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Multimodal admittance method in waveguides and singularity behavior at high frequencies

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ABSTRACT

This work presents a multimodal method for the propagation in a waveguide with varying height and its relation to trapped modes or quasi-trapped modes. The coupled mode equations are obtained by projecting the Helmholtz equation on the local transverse modes. To solve this problem we integrate the Riccati equation governing the admittance matrix (Dirichlet-to-Neumann operator). For many propagating modes, *i.e.* at high frequencies, the numerical integration of the Riccati equation shows that the rule is that this matrix has quasi-singularities associated to quasi-trapped modes.

1. Introduction

The computation of wave propagation in waveguides is a classical problem in many fields of Physics such as Electromagnetics and Acoustics [1], with a renewed interest during the last two decades because of the emergence of the study of quantum waveguides [2,3] and of elastic waveguides (see [4,5] and the references therein). Classical numerical techniques such as the finite element methods or the boundary element methods can be used to calculate the solutions of the Helmholtz equation in the waveguides, but multimodal methods are particularly well suited in this situation [6–10]. The multimodal methods consist in projecting the solution on the local transverse modes of the waveguide and then solving the coupled mode equations governing the evolution of the components on the transverse modes. In the case where these coupled mode equations are to be integrated numerically, two problems appear: firstly they are numerically unstable because of the presence of evanescent modes and secondly they cannot be integrated as an initial value problem since the Helmholtz equation imposes the form of a boundary value problem with a source and a radiation condition. This impossibility leads directly to the introduction of an admittance matrix [11,12] that corresponds to the Dirichlet-to-Neumann (DtN) operator in the multimodal context. This matrix represents the radiation condition (the outlet boundary condition) and is governed by a Riccati equation. It enables us to obtain an efficient and stable numerical method to solve the Helmholtz equation in waveguides [11,13,14,12,4,5].

In this paper, we present the multimodal admittance method and the way to integrate it. It is shown that the Riccati equation presents many quasi-singularities at high frequencies. The numerical integration through the singularities is possible owing to a "Möbius scheme" [15] that we perform with a Magnus exponential method [16]. Besides, we show that these singularities (quasi) are related to trapped modes (quasi) that correspond to situation where the DtN operator cannot be defined. The plan of the paper is as follows: in Section 2 we present the multimodal admittance method, Section 3 is devoted to the numerical schemes to integrate the equations and in Section 4 we show some results with a focus on the quasi-trapped modes associated to quasi-singularities.

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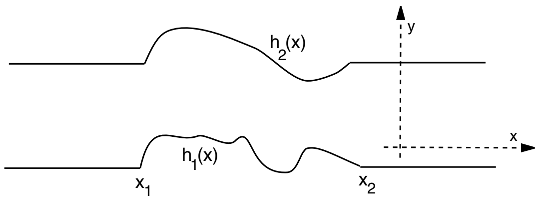


Fig. 1. Geometry of the 2D waveguide.

2. Multimodal admittance method

The aim is to solve the Helmholtz equation

$$\triangle\phi + k^2\phi = 0 \tag{1}$$

in the waveguide shown in Fig. 1 with Dirichlet boundary conditions at the wall ($\phi = 0$ for $y = h_1(x)$ and for $y = h_2(x)$). The same method could be also applied for Neumann or mixed boundary conditions but we take here the Dirichlet condition for the sake of clarity. Note also that here k is constant but it is possible to adapt the method for inhomogeneous k. The boundary conditions along the x-axis will be that of outgoing waves at the right ($x = x_2$) and a source condition at the left ($x = x_1$). A source condition will be a mixed Robin boundary condition involving ϕ, $\partial_x\phi$ and some given non-zero function.

