RELATIONS BETWEEN TRANSFER MATRICES AND NUMERICAL STABILITY ANALYSIS TO AVOID THE $\Omega d$ PROBLEM

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Abstract. The transfer matrix method is usually employed to study problems described by $N$ equations of matrix Sturm-Liouville (MSL) kind. In some cases a numerical degradation (the so called $\Omega d$ problem) appears thus impairing the performance of the method. We present here a procedure that can overcome this problem in the case of multilayer systems having piecewise constant coefficients. This is performed by studying the relations between the associated transfer matrix ($T$) and other transfer matrix variants. In this way it was possible to obtain the matrices which can overcome the $\Omega d$ problem in the general case and then in problems which are particular cases of the general one. In this framework different strategies are put forward to solve different boundary condition problems by means of these numerically stable matrices. Numerical and analytic examples are presented to show that these stable variants are more adequate than other matrix methods to overcome the $\Omega d$ problem. Due to the ubiquity of the MSL system, these results can be applied to the study of many elementary excitations in multilayer structures.

Key words. Transfer matrix, matrix Sturm-Liouville problem, numerical stability, quadratic eigenvalues, $\Omega d$ problem

AMS subject classifications. 34L16

1. Introduction. The study of elementary excitations in multilayer systems (heterostructures) continues to be a very active field of research due to the multiple applications of these systems for the design of devices with composite materials. In recent years magneto-electro-elastic materials [1] and piezoelectric multilayer structures [2, 3], among other systems, have been the object of many studies. The associated transfer matrix method [4] $T$ is one of the theoretical techniques most employed in the study of these systems. From the formal point of view this method is very adequate for the study of problems related with multilayer systems. It reflects in a very simple way the linearity of the problem, based on the fact that any solution can be expressed as a linear combination of a chosen basis of the corresponding functional space [4]. On the other hand, for several practical applications to different problems, the method is hampered by numerical instabilities, the most common one being called the $\Omega d$ problem [4]. The name associated to this numerical instability derives from the elastic waves studies where this instability is present at high frequencies $\Omega$ and/or big thicknesses ($d$) of the layers.

A description of this problem was given in [5] when studying wave propagation in layered elastic media at high frequencies. In this work the origin of the problem was assigned to the large frequency-thickness ($fd$) products. It was found that the modal calculations presented numerical difficulties and a matrix formulation, the $\delta$-matrix method, was proposed to deal with them. Another approach closely related with the scattering matrix method is the reflectivity matrix method [6]. Nevertheless the high frequency-thickness product instability has been a persistent feature in the study of

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*This work was supported by CONACYT (R. P.-S.), CONACYT grant 208108 (R. P.-A.) and the Spanish Ministerio de Ciencia y Economía through grant MAT2012-38045-C02-04 (V. R. V.)
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wave propagation in layered media as it can be seen in a later review [7]. The name Ωd problem was coined in [4]. There it was noticed that the expressions producing this instability are of the form Ωd where Ω stands for a function of the frequency or the equivalent magnitude for other elementary excitations.

Different techniques have been developed to deal with this problem. Some of them, as the global transfer matrix [4, 3], involve matrices with dimensions increasing with the number of layers forming the system. It is then clear that for systems including many layers the method will require big amounts of computer memory and time.

Other approaches employ transfer matrices with dimensions independent of the number of layers. Among them we can find the Stiffness matrix method [8, 9, 10, 11] (E), the Scattering matrix method [11, 12, 13] (S) and the method of the hybrid compliance-stiffness (or simply hybrid matrix) [11, 14, 15] (H). These methods have been mainly used in studies of elastic waves propagation in anisotropic systems and acoustic waves in piezoelectric systems.

All these studies have been performed in a separate way. There is no clear picture of the usefulness and limitations of the different approaches. Our aim is to give an unified view of the problem and present the most adequate transfer matrix variant to solve different problems. To this end we shall consider a general system of N differential equations of the matrix Sturm-Liouville (MSL) kind [4]. In this general framework the study of the expressions relating each different matrix with T will allow to understand how the different matrices elude the T numerical instabilities. To extend the use of these transfer matrix variants H, E and S to a wider range of physical problems involving multilayer systems we shall study the numerical stability of each matrix variant. In addition we shall present different strategies to be used in the case of common boundary value problems as superlattices or finite sandwiches in terms of H, E or S.

We must stress that our procedure can overcome this problem in the case of multilayer systems having piecewise constant coefficients. This is an important problem and covers many cases of practical interest.

Among the big amount of work done on this problem using other methods we can mention those based on the sextic formalism for the linear elasticity [16]. In this scheme the matricant matrix was introduced together with the impedance matrix and the two point impedance matrix [17]. This approach allows to deal with systems having inhomogeneous coefficients. Stable methods to compute the matricant and the impedance matrix with special integration schemes [18] and an alternative method based on the resolvent of a propagator have been presented recently [19, 20]. In these works the chain rule for the resolvent, together with a differential equation of Riccati kind for the obtention of the resolvent in continuous inhomogeneous media are presented. The resolvent is well adapted to get the spectrum and fields in these systems.

The general character of our approach allows the extension of the transfer matrix variants use to problems whose systems of equations are particular cases of the MSL. We shall illustrate, for example, the hybrid matrix numerical stability by numerical studies of the shear horizontal surface waves in piezoelectric multilayer systems.

In Section 2 we present the master equation of the matrix Sturm-Liouville system of equations. In Section 2.1 we introduce the quadratic eigenvalues problem leading to the linearly independent solutions of the system together with their eigenvalues for a homogeneous medium. We define in Section 2.2 the associated transfer matrix T and
introduce the form employed in the analysis of the numerical stability of the variants \( H \), \( E \) and \( S \). Section 2.3 introduces the \( \Omega \) problem together with the analysis of the \( T \) characteristics that can be the source of this numerical instability. Afterwards, the numerical stability of the hybrid matrix, Section 3.1, and the stiffness matrix, Section 3.2, are studied through their respective relations with \( T \) in an homogeneous domain. The analysis for the scattering matrix is presented in (Section 4.1). The composition rules for the different matrices considered here are analyzed in Section 4.2. Section 5 presents the strategies to solve several boundary problems in terms of \( H \), \( E \) or \( S \). A numerical example demonstrating the numerical stability of the hybrid matrix is also presented together with an analytic study of the well known Kronig-Penney model. Conclusions are presented in Section 6.

2. Matrix Sturm-Liouville system of equations (MLS). A matrix Sturm-Liouville problem emerges naturally in a wide range of physical and technological problems (see, for example Refs. [4, 21, 22], and citations therein). In this wide range of problems there are many belonging to the elasticity theory (see for example [23]), electromagnetism [24] and several other areas of classical physics. Some of these problems can be quite complicated as the magneto-electro-elastic waves [25]. A matrix Sturm-Liouville problem appears also in Quantum Mechanics and Solid State Physics. Particularly the Envelope Function Approximation (EFA) [26, 27] generates a massive class of systems of equations that follow the Sturm-Liouville equation in matrix form. Initially many of these systems of equations are three-dimensional, but in layered systems, as outlined in Figure 1, the normal modes can be chosen as exponential of \( i\vec{\kappa} \cdot \vec{\rho} \) multiplied by some function of the variable \( z \), the coordinate perpendicular to the interfaces. We denote by \( \vec{\rho} = xe_x + ye_y \) the position vector in the plane of the interfaces and by \( \vec{\kappa} = \kappa_x e_x + \kappa_y e_y \) the corresponding wavevector. In this way the equations of motion take the Sturm-Liouville form, namely:

\[
\frac{d}{dz} \left[ B(z) \cdot \frac{dF(z)}{dz} + P(z) \cdot F(z) \right] + Y(z) \cdot \frac{dF(z)}{dz} + W(z) \cdot F(z) = 0.
\]

This defines the matrix differential operator \( L(z) \). The unknown \( F(z) \) is the field under study: electronic wavefunctions, or envelope functions, if we deal with electronic states, vibration amplitude for elastic waves, or components of the electric field in some electrodynamic situations. In the case of the Full Phenomenological Model (FPM) for polar optical modes in heterostructures [21] the unknown field has several components: three mechanical amplitudes and a component which is interpreted as a coupled electrostatic potential [21]. The coefficients \( B(z) \), \( P(z) \), \( Y(z) \), and \( W(z) \) are square matrices of order \( N \), being \( N \) the number of coupled second order differential equations forming the system (2.1). These coefficients characterize the physical properties of the materials forming the multilayer system: dielectric constants, elastic coefficients, etc. As the multilayer structures studied here involve different materials these coefficients will be different for the different materials. The dot \( \cdot \) means standard matrix product.

As the linear differential form is defined from (2.1)

\[
A(z) = B(z) \cdot \frac{dF(z)}{dz} + P(z) \cdot F(z),
\]

then the first integration from \( z - \epsilon \) to \( z + \epsilon \) shows that \( A(z) \) is continuous for every \( z \) along the multilayer structure. The continuity of \( F(z) \) and \( A(z) \) along the structure
allows to obtain the composition rule for the transfer matrices defined from these magnitudes.

