Journal of Computational Physics **159,** 90–102 (2000)
doi:10.1006/jcph.2000.6434, available online at http://www.idealibrary.com on IDEAL®

Floquet Multipliers of Periodic Waveguides via Dirichlet-to-Neumann Maps

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Received August 30, 1999; revised December 27, 1999

A new approach to calculating Floquet spectra of multilayered periodic waveguides is presented. The problem is formulated as an eigenvalue problem of the Helmholtz equation on an infinite strip with discontinuous wavenumber. The strip is decomposed into a rectangle and two semi-infinite domains, and the problem is reduced to a nonlinear eigenvalue problem involving Dirichlet-to-Neumann (DtN) operators on the interfaces of the domains. A solution scheme based on the Taylor expansion of the DtN operator with respect to the Floquet exponent, whose order of convergence can be made arbitrarily large, is derived. An application to a typical waveguide geometry demonstrates the efficiency and accuracy of the approach.

Key Words: guided waves; Floquet spectrum; nonlinear eigenvalue problem.

1. INTRODUCTION

Thin film waveguides containing periodic corrugations are of considerable interest for integrated optics and millimeter waves. They have important applications in distributed feedback lasers [11], coupling of waveguides [4, 19], leaky-wave antennas [16] and many other fields.

The form of waves traveling along a z-periodic structure is described by Floquet's theorem. The theorem states that a time-harmonic electromagnetic field $F(x, y, z)$ of a normal mode has the property that

$$F(x, y, z + d) = e^{\gamma d} F(x, y, z), \tag{1}$$

where d is the length of the period for the physical corrugation. In the following we will assume that the problem is scaled so that $d = 1$.

The Floquet exponent (or propagation constant) γ is in general complex; its real part represents the attenuation and its imaginary part the phase shift in one period. The Floquet multiplier is given by e^{γ} and is the number by which the normal mode is multiplied under a

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shift. The mathematical problem common to the aforementioned applications is to determine the dominant modes for a given structure as a function of the the frequency.

A related problem is the calculation of Floquet spectra of doubly periodic structures such as photonic crystals; see, e.g., [2, 7, 8] and the references therein. There the unit cell of the period is a finite domain, which leads after discretization to a linear eigenvalue problem. Since multilayered waveguides are singly periodic the unit cell is an infinite strip and additional physical phenomena, such as leaky waves (i.e., radiation away from the grating region), can occur. The unbounded domain also requires special computational consideration, which leads, as we will describe below, to a nonlinear eigenvalue problem.

While the quantitative behavior of the Floquet spectrum of axially periodic multilayered structures is well understood [6, 13], good numerical schemes for finding the exact location of the Floquet exponents are difficult to obtain. Several methods have been investigated. The common feature of these approaches is that the field in the uniform layers surrounding the grating region is expanded as an infinite sum of spatial harmonics in the form $\exp[(2\pi ik+\gamma)x+i\gamma_k z]$, where γ_k depends on the unknown Floquet exponent through a dispersion relation. The field in the grating region is either again expanded in harmonics [15], converted to a system of ordinary differential equations [5], or, more recently, treated with a boundary element technique [9]. To ensure continuity, the fields inside and outside the grating region must be matched. The result is a nonlinear eigenvalue problem, i.e., the problem at hand is to find the Floquet exponent γ that makes the discretization matrix $A(\gamma)$ singular. Because of the dispersion relation some of the entries in the matrix depend on γ in a highly nonlinear fashion. The numerical method used for this problem is to solve $\det A(\gamma)=0$ by either Newton's or Muller's method [3]. However, discretizations lead to large ill-conditioned systems and hence the determinant is a bad indicator for the numerical rank of a matrix. For a description of some of the issues in this context see [17].

A commonly used method for unbounded spatial domains is to introduce an artificial boundary and use the Dirichlet-to-Neumann (DtN) map of the exterior domain as a boundary condition. The resulting problem is posed on a finite domain and can be treated with standard discretization methods. For artificial boundary conditions for scattering problems we refer to, e.g., [12], and in the context of waveguides to, e.g., [10]. When the Floquet spectrum is to be determined this approach leads to a nonlinear eigenvalue problem whose size is the number of degrees of freedom in the discretization of the interior problem.