We first write the Helmholtz as a first order evolution equation along the direction x of the waveguide

$$\partial_x \begin{pmatrix}\phi\\ \psi\end{pmatrix} = \begin{pmatrix}0 & 1\\ -(\partial_{y^2} + k^2) & 0\end{pmatrix}\begin{pmatrix}\phi\\ \psi\end{pmatrix}. \tag{2}$$

Then, the transverse modes of the waveguide are used to discretize the problem along the transverse direction y so that ϕ and ψ are projected on the modes as

$$\begin{aligned}\phi &= \sum_{n=1}^{+\infty} a_n(x) g_n(x; h)\\ \psi &= \sum_{n=1}^{+\infty} b_n(x) g_n(x; h)\end{aligned} \tag{3}$$

where

$$g_n(x; h) = \sqrt{\frac{2}{h}}\sin\left(\frac{n\pi y}{h}\right) \tag{4}$$

and $h(x) = h_2(x) - h_1(x)$. The projection of the evolution equation (2) yields the coupled mode equation for the components $a_n(x)$ and $b_n(x)$:

$$\begin{aligned}a' &= -Fa + b\\ b' &= -K^2 a + F^{\mathrm{T}} b\end{aligned} \tag{5}$$

where primes denote differentiation with respect to x, a (resp. b) is the vector of components a_n (resp. b_n) with $n \geq 1$, F is a matrix with non-diagonal elements ($n \neq m$) given by

$$F_{nm} = -\frac{nm}{m^2 - n^2}\frac{2}{h}\left((-1)^{n+m} h_2' - h_1'\right) \tag{6}$$

and $F_{nn} = 0$, and K is the diagonal matrix of the mode wavenumbers given by $K_{nm} = k_n \delta_{nm}$ with $k_n = \sqrt{k^2 - n^2\pi^2/h^2}$. Since the implicit harmonic time dependence here is $\mathrm{e}^{-\mathrm{i}\omega t}$ the square root for k_n is chosen such that $\mathrm{Re}(k_n) \geq 0$ and $\mathrm{Im}(k_n) \geq 0$. In Eq. (5) we see that the coupling between the modes is due to the matrix F that is non-zero for varying heights h_1 or h_2.

The coupled mode equations (5) cannot be integrated directly as an initial value problem for two reasons: (i) the problem is posed as a boundary value problem with a radiation condition given at the right ($x = x_2$), and a source given at the left ($x = x_1$) (ii) as an initial value problem the system (5) is unstable because of the evanescent modes that cause exponential divergence of the errors [12]. The method chosen here to solve this problem is to define the admittance matrix as

$$b = Ya. \tag{7}$$

This admittance matrix is the representation of the DtN operator on the mode basis. By inserting Eq. (7) into the system (5), a Riccati equation is obtained for the admittance matrix Y:

$$Y' = -K^2 - Y^2 + YF + F^{\mathrm{T}} Y. \tag{8}$$

The Riccati equation (8) is a first order differential equation that enables us to obtain the admittance matrix (DtN operator) for all x from the initial value of Y given by the radiation condition at the right of the waveguide ($x = x_2$ see Fig. 1). This initial condition is $Y(x_2) = Y_c$ for the radiation condition corresponding to only right-going waves in the region $x > x_2$, where the matrix Y_c is

$$Y_c = \mathrm{i}K$$

which is similar to the DtN condition imposed in finite elements method. Note that the same kind of method had been presented in [11,13,14,12,4,5].

2.1. Reflection and transmission matrix

To obtain the reflection matrix R from the calculated admittance matrix Y, the wave components are decomposed into right- and left-going parts as

$$a = a^+ + a^-$$

and

$$b = Y_c(a^+ - a^-).$$

Then from the definition of the reflection matrix $a^- = Ra^+$, we get

$$R = (Y_c + Y)^{-1}(Y_c - Y). \tag{9}$$

It is also possible to get the transmission matrix of the waveguide at the same time as the Y matrix by defining the propagator matrix G such that

$$a(x_2) = G(x_2, x)a(x), \tag{10}$$

where $x_2 \geq x$ and $G(x_2, x_2) = I$, where I is the identity matrix. The equation governing G is then found to be

$$G' = -G(-F + Y), \tag{11}$$

with the initial value $G(x_2, x = x_2) = I$. and the transmission matrix is given by

$$T = G(x_2, x = x_1)(I + R) \tag{12}$$

(the definition of the transmission matrix is the classical one: $a^+(x_2) = Ta^+(x_1)$).

To summarize, starting from $x = x_2$ Eqs. (8) and (11) are integrated for $x \leq x_2$ with the initial conditions $Y(x_2) = Y_c$ and $G(x_2, x = x_2) = I$ and they yield the reflection and transmission matrices by Eqs. (9) and (12). The verification of the conservation of energy taking into account the evanescent modes can be performed by algebraic computations [17] on the matrices R and T. The great advantage of the whole method is that the matrices (Y and G) do not have to be stored during the integration of the differential equation (8) and (11) along x.

