Computation of Plate Wave Dispersion Diagrams and Surface Wave Velocities Without Explicit Boundary Conditions

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***Abstract*—We discuss the computation of the band structure of plate waves using the plane wave expansion (PWE) method. This method is generally used to formulate eigenvalue problems to compute dispersion diagrams for solid-solid phononic crystals. We show how the free surface boundary condition can be included implicitly in the form of the PWE solution, thus leading to an efficient eigenvalue problem. This generic method for wave dispersion is non-iterative and does not require an initial guess for the solution. Furthermore, surface acoustic wave velocities can be estimated from the slowest wave for large wave vectors. Examples for a single plate and a multilayer plate are given, and extension to piezoelectric materials is discussed.**

I. Introduction

The rigorous evaluation of the dispersion relation for a particular type of wave is a numerical problem for which practical difficulty strongly depends on the algebraic form of the solution. For instance, the computation of the velocity of bulk acoustic waves in an arbitrary anisotropic material can be cast in the form of an eigenvalue problem and solved easily and reliably [1]. In contrast, in the case of SAW or plate waves, it is generally first necessary to form a determinant of the boundary conditions and then to seek its zeros as a function of the wave vector for a fixed frequency. Finding all zeros can be a numerically difficult problem and a cumbersome one for plate waves, because the number of allowed modes increases with the thickness of the plate.

To illustrate this line of thought, let us consider the simple plate depicted in Fig. 1(a). The solid constituting the plate can be an arbitrary homogeneous piezoelectric material. We are looking for monochromatic plane-wave modes of the plate propagating along its surface, so that we assume (inside the solid) a dependence for all displacements of the form

$$u_i(x_1, x_2, x_3, t) = u_i(x_3)\exp(i(\omega t - k_1 x_1 - k_2 x_2)). \quad (1)$$

Inserting this expression in the original wave equation results in a solution that is a superposition of 8 partial waves of exponential type [2]. Partial waves are modes of the unbounded homogeneous solid, but the modes of the plate themselves must satisfy the boundary conditions at the surfaces. In this paper, we will consider only the free surface boundary condition (for reasons discussed in the next section). The wave vector along the surface of the plate is obtained as a zero of a boundary condition determinant of the form $\Delta(k;\omega,\mathbf{n}) = 0$ which is of size 8×8. In this expression, $\mathbf{n}$ is a unit vector along the surface, so that we write $k_1 = kn_1$ and $k_2 = kn_2$. This discussion can be generalized to arbitrary multilayers of different materials [3]. Reliably finding all zeros of a function is not always a simple algorithmic task. The result is, in general, strongly dependent on the initial guess for the solution. Often an automated method is necessary to estimate the velocities of elastic waves of different types, especially if these are to be used in a subsequent computation, e.g., with FEM/BEM algorithms [4], [5]. As noted previously, finding bulk wave velocities can be fully automated because they can be obtained from a positive semi-definite eigenvalue problem and no initial guess is required. For finding Rayleigh surface wave velocities, using the slowest bulk wave as an initial guess value is generally a good idea, but one which fails in some cases. Finding the dispersion relation of all modes of an arbitrary multilayer is a difficult problem in most practical cases and is certainly difficult to automate.

The plane wave expansion (PWE) method is used in the field of phononic crystals to formulate eigenvalue problems to compute dispersion diagrams [6]. The method relies on Fourier expansions of the physical fields and of the material constants. Historically, the PWE method was limited to solid-solid compositions in which two or more solid materials are arranged periodically. Recently, it has been remarked that it can cope with solid-vacuum compositions where a vacuum is represented by a solid with zero mass density and elastic constants, and this result was employed to compute the dispersion of surface acoustic waves on a 2-D air-hole phononic crystal [7]. This idea was then used to compute the dispersion of waves in 2-D phononic crystals in the plate geometry [8]. However, the accuracy of the method has not been verified until now.