2.1. LI solutions. Quadratic Eigenvalues Problem. In the case of a homogeneous medium the differential equations system (2.1) takes the following form

\[ B \dddot{F} + (P + Y) \cdot \dot{F} + W \cdot F = 0. \]

In this simple case the linearly independent (LI) solutions of the differential equations system (2.1) can be expressed by means of exponentials [28, 29]

\[ F(z) = F_0 e^{ikz}. \]

The eigenvalues \( k \) are obtained from the zeros of the secular matrix determinant:

\[ \Theta(k) = -k^2 B + ik(P + Y) + W. \]

Now we are dealing with a quadratic eigenvalues problem (QEP) [22]. If matrix \( B \) is regular (\( \text{Det}[B] \neq 0 \)) we have a set of eigenvalues \( K = \{k_j, j = 1, 2, \ldots, 2N\} \) and the corresponding eigenfunctions \( F_j(z) = F_{j0} \exp[ik_jz] \). The amplitudes \( F_{j0} \) multiplied by a constant are obtained from the homogeneous linear equations system:

\[ \Theta(k_j) \cdot F_{j0} = 0. \]

The multiplicative constant is usually obtained by a normalization condition.

In the following, we shall always assume \( B^\dagger = B, \ W^\dagger = W \) and \( Y = -P^\dagger \), in order to ensure formal hermiticity of the operator \( L(z) \), see Ref. [4]. In this case the eigenvalues of the QEP satisfy the general property of being real or appearing in pairs: \( k_j \) and its complex conjugate \( k^*_j \).

2.2. Associated Transfer Matrix for the MSL equations system. We shall define the associated transfer matrix \( T(\alpha : z, z_0) \), which transfers the amplitudes \( F \) and the linear differential form \( A \) in a domain \( \alpha \), as in [4]:

\[ \begin{bmatrix} F(\alpha : z) \\ A(\alpha : z) \end{bmatrix} = T(\alpha : z, z_0) \cdot \begin{bmatrix} F(\alpha : z_0) \\ A(\alpha : z_0) \end{bmatrix}. \]

From now on we shall suppress the zonal argument \( \alpha \). Following the algebraic and analytic methods to calculate the matrix \( T(z, z_0) \), given in [4], we shall have:

\[ T(z, z_0) = Q(z) \cdot Q(z_0)^{-1}, \]

where the auxiliary matrix \( Q(z) \) is formed by a basis of eigenfunctions \( F_j(z) \) and of the linear differential forms \( A_j(z) = B(z) \cdot \frac{dF_j(z)}{dz} + P(z) \cdot F_j(z) \):

\[ Q(z) = \begin{bmatrix} F_1(z) & F_2(z) & \cdots & F_{2N}(z) \\ A_1(z) & A_2(z) & \cdots & A_{2N}(z) \end{bmatrix}. \]
For an homogeneous domain $\alpha$, with constant $B$, $P$ and $W$, we can choose the eigenfunctions $F_j(z) = F_{j0} e^{ikz}$, and after some manipulations on (2.9), we can separate the factors $F_{j0}$ from the exponentials $e^{ikz}$ in the form:

$$Q(z) = \begin{bmatrix} F_{0N} & F_{02N} \\ A_{0N} & A_{02N} \end{bmatrix} \cdot \begin{bmatrix} \Pi_{kN}(z-z_0) & 0 \\ 0 & \Pi_{k2N}(z-z_0) \end{bmatrix} \cdot \begin{bmatrix} \Pi_{kN}(z_0) & 0 \\ 0 & \Pi_{k2N}(z_0) \end{bmatrix}.$$

The submatrices $\Pi_{kN}(d)$ and $\Pi_{k2N}(d)$ are diagonal and the $j$th element is the exponential $e^{ikj} d$. $F_{0N}$, $A_{0N}$, $F_{02N}$ and $A_{02N}$ are square matrices of order $N$ whose elements are obtained in terms of the constant $F_{j0}$ and the corresponding $A_{j0}$. In our notation the subindex $\{N\}$ denotes that $j = 1, 2, \ldots, N$ and the subindex $\{2N\}$ means that $j = N + 1, N + 2, \ldots, 2N$.

By substituting $Q(z)$ in (2.8) and considering $d = z - z_0$ we have:

$$T(d) = \begin{bmatrix} F_{0N} & F_{02N} \\ A_{0N} & A_{02N} \end{bmatrix} \cdot \begin{bmatrix} \Pi_{kN}(d) & 0 \\ 0 & \Pi_{k2N}(d) \end{bmatrix} \cdot \begin{bmatrix} F_{0N} & F_{02N} \\ A_{0N} & A_{02N} \end{bmatrix}^{-1}.$$

The matrix $T(d)$ appearing in (2.10) can be interpreted as the associated transfer matrix (ATM) relating the vector $[F(z) \ A(z)]^T$ in the boundaries of an homogeneous domain with thickness $d$.

As the linear form $A(z)$ is continuous along the interface separating two adjacent domains, the ATM has the chain property. Then for an ensemble of $\mu$ layers sketched in Figure 1, the system ATM is obtained from the following matrix product:

$$T(z_r, z_\ell) = T(z_r - z_{\mu-1}) \ldots T(z_2 - z_1) \cdot T(z_1 - z_\ell),$$

where $z_\ell, z_1, z_2, \ldots, z_r$ are coordinates of the interfaces matching the different domains of the multilayer structure.

We shall start now the study of the $T$ characteristics which can be the source of the $\Omega d$ problem in the numerical calculations. With this knowledge we shall study later the numerical stability of the $H$, $E$ and $S$ matrices, by means of their relations with $T$.

2.3. $\Omega d$ problem. From (2.10) we can obtain expressions for the analysis of the numerical instability of the $T$ matrix elements for any $N$. For real eigenvalues (allowed regions) we have:

$$T_{ls} = \sum_{j=1}^{2N} A_{lsj} \cos(k_j d) + i \sin(k_j d),$$

whereas for complex eigenvalues (forbidden regions) we shall have combinations of decreasing and increasing exponentials:

$$T_{ls} = \sum_{j=1}^{N} C_{lsj} \tau_j e^{i|3(k_j)| d} \left(1 \pm D_{lsj} e^{-2|3(k_j)| |d|}\right).$$

The coefficients $A_{lsj}, C_{lsj}$ and $D_{lsj}$ are expressed in terms of the elements of $F_{0N}, A_{02N}, F_{02N}$ and $A_{02N}$. In (2.13) we have separated the $k_j$ eigenvalue real $\Re(k_j)$ and
imaginary $\Im(k_j)$ parts. The real part is included in the $\tau_j = e^{i\Re(k_j)}d$ factor having a bounded value.

For real eigenvalues the $T$ elements are represented by means of trigonometric functions which are bounded by $\pm 1$. In this case the $\Omega d$ problem does not appear when the product $(k_j d)$ increases. On the other hand, for complex eigenvalues the mixing of terms with increasing and decreasing exponential values present in (2.13) may give rise to this numerical instability.

For increasing $k_j d$ leading to $D_{lsj}e^{-2|\Im(k_j)|}d \approx u$ (unit roundoff) the $(1 \pm D_{lsj}e^{-2|\Im(k_j)|}d)$ operation is rounded to 1.0 by the computer. Thus the result (1.0) will have a roundoff error. The number $u$ (unit roundoff) is the machine precision, that is, the value to be added to 1.0 to produce a result different from 1.0. This number can be calculated as $u = \frac{1}{2}\beta^{1-t}$ [30], where $\beta$ is the base of the floating point number system and $t$ its precision (can be understood as the number of digits used to give a value). The roundoff error is defined as the difference between the calculated approximation of a number and its exact mathematical value. When the roundoff result is 1.0 the absolute value of this error $E_{abs}$ is bounded $E_{abs} \leq u$ [30]. In the double precision decimal system ($\beta = 10$, $t = 16$) we have $u = 5 \times 10^{-16}$.

If we assume that the calculation of a term $C_{lsj} \tau_j e^{i\Im(k_j)}d (1 \pm D_{lsj}e^{-2|\Im(k_j)|}d)$ of (2.13) is performed with roundoff, then the result will be affected by a roundoff error with absolute value $E_r$ given by:

\[(2.14) \quad E_r \leq C_{lsj} \tau_j e^{i\Im(k_j)}d u.\]

Depending on the numerical problem under study the right-hand side in (2.14) can
have a high value and also a big $E_r$ error. The roundoff error can be accumulated when the final result to be obtained (e.g., eigenvalues or parameters of a given problem) is preceded by a sequence of calculations prone to roundoff errors. In these cases the error can dominate the calculations thus giving a very inaccurate final result. When this happens we are in the presence of the numerical instability called Ωd problem.