2.2. Calculation of the wave field

If one is interested in the calculation of the whole field in the waveguide the method is as follows. Once the Riccati equation (8) has been solved and the matrix Y has been stored along x, it is sufficient to solve the first equation of the coupled mode equations (5) where b is replaced by its value $b = Ya$:

$$a' = (Y - F)a. \tag{13}$$

This first order equation for the vector a resembles the parabolic approximation equation but here the factorization of the second order Helmholtz equation has been done exactly owing to the integration of the Riccati equation for Y. Thus it can be noticed that once the matrix Y is computed and stored (independently of the source condition) we can use the simple first order equation of the field (13) for several source conditions.

3. Numerical integration

The Riccati equation (8) can be numerically integrated owing to a classical scheme as the Runge–Kutta method for instance. Nevertheless, the Riccati equation is known to have movable singularities (*i.e.* depending on the initial condition) in the complex x-plane [18,15]. In the sequel, we will call quasi-singularities the movable singularities x_c of Y with non-zero imaginary part. As the frequency k is increased the admittance matrix Y shows more and more quasi-singularities that makes this kind of numerical method very time consuming or even useless. Fig. 2 displays the behavior of the real part of the diagonal element $Y_{5,5}$ for a frequency corresponding to 20 to 40 locally propagating modes in a waveguide with a semi-circular enlargement. The quasi-singularities are apparent and necessitate a very small step size with a Runge–Kutta method. An alternative has been proposed to avoid this problem in [15]: they called it a “Möbius scheme” and it consists

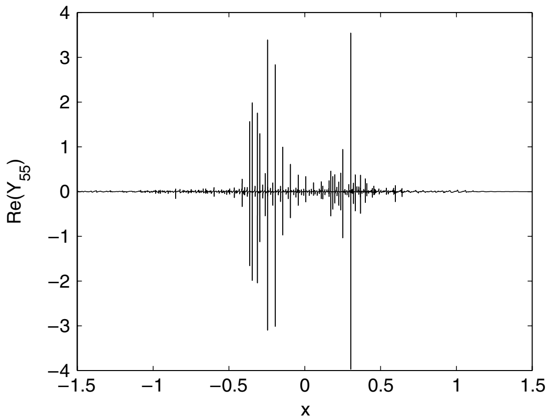


Fig. 2. Real part of $Y_{5,5}$ as a function of x for a case with at most 40 locally propagating modes and showing the quasi-singularities.

in using the numerical integration of the linear system from which the Riccati equation comes from (here the system (5)). Besides, we use the Magnus method [16,19] for the numerical integration of the linear differential equation. It is a very efficient method that necessitates very few points to describe wildly oscillating solutions and is particularly well suited for high frequencies computations. Similar ideas were presented in [14,5].

We now present the details of this "Magnus–Möbius scheme". With the radiation condition at $x = x_2$ the boundary condition for Y is given at the right by $Y(x_2) = Y_c$ and the source a is imposed at x_1. The interval $[x_1, x_2]$ is discretized by a series of longitudinal coordinates $\tilde{x}_1 > \tilde{x}_2 > \cdots > \tilde{x}_N$ such that $\tilde{x}_1 = x_2$ and $\tilde{x}_N = x_1$.

We start from Eq. (5) rewritten in the form

$$\frac{\mathrm{d}}{\mathrm{d}x}\begin{pmatrix} a(x) \\ b(x) \end{pmatrix} = H(x)\begin{pmatrix} a(x) \\ b(x) \end{pmatrix},$$

so that the numerical scheme of the Magnus method yields

$$\begin{pmatrix} a(\tilde{x}_{n+1}) \\ b(\tilde{x}_{n+1}) \end{pmatrix} = \mathrm{e}^{\Omega_n}\begin{pmatrix} a(\tilde{x}_n) \\ b(\tilde{x}_n) \end{pmatrix}. \tag{14}$$