Fig. 1(b) describes how a plate surrounded by a vacuum can be artificially repeated periodically to create a periodic system, similar to a 1-D phononic crystal. Because there is no elastic energy in a vacuum, the replicas of the plate are theoretically completely isolated and waves cannot be transmitted from one plate to another. Hence, the

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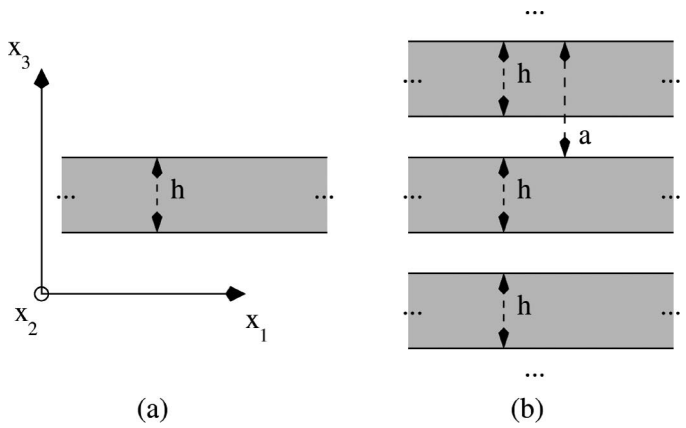

Fig. 1. (a) A solid plate with finite thickness h supposed to be surrounded by a vacuum, shown together with the definition of axes. (b) The same plate is artificially repeated periodically in the vertical direction, x_3. The structure is assumed to be periodic in the x_3 direction (with period a) and infinite in the x_1 and x_2 directions. Vacuum alternates with the solid material.

isolated plate and the periodically repeated plate wave problems have formally identical solutions. We discuss in this paper how the boundary conditions at the surfaces of the plate can be included implicitly in the form of the PWE solution, thus leading to an efficient eigenvalue problem that will systematically give the dispersion of all waves inside the plate. We have specifically implemented a PWE method to solve the plate wave problem for arbitrary anisotropic elastic materials. In the limit of a large number of Fourier harmonics, the condition that there are no elastic waves in the vacuum part can be satisfied, and the solutions of the eigenvalue problem represent waves propagating in the plate with a given wave vector along the surface. By comparing with a classical determinant-based method, it is verified that all solutions are found with excellent accuracy. Furthermore, SAW velocities can be safely estimated from the slowest wave for large wave vectors. The PWE numerical algorithm we propose is fast and accurate. We discuss the issue of convergence (the number of harmonics that have to be included in the computation) and the extension of the method to multilayered plates and to piezoelectric materials, where an additional difficulty appears because of the existence of an electromagnetic field in a vacuum.

II. Solid-Vacuum PWE Method

The PWE method is based on a direct application of the Bloch-Floquet theorem to the representation of Bloch waves as the product of a periodic function, given by a discrete sum over Fourier harmonics in the reciprocal-lattice space, with a time-harmonic exponential function with frequency ω and Bloch wave vector k. Specifically, the displacements in the x_i direction read

$$u_i(r) = \left(\sum_{n=1}^{N} U_{in} \exp(-iG^n r) \exp(-ik \cdot r) \right), \tag{2}$$

where G^n are the reciprocal lattice vectors and $i^2 = -1$. Similarly, the stresses are expressed as

$$T_{ij}(r) = \left(\sum_{n=1}^{N} T_{ijn} \exp(-iG^n r) \exp(-ik \cdot r) \right). \tag{3}$$

We specifically use the formulation by Wilm *et al.* for bulk and plate waves in piezoelectric media [9], which was later extended to surface waves in anisotropic and piezoelectric media [7], [10]. The secular equation ([7, Eq. (5)]),

$$\omega^2 \tilde{R} \tilde{U} = \left(\sum_{i,j=1,3} \Gamma_i \tilde{A}_{ij} \Gamma_j \right) \tilde{U}, \tag{4}$$

defines a generalized eigenvalue problem for the frequency as a function of the wave vector and is used to obtain band structures. In this expression, $\tilde{U}$ is a vector gathering the Fourier coefficients of the three displacements and the electric potential, and the matrices Γ_i, $\tilde{A}_{ij}$, and $\tilde{R}$ contain $4N \times 4N$ Fourier coefficients. These matrices read

