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Scattering matrix analysis of photonic crystals

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ABSTRACT

SCATTERING MATRIX ANALYSIS OF PHOTONIC CRYSTALS

by
Valeriy Lukyanov

Using a scattering matrix approach we analyze and study the scattering and transmission of waves through a two-dimensional photonic crystal which consists of a periodic array of parallel rods with circular cross sections. Without making any assumptions about normal incidence, single mode propagation, and sufficient inter-scatter separation in the direction of propagation, we show how to compute the transmission and reflection coefficients of these periodic structures. The method is based on the computation of a generalized scattering matrix for one column of the periodic structure.

We also develop an analytical method to analyze and to study the scattering and transmission of waves through a two-dimensional photonic crystal which consists of a periodic array of parallel metallic rods with rectangular cross sections. The method is based on the computation of generalized scattering matrices for several parts of the periodic entire structure, and their composition to form the scattering matrix for the structure. We derive an explicit formula for the reflection and transmission coefficients when we take into account only one propagating mode in a specific portion of the periodic structure.

Finally, we develop an analytical method to analyze and to study Rayleigh-Bloch surface waves propagating along a two-dimensional diffraction grating which again consists of a periodic array of rods with rectangular cross sections. The method is based on mode matching. By taking into account all propagating and only a finite number of evanescent modes in a specific portion of the waveguide we show that the surface waves correspond to the zeros of the determinant of a Hermitian matrix.

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by
Valeriy Lukyanov

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V. M. Babich, V. V. Lukyanov,
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Wave Motion, vol. 26, no. 4, pp. 379-397, 1997.

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To my parents,
Lyudmyla Nosova and Valeriy D. Lukyanov

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CHAPTER 1

INTRODUCTION

1.1 Photonic Crystals

In the past decade, a great deal of effort has been devoted to the study of photonic crystals. Photonic crystals are periodic structures of dielectric or metallic materials which are designed to control the propagation of light. The characteristic feature of a photonic crystals is that it has a spectral gap in its dispersion relationship. Light can not propagate in the crystal when its frequency is in this gap. This effect has long been used in dielectric mirrors and optical filters, which are made from alternating dielectric layers. Photonic crystals allow the extension of this idea to two and three dimensions. Some periodic structures have a complete band gap in which light can not propagate in any directions. This property is the optical analog of electronic band gaps in semiconductors caused by their periodic atomic lattice structures. This similarity has many potential applications in designing of optical devices. For example, it is believed that by replacing electrons with photons the speed and band-width of communication system will be dramatically increased. Other applications might be designing entirely optical computers, high efficiency lasers, laser diodes, highly efficient wave guides, high speed optical switches, and more.

A two-dimensional photonic crystal can be constructed from a lattice of parallel dielectric rods. A commonly used material for rods is GaAs with a dielectric constant $\epsilon = 13$. The rods are separated by air for which $\epsilon = 1$. The computation of band gaps for 2D photonic crystals (moreover, for 3D crystals) is a challenging numerical problem. The theory of 2D photonic crystals reduces to the solution of two scalar equations for the E- and H-polarized electromagnetic fields. The common approach to the computations of band gaps is based on the decomposition of the fields into plane waves with a consequent series truncation. Although this approach can be applied to any periodic dielectric structure, in practice, the truncation severely limits the accuracy of the plane-wave method. The reason for this is that usually dielectric constant $\epsilon(x)$ is discontinuous for photonic crystals as function of x and, hence, the series of plane waves for it converges very slowly. Therefore, to get accurate results we should keep enormous number plane waves and deal with extremely large matrixes. Another numerical approach is to apply finite difference time domain method (FDTD). Although it can be applied to any photonic crystals this method is also requires significant computer resources and it only clarify the "physics" of photonic crystal after many numerical simulations.