The Magnus matrix Ω_n has different expression for different orders of the Magnus integration scheme. For the second order it is given [19] by

$$\Omega_n = \delta_n \quad H\left(\frac{\tilde{x}_n + \tilde{x}_{n+1}}{2}\right),$$

where $\delta_n = \tilde{x}_{n+1} - \tilde{x}_n$, and which corresponds to the classical midpoint rule. For the fourth order [19], the Magnus matrix is

$$\Omega_n = \frac{1}{2}\delta_n(H_1 + H_2) + \frac{\sqrt{3}}{12}\delta_n^2[H_2, H_1],$$

where

$$H_1 = H\left(\tilde{x}_n + \left(\frac{1}{2} - \frac{\sqrt{3}}{6}\right)\delta_n\right)$$

and

$$H_2 = H\left(\tilde{x}_n + \left(\frac{1}{2} + \frac{\sqrt{3}}{6}\right)\delta_n\right)$$

are the evaluations of the matrix H at the nodes of the fourth order Gauss–Legendre quadrature in the segment joining $\tilde{x}_n$ and $\tilde{x}_{n+1}$. We can notice that the commutator $[H_2, H_1]$ between H_2 and H_1 appears in this fourth order scheme.

Then, this Magnus step eventually permits to obtain the following scheme to solve the Riccati equation for Y

$$Y(\tilde{x}_{n+1}) = [E_3 + E_4 Y(\tilde{x}_n)][E_1 + E_2 Y(\tilde{x}_n)]^{-1}, \tag{15}$$

where the matrices E_1 to E_4 are defined from the exponential propagator

$$\mathrm{e}^{\Omega_n} = \begin{pmatrix} E_1 & E_2 \\ E_3 & E_4 \end{pmatrix}.$$

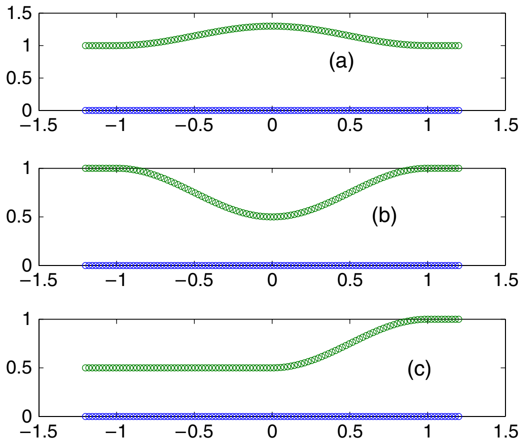
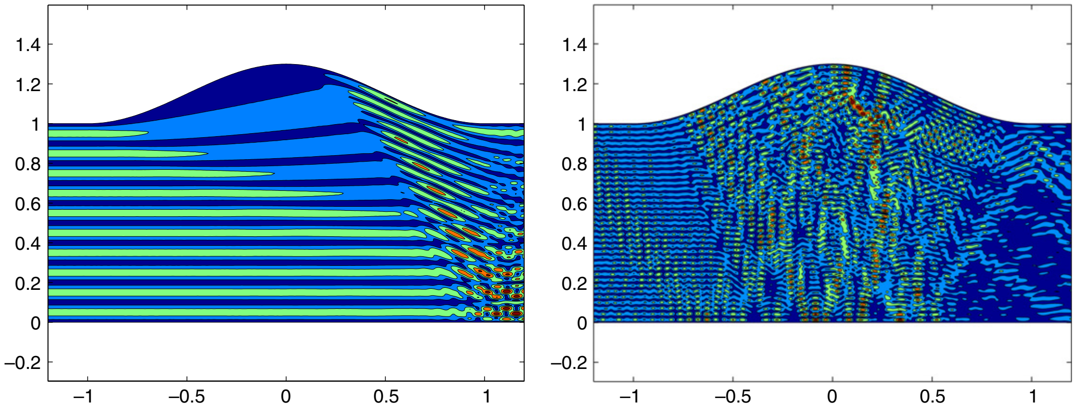


Fig. 3. Geometries (A), (B) and (C) chosen for the computation.



(a) Mode 10 incident.

(b) Mode 35 incident.

Fig. 4. Computed solutions for $k = 40.3$ in (A)-geometry with the Magnus–Möbius scheme.