$$\begin{aligned}
\tilde{A}_{ij} &= \begin{bmatrix} A_{ij0} & A_{ijG^1-G^2} & \cdots & A_{ijG^1-G^N} \\ A_{ijG^2-G^1} & A_{ij0} & \cdots & A_{ijG^2-G^N} \\ \vdots & \vdots & \ddots & \vdots \\ A_{ijG^N-G^1} & A_{ijG^N-G^2} & \cdots & A_{ij0} \end{bmatrix}, \\
\Gamma_i &= \begin{bmatrix} (k_i + G_i^1) I_d & & 0 \\ & \ddots & \\ 0 & & (k_i + G_i^N) I_d \end{bmatrix}, \\
\tilde{R} &= \begin{bmatrix} \rho_0 \tilde{I} & \rho_{G^1-G^2} \tilde{I} & \cdots & \rho_{G^1-G^N} \tilde{I} \\ \rho_{G^2-G^1} \tilde{I} & \rho_0 \tilde{I} & \cdots & \rho_{G^2-G^N} \tilde{I} \\ \vdots & \vdots & \ddots & \vdots \\ \rho_{G^N-G^1} \tilde{I} & \rho_{G^N-G^2} \tilde{I} & \cdots & \rho_0 \tilde{I} \end{bmatrix},
\end{aligned} \tag{5}$$

with $A_{ilG}(j,k) = c_{ijklG}$, $A_{ilG}(j,4) = e_{lijG}$, $A_{ilG}(4,k) = e_{iklG}$, $A_{ilG}(4,4) = -\varepsilon_{ilG}$. I_d is the 4×4 identity matrix and $\tilde{I} = I_d$, but for $\tilde{I}(4,4) = 0$. c_{ijkl}, e_{ijk}, and ε_{ij} are the elastic, piezoelectric, and dielectric tensors, respectively. The Γ_i and $\tilde{R}$ matrices are each formed of N^2 4×4 diagonal blocks. Note that all material constants enter the equations through their Fourier series, and are linear combinations of the Fourier series of the material constants of each involved solid.

To describe solid-vacuum compositions using only solids, the equivalent material constants of a vacuum should be defined. More precisely, this modification must be such that the interfaces between the solid material (solid 1) and vacuum (solid 2) are free of tractions. In this way, the free (or natural, or Neumann) boundary condition is automatically satisfied. We first let the piezoelectric constants in solid 2 vanish and impose $\varepsilon_{ij}^{(2)} = \varepsilon_0$. The equations of motion in solid 2 are then purely elastic and can be written

$$T_{ij}^{(2)} = \sum_{k,l=1}^{3} c_{ijkl}^{(2)} \frac{\partial u_k^{(2)}}{\partial x_l}, \tag{6}$$

$$\rho^{(2)} \frac{\partial^2 u_j^{(2)}}{\partial t^2} = \sum_{i=1}^{3} \frac{\partial T_{ij}^{(2)}}{\partial x_i}. \tag{7}$$

Because there are no stresses in a vacuum, we set $c_{ijkl}^{(2)} = 0$ to impose $T_{ij}^{(2)} = 0$ independently of the displacements, which have a physical meaning in solid 2 only at the interfaces. As a consequence, we have to set $\rho^{(2)} = 0$, otherwise the displacements at the interface would not be free. Because the stresses are uniformly zero inside solid 2, even if the displacements can assume any value (the equations do not constrain them), then the elastic energy is exactly zero everywhere as should be expected.

Let us now emphasize that the PWE method implicitly requires that all physical fields are continuous. This property is obvious for the displacements from (2) and is physically required at the interface between two solids or a solid and a vacuum. However, the situation is different for the stresses. According to (3), the stresses are also expanded according to the Bloch-Floquet theorem and are thus made continuous everywhere. But the boundary condition is only that the normal stress (the traction) is continuous at an interface between two solids. The transverse stresses are not specified and are, in effect, generally non-vanishing at the interface between a solid and a vacuum. However, despite the fact that the PWE solution is continuous, the local variations of the solution are directly dictated by the number of Fourier harmonics that are included in the computation and sharp transitions can still be approximated. Using N harmonics, the moduli of the reciprocal lattice wavevectors in the solution span a range equal to $N2\pi/a$. However, the Fourier coefficients of the material constants appearing in (5) span twice this range. In a sense, it can be said that the PWE method replaces the abrupt transition between two solids by a smoothed and continuous interface between them, whose thickness can be approximated by $a/(2N)$.

