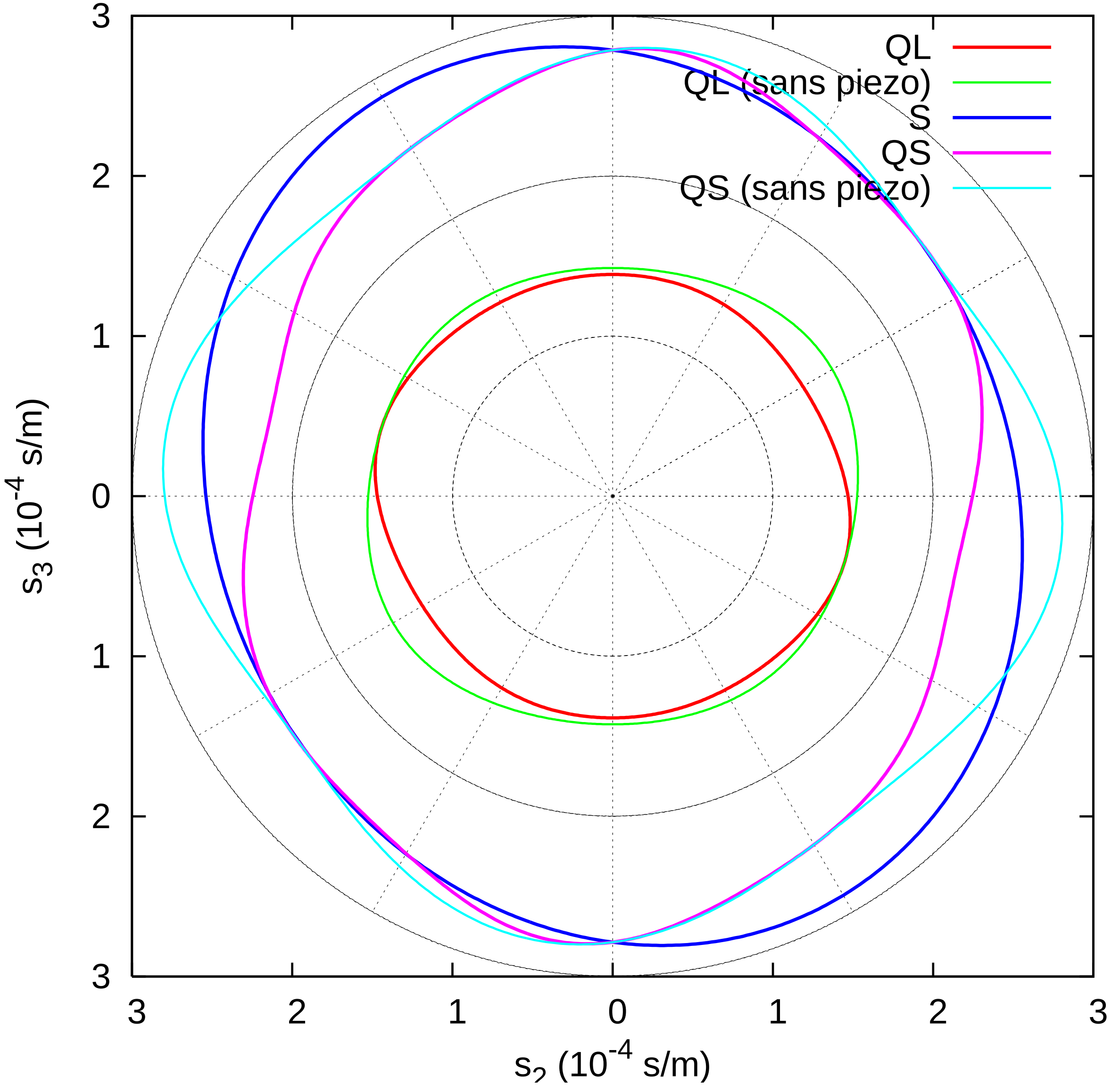
4.3 ZnO (hexagonal 6mm)



4.4 Quartz (trigonal 32)



4.5 $LiNbO_3$ (trigonal 3m)