In this thesis, we show how to apply a scattering matrix approach for the investigation of photonic crystals. This method is based on a natural representation of the electromagnetic field in terms of plane waves and allows a considerably reduction of computations. This is because only one generalized scattering matrix is required. In Ref. [3], Kriegsmann applied it to compute the reflection and transmission coefficients in one mode regime, by neglecting evanescent modes. Here we apply scattering matrix theory without these assumption to photonic crystal consisted of metallic or dielectric cylinders. In Ref. [2], Venakides et al. solved the problem, with an incident wave, using a boundary integral method technique. They reduced the problem to the boundary integral equation on n cylinders, where n is the number of columns of a periodic structure. The scattering matrix approach reduces the problem to a boundary integral equation on only one cylinder. We describe how to solve this integral equation by means of Nostrem method with quadrature formulae based on Lagrange polynomials and Ewald representation of the Green's function.

Although in this thesis the scattering matrix theory is applied only to 2D photonic crystals it can be extended for 3D case and this is a goal of my future research. For 3D photonic crystals the advantages of this theory become more obvious.

1.2 Dissertation Overview

This thesis is organized in the following way. In Chapter 2, we analyze and study the scattering and transmission of waves through a two-dimensional photonic crystal which consists of a periodic array of parallel rods of a circular cross section. Without making any assumptions about normal incidence, single mode propagation, and sufficient inter-scatterer separation in the direction of propagation, we show how to compute the transmission and reflection coefficients of periodic structures. The method is based on computation of generalized scattering matrix for one column of the periodic structure. We show that evanescent waves play an important role in periodic structures such as photonic crystals and that taking into account several of them gives good approximation for the solution.

In Chapter 3, we show how to solve the problem on scattering of plane wave by one column of metallic and dielectric cylinders. We reduce the problem to boundary integral equation on one cylinder using periodic Green's function and show how to discretize it.

In Chapter 4, we develop an analytical method to analyze and to study the scattering and transmission of waves through a two-dimensional photonic crystal which consists of a periodic array of parallel rods of a rectangular cross section. The method is based on the computation of generalized scattering matrices for several parts of the periodic structure, and their composition to form the scattering matrix for the structure. We show that an explicit formula for the reflection and transmission coefficients can be obtained if we take into account only one propagating mode in a specific portion of the periodic structure. We demonstrate numerically that the formula gives good results under certain conditions on the wave number and the distance between rectangular rods.

In Chapter 5, we develop an analytical method to analyze and to study the Rayleigh-Bloch surface waves propagating along two-dimensional diffraction grating which consists of a periodic array of rods of a rectangular cross section. The method is based on the mode matching. By taking into account all propagating and only finite number of evanescent modes in a specific portion of the waveguide we show that the surface waves correspond to the singularities of a Hermitian matrix. We demonstrate numerically that the method gives accurate results if we take into account only several evanescent waves.

CHAPTER 2

COMPUTATION OF ELECTROMAGNETIC FIELDS IN PERIODIC STRUCTURES

2.1 Introduction

Two-dimensional photonic crystals are man made periodic structures made of either dielectric or metallic cylinders. These crystals are used in many technological fields, such as optics and microwaves. Examples of the former are optical filters and Fabry-Perot resonators, and of the latter are antenna and filter design. A typical crystal structure is shown in Fig. 2.1.

The problem of finding transmission and reflection coefficients for periodic structures has been successively studied by researchers employing boundary integral equation methods [1,2]. These techniques produce accurate approximations, but become computationally intensive when the number of columns making up the periodic structures become moderate to large. Because of this fact these techniques are costly when used as a design tool for periodic structures.

In a recent paper [3], the scattering and transmission of waves through a two-dimensional photonic crystal were studied using scattering matrix theory. This is computationally more efficient than those reported in [1,2] because it requires solution of the problem only for one layer of periodic structure. However, the application of this theory required two assumption, which limits its applicability. The first required the scatterers to be sufficiently far apart in x-direction to neglect evanescent waves. The second required them to be sufficiently close together in the y-direction for a fixed frequency, to ensure single mode propagation in a fundamental waveguide-cell.