III. Elastic Plates

Let us consider as a first example a silicon plate with the crystallographic axes aligned with the reference axes of Fig. 1. Fig. 2 shows the dispersion diagram $\omega(k)$ of the periodized plate. Though the computation was conducted for the periodized plate, the band structure of the isolated plate is retrieved. This is because, as we indicated in the introduction, there is no elastic energy in a vacuum up to numerical errors, and consequently the periodized plates are isolated from each other. In practice, the band structure is generated by varying k_1 while maintaining $k_2 = k_3 = 0$, and the frequencies of the modes are obtained by solving the eigenvalue problem of (4). In the example of Fig. 2, $N = 31$ harmonics are used in the Fourier series and a/h equals 1.5. The size of the matrices

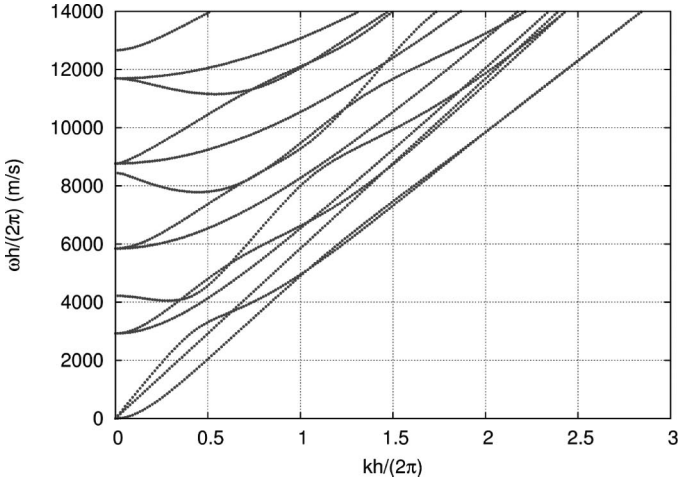

Fig. 2. Band structure computed by the PWE method for the single elastic plate of Fig. 1. The considered material is (100) silicon. Thirty-one harmonics are used and $a/h = 1.5$.

in the eigenvalue problem is 93×93 because there are 3 independent unknowns, the mechanical displacements. For such matrix sizes, the computation of the full band diagram takes only a few seconds on a personal computer. An eigenvalue solver will return up to $3N$ eigenvalues and eigenvectors. The band structures plotted in this paper include all eigenmodes within the frequency range chosen for display, without any further selection among the solutions returned by the eigenvalue solver.

When using more harmonics, it was checked that the results are not changed appreciably in the (k_1, ω) range of Fig. 2. Using fewer harmonics can lead to a slightly degraded convergence, depending on the choice of the value of the ratio of the period a to the plate thickness h. In the particular case of Fig. 2, convergence is achieved for $N \geq 11$ if $a/h = 1.5$, for $N \geq 21$ if $a/h = 1.2$, and for $N \geq 31$ if $a/h = 1.1$. This numerical observation is directly connected to the previous observation that sharp interfaces are replaced in the PWE method by smoothed interfaces with a resolution inversely proportional to the number of harmonics.

Fig. 3 displays the phase velocity $v = \omega/k$ computed from Fig. 2. It can be seen that the velocity of the slowest plate mode tends to that of the Rayleigh wave, $v = 4921.9$ m/s, as should be expected. This is an important test of the consistency of the method and of its convergence. It also proves that the SAW velocity can be obtained directly from an eigenvalue problem by considering a large value of k and keeping only the slowest mode.

The modal distribution at any point of the band structure can be obtained by examining the corresponding eigenvector. The modal distribution of the mode at $kh/(2\pi) = 2$ and $\omega h/(2\pi) = 11\,490$ m/s in Fig. 1 is displayed, for example, in Fig. 4. This mode is a Lamb wave polarized in the (x_1, x_3) plane. The displacement u_2 is exactly zero in the case of silicon as a result of the symmetry of the matrices involved in the eigenvalue problem. It can be observed that the displacements u_1 and u_3 have non-