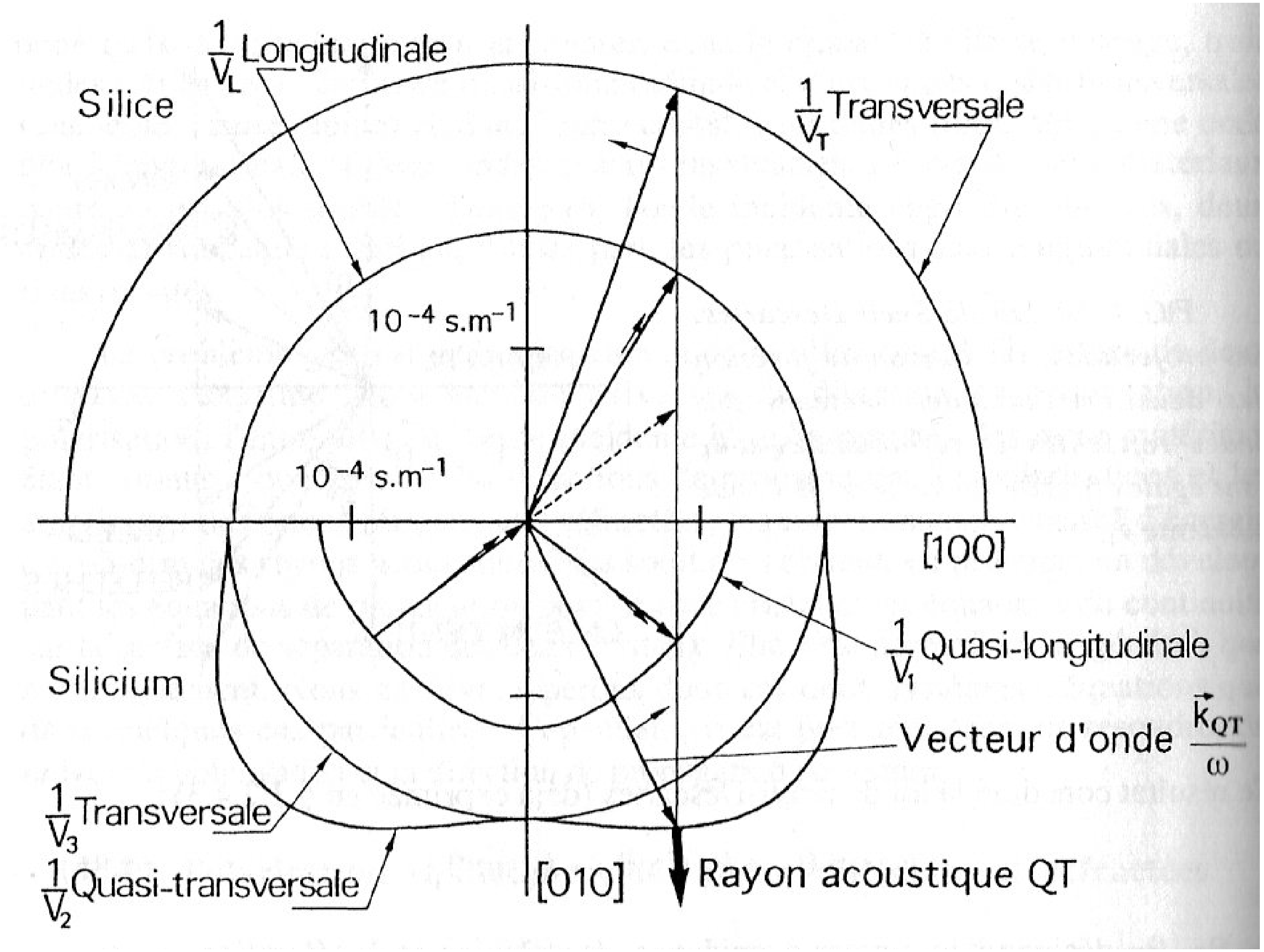


5 Reflection and refraction

5.1 General properties

- The polarization of waves in an ideal fluid medium has only an acoustic longitudinal component.
- The polarization of elastic waves in a solid has 3 acoustic components, 1 QL and 2 QS waves.
- The polarization of elastic waves in piezoelectric media has 4 components, the combination of 3 elastic degrees of freedom (u_i) and 1 electrical degree of freedom (ϕ). There are 1 QL, 2 QS, and 1 quasi-electrostatic (QE) waves.
- An incident wave with a pure polarization can give rise to 4 reflected waves and 4 transmitted waves in a piezoelectric medium (1 and 1 in a fluid; 3 and 3 in an elastic solid).
- The frequency and the projection of the wavevector onto the interface are conserved.