In this paper, we show how to solve such problems without these assumptions. Specifically, we remove the requirement that scatterers are far apart and take into account the evanescent modes and eliminate the restriction of single mode propagation.

Accordingly, the resulting theory becomes more involved than the one presented in Ref [3]. Our new theory is based upon the computation of a generalized scattering matrix which in principal takes into account any finite number of propagating and evanescent modes. The number of the former is determined by the frequency and the spacing of the cylinders in y-direction. However, the required number of evanescent modes is determined by the spacing in the x-direction and the amount of accuracy needed.

In order to estimate the number of evanescent modes to include we consider the structure shown in Fig. 2.1 with $N = 2$. We first approximately solve this problem by employing a boundary integral equation technique which yields very accurate approximations to the transmission and reflection coefficients for this grating. In the second approximation, we first compute the generalized scattering matrix for the structure, when $N = 1$, which incorporates m evanescent modes. Again the same boundary integral technique is employed. Then, we apply our generalized scattering matrix method to approximate the reflection and transmission coefficients for the case $N = 2$. These are compared with those of our first approximation to obtain the error. The dependence of this error on the x-spacing, m, and the frequency is then studied and trends are observed. Specifically, we can systematically estimate m for a prescribed accuracy in the reflection and transmission coefficients.

Finally, we apply our generalized scattering matrix theory to the problem with $N = 10$ columns. The dependence of the modulus of the transmission coefficient upon m, k, and the x-direction spacing is presented and discussed. In particular, their effects on the pass and stop bands are exhibited. Since our technique depends only upon determining the generalized scattering matrix for a single column, i.e., $N = 1$, our results do not suffer the computational burden of a straightfoward application of the boundary integral method. Because of this fact, our method may be useful as a design tool for periodic structure when the frequency is fixed and the inter-column distance is varied.

2.2 Statement of the Problem

Consider an infinite array made up of N columns of identical metallic cylinders. The cylinders have radius 1 and their centers are located at points $(hm, 2dn)$, $m = 1, ..., N$, $n = 0, \pm 1, \pm 2, ...$, where h is the spacing between cylinders in the x-direction and $2d$ is the spacing in the y (see Fig. 2.1).

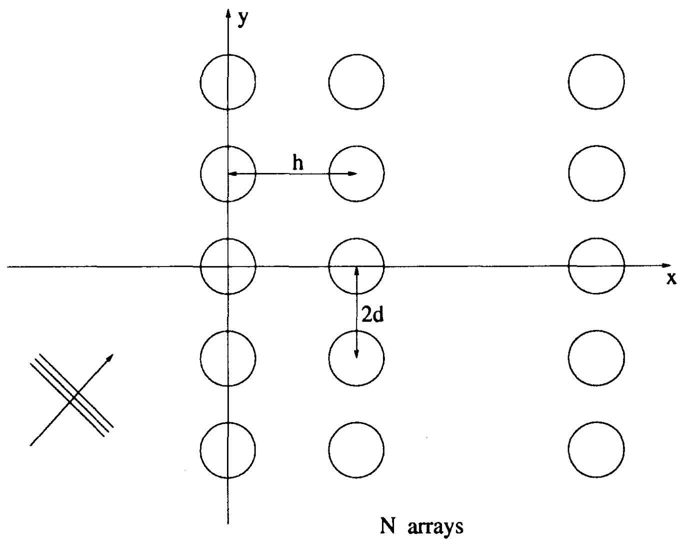

Figure 2.1 Geometry of the problem.