To decrease the size and to improve the conditioning of the nonlinear eigenvalue problem, we consider in this article using DtN operators for the exterior *and* the interior domain. We will show in Section 3 that this approach leads to a nonlinear eigenvalue problem $T(\gamma)$ which is posed on the artificial boundary. Since typically only a few harmonics will suffice for its discretization, the resulting nonlinear eigenvalue problem is very small and well-conditioned. Instead of solving for roots of the determinant, we will derive a matrix–Newton scheme that, for a given iterate $\bar{\gamma}$, finds a new approximation of γ that makes the mth order truncated Taylor expansion of $T(\gamma)$ at $\bar{\gamma}$ singular. We will describe how the Taylor coefficients can be calculated stably without using derivatives in Section 4. Section 5 discusses how the Taylor expansion of the exterior DtN operators can be calculated if the exterior problems contain an arbitrary number of uniform layers. This is important to keep the interior problem as small as possible. Finally, Section 6 concludes with a numerical example that demonstrates the convergence properties of the discretization scheme and the nonlinear solver.

2. PROBLEM DESCRIPTION AND NOTATIONS

We consider the propagation of polarized electromagnetic waves through a structure which is homogeneous in y-direction and periodic in z-direction with period one. In the TE case the electric field only has a component in the y-direction, i.e., $\mathbf{E}(x, y, z) = u(x, z)\mathbf{e}_y$, where the wave function u satisfies the Helmholtz equation

$$\Delta u + \kappa^2 u = 0. \tag{2}$$

A typical waveguide geometry consists of a substrate region, several stratified layers, a small grating layer, and an air superstrate region. The different layers are denoted by Ω_j, $j = 0, \ldots, J$. The super- and substrate regions, Ω_0 and Ω_J, respectively, have infinite extent. A typical geometry is shown in Fig. 1.

We assume that the magnetic permeability μ is constant and that the electric permittivity ϵ is constant within each layer. Therefore the wave number κ is a piecewise constant function,

$$\kappa(x, z) = \kappa_j := \omega\sqrt{\mu_0 \epsilon_j}, \quad (x, z) \in \Omega_j. \tag{3}$$

On the interfaces of two layers the wave potential and its normal derivative are continuous, i.e.,

$$u^+ = u^- \quad \text{and} \quad \frac{\partial}{\partial n} u^+ = \frac{\partial}{\partial n} u^-. \tag{4}$$

Using Floquet theory, PDEs with periodic coefficients can be reduced to problems posed on one periodic cell (for a description of the theory for PDEs see, for instance, [14]). In that cell, the solutions of the Helmholtz equation (2) are of the form

$$u(x, z) = \exp(\gamma z) v(x, z) \tag{5}$$

where v is periodic in z and γ is an unknown complex number, usually referred to as the fundamental propagation constant or as the Floquet exponent.

Substituting the form of u in (5) into the Helmholtz equation (2) results in the following PDE for v

$$\Delta v + 2\gamma v_z + (\gamma^2 + \kappa^2) v = 0. \tag{6}$$

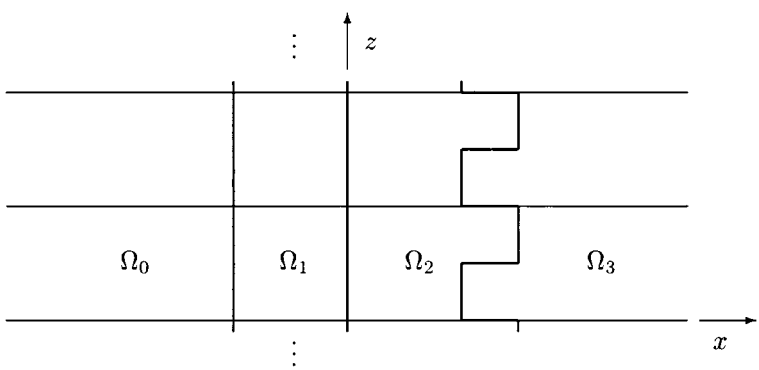

FIG. 1. Typical waveguide geometry.

Because of periodicity, (6) can be solved in the unit strip $\mathbf{R} \times [0, 1]$ with periodic boundary conditions. The core problem that must be solved is to find the characteristic values of γ for which Eq. (6) has a nontrivial solution.

For the infinite and stratified layers the solution of (6) can be obtained by separation of variables. In the jth layer the wave function is a linear superposition of spatial harmonics in the form

$$v_k^{\pm j}(x, z) = \exp\left(\pm i \gamma_k^j x\right) \exp(2\pi i k z), \tag{7}$$

where γ_k^j is the transverse wave number and is given by the dispersion relation

$$\gamma_k^j = \sqrt{(\gamma + 2\pi i k)^2 + \kappa_j^2}. \tag{8}$$

While in each finite layer there are two fundamental modes corresponding to the sign in (7), there is only one mode in the semi-infinite layers. Usually the sign is chosen so that energy flows or decays away from the structure [15].

Inside the grating layer the wave number is a function of x and z. Hence solutions can no longer be expressed in closed form and must be determined numerically, for instance with a finite element scheme. As it is not possible to discretize the whole strip, the solution for the grating layer must be coupled with the analytical solution in the uniform layers. The method used in this paper is based on matching the Dirichlet-to-Neumann operators on the interfaces of the domain and will be described below.