5.2 Example: interface between silicon - silica



5.3 Generalized displacements and constraints

We define generalized constraints by $\bar{T}_{ij} = T_{ij}$ for $i = 1, 2, 3$ and $\bar{T}_{4j} = D_j$ for $i = 4$. Similarly, we define generalized displacements by $\bar{u}_i = u_i$ for $i = 1, 2, 3$ and $\bar{u}_4 = \phi$. We can thus write the constitutive relations as

$$\bar{T}_{ij} = \bar{c}_{ijkl} \frac{\partial \bar{u}_l}{\partial x_k} \text{ with } \bar{c}_{ijkl} = c_{ijkl}, \bar{c}_{ijk4} = +e_{kij}, \bar{c}_{4jkl} = e_{jkl}, \bar{c}_{4jk4} = -\varepsilon_{jk} \qquad (12)$$

and the elastodynamic and the Poisson equations

$$\frac{\partial \bar{T}_{ij}}{\partial x_j} = \bar{\rho}_{ij} \frac{\partial^2 \bar{u}_j}{\partial t^2} \text{ with } \bar{\rho} = \rho \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \qquad (13)$$

As a result, pseudo-mechanical equations similar to elastic solids are obtained. In particular, the piezoelectric Christoffel equation can be written $\bar{\rho}_{ij} \, \bar{u}_j = s^2 \, (\bar{c}_{ijkl} \, n_j \, n_k) \, \bar{u}_l$, which has the form of a generalized eigenvalue problem (of the type $A\boldsymbol{x} = \lambda B\boldsymbol{x}$).

5.4 Eigenvalue equation

Let us consider a reflection-transmission problem on a plane interface normal to x_1. The slownesses s_2 and s_3 are conserved. What are the possible walues for s_1? Relations (12) et (13) can be arranged as

$$\begin{pmatrix} -\bar{c}_{i12l}\,s_2 - \bar{c}_{i13l}\,s_3 & \delta_{il} \\ \sum_{j,k=2}^{3} \bar{c}_{ijkl}\,s_j\,s_k + \bar{\rho}_{il} & 0 \end{pmatrix} \begin{pmatrix} \bar{u}_l \\ \tau_{l1} \end{pmatrix} = s_1 \begin{pmatrix} c_{i11l} & 0 \\ \bar{c}_{i21l}\,s_2 + \bar{c}_{i31l}\,s_3 & \delta_{il} \end{pmatrix} \begin{pmatrix} \bar{u}_l \\ \tau_{l1} \end{pmatrix} \tag{14}$$

with $\tau_{ij} = T_{ij}/(-\mathrm{i}\omega)$.