The scheme to compute the matrix G follows the same line:

$$G_{n+1} = G_n[E_1 + E_2 Y(\tilde{x}_n)]^{-1}.$$

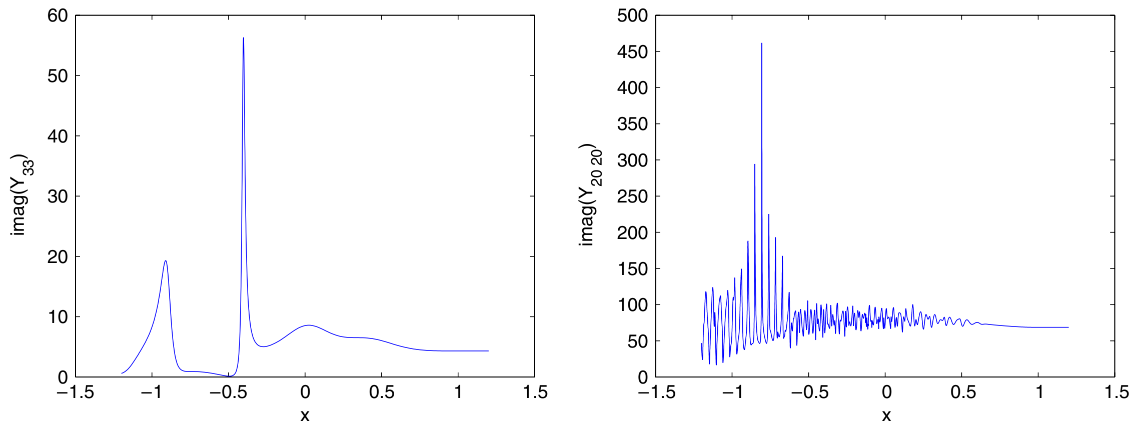
Note that the integration is performed from right at $x = x_2$ to left at $x = x_1$. When not only the scattering properties but also the whole solution is sought in the geometry, then, Eq. (14) is used once again to get

$$a(\tilde{x}_n) = [E_1 + E_2 Y(\tilde{x}_n)]^{-1} a(\tilde{x}_{n+1}), \tag{16}$$

where the calculation is done from left to right, starting from the source boundary condition $a(x_1)$. In the computation, the projection (3) is truncated to a finite number of terms N. Numerically it is found that the convergence for the total field ϕ follows a $1/N^3$ law; in the case of Neumann boundary condition at the wall the convergence follows a $1/N^2$ law [8].

4. Quasi-singularities of *Y* and quasi-trapped modes

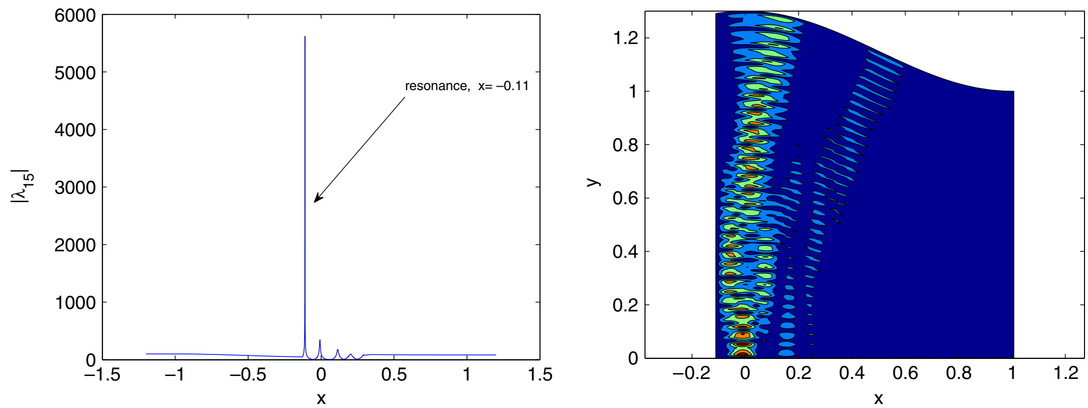
In this section we will display the behavior of our method for three different geometries of the waveguide with varying height (Fig. 3). The geometry (A) corresponding to a local enlargement of the height is defined by $h_1 = 0$ and $h_2 = 1 + 0.15(1 + \cos(\pi x/b))$ for $|x| \leq 1$ and $h_2 = 1$ for $|x| > 1$. The geometry (B), corresponding to a contraction of the waveguide, is defined by $h_1 = 0$ and $h_2 = 1 - 0.25(1 + \cos(\pi x/b))$ for $|x| \leq 1$ and $h_2 = 1$ for $|x| > 1$. Finally, the geometry (C) which represents a step waveguide is defined by $h_1 = 0$ and $h_2 = 1 - 0.25(1 + \cos(\pi x/b))$ for $0 \leq x \leq 1$, $h_2 = 1$ for $x > 1$ and $h_2 = 1/2$ for $x < 0$ (in the three geometries $b = 1$). First we show a routinely obtained result with the Magnus–Möbius scheme in Fig. 4. It corresponds to a frequency $k = 40.3\pi$ in geometry-(A) with a given incident mode and, thus, is a typical high frequency result with 40 modes propagating in the constant waveguide leads at right and left. The total number of modes that gives the dimension of the matrix Y is 60 and the number of discretization along $-1.2 < x < 1.2$ is only 334 which means that there are here 6 points per wavelength. Needless to say that this kind of computation would