Two dimensional scattering problem we wish to solve is governed by the Helmholtz equation

$$\Delta u + k^2 u = 0, \tag{2.1}$$

$$u = u_i + u_s,$$

where u represents the z-component of the magnetic field, u_s is unknown scattered field, and u_i is an incident plane wave impinging upon our structure

$$u_i = e^{ik(x\cos\theta + y\sin\theta)}. \tag{2.2}$$

We assume that on the surface of each cylinder Neumann boundary conditions are satisfied, i.e.,

$$\frac{\partial u}{\partial n} = 0. \tag{2.3}$$

Because of periodicity of the problem, we can represent the incident and scattered fields in the form

$$u_i = e^{i\beta y}\tilde{u}_i, \quad u_s = e^{i\beta y}\tilde{u}_s, \tag{2.4}$$

where β is a real number and $\tilde{u}_i$ and $\tilde{u}_e$ are periodic functions with respect to y and consider only a single interval of length $2d$ in the y-direction

$$R = \{(x, y) : -\infty < x < \infty, -d \le y \le d\}. \tag{2.5}$$

This is the fundamental waveguide in which we formulate and study our problem. The periodic function u_s satisfies the equation

$$\Delta\tilde{u}_s + 2i\beta\frac{\partial\tilde{u}_s}{\partial y} + \left(k^2 - \beta^2\right)\tilde{u}_s = 0 \tag{2.6}$$

with the periodic boundary conditions

$$\tilde{u}_s\big|_{y=-d} = \tilde{u}_s\big|_{y=d}, \quad \left.\frac{\partial\tilde{u}_s}{\partial y}\right|_{y=-d} = \left.\frac{\partial\tilde{u}_s}{\partial y}\right|_{y=d}. \tag{2.7}$$

Taking into account Eqs. (2.4) we can recast the problem (2.1)-(2.3) in the fundamental waveguide R with quasi periodic boundary conditions

$$u_s\big|_{y=-d} = e^{2i\beta d}\, u_s\big|_{y=d}, \quad \left.\frac{\partial u_s}{\partial y}\right|_{y=-d} = e^{2i\beta d}\left.\frac{\partial u_s}{\partial y}\right|_{y=d}. \tag{2.8}$$

To solve this problem we split it into two parts. In the first we consider only one cylinder in the fundamental waveguide,i.e., $N = 1$. In the appendix we show how this problem can be solved numerically by using boundary integral equation technique. In the second, we solve the problem with N cylinders by using the generalized scattering matrix, introduced in Section 2.3. Specifically, we employ this matrix to obtain difference equations for the Fourier's coefficients of the scattered field. By solving these equations we find approximate reflection and transmission coefficients for this photonic structure.

2.3 The generalized scattering matrix and its calculation

In order to introduce the scattering matrix we consider one cylinder in the fundamental waveguide. Let u_i and v_i be incident waves (see Fig. 2.2) impinging upon the cylinder from the left and right respectively. These waves contain both propagating and

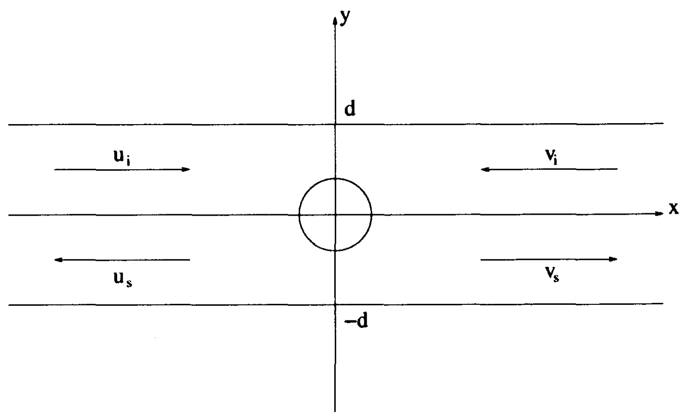

Figure 2.2 One scatterer in the waveguide.

evanescent modes. Similarly u_s and v_s are the scattered waves. In the appendix we briefly explain how to find the scattered fields u_s and v_s. To find them we employ the boundary integral equation method.