In practice it is quite easy to deal with problems in which the $T$ determinant is constant and equal to one. This can be used as a test of the numerical accuracy in the real calculations. When the numerical instability is present the Det[$T$] takes values quite different from the exact one, being in some cases several orders of magnitude bigger or smaller than 1.0.

The expression (2.13) shows also clearly that the $T_{ts}$ elements increase indefinitely when exponential argument $|\Im(k_j)| \to \infty$. In this case the $T$ matrix overflows and cannot be calculated numerically. Thus it is clear that in the $T$ numerical applications we can find two kinds of numerical instability: the Ωd problem and the matrix overflow.

3. Hybrid matrix and Stiffness matrix of the MSL system. We can define new matrices in the domain $\alpha$, where $T$ was defined, by changing the arrangement of the $F(z)$, $A(z)$, $F(z_0)$ and $A(z_0)$ vectors in (2.7). Some examples are the Hybrid Compliance-Stiffness matrix ($H$) and the Stiffness matrix ($E$):

\begin{equation}
\begin{vmatrix}
F(\alpha : z_0) \\
A(\alpha : z)
\end{vmatrix} =
\begin{vmatrix}
H(\alpha : z; z_0) \\
A(\alpha : z_0)
\end{vmatrix}.
\end{equation}

\begin{equation}
\begin{vmatrix}
A(\alpha : z_0) \\
A(\alpha : z)
\end{vmatrix} =
\begin{vmatrix}
E(\alpha : z; z_0) \\
F(\alpha : z_0)
\end{vmatrix}.
\end{equation}

The Hybrid Compliance-Stiffness matrix was employed in Ref. [14] as a stable variant to study the propagation of an acoustic wave in an anisotropic multilayer system. The acoustic wave equations of motion are a particular case of the system (2.1) including the displacement vector as $F(z)$ and the force vector normal to the interfaces as $A(z)$.

Following this procedure we can define up to 24 interrelated matrices related among them. In fact we obtain 12 different matrices and their respective inverses. Among them we find $T^{-1}$, $H^{-1}$ and $E^{-1}$. The matrix $E^{-1}$ is known as Compliance matrix, see Refs. [14, 8]. By taking as reference the expressions defining $T$, $H$, $E$, $T^{-1}$, $H^{-1}$ and $E^{-1}$ is possible to obtain from them other three different matrices which will exhibit a similar numerical behaviour. A first matrix is obtained by permuting among them the positions of the vectors in the right-hand side of the matrix taken as reference (e.g., the $A(\alpha : z_0)$ and $F(\alpha : z)$ vectors in the right-hand side of (3.1)). The second matrix is obtained by means of the other operation applied to the vectors in the left-hand side of the matrix taken as reference. The third one is the result of both permutations. The Appendix A shows, by means of the relations between the matrices, that the matrices defined in this way will have a similar behaviour from the numerical point of view.

We obtain $T(-d)$ by inversion of (2.10). Thus $T^{-1}$ will have the same numerical behaviour than $T$. When inverting the expressions for $H(d)$ and $E(d)$ the result is the permutation of the $F_{0\infty}$ submatrix with the $A_{0\infty}$ one and of the $F_{\infty 0}$ submatrix with the $A_{\infty 0}$ one. Thus $H^{-1}$ and $E^{-1}$ will have also a numerical behaviour similar to those of their counterparts.
3.1. Analysis of the numerical instability of the Hybrid matrix of the MSL system. The following relations can be obtained from Eqs. (2.7) and (3.1):

\begin{equation}
H = \begin{bmatrix}
-T_{11}^{-1} & T_{12} \\
T_{22} - T_{21} \cdot [T_{11}]^{-1} - T_{12} & T_{21} \cdot [T_{11}]^{-1}
\end{bmatrix},
\end{equation}

On the other hand, equations (2.7) and (2.8) exhibit an important property. Equation (2.8) leads to a unique ATM expression (2.10) was built from a base of solutions $F_j(z) = F_{j0} e^{i k_j z}$, in such a way that $\Pi_{kN}(d)$ contains the eigenvalues with positive imaginary part $\Im(k_1, k_2, \ldots, k_N) > 0$ and $\Pi_{k2N}(d)$ the eigenvalues with negative imaginary part $\Im(k_{N+1}, k_{N+2}, \ldots, k_{2N}) < 0$. In this way the submatrices $\Pi_{kN}(d)$ and $\Pi_{k2N}(d)$ reduce to the order $N$ nil matrix (0N) when the thickness $d \rightarrow \infty$ whereas the elements of $\Pi_{kN}(d)$ and $\Pi_{k2N}(d)$ tend to infinity.

Appendix B contains the expressions for the $N$ order partitions: $T_{11}, T_{12}, T_{21}$ and $T_{22}$ obtained from (2.10). With the help of (3.3) we have:

\begin{equation}
H_{11} = \begin{bmatrix}
A_{0N} \cdot F_{02N}^{-1} - \gamma_{21} \cdot \Pi_{kN}(-d) \cdot F_{0N}^{-1} \cdot F_{02N} \cdot \Pi_{k2N}(d) \cdot \gamma_{12}^{-1}
\end{bmatrix}^{-1} + \\
A_{0N} \cdot F_{0N}^{-1} - \gamma_{22} \cdot \Pi_{k2N}(-d) \cdot F_{0N}^{-1} \cdot F_{02N} \cdot \Pi_{kN}(d) \cdot \gamma_{11}^{-1}
\end{equation}

\begin{equation}
H_{12} = \gamma_{12} \cdot \Pi_{k2N}(-d) \cdot F_{02N}^{-1}
\end{equation}

\begin{equation}
H_{21} = \begin{bmatrix}
A_{0N} - H_{22} \cdot F_{0N} \cdot \Pi_{kN}(d) \cdot \gamma_{21}^{-1} + \\
A_{02N} - H_{22} \cdot F_{02N} \cdot \Pi_{k2N}(d) \cdot \gamma_{22}^{-1}
\end{bmatrix}^{-1}
\end{equation}

\begin{equation}
H_{22} = \begin{bmatrix}
F_{0N} \cdot A_{02N}^{-1} - F_{02N} \cdot \Pi_{k2N}(d) \cdot A_{0N}^{-1} \cdot A_{02N} \cdot \Pi_{kN}(d) \cdot A_{0N}^{-1}
\end{bmatrix}^{-1} + \\
\begin{bmatrix}
F_{02N} \cdot A_{02N}^{-1} - F_{0N} \cdot \Pi_{kN}(d) \cdot A_{02N}^{-1} \cdot A_{0N} \cdot \Pi_{k2N}(-d) \cdot A_{02N}^{-1}
\end{bmatrix}^{-1}
\end{equation}

The coefficients $\gamma_{11}, \gamma_{12}, \gamma_{21}$ and $\gamma_{22}$ are obtained in terms of $F_{0N}, F_{02N}, A_{0N}$ and $A_{02N}$ as indicated in Appendix B.

When $d$ increases indefinitely the expressions (3.4-3.6) are reduced to:

\begin{equation}
H_{11}|_{d \rightarrow \infty} = F_{0N} \cdot A_{0N}^{-1} \cdot [I_N - 0_N]^{-1} = F_{0N} \cdot A_{0N}^{-1}
\end{equation}

\begin{equation}
H_{12}|_{d \rightarrow \infty} = 0_N \cdot [I_N - 0_N]^{-1} = 0_N
\end{equation}

\begin{equation}
H_{21}|_{d \rightarrow \infty} = \begin{bmatrix}
A_{02N} - A_{0N} \cdot F_{02N}^{-1} \cdot [I_N - 0_N]^{-1} \cdot F_{0N}
\end{bmatrix} \cdot 0_N
\end{equation}

\begin{equation}
H_{22}|_{d \rightarrow \infty} = A_{02N} \cdot F_{02N}^{-1} \cdot [I_N - 0_N]^{-1} = A_{02N} \cdot F_{02N}^{-1}.
\end{equation}
We denote by \([I_N - 0_N]\) the \(N\) order identity matrix obtained with roundoff, whose elements are characterized by a roundoff error with absolute value \(Er \leq u\) (unit roundoff). Thus, the \(H\) matrix elements will be characterized by an error whose absolute value is of order of \(u\). These results show that the MLS matrix \(H\) converges to finite values, without significant precision loss, when \(d\) increases indefinitely.

On the other hand when \(d \to 0\) we obtain immediately from (2.10) that \(T = I_{2N}\) and by substituting its partitions of order \(N\) in (3.3) we obtain:

\[
H|_{d \to 0} = \begin{bmatrix} 0_N & I_N \\ I_N & 0_N \end{bmatrix}, \tag{3.12}
\]

thus \(H\) also converges in a numerically stable way when \(d \to 0\).