3. PROBLEM REDUCTION USING DIRICHLET-TO-NEUMANN MAPS

Decompose the infinite strip into three rectangular domains D_+, D_-, and D_0 as illustrated in Fig. 2. Domain D_0 contains the grating region; D_+, D_- have infinite extend in positive and negative x-direction, respectively. The interfaces between D_0 and $D_\pm$ are denoted by $S_\pm$. For now we stipulate that the semi-infinite domains are subsets of Ω_0 and Ω_J, respectively; that is, the wave number κ is constant in both domains. For structures that contain a large number of layers it is desirable to include the uniform layers in D_+ and D_- to save on computational work for D_0. The alteration of the method for this case will be discussed in Section 5.

Assume that γ is a number for which the interior problem

$$\begin{aligned} \Delta v + 2\gamma v_z + (\gamma^2 + \kappa^2) v &= 0 \quad \text{in } D_0 \\ v &= f_\pm \quad \text{on } S_\pm \\ v \text{ periodic in } z & \end{aligned} \tag{9}$$

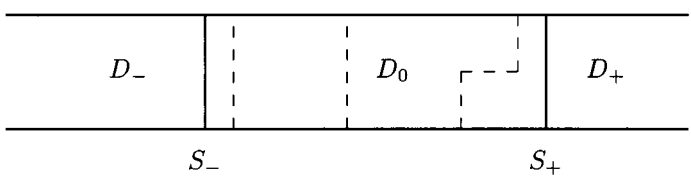

FIG. 2. Decomposition of the infinite strip.

is uniquely solvable. Then a pair of functions $f_\pm$ maps onto the normal derivatives $\partial v_\pm/\partial n$ of the solution to (9) restricted to S_+ and S_-. For γ fixed this is the Dirichlet-to-Neumann (DtN) operator which will be denoted by $T_{\text{int}}(\gamma)$ in the following. Similarly, the exterior problems

$$\begin{aligned} \Delta v + 2\gamma v_z + (\gamma^2 + \kappa^2)v = 0 \quad & \text{in } D_\pm \\ v = f_\pm \quad & \text{on } S_\pm \\ v \text{ periodic in } z & \end{aligned} \tag{10}$$

give rise to a DtN map which is denoted by $T_{\text{ext}}(\gamma)$. The numerical method for determine the characteristic values of the full problem (6) is based on the following observation.

LEMMA 1. *Suppose γ is such that the interior and exterior problems are uniquely solvable. Then γ is a characteristic value of* (6) *if and only if $T(\gamma) := T_{\text{int}}(\gamma) - T_{\text{ext}}(\gamma)$ is singular.*

Proof. Let v, γ be an eigenpair of the full problem (6). Then the derivative $\partial v/\partial x$ is continuous and hence $T(\gamma)v = 0$, i.e., the DtN map is singular. On the other hand, let $T(\gamma)v = 0$ for a $v \neq 0$. Since the problems in D_0 and $D_\pm$ are uniquely solvable, v extends to a solution of the interior and exterior problems, and, as v is continuous and differentiable across the interfaces $S_\pm$, the extension is also a solution of (6). ∎

Instead of solving (6) directly, our numerical method is based on finding the values of γ for which the DtN-map $T(\gamma)$ is singular. This is a nonlinear eigenvalue problem in a vector space of functions on the interfaces $S_\pm$.

Functions on the interfaces can be expanded in terms of the Fourier modes

$$e_k^\pm(z) = \begin{cases} \exp(2\pi i k z) & \text{on } S_\pm, \\ 0 & \text{on } S_\mp, \end{cases} \quad k \in \mathbf{Z}. \tag{11}$$

In this basis the exterior DtN-map is a diagonal operator

$$T_{\text{ext}}(\gamma)e_k^\pm = i s_k^\pm \gamma_k^\pm e_k^\pm, \quad k \in \mathbf{Z}, \tag{12}$$

where γ_k^+ and γ_k^- follow from the dispersion relation (8) and $s_k^\pm$ is the sign of the solution (7) for the infinite layer.