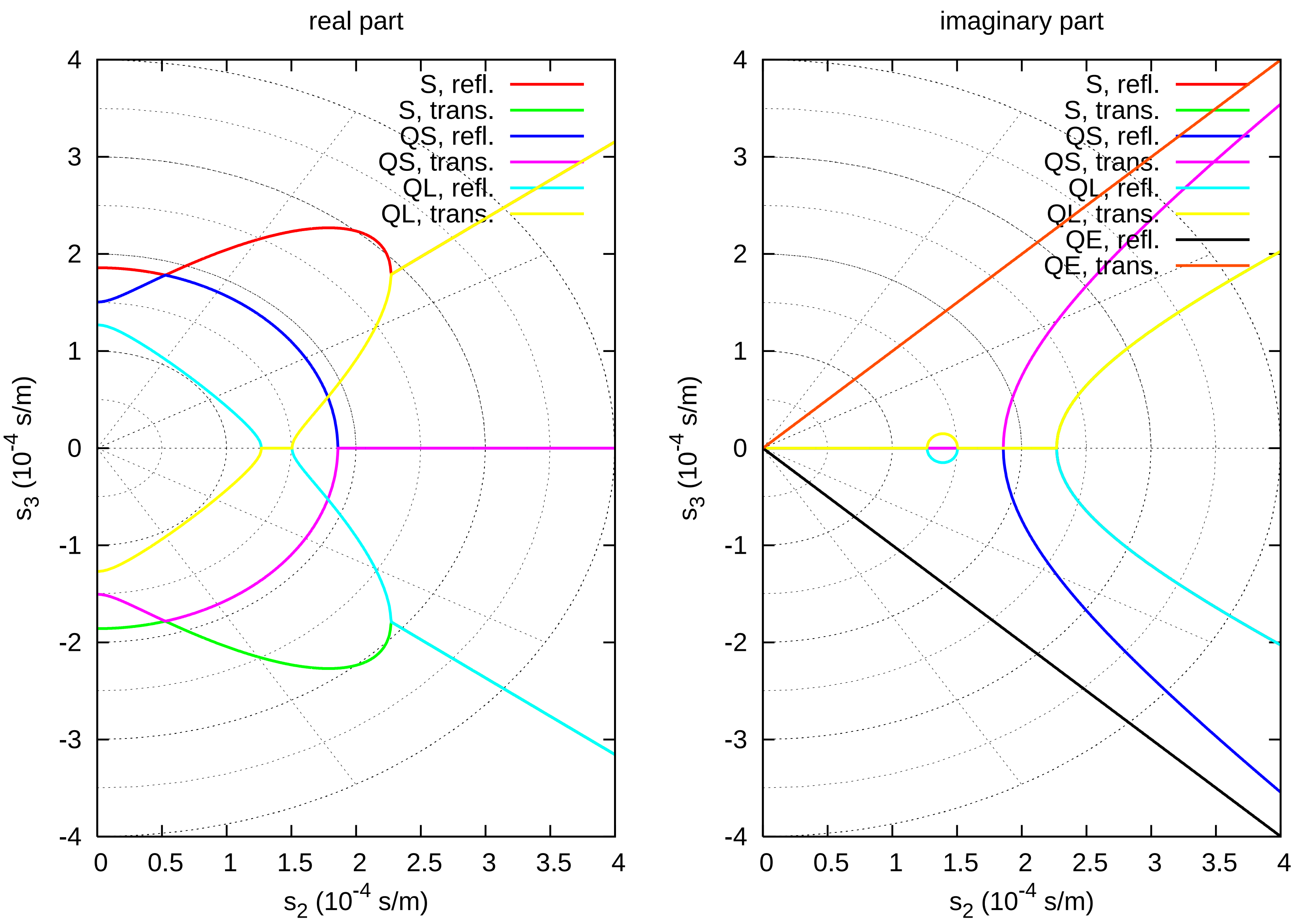
This is a generalized eigenvalue problem, of the form