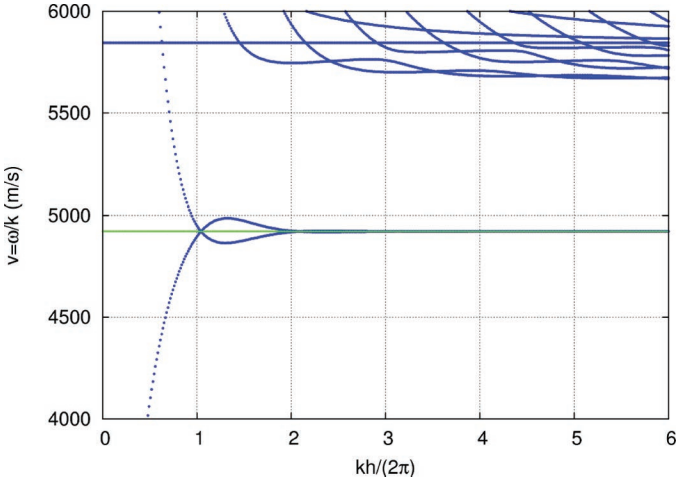

Fig. 3. Plate wave velocities as a function of the normalized wave vector kh computed by the PWE method for the single elastic plate of Fig. 1. The considered material is (100) silicon. The green line shows the Rayleigh SAW velocity for comparison (v = 4921.2 m/s). Thirty-one harmonics are used and $a/h = 1.5$.

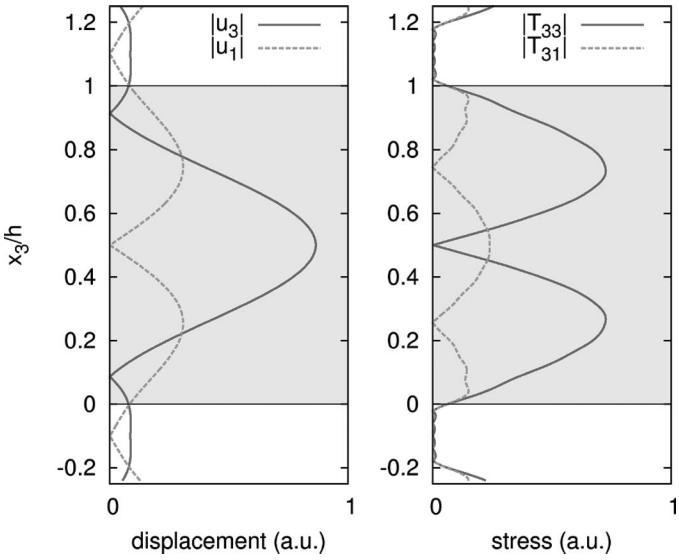

Fig. 4. Displacement and stress modal distribution for the mode at $kh/(2\pi) = 2$ and $\omega h/(2\pi) = 11\,490$ m/s in Fig. 2. Thirty-one harmonics are used and $a/h = 1.5$. The gray region indicates the position of the silicon plate extending between $x_3 = 0$ and $x_3 = h$.

vanishing values outside the plate. These values have no special physical meaning and are absent from the kinetic or elastic energy of the modes because $\rho = 0$ and $c_{ijkl} = 0$ outside the plate. The stresses outside the plate are found to be close to zero, but not to vanish because of the approximate nature of the solution. The observed oscillations are characteristic of the number of harmonics used.

We also checked the consistency of the PWE method in comparison with the dispersion diagram of Lamb waves of a steel plate given in [1, ch. 5] and obtained no apparent difference. Intuitively, it can be expected that the accuracy of the method will be reduced for higher-order plate modes, because they have sharper spatial variations along axis x_3 and hence require more harmonics to be captured in the solution. Estimating from the equations the number of modes that are correctly converged for a given number of harmonics is not straightforward. However, convergence in a given (k_1, ω) window can always be estimated numerically by increasing the number of harmonics until the dispersion diagram remains unchanged.

Regarding multilayer systems, obtaining the exact dispersion relation for all modes is a difficult problem for most practical cases. There exist many rigorous methods to deal with wave propagation in such structures. To cite a few, and especially those that can cope with piezoelectric materials, we can mention transmission matrix methods [2], [11] or the Campbell and Jones method [12], whereby the SAW phase velocity in multilayer system can be obtained. Various improvements of the matrix method have been proposed to ensure numerical stability [13]–[16]. In all of these methods, plane wave propagation in the individual layers is solved very accurately, however the plate modes must satisfy boundary conditions which are considered at the end of the computation in the form of determinants. Finding all the zeros of such determinants is certainly possible numerically, but sometimes requires a very fine sampling in terms of frequency and wavevectors, otherwise some modes can be missed. The correct sampling rate can hardly be predicted and has to be found by trial-and-error in practice. Alternatively, the PWE method presented previously yields the band structure of all plate modes at once as an eigenvalue problem, with the boundary conditions again satisfied implicitly. As an illustration, we consider in Fig. 5 the case of a SiO_2/diamond/Si multilayer. This multilayer is composed of a 20 μm-thick layer of silicon, a 10 μm-thick layer of diamond, and a layer of SiO_2 with a thickness $t_3 = 20$, 40, or 60 μm. It can be further checked that the SAW velocities of the two outer materials, Si and SiO_2, are found as limiting values for large k, whatever the thickness of the layers. It is worth mentioning that the computation requirements for the single plate and the multilayer are not significantly different, and no parametric adjustment other than selecting an adequate number of harmonics has been performed to obtain Fig. 5.