Since there is a non-uniform layer in the domain D_0, the Fourier modes of the interior DtN-map are coupled and therefore $T_{\text{int}}(\gamma)$ is not a diagonal operator in basis (11). The coefficients of $T_{\text{int}}(\gamma)$ must be determined by first solving the interior problem (9) with boundary condition $f_\pm = e_k^\pm$ and then calculating the Fourier coefficients of the solution $v_k^\pm$, i.e.,

$$T_{\text{int}}(\gamma)_{l,k}^{\pm,\pm} = \left\langle e_l^\pm, \frac{\partial v_k^\pm}{\partial n} \right\rangle, \quad k, l \in \mathbf{Z}. \tag{13}$$

In order to calculate the Floquet exponents numerically, two discretizations are necessary. First, only Fourier modes of order $|k| \leq p$ are used to approximate the DtN maps. The

truncation can be regarded as the Galerkin discretization of $T(\gamma)v = 0$ using the Fourier modes up to a given order as the trial- and test space. Solving the interior problem numerically involves a second discretization step. A large number of options are available, in our implementation we have used the finite element method [18].

4. MATRIX-NEWTON SOLVER

After discretizing the DtN operators the problem on the interfaces reduces to a matrix problem of size $4p+2$. The matrix entries depend nonlinearly on the Floquet exponent γ and the problem at hand is to find γ such that $T(\gamma)$ is singular. In principle, this problem can be rewritten as $\det T(\gamma) = 0$ and solved by the Newton method, but the iteration can be slow, especially near Bragg conditions where solution branches intersect or nearly intersect.

Instead of dealing with the determinant, consider the truncated Taylor expansion of the DtN operator

$$T_m(\sigma) = \bar{T}_0 + \sigma \bar{T}_1 + \cdots + \sigma^m \bar{T}_m, \tag{14}$$

where $\gamma = \bar{\gamma} + \sigma$ and

$$\bar{T}_l = \frac{1}{l!}\frac{\partial^l}{\partial \gamma^l} T(\bar{\gamma}), \quad l = 0, \ldots, m. \tag{15}$$

For the current iterate $\bar{\gamma}$ the next iterate is determined from the smallest value (in modulus) of σ that makes the matrix polynomial (14) singular. For that, write

$$\bar{T}_m(\sigma) = \sigma^m \bar{T}_0 \, S_m\left(\frac{1}{\sigma}\right), \tag{16}$$

where

$$S_m(\lambda) = A_0 + \lambda A_1 + \cdots + \lambda^{m-1} A_{m-1} + \lambda^m I \tag{17}$$

and $A_k = \bar{T}_0^{-1}\bar{T}_{m-k}$. Since $\bar{T}_0$ is nonsingular (otherwise $\bar{\gamma}$ would be a Floquet exponent), the matrix polynomial $T_m(\sigma)$ becomes singular only if $S_m(1/\sigma)$ is singular. It follows that the correction of the current iterate is given by the reciprocal of the largest eigenvalue of the companion matrix

$$\begin{bmatrix} & & & -A_0 \\ I & & & -A_1 \\ & I & & -A_2 \\ & & \ddots & \vdots \\ & & I & -A_{m-1} \end{bmatrix} \tag{18}$$

of the matrix polynomial S_m. Thus the companion matrix has size $m(4p+2)$ and hence, since p and m are typically small, the eigenvalue problem can be solved inexpensively using standard linear algebra routines.

It remains to determine the expansion coefficients $\bar{T}_0, \bar{T}_1, \ldots, \bar{T}_m$. In the following we will describe how these terms can be calculated stably without evaluating numerical derivatives.

Expansion of the Exterior DtN-Map

The diagonal coefficients of the exterior DtN-map are determined by the dispersion relation (8) for which the Taylor expansion must be determined. If $\gamma = \bar{\gamma} + \sigma$ then the transverse wave number can be considered as a function of the perturbation, i.e., $\gamma_k^{\pm} = \gamma_k^{\pm}(\sigma)$. Dropping obvious super- and subscripts and setting $\bar{\gamma}_k = \sqrt{(2\pi i k + \bar{\gamma})^2 + \kappa^2}$ and $\mu_k = -(2\pi i k + \bar{\gamma})/\bar{\gamma}_k$, one obtains the expansion

$$\gamma_k(\sigma) = \bar{\gamma}_k \sqrt{1 - 2\mu_k \frac{\sigma}{\bar{\gamma}_k} + \left(\frac{\sigma}{\bar{\gamma}_k}\right)^2} \tag{19}$$

$$= \bar{\gamma}_k \sum_{n=0}^{\infty} C_n(\mu_k) \left(\frac{\sigma}{\bar{\gamma}_k}\right)^n. \tag{20}$$

The functions $C_n(\mu)$ are orthogonal polynomials which have three-term recurrence relations; see, e.g., Abramowitz and Stegun [1, Formulas 22.9.4 and 22.7.3].