(a) Imaginary part of $Y_{3,3}$ at $k = 3.3\pi$.

(b) Imaginary part of $Y_{20,20}$ at $k = 30.3\pi$.

Fig. 5. Behavior of diagonal elements of the admittance matrix in the geometry (A) for low and high frequencies.



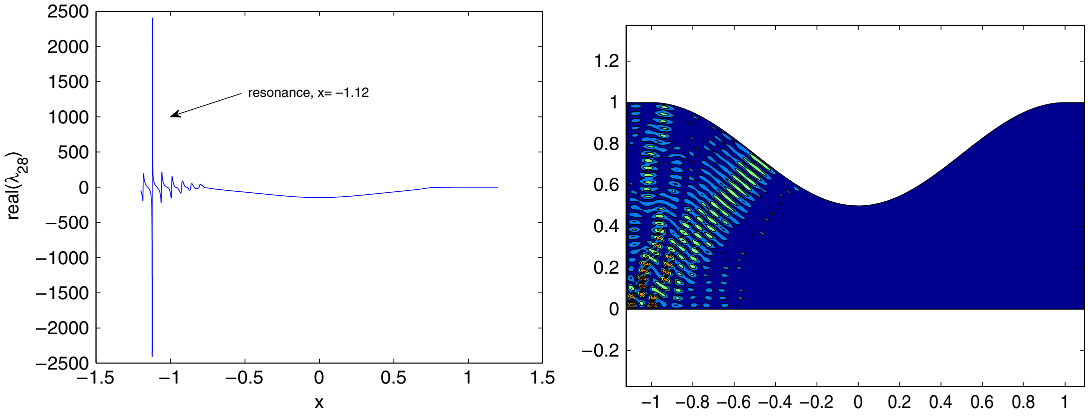
(a) Evolution of the imaginary part of eigenvalue λ_{20} of Y.

(b) Quasi-trapped mode for a quasi-singularity at $x_c = -0.11$ for the geometry (A) at $kh_0 = 30.3\pi$.

Fig. 6. Y-eigenvalue behavior and associated quasi-trapped mode for the (A)-geometry with $k = 30.3\pi$.

very time and storage consuming if the Riccati were integrated using a classical numerical method such as the Runge–Kutta scheme for instance because there are many quasi-singularities of the Y matrix.