3.2. Numerical stability of the Stiffness matrix of the MSL system.

From the expressions (2.7) and (3.2) we derive the following relations:

\[
E = \begin{bmatrix} \begin{bmatrix} T_{12} \end{bmatrix}^{-1} \cdot T_{11} & \begin{bmatrix} T_{12} \end{bmatrix}^{-1} \\ T_{21} - T_{22} \cdot \begin{bmatrix} T_{12} \end{bmatrix}^{-1} \cdot T_{11} & T_{22} \cdot \begin{bmatrix} T_{12} \end{bmatrix}^{-1} \end{bmatrix}. \tag{3.13}
\]

The Stiffness matrix obtained from equation (3.13) will be, as the \(H\) matrix, independent of the base of the LI solutions chosen to build \(T\). Because of this we consider also the ATM coming from the expression (2.10), which was obtained from a base of solutions \(F_j(z) = F_{j0} e^{ik_j z}\), where \(\Pi_{k_N}(d)\) contains the eigenvalues with positive imaginary part: \(\Im(k_1, k_2, \ldots k_N) > 0\) and \(\Pi_{k_{2N}}(d)\) contains the eigenvalues with negative imaginary part: \(\Im(k_{N+1}, k_{N+2}, \ldots k_{2N}) < 0\).

Following the same procedure employed for \(H\) we substitute in (3.13) the expression of the partitions \(T_{11}, T_{12}, T_{21}\) and \(T_{22}\) given in the Appendix B and calculate the limit of the partitions of \(E\) when \(d \to \infty\), to obtain:

\[
E_{11}|_{d \to \infty} = A_{0_N} \cdot F_{0_N}^{-1} \cdot [I_N - 0_N]^{-1} = A_{0_N} \cdot F_{0_N}^{-1} \tag{3.14}
\]

\[
E_{12}|_{d \to \infty} = 0_N \cdot [I_N - 0_N]^{-1} = 0_N \tag{3.15}
\]

\[
E_{21}|_{d \to \infty} = \begin{bmatrix} A_{0_N} - A_{0_{2N}} \cdot F_{0_{2N}}^{-1} \cdot [I_N - 0_N]^{-1} \cdot F_{0_N} \end{bmatrix} \cdot 0_N \tag{3.16}
\]

\[
E_{22}|_{d \to \infty} = A_{0_{2N}} \cdot F_{0_{2N}}^{-1} \cdot [I_N - 0_N]^{-1} = A_{0_{2N}} \cdot F_{0_{2N}}^{-1}. \tag{3.17}
\]

These results show that the \(E\) matrix also converges to finite values without a significant precision loss when \(d\) grows indefinitely. On the other hand, when \(d \to 0\), we know that \(T = I_{2N}\), which means that \(T_{12} = T_{21} = 0_N\) and then the \(E\) matrix is not numerically computable (overflow) as is directly obtained from the relations (3.13).

Let us now assume that \(d\) is very small but not enough to provoke the overflow state. From (3.13) we can express the partition \(E_{21}\) in the following form:

\[
E_{21} = - (I_N - T_{21} \cdot T_{11}^{-1} \cdot T_{12} \cdot T_{22}^{-1}) \cdot T_{22} \cdot T_{12}^{-1} \cdot T_{11}, \tag{3.18}
\]

then for a sufficiently small \(d\) this partition will be the object of the roundoff in the first place, giving:
Unlike the limits given in (3.14)-(3.16) the term \( T_{12}^{-1} \) subjected to the round-off, multiplies now a term \( T_{12}^{-1} \) whose value can be big enough to affect the Stiffness matrix due to the roundoff error and then gives rise to the \( \Omega_d \) problem.

4. Scattering Matrix and Coefficients Transfer Matrix for the MSL system. In the case of the Scattering Matrix (\( S \)) its relation with \( T \) is not a direct one (because there are other matrices involved) as in the relations studied previously. A possible way to relate \( S \) with \( T \) is by using the Coefficients Transfer Matrix (\( K \)). We need to use the direct relation \( S - K \) and the indirect one \( K - T \). Being known a base of solutions \( F_j(\alpha, z) \) in a domain \( \alpha \) the general solution \( F_p(\alpha, z) \) of the differential system (2.1) can be written as:

\[
F(\alpha, z) = \sum_{j} a_j(\alpha) F_j(\alpha, z) .
\]

Let be \( a^{+/-}(\alpha) \) the \( N \)-vector formed by the coefficients \( a_j(\alpha) \) of the amplitudes travelling to the right/left. Then we shall denote as \( K(R, L) \) the Coefficients Transfer Matrix transferring the ensemble of coefficients \( a^{+/-} \) from domain \( L \) to domain \( R \):

\[
\begin{bmatrix}
  a^{+}(R) \\
  a^{-}(R)
\end{bmatrix}
= K(R, L) \cdot
\begin{bmatrix}
  a^{+}(L) \\
  a^{-}(L)
\end{bmatrix} .
\]

The term Scattering Matrix is widely used in the literature and can be defined in different ways. Here we shall use the definition and notation \( S(R; L) \) employed in [4]:

\[
\begin{bmatrix}
  a^{-}(L) \\
  a^{+}(L)
\end{bmatrix}
= S(R; L) \cdot
\begin{bmatrix}
  a^{+}(R) \\
  a^{-}(R)
\end{bmatrix} .
\]

From these definitions we obtain a direct relation between \( S \) and \( K \):

\[
S = \begin{bmatrix}
  \frac{1}{[K_{22}]^{-1}} \cdot K_{21} & \frac{1}{[K_{22}]^{-1}} \\
  K_{11} - \frac{1}{K_{12} \cdot [K_{22}]^{-1}} \cdot K_{21} & \frac{1}{K_{12} \cdot [K_{22}]^{-1}}
\end{bmatrix} .
\]

By taking into account that between the domains \( R \) and \( L \) there is an intermediate region \( M \) (can be a single or a multiple layer) described by a \( T \) matrix, it is possible to obtain [4]:

\[
K(R, L) = \left[ Q(R : z_r) \right]^{-1} \cdot T(z_r, z_\ell) \cdot Q(L : z_\ell) ,
\]

where \( z_r/\ell \) are the coordinates of the interfaces matching the intermediate region \( M \) with the external domains \( R \) (to the right)/\( L \) (to the left). The matrix \( Q(z) \) for an arbitrary domain is given in (2.9). Expression (4.5) shows clearly that the matrix \( K \) and consequently \( S \) depends on the base of LI solutions chosen to build the matrix \( Q \). It is a common practice to choose a reduced base in \( z_r/\ell \), that is a base tending to unity in \( z_r/\ell \).
4.1. Analysis of the numerical stability of the Scattering Matrix (SM).

In the first place we substitute in (4.5) the expressions (B.2) giving the $T$ partitions when $d \to \infty$. Now we substitute in (4.4) the expressions obtained for the partitions of $K$ and obtain:

\begin{align*}
S_{11}|_{d \to \infty} &= -\left[\gamma_{12}^{-1} \cdot (I_N + 0_N) \cdot Q(z_\ell)_{12} + \gamma_{22}^{-1} \cdot (I_N + 0_N) \cdot Q(z_\ell)_{22}\right]^{-1} \\
&\cdot \left[\gamma_{12}^{-1} \cdot (I_N + 0_N) \cdot Q(z_\ell)_{11} + \gamma_{22}^{-1} \cdot (I_N + 0_N) \cdot Q(z_\ell)_{21}\right] ; \\
S_{12}|_{d \to \infty} &= \left[\gamma_{12}^{-1} \cdot (I_N + 0_N) \cdot Q(z_\ell)_{12} + \gamma_{22}^{-1} \cdot (I_N + 0_N) \cdot Q(z_\ell)_{22}\right]^{-1} \\
&\cdot \Pi_{b_{2N}}(d)|_{d \to \infty} \cdot [(Q(z_r)^{-1})_{21} \cdot F_{02N} + (Q(z_r)^{-1})_{22} \cdot A_{02N}]^{-1} \\
S_{21}|_{d \to \infty} &= 0_N ; \\
S_{22}|_{d \to \infty} &= [(Q(z_r)^{-1})_{11} \cdot F_{02N} + (Q(z_r)^{-1})_{12} \cdot A_{02N}] \\
&\cdot [(Q(z_r)^{-1})_{21} \cdot F_{02N} + (Q(z_r)^{-1})_{22} \cdot A_{02N}]^{-1}.
\end{align*}

We have used the notation $Q(z_r)$ instead of $Q(R : z_r)$ and $Q(z_\ell)$ instead of $Q(L : z_\ell)$ to simplify the expressions. The term $[I_N + 0_N]$ is an identity matrix of order $N$ obtained by roundoff whose elements have a roundoff error with absolute value $Eu \leq u$ (unit roundoff). Because of this the matrix elements of $S$ will have an error with absolute value of the order of $u$. These results show that the $S$ matrix of a MSL system converges also to finite values without significant precision loss when $d$ increases indefinitely.

On the other hand, if the intermediate region $M$ thickness is nil (no $M$ region, $z_\ell = z_r = z_s$) we obtain from (4.5) that $K(R, L) = [Q(R : z_s)]^{-1} \cdot Q(L : z_s)$ and we can obtain $S$ without trouble. This means that the $S$ matrix of the MSL can avoid the $\Omega d$ problem and converge in a stable numerical way when $d \to 0$.