Expansion of the Interior DtN-Map

The interior DtN-map and its expansion coefficients have no closed form. Therefore the coefficients must be determined from an expansion of the solution of the interior problem in terms of the perturbation σ. For this, write (9) symbolically in the form

$$\left(A + \sigma B + \sigma^2 I\right) v = 0, \quad \text{in } D_0 \tag{21}$$

$$v = f, \quad \text{on } S_{\pm}, \tag{22}$$

where $\gamma = \bar{\gamma} + \sigma$ and

$$Av = \Delta v + 2\bar{\gamma} v_z + (\bar{\gamma}^2 + \kappa^2) v, \tag{23}$$

$$Bv = 2\bar{\gamma}(v_z + v). \tag{24}$$

Thus the solution of (9) is a function of the perturbation $v = v(\sigma, x, z)$ with expansion

$$v(\sigma, x, z) = \sum_{n=0}^{\infty} \sigma^n v_n(x, z). \tag{25}$$

If the above series is substituted into the partial differential equation, it can be seen that the coefficients v_n satisfy

$$\begin{aligned} Av_0 &= 0, \quad \text{in } D_0, \\ v_0 &= f, \quad \text{on } S_{\pm}, \end{aligned} \tag{26}$$

$$\begin{aligned} Av_1 &= -Bv_0, \quad \text{in } D_0, \\ v_1 &= 0, \qquad \text{on } S_{\pm}, \end{aligned} \tag{27}$$

$$\begin{aligned} Av_n &= -Bv_{n-1} - v_{n-2}, \quad \text{in } D_0, \\ v_n &= 0, \qquad\qquad\quad \text{on } S_{\pm}, \end{aligned} \qquad n = 2, 3, \ldots. \tag{28}$$

Thus the functions v_n and the expansion coefficients of the interior DtN-map can be calculated iteratively. Each step of the iteration involves an inversion of the interior problem

for the current iterate $\bar{\gamma}$ with an inhomogeneity which depends on the previously calculated functions. Since this iteration has to be done for the $4p+2$ harmonics in the discretization of $T(\gamma)$, the calculation of the entries in the companion matrix (18) takes $(m+1)(4p+2)$ solutions of the interior problem.

5. EXPANSION OF TRANSLATION OPERATORS

Since the interior problem must be solved repeatedly for each step of the nonlinear solver, it is important for the efficiency of the method that the domain D_0 is kept as small as possible. This can be achieved by including the uniform layers in the exterior domains D_+ and D_-. In that case, the exterior DtN-map is still a diagonal operator, because no mode coupling occurs, but it is no longer given by the dispersion relation (8). In this section we will derive the form of the DtN-map and its expansion coefficients. For this it is convenient to write the solution in the uniform layers (7) for mode k and layer j in the form

$$v_k^j(x) = \phi_k^j(\sigma)c_k^j(\sigma, x) + \psi_k^j(\sigma)s_k^j(\sigma, x), \quad x_{j-1} \le x \le x_j, \tag{29}$$

where σ is the perturbation of γ and

$$c_k^j(\sigma, x) = \cos\big(\gamma_k^j(\sigma)(x - x_{j-1})\big), \tag{30}$$

$$s_k^j(\sigma, x) = \sin\big(\gamma_k^j(\sigma)(x - x_{j-1})\big)/\gamma_k^j(\sigma). \tag{31}$$

Hence the state variables ϕ^j and ψ^j describe the system at the interface of two layers

$$v_k^j(x_{j-1}) = \phi_k^{j-1}(\sigma), \tag{32}$$

$$\frac{d}{dx}v_k^j(x_{j-1}) = \psi_k^{j-1}(\sigma). \tag{33}$$

Since v and its derivative are continuous functions the state variables of two adjacent layers are coupled,

$$\begin{bmatrix} \phi_k^j(\sigma) \\ \psi_k^j(\sigma) \end{bmatrix} = T_k^j(\sigma) \begin{bmatrix} \phi_k^{j-1}(\sigma) \\ \psi_k^{j-1}(\sigma) \end{bmatrix}, \tag{34}$$

where T_k^j is the translation of the state variables across layer j, which is the matrix

$$T_k^j(\sigma) = \begin{bmatrix} c_k^j(\sigma, x_j) & s_k^j(\sigma, x_j) \\ \frac{d}{dx}c_k^j(\sigma, x_j) & \frac{d}{dx}s_k^j(\sigma, x_j) \end{bmatrix}. \tag{35}$$

Thus the translation of the state variables from the outer- to the innermost layer (i.e., the interface S_- located at x_{j^-}) is the product of the translation operators across all layers

$$\begin{bmatrix} \phi_k^{j^-}(\sigma) \\ \psi_k^{j^-}(\sigma) \end{bmatrix} = T_k^{j^-}(\sigma) \cdot \cdots \cdot T_k^1(\sigma) \begin{bmatrix} 1 \\ \gamma_k^-(\sigma) \end{bmatrix}. \tag{36}$$