We turn now to the study of the singularities of the admittance matrix. When Y has been introduced in Eq. (7) it has been assumed implicitly that it was possible to define the DtN operator mapping ϕ to $\partial_x\phi$ on the vertical x_c with $x_c < x_2$. Indeed this is possible when there is uniqueness of the solution of the Helmholtz equation with Dirichlet boundary conditions in the domain $x \geq x_c$ (with outgoing wave at x_2). That means that if there exists a trapped mode [20–22] in the domain $x \geq x_c$ the matrix Y cannot be defined at $x = x_c$. Thus the movable singularities of Y at real x_c correspond to trapped modes at the right of x_c. The movable singularities of the Riccati equation are generally located in the complex x-plane and when the singularities are near the real x-axis they correspond to very high peaks that are shown in Fig. 5 (in such a case we call them quasi-singularities). This result is obtained with a Runge–Kutta scheme with an adaptive step in order to follow precisely the locations of the quasi-singularities. It can be seen that as the frequency increases there are more and more quasi-singularities, closer and closer to the real x-axis. The observed quasi-singularities of the matrix Y correspond to quasi-trapped modes (or complex resonance [23]) that can be found owing to the eigenvectors of Y. Let a_0 be an eigenvector of Y at $x = x_c$ with eigenvalue λ, $Ya_0 = \lambda a_0$ and if we choose the source to be given at $x = x_c$ by $a(x_c) = a_0$ then $b(x_c) = Ya(x_c) = \lambda a(x_c)$. Suppose now that the eigenvector a_0 of Y has a very high eigenvalue with $\lambda \to \infty$. If the source is chosen to be collinear to the eigenvector a_0 then $a(x_c) = 1/\lambda b(x_c)$ and thus this source has $a(x_c) \to 0$ and $b(x_c)$ finite. That means that the eigenvector associated to a quasi-singularity can be also associated to a quasi-trapped mode of the geometry. Practically, if there is a quasi-singularity at $x = x_c$ for Y, we take the associated eigenvector a_0 as an initial condition of the evolution equation (13) and we calculate the values of $a(x)$ for $x_c \leq x \leq x_2$. Fig. 6(a) shows the behavior of one of the eigenvalues λ with a quasi-singularities at $x_c = -0.11$ for the geometry (A) with $k = 30.3\pi$ and the quasi-trapped mode associated to this eigenvalue is displayed in Fig. 6(b). No difference can be noticed between this solution and a genuine trapped mode. The same kind of results is presented in Fig. 7 for the geometry (B) for which there is a contraction of the



(a) Evolution of the imaginary part of eigenvalue λ_{28} of Y.

(b) Quasi-trapped mode for a quasi-singularity at $x_c = -1.12$ for the (B)-geometry at $kh_0 = 30.3\pi$.

Fig. 7. Y-eigenvalue behavior and associated quasi-trapped mode for the (A)-geometry with $k = 30.3\pi$.

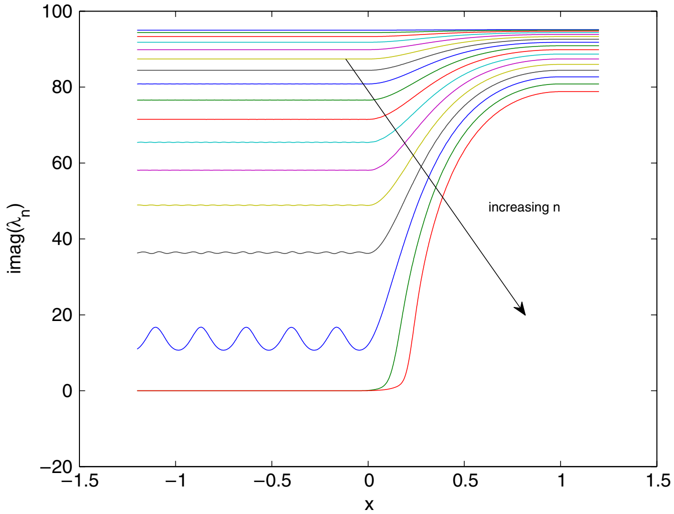


Fig. 8. Behavior of the Y-eigenvalues λ_n ($1 \le n \le 17$) for the (C)-geometry with $kh_0 = 30.3\pi$.

waveguide. In this case there are no quasi-singularities for $x > 0$ where the height h_2 is decreasing. It agrees with the intuition that would tell us that the wave cannot be trapped in this repulsing region. Accordingly, the obtained quasi-trapped mode (Fig. 7(b)) is localized in the "open box" at $x < 0$. This relation between the x region with quasi-singularities and the shape of the waveguide is confirmed in Fig. 8 where the behavior of the first seventeen eigenvalues of Y is displayed for the case of geometry (C) at $k = 30.3\pi$. Here, we see that there are no quasi-singularities at all, in agreement with the intuition that this step geometry is not a good candidate to trap a wave which is outgoing at the right. For this case the matrix Y remains always close to the adiabatic value given by $Y_c(x)$.

5. Concluding remarks

The movable singularities of the admittance matrix (DtN operator) have been shown to be linked to quasi-trapped modes in waveguide. It appears that these modes are the rule rather than the exception when the frequency increases. Ironically, the singularities that could be thought to create trouble for the use of the admittance matrix method might also be an efficient method to find trapped modes in complicated geometries.

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