4.2. Composition rules. The hybrid matrix $H^{(m)}$ relating the field and the linear form in the positions $z_{m-1}$ and $z_r$ of the sketch shown in Figure 1 can be described as the hybrid matrix of the structure formed by the layers $m, m + 1, \ldots, \mu$:

\begin{equation}
\begin{bmatrix}
F(m : z_{m-1}) \\
A(\mu : z_r)
\end{bmatrix} = H^{(m)} \\
\begin{bmatrix}
A(m : z_{m-1}) \\
F(\mu : z_r)
\end{bmatrix}.
\end{equation}

We use here the supraindex $m$ among parentheses to denote the hybrid matrix of the structure being considered in a similar way to that employed in Ref. [14]. The partitions of the matrix given in (4.10) can be expressed in terms of the $H^{(m+1)}$ matrix partitions corresponding to the structure including the layers from $m + 1$ to $\mu$ and of the matrix $H^m$ given by (3.1) relating the field and the linear form in the layer $m$ borders $z_0 = z_{m-1}$ and $z = z_m$. We must take into account the continuity of the field and the associated linear form in $z_m$, $F/A(m+1 : z_m) = F/A(m : z_m)$.

Then we obtain the following composition rule:
\[ H_{11}^{(m)} = H_{11}^{m} + H_{12}^{m} \cdot H_{11}^{(m+1)} \cdot \left[I_N - H_{22}^{m} \cdot H_{11}^{(m+1)}\right]^{-1} \cdot H_{21}^{m} \]
\[ H_{12}^{(m)} = H_{12}^{m} \cdot \left[I_N + H_{11}^{(m+1)} \cdot \left[I_N - H_{22}^{m} \cdot H_{11}^{(m+1)}\right]^{-1} \cdot H_{22}^{m}\right] \cdot H_{12}^{(m+1)}; \]
\[ H_{21}^{(m)} = H_{21}^{(m+1)} \cdot \left[I - H_{22}^{m} \cdot H_{11}^{(m+1)}\right]^{-1} \cdot H_{21}^{m}; \]
\[ (4.11) H_{22}^{(m)} = H_{22}^{(m+1)} + H_{21}^{(m+1)} \cdot \left[I_N - H_{22}^{m} \cdot H_{11}^{(m+1)}\right]^{-1} \cdot H_{22}^{m} \cdot H_{12}^{(m+1)}. \]

In the same way the Stiffness matrix relating the field and the linear form in the positions \( z_{m-1} \) and \( z_r \) can be described as the Stiffness matrix of the structure formed by the layers \( m, m+1, \ldots, \mu \):

\[ (4.12) \begin{bmatrix} A(m : z_{m-1}) \\ A(\mu : z_r) \end{bmatrix} = E^{(m)} \begin{bmatrix} F(m : z_{m-1}) \\ F(\mu : z_r) \end{bmatrix}, \]

and its composition rule in terms of \( E^{(m+1)} \) and \( E^m \) is given by:

\[ E_1^{(m)} = E_{11}^m + E_{12}^m \cdot \left[E_{11}^{(m+1)} - E_{22}^m\right]^{-1} \cdot E_{21}^m; \]
\[ E_2^{(m)} = -E_{12}^m \cdot \left[E_{11}^{(m+1)} - E_{22}^m\right]^{-1} \cdot E_{12}^{(m+1)}; \]
\[ E_2^{(m+1)} = E_{21}^{(m+1)} \cdot \left[E_{11}^{(m+1)} - E_{22}^m\right]^{-1} \cdot E_{21}^m; \]
\[ (4.13) E_{22}^{(m)} = E_{22}^{(m+1)} - E_{21}^{(m+1)} \cdot \left[E_{11}^{(m+1)} - E_{22}^m\right]^{-1} \cdot E_{12}^{(m+1)} \]

Analogously, the composition rule for the Scattering matrix \( S(R; m) \), can be expressed in terms of the matrices \( S(R; m + 1) \) and \( S(m + 1; m) \), each one defined in agreement with (4.3) for the interfaces placed between the domains \( m \) and \( R \), between \( m + 1 \) and \( R \) and between \( m \) and \( m + 1 \), respectively. This composition rule can be expressed by means of the product denoted by \( \otimes \), in the form:

\[ (4.14) S(R; m) = S(R; m + 1) \otimes S(m + 1; m). \]

Given three matrices \( Z, Y \) and \( X \) of order \( 2N \) subdivided in their \( N \times N \) partitions the product \( \otimes \) expressing \( Z = Y \otimes X \) is defined in [4] by means of the composition rule:

\[ Z_{11} = X_{11} + X_{12} \cdot Y_{11} \cdot \left[I_N - X_{22} \cdot Y_{11}\right]^{-1} \cdot X_{21}; \]
\[ Z_{12} = X_{12} \cdot Y_{12} + X_{12} \cdot Y_{11} \cdot \left[I_N - X_{22} \cdot Y_{11}\right]^{-1} \cdot X_{22} \cdot Y_{12}; \]
\[ Z_{21} = Y_{21} \cdot \left[I_N - X_{22} \cdot Y_{11}\right]^{-1} \cdot X_{21}; \]
\[ Z_{22} = Y_{22} + Y_{21} \cdot \left[I_N - X_{22} \cdot Y_{11}\right]^{-1} \cdot X_{22} \cdot Y_{12}. \]

We must note that the composition rules (4.11) and (4.15) include the inverses \( \left[I_N - H_{22}^{m} \cdot H_{11}^{(m+1)}\right]^{-1} \) and \( \left[I_N - S_{22}^{(m + 1; m)} \cdot S_{11}^{(R; m + 1)}\right]^{-1} \) respectively, which
are regular even when the thickness of the layer or of the multilayer goes to infinity or to zero. The composition rule (4.13) includes the term $\left[E_{11}^{(m+1)} - E_{22}^m\right]^{-1}$, which is regular when the thickness of the layer or of the multilayer goes to infinity. For very small thicknesses this composition rule will lead to the accumulation of the roundoff errors.

5. General formulation of some typical boundary problems. Numerical examples. The boundary problems can be formulated in terms of the $T$, hybrid, scattering or stiffness matrices. We consider a system formed by three domains $L - M - R$. The internal domain $M$ can be formed by one or several homogeneous layers in whose case the matrix of the structure $M$ must be obtained through composition rules (see Section 4.2). In the external domains $L$ and $R$ we can have different media and even the vacuum. Depending on the problem under study we shall employ different boundary conditions at the interface $L|M$ with coordinate $z_\ell$ and at $M|R$ with coordinate $z_r$. We denote by $F(\ell/r), A(\ell/r)$ the field and the associated linear form at the coordinate $z_\ell/z_r$. In all the cases here considered we avoid to use submatrices which can exhibit numerical instabilities when $d \to \infty$, as it happens for $H_{12}^{-1}$ or $E_{12}^{-1}$.

5.1. Escape problem. We shall study the escape problem in a system formed by three domains $L - M - R$ having full matching conditions (FMC) at the interface $L|M$ with coordinate $z_\ell$ and at the interface $M|R$ with coordinate $z_r$. In the escape problem we shall have only outgoing waves in $M$. Applying the continuity conditions at the interface we can write:

$$
\begin{bmatrix}
F(\ell^-) \\
A(\ell)^+ 
\end{bmatrix} = 
\begin{bmatrix}
H(r, \ell) \\
A(r)^- 
\end{bmatrix} \cdot 
\begin{bmatrix}
A(\ell^-) \\
F(r)^+ 
\end{bmatrix}.
$$

(5.1)

The superindex $\pm$ denote the vectors related with the wave travelling in $R/L$ towards the right/left. From the two matrix equations coming from (5.1) we can write:

$$
0 = 
\begin{pmatrix}
-I_N & H_{11}(r, \ell) & H_{12}(r, \ell) & 0_N \\
0_N & H_{21}(r, \ell) & H_{22}(r, \ell) & -I_N
\end{pmatrix} \cdot 
\begin{bmatrix}
F(\ell)^- \\
A(\ell)^- \\
0_N \\
A(r)^+
\end{bmatrix}.
$$

(5.2)

We can express the vectors appearing in the right-hand side of (5.2) in the form:

$$
\begin{bmatrix}
F(\ell)^- \\
A(\ell)^-
\end{bmatrix} = 
\begin{bmatrix}
F_1(\ell)^- & \ldots & F_N(\ell)^- \\
A_1(\ell)^- & \ldots & A_N(\ell)^-
\end{bmatrix} \cdot 
\begin{bmatrix}
a_1(L)^- \\
\vdots \\
a_N(L)^-
\end{bmatrix} = LI(\ell)^- \cdot a(L)^-,
$$

(5.3)

$$
\begin{bmatrix}
F(\ell)^- \\
A(\ell)^-
\end{bmatrix} = 
\begin{bmatrix}
F_1(\ell)^+ & \ldots & F_N(\ell)^+ \\
A_1(\ell)^+ & \ldots & A_N(\ell)^+
\end{bmatrix} \cdot 
\begin{bmatrix}
a_1(R)^+ \\
\vdots \\
a_N(R)^+
\end{bmatrix} = LI(r)^+ \cdot a(R)^+,
$$

(5.4)

where $F_j(\ell)^-$ are LI solutions belonging to the $L$ domain, evaluated at $z_\ell$ and $F_j(r)^+$ are LI solutions belonging to the $R$ domain, evaluated at $z_r$. The $N$-vector $a(R)^+$ is
formed by the coefficients $a_j(R)^+$ from those waves travelling to the right at $R$ and $a_j(L)^-$ by the coefficients $a_j(L)^-$ from those waves travelling to the left at $L$.