$$A\boldsymbol{h} = s_1\,B\boldsymbol{h} \tag{15}$$

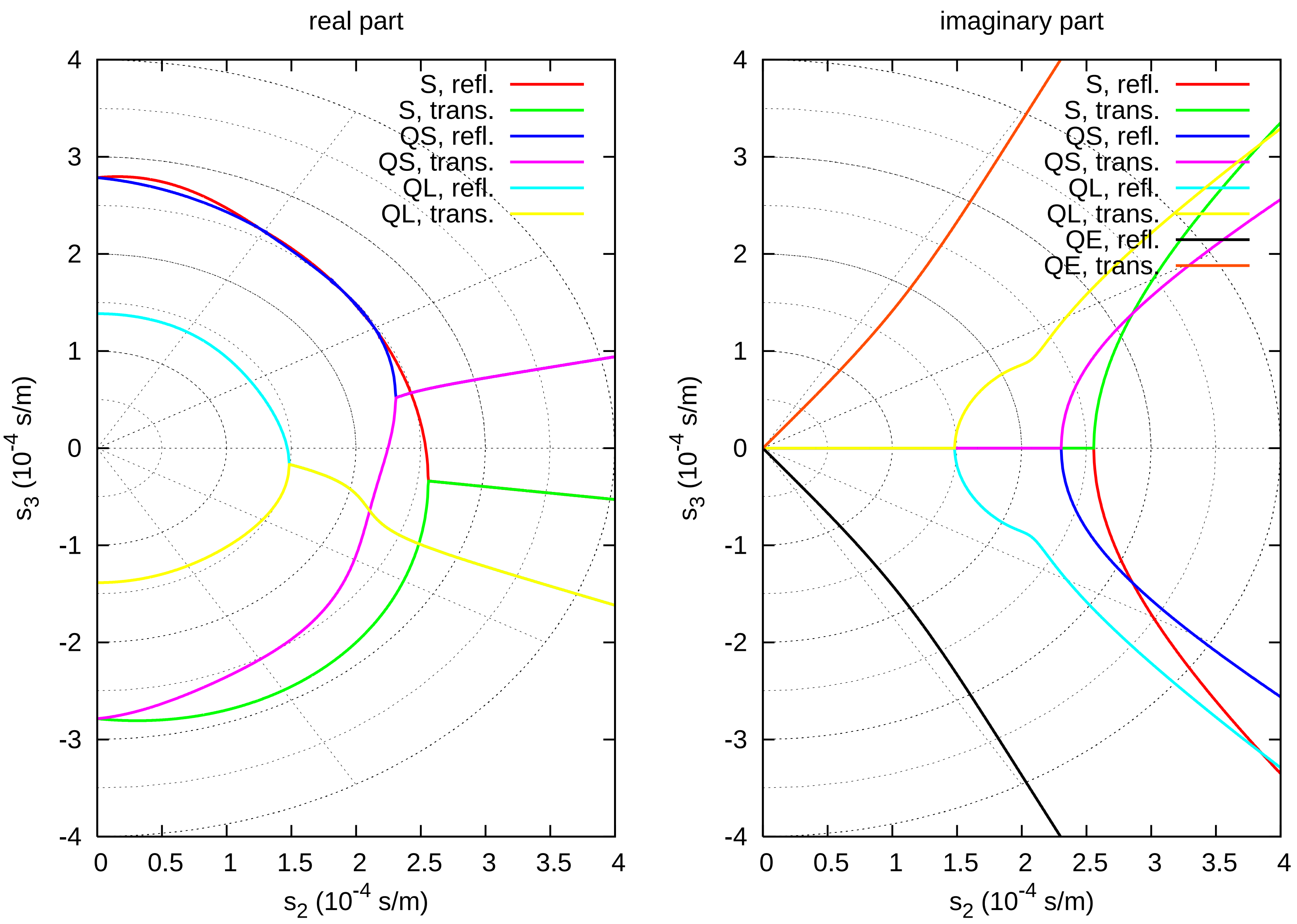
in which matrices A and B depend on s_2 and s_3 (and on the constants of the medium). Vector $\boldsymbol{h}$ has 8 components, the 4 $\bar{u}_l$ and the 4 τ_{l1}.

- There are 8 eigenvalues, corresponding to the 8 possible values of s_1. These eigenvalues belong in pairs to each of the 4 slowness surfaces (possibly to their imaginary branches). Those pairs are either real of opposite signs or complex conjugate.
- The 8 eigenvectors are called partial waves. There are 4 reflected and 4 transmitted partial waves.

5.5 Example: partial waves for rutile



5.6 Example: partial waves of $LiNbO_3$



5.7 Numerical solution method

1. Solve the eigenvalue equation (15) in each media 1 and 2, leading for each to 8 eigenvalues ($s_{1r}^{(1)}$ et $s_{1r}^{(2)}$) and 8 eigenvectors or polarizations ($\boldsymbol{h}_r^{(1)}$ and $\boldsymbol{h}_r^{(2)}$).