The translation to the interface S_+ located at x_{j^+} follows in a similar fashion. The DtN maps at $S_\pm$ are then given by

$$T_{\text{ext}}(\sigma)\, e_k^\pm = \frac{\psi_k^{j^\pm}(\sigma)}{\phi_k^{j^\pm}(\sigma)}\, e_k^\pm. \tag{37}$$

Beginning with the dispersion relation (8), the DtN operator for the exterior problem consists of several applications (products) of translations followed by a division. To obtain the Taylor expansion of $T_{\text{ext}}(\sigma)$, power series expansions must be multiplied and divided, which reduces to convolutions and deconvolutions of the expansion coefficients. Thus the expansion of the dispersion relation (20) must be repeatedly convolved with the expansion of the translation matrices. Finally, the resulting series must be divided (i.e., deconvolved) to obtain the expansion of the DtN map at the interfaces $S_{\pm}$.

Since the expansion of $\gamma^{\pm}(\sigma)$ has already been derived in (20), it remains to obtain the expansion of the translation matrices $T_k^j(\sigma)$. This reduces to finding the Taylor series of the functions c_k^j and s_k^j. The explicit form of the coefficients is a rather complicated expression, but the coefficients can also be calculated iteratively in a similar way as for the interior problem in (26)–(28). The details of the derivation are described in the appendix.

6. NUMERICAL EXAMPLE

To demonstrate the feasibility of this approach to calculating Floquet exponents associated with periodic dielectric waveguides we include a simple example with geometry similar to that in Fig. 1, which consists of three layers whose wavenumbers are given by $\kappa_0 = \sqrt{2.3}\,\omega$, $\kappa_1 = \sqrt{3}\,\omega$, and $\kappa_2 = \omega$. The layer Ω_1 contains a rectangular corrugation 0.4 units in height. The smaller x-extent of Ω_1 is $2/\pi$. This example makes frequent appearances in the literature; see, e.g., [3].

For our calculations, the interfaces $S_{\pm}$ coincide with the grating layer. Thus there is one translation operation across the guiding layer for the state variables. The interior problem was discretized into rectangles with piecewise bilinear basis functions.

Figure 3 shows the dependence of the phase shift $-\text{Im}\,\gamma$ of the frequency ω. There are three solution branches in the displayed frequency range, they intersect at the first and second

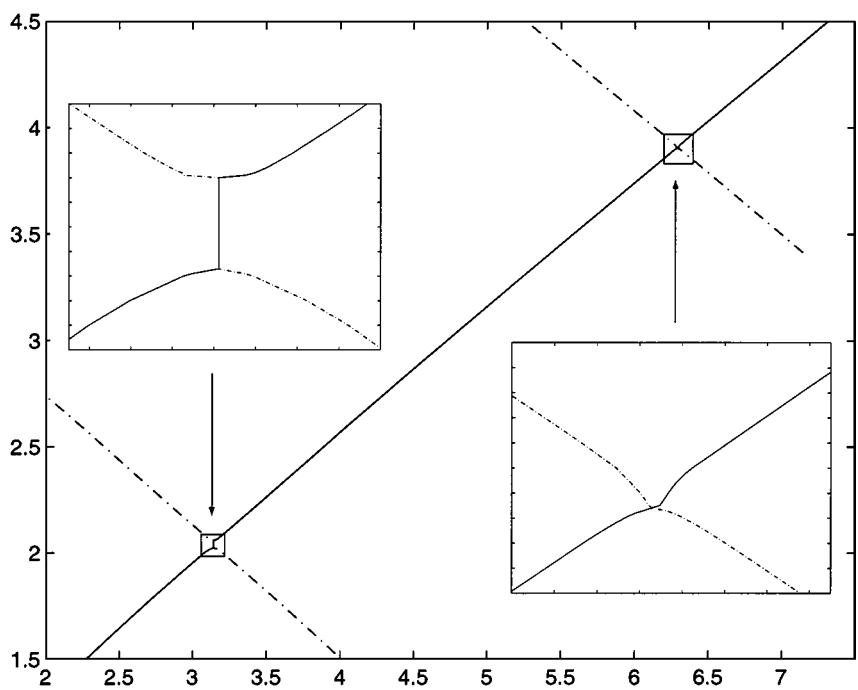

FIG. 3. ω–β Plot.