Then by using (5.3) and (5.4) we transform (5.2) into the secular system:

\[
0 = \begin{pmatrix}
Ms_{11} & Ms_{12} \\
Ms_{21} & Ms_{22}
\end{pmatrix} \cdot \begin{pmatrix}
a(L)^- \\
a(R)^+
\end{pmatrix}.
\]

(5.5)

\[
Ms_{11} = \begin{bmatrix}
-I_N & H_{11}(r, \ell) \end{bmatrix} \cdot LI(\ell)^-,
\]

(5.6)

\[
Ms_{12} = \begin{bmatrix}
H_{12}(r, \ell) & 0_N \end{bmatrix} \cdot LI(r)^+,
\]

(5.7)

\[
Ms_{21} = \begin{bmatrix}
0_N & H_{21}(r, \ell) \end{bmatrix} \cdot LI(\ell)^-,
\]

(5.8)

\[
Ms_{22} = \begin{bmatrix}
H_{22}(r, \ell) & -I_N \end{bmatrix} \cdot LI(r)^+.
\]

(5.9)

The problem eigenvalues are obtained from the secular equation $\text{Det}[Ms] = 0$.

In terms of the Stiffness matrix we have:

\[
Ms_{11} = \begin{bmatrix}
E_{11}(r, \ell) & -I_N \end{bmatrix} \cdot LI(\ell)^-,
\]

(5.10)

\[
Ms_{12} = \begin{bmatrix}
E_{12}(r, \ell) & 0_N \end{bmatrix} \cdot LI(r)^+,
\]

(5.11)

\[
Ms_{21} = \begin{bmatrix}
E_{21}(r, \ell) & 0_N \end{bmatrix} \cdot LI(\ell)^-,
\]

(5.12)

\[
Ms_{22} = \begin{bmatrix}
E_{22}(r, \ell) & -I_N \end{bmatrix} \cdot LI(r)^+.
\]

(5.13)

As a numerical example we use the secular equation in terms of the hybrid matrix $H(r, \ell)$ to obtain the velocities of shear horizontal (SH) acoustic waves in piezoelectric multilayers systems. These curves were obtained in Ref. [3] by using the singular value decomposition (SVD) method together with a variant of the Global Matrix Method (GMM) as an alternative technique to avoid the numerical instabilities found by the authors.

The piezoelectric systems studied there, are formed by two different materials, A (PZT4) and B (PZT5A), and have different layer configurations: $n = 3$ (ABA), $n = 5$ (ABABA), $n = 7$ (ABABABA) and $n = 9$ (ABABABABA). All these systems have the $L - M - R$ structure, with $L = R = A$. The external domains are semi-infinite and to obtain confined modes it was assumed that there are no ingoing waves in the inner region $M$, whereas the outgoing waves are evanescent. It is then clear that this problem can be studied as a particular case of the escape problem considered in this section. In order to get evanescent waves the eigenvalues $k_j$ appearing in the exponential terms of these waves were assumed to be pure imaginary.

Except for $n = 3$, the hybrid matrix $H(r, \ell)$ in the inner region $M$ was obtained by means of the composition rule (4.11). To solve this problem it was necessary to transform the original system of two equations of motion [3] in a matrix Sturm-Liouville system (2.1) with $N=2$. In this problem $F(z)$ has two components, the transverse displacement $u$ and the electric potential $\phi$. The $z$ axis is oriented in the direction normal to the multilayer interfaces in such a way that it coincides with the $y$ axis in the scheme of Figure 1 in Ref. [3]. The $x$ axis coincides in both cases.

The quadratic eigenvalues problem solution (QEP, Section 2.1) for one layer is:
transfer matrix numerical stability and the \( \Omega d \) problem

\[
\begin{align*}
(5.14) & \quad k_1 = -ik_x = -i \frac{\omega}{v_s} \\
(5.15) & \quad k_2 = -k_1 \\
(5.16) & \quad k_3 = \sqrt{-k_x^2 + \frac{\rho}{\rho:\epsilon_44} \left( \frac{\epsilon_{15}}{\epsilon_{11}} \right)} = -i \omega \sqrt{\frac{1}{v_s^2} - \frac{1}{v^2}} \\
(5.17) & \quad k_4 = -k_3,
\end{align*}
\]

where \( v_s \) is the velocity of the surface wave we are studying, whereas \( v \) is the SH wave velocity. The material parameters of the layer needed for this study are the mass density \( \rho \), the elastic constant \( c_{44} \), the piezoelectric constant \( e_{15} \) and the dielectric constant \( \epsilon_{11} \). The eigenfunctions can be chosen in the form:

\[
(5.18) \quad F_j(z) = F_{j0} e^{ik_j(z-z_0)} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{ik_j(z-z_0)}, \quad j = 1, 2
\]

and:

\[
(5.19) \quad F_j(z) = F_{j0} e^{ik_j(z-z_0)} = \begin{pmatrix} 1 \\ e_{15}/\epsilon_{11} \end{pmatrix} e^{ik_j(z-z_0)}, \quad j = 3, 4.
\]

\( k_3 \) and \( k_4 \) must be pure imaginary to obtain evanescent outgoing waves. As these waves travel in material A (PZT4) layers the expression (5.16) shows that this happens for \( v_s < v_A \). It is also possible to obtain confined modes when there are layers in the domain M with \( k_3 \) and \( k_4 \) real. This is only possible in material B (PZT5A) layers when \( v_B < v_s \).

The hybrid matrix of an independent layer was obtained by a method analogous to that employed in [4] to get the expression (2.8). For the \( H \) matrix we have:

\[
(5.20) \quad H(z, z_0) = U^{FA}(z, z_0) \cdot \left[ U^{AF}(z, z_0) \right]^{-1}.
\]

\[
(5.21) \quad U^{FA}(z, z_0) = \begin{bmatrix} F_1(z_0) & F_2(z_0) & \ldots & F_{2N}(z_0) \\ A_1(z) & A_2(z) & \ldots & A_{2N}(z) \end{bmatrix};
\]

\[
(5.22) \quad U^{AF}(z, z_0) = \begin{bmatrix} A_1(z_0) & A_2(z_0) & \ldots & A_{2N}(z_0) \\ F_1(z) & F_2(z) & \ldots & F_{2N}(z) \end{bmatrix}.
\]

The secular matrix \( M_s \) was obtained from the expressions (5.6-5.9) and then we obtained the values of the surface wave velocities zeroing the secular determinant at different frequency values. Table 1 shows the values obtained in our calculation, those obtained in [3] together with the corresponding frequencies. The values in [3] were obtained by using the (SVD) method and a Global Matrix of order \( 4(N_L-1) \times 4(N_L - 1) \), \( N_L \) being the number of layers in the structure. Thus for \( N_L = 3 \) the matrix would
Table 1

| No. of layers | ω (MHz) | MG and SVD vs (m/s) | Hs vs (m/s) |
|---------------|---------|---------------------|-------------|
|               |         | 2324                | 2324.08     |
| 3             | 123.1   | 2286                | 2285.94     |
| 5             | 123.1   | 2313.6/ 2340.5      | 2313.9/ 2340.8 |
|               | 279.1   | 2292.6/ 2294.5      | 2292.5/ 2294.7 |
|               | 318.1   | 2343.1/ 2350.7      | 2344.1/ 2351 |
|               | 396.1   | 2330.3/ 2333.6      | 2330.3/ 2333.8 |
| 9             | 20      | 2339                | 2339.4      |
|               | 80      | 2314/ 2335          | 2314/ 2335.2 |

Comparison between the surface wave velocity values for different frequency values obtained by two different theoretical methods: (GM) Global Matrix Method and (SVD) Singular Value Decomposition method. (Hs) Hybrid compliance-stiffness Matrix Method.