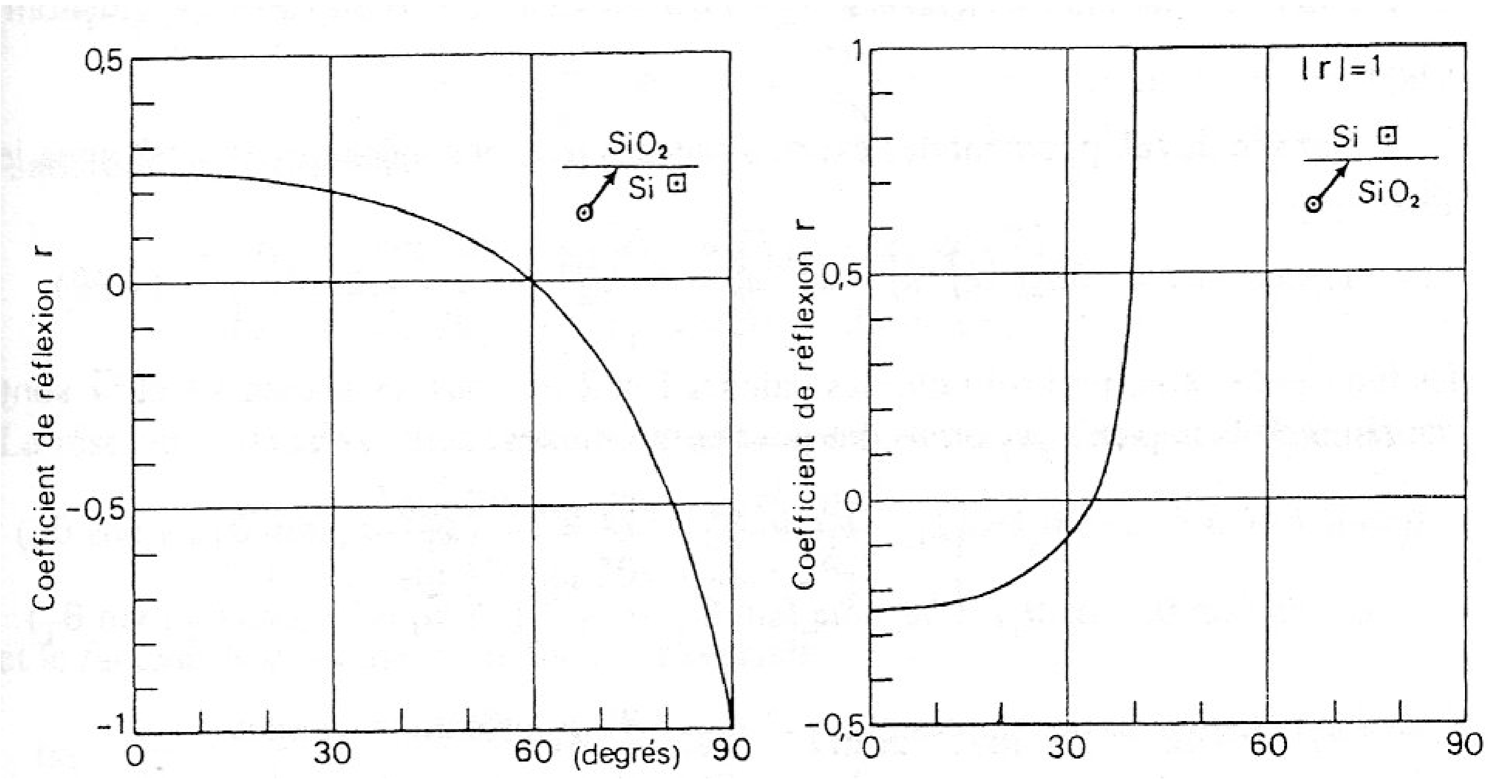
2. The general solution in each medium is a superposition of 8 partial waves

$$\boldsymbol{h}(t,\boldsymbol{x}) = \sum_{r=1}^{8} a_r \, \boldsymbol{h}_r^{(1\text{ou}2)} \exp(\mathrm{i}\omega\,(t - s_{1r}^{(1\text{ou}2)}\,x_1 - s_2\,x_2 - s_3\,x_3)) \tag{16}$$

3. Partial waves (PW) in incident medium 1 are separated into 4 incidents PW (their amplitudes are supposedly known) and into 4 reflected PW. Partial waves in medium 2 are separated into 4 transmitted PW and 4 incident PW (their amplitudes vanish).