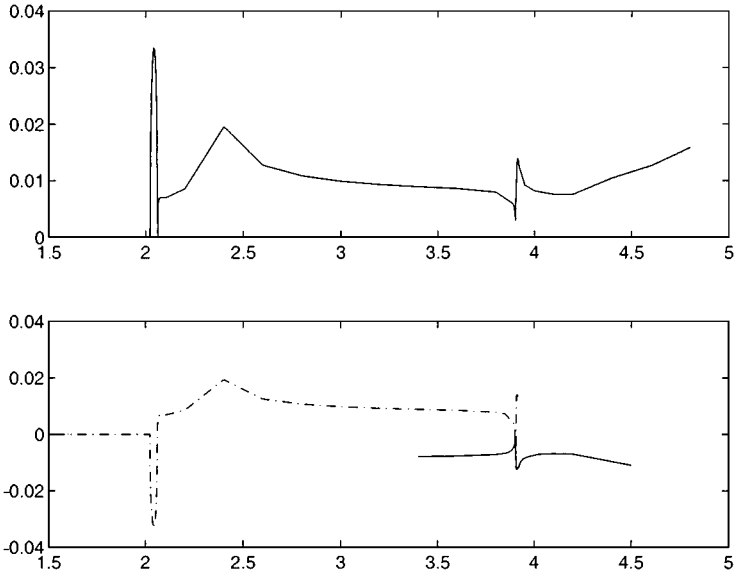

FIG. 4. α–ω plot for the main branch (top) and the other two branches (bottom).

Bragg condition. Figure 4 shows the attenuation factor $-\alpha$ for the three solution branches as a function of ω. Before the first Bragg there is no radiation and since the materials have been assumed to be lossless, the attenuation is zero. At the first Bragg a stopband appears, at the second Bragg a sharp drop occurs before the attenuation goes back to normal.

TABLE I

Convergence of the Dominant Floquet Exponent, $\omega = \pi$

	$-\mathrm{Re}(\gamma)$				
h	0.1	0.05	0.025	0.0125	0.00625
$p = 0$	−7.77e-15	−3.47e-13	−7.68e-13	1.08e-11	1.36e-11
$p = 1$	0.010576	0.0098030	0.0096199	0.0095745	0.0095631
$p = 2$	0.010458	0.0096259	0.0094239	0.0093737	0.0093611
$p = 3$	0.010459	0.0096259	0.0094248	0.0093746	0.0093620
$p = 4$	0.010459	0.0096254	0.0094241	0.0093738	0.0093612
$p = 5$	0.010459	0.0096255	0.0094242	0.0093739	0.0093613
$p = 6$	0.010459	0.0096254	0.0094241	0.0093738	0.0093612
$p = 7$	0.010459	0.0096254	0.0094241	0.0093738	0.0093612
	$-\mathrm{Im}(\gamma)$				
h	0.1	0.05	0.025	0.0125	0.00625
$p = 0$	4.98213	4.98100	4.98059	4.98046	4.98043
$p = 1$	4.96719	4.96633	4.96608	4.96601	4.96599
$p = 2$	4.96719	4.96639	4.96610	4.96604	4.96602
$p = 3$	4.96720	4.96639	4.96615	4.96609	4.96607
$p = 4$	4.96720	4.96639	4.96615	4.96609	4.96607
$p = 5$	4.96720	4.96639	4.96616	4.96609	4.96607
$p = 6$	4.96720	4.96639	4.96616	4.96609	4.96607
$p = 7$	4.96720	4.96639	4.96616	4.96609	4.96607

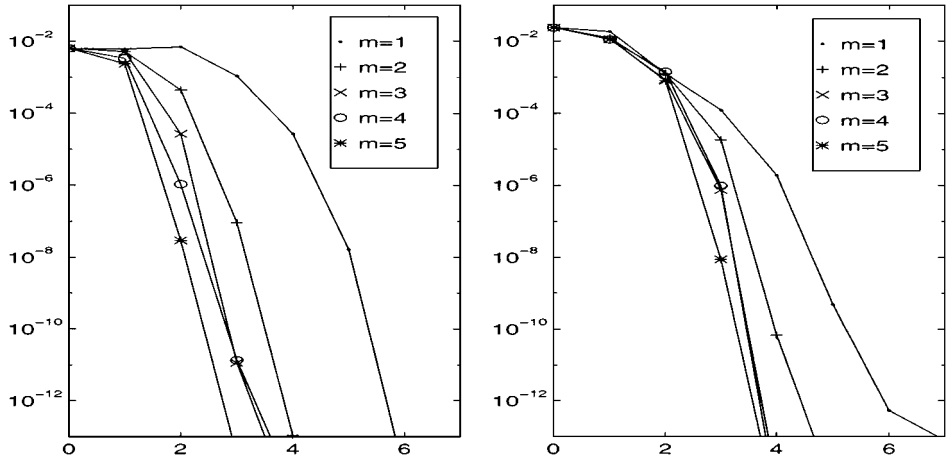

FIG. 5. Convergence of nonlinear solver $\mathrm{cond}^{-1}T(\gamma)$ vs iterate, $\omega = 3.14$ (left) and $\omega = 2.02$ (right).