Figure 2 shows the values of the surface wave velocity for the corresponding frequency values for the three and nine layer systems coming from our calculations. We can observe two bands, the first of the even modes and the first of the odd modes, together with the convergence of the modes of the system N=9 towards those of the system N=3 when the frequency is increased. This behaviour is present in the curves given in [3].
5.2. Periodic systems. Let us consider a periodic system along the $z$ direction with arbitrary period $d$. This could be a periodic bulk crystal or a superlattice. The matrices $H(z + d, z)$, $E(z + d, z)$ transfer along a given period. The Bloch-Floquet conditions are satisfied for both $F(z)$ and $A(z)$, in such a way that $F(z + d) = F(z) \cdot e^{i q d}$ and $A(z + d) = A(z) \cdot e^{i q d}$.

We can write this in terms of the hybrid matrix as:

\begin{equation}
\begin{pmatrix}
F(z) \\
A(z + d)
\end{pmatrix} = H(z + d, z) \cdot 
\begin{pmatrix}
A(z) \\
F(z + d)
\end{pmatrix}.
\end{equation}

The Bloch-Floquet conditions for $F(z)$ and $A(z)$ in (5.23) lead to:

\begin{equation}
A(z) = H_{11}^{-1} \cdot [I - H_{12} e^{i q d}] \cdot F(z)
\end{equation}

\begin{equation}
A(z) = [I - H_{21} e^{-i q d}] \cdot H_{22} \cdot F(z).
\end{equation}

We write $H$ instead of $H(z + d, z)$ to simplify. The secular system is obtained from expressions equations (5.24) and (5.25):

\begin{equation}
\{[I - H_{21} e^{-i q d}] \cdot H_{22} - H_{11}^{-1} \cdot [I - H_{12} e^{i q d}]\} \cdot F(z) = 0_N.
\end{equation}

It will have nontrivial solutions if:

\begin{equation}
\text{Det} \{[I - H_{21} e^{-i q d}] \cdot H_{22} - H_{11}^{-1} \cdot [I - H_{12} e^{i q d}]\} = 0.
\end{equation}

This equation gives a dispersion relation in terms of the $H$ matrix elements for any $N$.

Following the same procedure with $E(z + d, z)$ we obtain the following secular system:

\begin{equation}
\{[E_{11} + E_{12} e^{i q d}] - [E_{21} e^{-i q d} + E_{22}]\} \cdot F(z) = 0_N,
\end{equation}

and the dispersion relation:

\begin{equation}
\text{Det} \{[E_{11} + E_{12} e^{i q d}] - [E_{21} e^{-i q d} + E_{22}]\} = 0.
\end{equation}

We assume that in our periodic system the inner domain M (containing one or several homogeneous layers) coincides with the period $d$. Now we shall pose the problem in terms of the Scattering matrix $S(R; L)$.

For the external domains L and R we have:

\begin{equation}
\begin{pmatrix}
F(L : z_L) \\
A(L : z_L)
\end{pmatrix} = Q(L : z_L) \cdot 
\begin{pmatrix}
\alpha^+(L) \\
\alpha^-(L)
\end{pmatrix}.
\end{equation}

\begin{equation}
\begin{pmatrix}
F(R : z_r) \\
A(R : z_r)
\end{pmatrix} = Q(R : z_r) \cdot 
\begin{pmatrix}
\alpha^+(R) \\
\alpha^-(R)
\end{pmatrix}.
\end{equation}
From now on we shall employ $Q_L$ instead of $Q(L : z_\ell)$ and $Q_R$ instead of $Q(R : z_r)$ to simplify the notation. Usually a reduced base in $z_\ell$ is employed to obtain $Q_L$ and a reduced base in $z_r$ is used to obtain $Q_R$. From these matrices we can obtain the matrix $K(R,L)$ by means of (4.5) and then from (4.4) we can obtain $S(R;L)$.

From the Bloch-Floquet condition we obtain:

$$F(R : z_r) = F(L : z_\ell) e^{iqd}$$

$$A(R : z_r) = A(L : z_\ell) e^{iqd}$$

Combining (5.30), (5.31) and (5.32) with the expression (4.3) defining the scattering matrix we can write the following expressions:

$$a^+(L) = [QR_{11} \cdot S_{21} - QL_{11} e^{iqd} - QL_{12} \cdot S_{11} e^{iqd}]^{-1} \cdot [QL_{12} \cdot S_{12} e^{iqd} - QR_{11} \cdot S_{22} - QR_{12}] \cdot a^-(R).$$

(5.33)

$$a^+(L) = [QR_{21} \cdot S_{21} - QL_{21} e^{iqd} - QL_{22} \cdot S_{11} e^{iqd}]^{-1} \cdot [QL_{22} \cdot S_{12} e^{iqd} - QR_{21} \cdot S_{22} - QR_{22}] \cdot a^-(R).$$

(5.34)

Subtracting these equations we arrive to the secular system:

$$0_N = M s \cdot a^-(R),$$

and from it we obtain the secular determinant:

$$\det \left\{ [QR_{11} \cdot S_{21} - QL_{11} e^{iqd} - QL_{12} \cdot S_{11} e^{iqd}]^{-1} \cdot [QL_{12} \cdot S_{12} e^{iqd} - QR_{11} \cdot S_{22} - QR_{12}] - [QR_{21} \cdot S_{21} - QL_{21} e^{iqd} - QL_{22} \cdot S_{11} e^{iqd}]^{-1} \cdot [QL_{22} \cdot S_{12} e^{iqd} - QR_{21} \cdot S_{22} - QR_{22}] \right\} = 0.$$  

(5.35)

We note that the equations (5.27), (5.29) and (5.35) are given in terms of matrix blocks that can overcome the numerical instability known as $\Omega d$ problem. This is not the case for the secular equation in terms of $T(z + d, z)$:

$$\det [T(z + d, z) - I e^{iqd}] = 0,$$

(5.36)

We shall consider now as an example the motion of electrons in a periodic one-dimensional potential such as that of a superlattice formed by barriers of $B$ material with effective mass $m_B$, thickness $b$ and height $V_0$ and wells of $A$ material with effective mass $m_A$ and thickness $a$. In this case the equations (5.27), (5.29), (5.35) and (5.36) are given by:
\[ 2 \cos(qd) H_{12} = 1 - H_{11} H_{22} + H_{12}^2 \] (5.37)

\[ 2 \cos(qd) E_{12} = E_{22} - E_{11} \] (5.38)

\[ 2 \cos(qd) S_{12} = \frac{k_A m_+}{k_A m_0} (S_{21} S_{12} - S_{11} S_{22}) + 1 \] (5.39)

\[ \cos(qd) = \frac{1}{2} (T_{11} + T_{22}), \] (5.40)

where

\[ k_A = \sqrt{\frac{2m_A}{\hbar^2} E} \] (5.41)

\[ k_B = \sqrt{\frac{2m_B}{\hbar^2} (E - V_0)}. \] (5.42)

We used the \( \sin k(z - z/|z|) \) and \( \cos k(z - z/|z|) \) base in the L/R domain to obtain (5.39). When we use the matrix elements of \( T \) for this problem in the period \( d = a + b \) in (5.40) we arrive to the well known Kronig-Penney equation [31]. The expressions (5.37)-(5.39) are variations of this equation if we notice that the matrices \( H, E \) and \( S \) can be calculated from their relations with \( T \).

Expressions (5.37)-(5.39) are variations of (5.40) to calculate the system energy levels for any barrier width \( b \). When the barrier thickness \( b \rightarrow \infty \) (limit of isolated symmetric rectangular wells) the secular equation in terms of \( T \) diverges. On the other hand its variations lead directly to the well known transcendental equations giving the energy levels for even and odd states of a symmetric rectangular well of width \( a \) and depth \( V_0 \).

After some algebra it can be shown that equation (5.37) coincides with the equation (32) in [32] for the Kronig-Penney equation. In the same way it coincides with the equation (20) of Ref. [33]. Refs. [32, 33] give results for the Kronig-Penney equation to avoid the \( \Omega^d \) problem.

6. Conclusions. In the general framework of \( N \) equation systems of the Sturm-Liouville matrix kind with piecewise constant coefficients we have shown that there are transfer matrix variants with dimensions independent of the number of layers in the structure which can avoid the numerical instabilities present in the ATM. The hybrid compliance-stiffness matrix and the scattering matrix can avoid the so called \( \Omega^d \) problem, being numerically stable independently of how big or small be the thicknesses in the multilayer structure. The Stiffness matrix and its inverse the compliance matrix are numerically stable for big thicknesses of the layers or of the multilayer structure. On the other hand, in the case of very small layer thicknesses these two matrices can exhibit the \( \Omega^d \) problem due to the roundoff errors accumulation. For zero thicknesses both matrices exhibit a numerical singularity (overflow).

Given the big variety of boundary problems which can be studied with these numerically stable variants of the ATM and the generality and ubiquity of the matrix Sturm-Liouville system, the results obtained here can be applied to the study of various elementary excitations in multilayer systems.

The relations between the different matrices studied here has proven to be an useful instrument in the study of the numerical stability of transfer matrices.
this technique it was possible to show analytically the capability of some of these
variants of the transfer matrix to avoid the numerical degradation leading to the Ωd
problem.