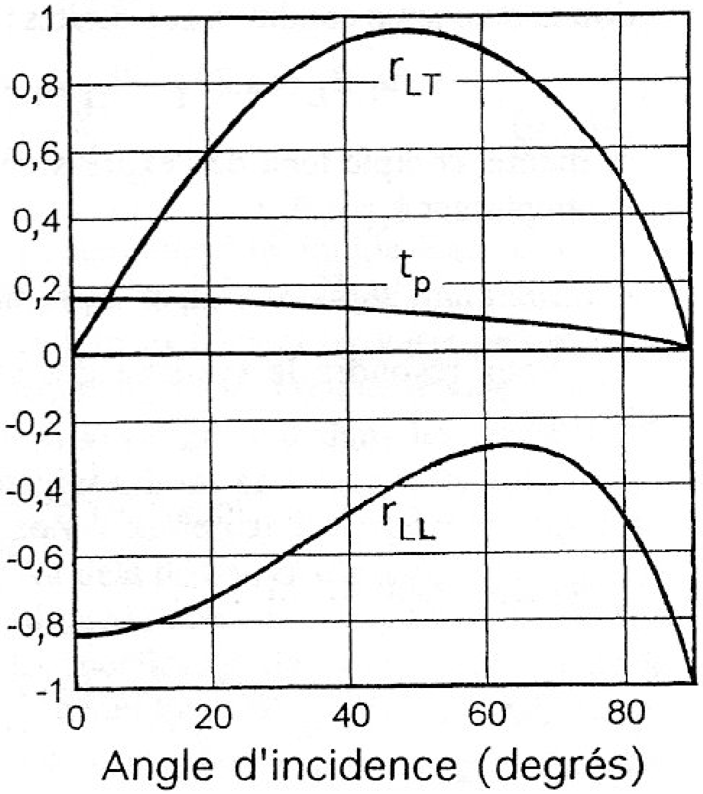
4. The 8 components of $\boldsymbol{h}$ are continuous at the interface, leading to 8 linear equations for 8 unknowns (the amplitudes of the reflected and trasnmitted PW). The problem is thus completely determined.

5.8 Example: interface silicon - silica, and reciprocally

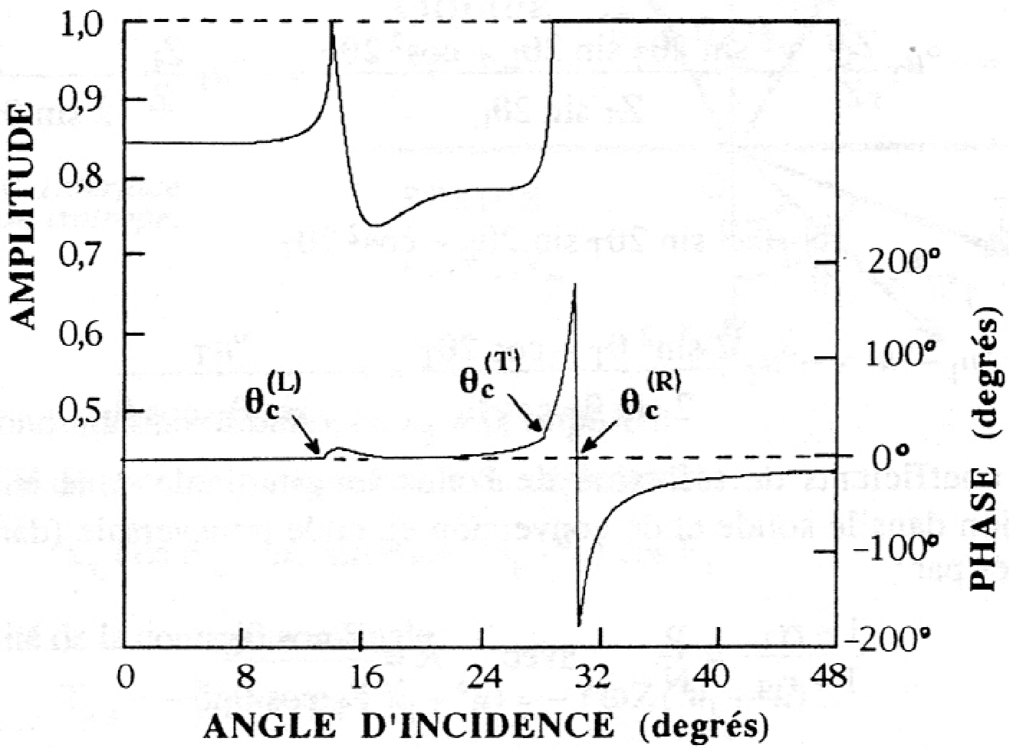


Pure shear incident wave (S)

5.9 Example: interface duralumin - water, and reciprocally



L incident wave in duralumin



Reflection coefficient r_{LL} in water