Table I displays the real and imaginary parts of the dominant Floquet exponent as a function of the number of modes and the mesh width used in the discretization of the DtN-map. Even for a very coarse mesh and a small number of modes the approximation is close to the one obtained with fine meshes and high p. The convergence in p is much faster than that in h; therefore even for fine meshes a low p will suffice. The results in the table are shown for $\omega = \pi$, the convergence behavior at the other frequencies is similar.

In Fig. 5 we show the behavior of the nonlinear solver as a function of the number of moments in the expansion of the DtN-map. For $\omega = 3.14$ the convergence is faster as the number of moments is increased, but even a small number of moments suffices to achieve rapid convergence. Where solution branches intersect or nearly intersect one would expect the convergence rate of the nonlinear solver to deteriorate. However, our experiments revealed that once the iterate is sufficiently close to the actual solution, the convergence near the Bragg conditions is almost as rapid in regions where there is only one solution branch.

7. CONCLUSIONS

In this paper we have introduced a new approach to calculating the Floquet modes of two-dimensional waveguides. The main feature of our method is the reduction of the eigenvalue problem posed in an infinite strip to an eigenvalue problem posed on two intervals of unit length. The matrix–Newton method is better suited for nonlinear eigenvalue problems associated with Floquet-type wave phenomena than methods that are based on setting the determinant to zero. The numerical results demonstrate that Floquet modes can be calculated accurately and efficiently by retaining a small number of harmonics in (11) and a small number of expansion terms in (14). The approach of finding the characteristic values of the DtN map rather than the PDE can readily be extended to problems which are inherently three-dimensional.

The method presented of determining the eigenvalues assumes that the assumptions of Lemma 1, namely that the interior and exterior problems are uniquely solvable, hold in a neighborhood of the Floquet exponent. The exterior problem is always solvable as soon as

the sign in (7) is determined, and the solvability of the interior problem can be controlled by the extend of the domain D_0. In our experiments the assumptions of the lemma never appeared to cause any problems.

APPENDIX

The expansion coefficients of the functions c_k^j and s_k^j defined in (30) and (31) can be obtained recursively. The calculation is based on the observation that both functions satisfy the differential equation

$$y'' + \left((\gamma + 2\pi ik)^2 + \kappa_j^2\right) y = 0 \tag{38}$$

with boundary conditions

$$y(x_{j-1}) = 1, \quad y'(x_{j-1}) = 0, \quad \text{for } c_j^k, \tag{39}$$

$$y(x_{j-1}) = 0, \quad y'(x_{j-1}) = 1, \quad \text{for } s_j^k. \tag{40}$$

If $\gamma = \bar{\gamma} + \sigma$ both functions can be expanded in the form

$$\sum_{n=0}^{\infty} \sigma^n y_n(x). \tag{41}$$

Substituting this expansion into the differential equation, it follows that the y_n's solve the recurrence relation

$$y_n'' + \left(\bar{\gamma}_k^j\right)^2 y_n = -2\bar{\gamma}_k^j y_{n-1} - y_{n-2}, \quad n = 1, 2, \ldots \tag{42}$$

$$y_n(x_{j-1}) = y_n'(x_{j-1}) = 0, \tag{43}$$

where $y_{-1} = 0$ and $y_0(x) = \cos(\bar{\gamma}_k^j (x - x_{j-1}))$ for c_k^j or $y_0(x) = \sin(\bar{\gamma}_k^j (x - x_{j-1}))/\bar{\gamma}_k^j$ for s_j^k. The solution of the above differential equation with right hand side f can be expressed using the Green's function for this problem,

$$y(x) = \frac{1}{\bar{\gamma}_k^j} \int_0^x \sin\left(\bar{\gamma}_k^j (x - t)\right) f(t)\, dt \equiv Sf(x). \tag{44}$$

Setting $c_n(x) = \cos(\bar{\gamma}_k^j x) x^n$ and $s_n(x) = \sin(\bar{\gamma}_k^j x) x^n$, we see that

$$Sc_n = \frac{1}{\bar{\gamma}_k^j} \left(\frac{1}{n+1} s_{n+1} - \frac{n}{2} S s_{n-1} \right), \tag{45}$$

$$Ss_n = \frac{1}{\bar{\gamma}_k^j} \left(\frac{-1}{n+1} c_{n+1} + \frac{n}{2} S c_{n-1} \right). \tag{46}$$

By combining Eqs. (44), (45), and (42), it follows that the expansion coefficients $y_n(x)$ are linear combinations of the functions $c_0, \ldots, c_n$ and $s_0, \ldots, s_n$, whose weights can be again recursively determined.

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