In recent years some methods able to deal with systems having inhomogeneous
coefficients have been developed. We present in Appendix C the link of the N equation
systems of the Sturm-Liouville matrix kind to the corresponding differential forms of
those problems.

Appendix A. Example of a matrix subset with a similar behaviour from
the numerical point of view.

Let us denote by $X$, $Y$, $Z$ and $R$ four matrices in whose definition enter the
vectors $F(z)$, $F(z_0)$, $A(z)$ and $A(z_0)$, as for example:

$$
\begin{align*}
  \begin{bmatrix}
    A(z_0) \\
    F(z)
  \end{bmatrix}
  &=
  \begin{bmatrix}
    X \\
    Z
  \end{bmatrix}
  \begin{bmatrix}
    F(z_0) \\
    A(z)
  \end{bmatrix}
  =
  \begin{bmatrix}
    Y \\
    R
  \end{bmatrix}
  \begin{bmatrix}
    F(z_0) \\
    A(z)
  \end{bmatrix},
\end{align*}
$$

(A.1)

If we take as the reference matrix any one of them it can be shown that one of
the remaining matrices is obtained by permutations among them of the vectors in the
right-hand side of the reference matrix. A second one is obtained by following this
method among the vectors in the left-hand side of the reference matrix. Finally the
third one is obtained with both permutations. The relations between these matrices
can be resumed as:

$$
\begin{align*}
  (X)_{11} &= (Y)_{21} = (R)_{22} = (Z)_{12} \\
  (X)_{12} &= (Y)_{22} = (R)_{21} = (Z)_{11} \\
  (X)_{21} &= (Y)_{11} = (R)_{12} = (Z)_{22} \\
  (X)_{22} &= (Y)_{12} = (R)_{11} = (Z)_{21}
\end{align*}
$$

(A.2) (A.3) (A.4) (A.5)

These relations show that the matrices $X$, $Y$, $Z$ and $R$ will have a similar
behaviour from the numerical point of view.

Appendix B. Matrix $T$ partitions of order $N$.

Starting with the expression:

$$
\begin{align*}
  T(d) &= \begin{bmatrix}
    F_{0_N} & F_{0_2N} \\
    A_{0_N} & A_{0_2N}
  \end{bmatrix}
  \begin{bmatrix}
    \Pi_{kN}(d) & 0 \\
    0 & \Pi_{k2N}(d)
  \end{bmatrix}
  \begin{bmatrix}
    F_{0_N} & F_{0_2N} \\
    A_{0_N} & A_{0_2N}
  \end{bmatrix}^{-1},
\end{align*}
$$

(B.1)

we have:

$$
\begin{align*}
  T_{11} &= F_{0_N} \cdot \Pi_{kN}(d) \cdot \gamma_{11}^{-1} + F_{0_2N} \cdot \Pi_{k2N}(d) \gamma_{12}^{-1}, \\
  T_{12} &= F_{0_N} \cdot \Pi_{kN}(d) \cdot \gamma_{21}^{-1} + F_{0_2N} \cdot \Pi_{k2N}(d) \gamma_{22}^{-1}, \\
  T_{21} &= A_{0_N} \cdot \Pi_{kN}(d) \cdot \gamma_{11}^{-1} + A_{0_2N} \cdot \Pi_{k2N}(d) \gamma_{12}^{-1}, \\
  T_{22} &= A_{0_N} \cdot \Pi_{kN}(d) \cdot \gamma_{21}^{-1} + A_{0_2N} \cdot \Pi_{k2N}(d) \gamma_{22}^{-1}.
\end{align*}
$$

(B.2)
\( \gamma_{11} = [F_{0_2N} - F_{0_2N} \cdot A_{0_2N}^{-1} \cdot A_{0_N}] \),
\( \gamma_{12} = [F_{0_2N} - F_{0_N} \cdot A_{0_2N}^{-1} \cdot A_{0_2N}] \),
\( \gamma_{21} = [A_{0_N} - A_{0_2N} \cdot F_{0_2N}^{-1} \cdot F_{0_N}] \),
\( \gamma_{22} = [A_{0_2N} - A_{0_N} \cdot F_{0_N}^{-1} \cdot F_{0_2N}] \).

**Appendix C. Sturm-Liouville matrix form for inhomogeneous media.**

The matrix Sturm-Liouville equation

\[
\frac{d}{dz} \left[ B(z) \cdot \frac{dF(z)}{dz} \right] + P(z) \cdot F(z) + Y(z) \cdot \frac{dF(z)}{dz} + W(z) \cdot F(z) = L(z) \cdot F(z) = 0_{N \times 1},
\]

can be written as:

\[
\frac{d}{dz} \left| F(z) \right| A(z) = \left( \begin{array}{cc} -B(z)^{-1}P(z) & B(z)^{-1} \\ Y(z) \cdot B(z)^{-1} \cdot P(z) - W(z) & -Y(z) \cdot B(z)^{-1} \end{array} \right) \cdot \left| F(z) \right| A(z).
\]

Here \( A(z) = B(z) \cdot \frac{dF(z)}{dz} + P(z) \cdot F(z) \) is the SLM operator matrix differential form.

The equation (C.2) is the link with the first order differential equations systems given in eq.(2.10) of [16], eq.(3.3) of [17], eq.(2) and (A.6) of [18], eq.(3) of [19] and eq.(8) of [20].

These equations cover different inhomogeneous systems.

**C.1. Radially inhomogeneous cylindrically anisotropic systems.** This is the case considered in [16]. In this work the mass density and the elements of the stiffness tensor depend only on the radial coordinate \( r \). It is then possible to write:

\[
u = CU^{(n)}(r)e^{i(n\theta + \kappa_z \cdot \omega t)},
\]

to obtain:

\[
\frac{d}{dr} \left[ r \overline{Q} \frac{d(CU)}{dr} + (\overline{R}k + i\kappa_z r \overline{P}) \right] + \left( kR^T + i\kappa_z r \overline{P}^T \right) \frac{d(CU)}{dr} \]

\[
+ \frac{1}{r} \left[ kT_k + i\kappa_z r (k \overline{S} + \overline{S}^T k) + (i\kappa_z r)^2 (\overline{M} - I \rho \omega^2 / \kappa_z^2) \right] (CU) = 0.
\]

Here \( C \) is a normalization constant. Equation (C.4) is of kind (C.1) for a cylindrical elastic material radially inhomogeneous. Here \( r \) plays the role of \( z \) in the planar systems. With the properties imposed on \( k, \overline{Q}, \overline{P}, \overline{R}, \overline{S}, \overline{T} \) and \( \overline{M} \) in [16] we have \( Y = -P^T, B = B^T \) and \( W = W^T \).

In this case the linear differential form in (C.4) is \( A = rt_r \) (where \( t_r \) is the stress radial component and from eq.(2.7) from [16] we obtain \( A(r) = Cr \cdot \overline{X}^{(n)}(r) \). We see also that \( F(r) = CU^{(n)}(r) \). By identifying the \( B, P, Y \) and \( W \) matrices in (C.4) and substitution in (C.2) we arrive to eq.(2.10) of [16], eq.(3.3) of [17] and eq.(A.6) of [18]:
\[
\frac{d}{dr}(r^{(n)}) = \frac{i}{r} G(r) \eta(r^{(n)}); \\
\eta(r^{(n)}) = C \left( \begin{array}{c} U^{(n)}(r) \\ ir Y^{(n)}(r) \end{array} \right); \\
i r G(r) = \left( \begin{array}{cc} -B(r)^{-1} P(r) & B(r)^{-1} \\ Y(r) \cdot B(r)^{-1} \cdot P(r) & -Y(r) \cdot B(r)^{-1} \end{array} \right).
\]

C.2. Shear-horizontal elastic waves in phononic crystals formed by inhomogeneous anisotropic materials. Cartesian coordinates. This is studied in [20] where the displacement \( u \) depends on \( x_1 \) and \( x_2 \), but after expanding \( x_1 \) in plane waves they obtain the following ordinary differential equation in \( x_2 \)

\[
-(\partial_1 + ik_1)(\mu \partial_1 + ik_1)u + \partial_2(\mu \partial_2 u) = -\rho \omega^2 u.
\]

We can then identify \( F(x_2) = u(x_2) \) and \( A(x_2) = \mu \partial_2 u, P = 0, Y = 0, B = \mu^{-1} \) and \( W = \rho \omega^2 - (\partial_1 + ik_1)\mu(\partial_1 + ik_1) \). After substitution of these expressions in (C.2) \( W \) acts on the displacement \( u(x_2) \) and we obtain eq.(8) of [20] which is essentially the same than eq.(3) of [19].

We have seen that in all these cases involving inhomogeneous elastic anisotropic media we can put the matrix Sturm-Liouville in the (C.2) form. Then it would be possible to apply the stable integration methods of [16, 17, 18] for cylindrical geometry and those of [19, 20] for layered systems.

Acknowledgments. We thank the Associate Editor and the referees for valuable comments and useful suggestions.

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