IV. Extension to Piezoelectric Materials

The extension of the method to piezoelectric materials requires some adjustment because of the fact that the dielectric tensor does not vanish in a vacuum. This creates a possibility of numerical coupling between the periodic replicas of the plate through evanescent electromagnetic waves, even though they transport no energy away from the plate surfaces. In practice, numerical instability is observed for large k values if the formulas of Section II are directly applied. To preserve the numerical characteristics of the solution, we choose to work with the polarization $\mathbf{P}$ instead of the electric displacement $\mathbf{D}$. Both are simply related by $\mathbf{D} = \varepsilon_0\mathbf{E} + \mathbf{P}$, so that $\mathbf{P}$ vanishes in a vacuum. By straightforward algebra, it can be shown that the

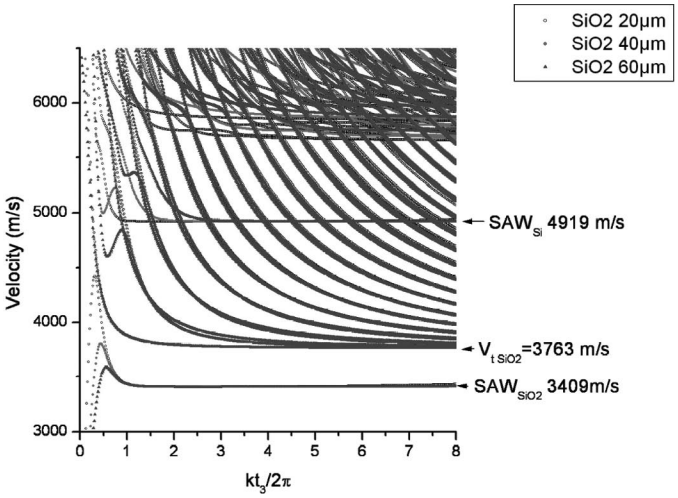

Fig. 5. Band structure computed by the PWE method for a SiO_2/diamond/Si multilayer elastic plate. This multilayer is composed of a silicon layer (20 µm thick), a diamond layer (10 µm thick), and a SiO_2 layer (thickness t_3 = 20, 40, and 60 µm). Sixty-one harmonics are used and $a/h = 1.2$.

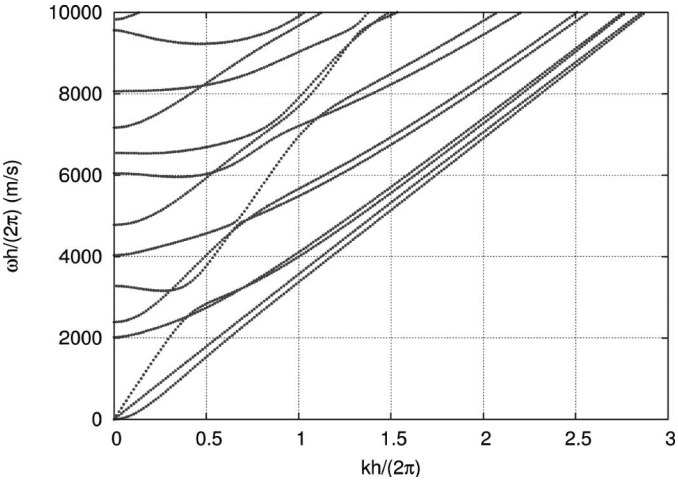

Fig. 6. Band structure computed by the PWE method for an *X*-cut lithium niobate plate (*Z* propagation).

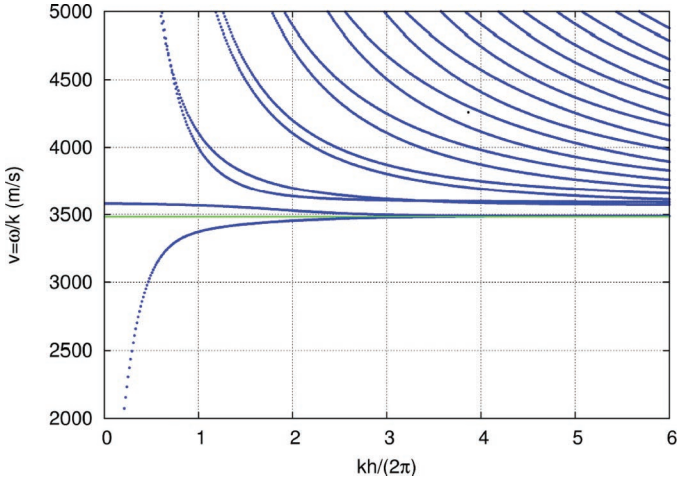

Fig. 7. Plate wave velocities as a function of the normalized wave vector *kh* computed by the PWE method for an *X*-cut lithium niobate plate (*Z* propagation). The SAW velocity (v = 3483.3 m/s) is shown as a solid line.

TABLE I. Estimation of the Error in the Evaluation of the SAW Velocity for Some Lithium Niobate Cuts.

	LN cut			
	(XZ)	(XY)	(ZX)	(ZY)
SAW velocity (m/s)	3483	3696	3779	3902
PWE error (m/s)	4	3	11	9
PWE error (%)	0.11	0.08	0.29	0.23

The reference SAW velocity has been obtained by searching for the zero of the boundary condition determinant. The PWE estimates (31 harmonics) are all slightly above the reference value (convergence from above in energy).

eigenvalue problem of (4) is unchanged, except that $\varepsilon_{ij} - \varepsilon_0$ must be considered instead of ε_{ij} in the expression of matrix $\tilde{A}$. A consequence of this choice is that the free electrical boundary condition, which should be that D_3 is continuous at the solid-vacuum interface, is not strictly satisfied. Instead, the condition $P_3 = 0$ is continuously imposed (together with $P_1 = P_2 = 0$). In practice, this results in a bias in the eigenfrequency convergence.

As an illustration, we have considered a plate of lithium niobate. Figs. 6 and 7 display the band structure obtained for an *X*-cut plate with propagation along the *Z* direction. As opposed to the purely elastic case, convergence to the band structure of the isolated piezoelectric plate with free surfaces is only approximate. As Fig. 7 illustrates, the Rayleigh SAW velocity is slightly overshot by the slowest plate mode for large k values. Increasing the number of Fourier harmonics does not solve this problem. The convergence was checked for different cuts and propagation directions in lithium niobate. Table I summarizes the estimation error on the Rayleigh SAW velocity; it can be seen that this error remains well below 1% in all tested cases.

Before concluding, we attempt a short comparison with the polynomial approach popularized after the work of Datta and Hunsinger [17]. In this method, the $u_i(x_3)$ term in (1) is expanded over an orthogonal polynomial basis, the expansion being truncated to some number of polynomials N in practice. For surface acoustic waves in semi-infinite and possibly multilayered structures [17]–[19], Laguerre polynomials are used and an exponentially decreasing factor is included to fulfill the radiation condition at infinity. For plate waves, Hermite polynomials are used [20], [21]. As with the PWE method, the boundary conditions can easily be incorporated in the polynomial solution form and a generalized eigenvalue problem with a very moderate size is obtained for the mode frequencies. However, of the $3(N + 1)$ eigenmodes that are obtained, only those for which the eigenvalues and eigenvectors converge with increasing N are retained as solutions [17]. In contrast, we found no spurious eigenvalues with the PWE method. In addition, Lefebvre *et al.* [19], [20] mention that the polynomial approach works better under the restriction that the parameters of the constituent materials are close to each other. Such a study has yet to be performed for the PWE method and is left for future research.

V. Conclusion

We have discussed the computation of the band structure of plate waves using the plane wave expansion method. Boundary conditions at the surfaces of an elastic plate are included implicitly in the form of the solution, thus leading to an efficient eigenvalue problem. SAW velocities can be estimated from the slowest wave for large wave vectors. Examples for a single plate and a multilayer elastic plate were given, and extension to piezoelectric materials was discussed. We believe the method can be of value for numerical codes requiring a generic wave dispersion method that does not require an initial guess for the solution, as opposed to zero-finding procedures. We finally note that the method also applies to the computation of the complex band structure [22] of plate waves in multilayers, including both propagating and evanescent guided waves.

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