We shall now describe the generalized scattering matrix. The incident and scattered field can be expanded into

$$u_i(x,y) = \sum_{n=-\infty}^{\infty} a_n e^{i\gamma_n(x+1)+i\beta_n y}, \quad x < -1, \tag{2.9}$$

$$v_i(x,y) = \sum_{n=-\infty}^{\infty} b_n e^{-i\gamma_n(x-1)+i\beta_n y}, \quad x > 1, \tag{2.10}$$

$$u_s(x,y) = \sum_{n=-\infty}^{\infty} c_n e^{-i\gamma_n(x+1)+i\beta_n y}, \quad x < -1, \tag{2.11}$$

$$v_s(x,y) = \sum_{n=-\infty}^{\infty} d_n e^{-i\gamma_n(x-1)+i\beta_n y}, \quad x > 1, \tag{2.12}$$

$$\gamma_n = \sqrt{k^2 - \beta_n^2} = i\sqrt{\beta_n^2 - k^2}, \tag{2.13}$$

$$\beta_n = \beta + \pi n/d, \tag{2.14}$$

and describe their modal amplitudes by the infinite column vectors

$$\mathbf{a} = (..., a_{-L-1}, a_{-L}, ..., a_{-1}, a_0, a_1, ..., a_M, a_{M+1}, ...)^\top,$$

$$\mathbf{b} = (..., b_{-L-1}, b_{-L}, ..., b_{-1}, b_0, b_1, ..., b_M, b_{M+1}, ...)^\top,$$

$$\mathbf{c} = (..., c_{-L-1}, c_{-L}, ..., c_{-1}, c_0, c_1, ..., c_M, c_{M+1}, ...)^\top, \tag{2.15}$$

$$\mathbf{d} = (..., d_{-L-1}, d_{-L}, ..., d_{-1}, d_0, d_1, ..., d_M, d_{M+1}, ...)^\top,$$

where $\top$ denotes transposition. Here the amplitudes with the numbers $n = -L, -L+1, ..., M-1, M$ correspond to the amplitudes of the propagating plane waves and the other correspond to the amplitudes of the evanescent waves. Because of linearity of the problem there are infinite matrices S_{11}, S_{12}, S_{21}, S_{22}, which relate the amplitudes of incident waves **a**, **b** to the amplitudes of scattered waves **c**, **d**

$$\begin{pmatrix} \mathbf{c} \\ \mathbf{d} \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} \mathbf{a} \\ \mathbf{b} \end{pmatrix}. \tag{2.16}$$

The matrix

$$\mathbf{S} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \tag{2.17}$$

is called generalized scattering matrix. The difference between generalized scattering matrix and standard scattering matrix is that the former takes into account both propagating and evanescent modes while the latter just handles propagating modes.

To calculate **S** we consider incident waves, which may be evanescent,

$$\mathbf{a} = (..., 0, 1, 0, ...)^{\top}, \tag{2.18}$$

$$\mathbf{b} = (..., 0, 0, 0, ...)^{\top}, \tag{2.19}$$

where the m-th coordinate is equal to 1 in the vector **a**. Let c_n and d_n be the Fourier's coefficients of the scattered fields v_s and u_s. It follows from Eqs. (2.11)-(2.12) that for a fixed x

$$c_n = \frac{1}{2d} e^{-i\gamma_n x} \int_{-d}^{d} u_s(x,y) e^{-i\beta_n y}\, dy, \tag{2.20}$$

$$d_n = \frac{1}{2d} e^{i\gamma_n x} \int_{-d}^{d} v_s(x,y) e^{-i\beta_n y}\, dy. \tag{2.21}$$

It then follows from Eqs. (2.16), (2.20), and (2.21) that

$$(S_{11})_{nm} = c_n,$$

$$(S_{21})_{nm} = d_n.$$

Performing this procedure for each m we can find the matrices S_{11} and S_{12}. Because of the assumed symmetry of the scatterer we have

$$S_{12} = S_{21}, \quad S_{22} = S_{11}.$$

2.4 The Difference Equations for the N Arrays

In this section, we use the generalized scattering matrix and obtain difference equations for the Fourier's coefficients of scattered field. We begin by defining D_m the region between m^{th} and $(m+1)^{th}$ cylinders (see Fig. 2.3),

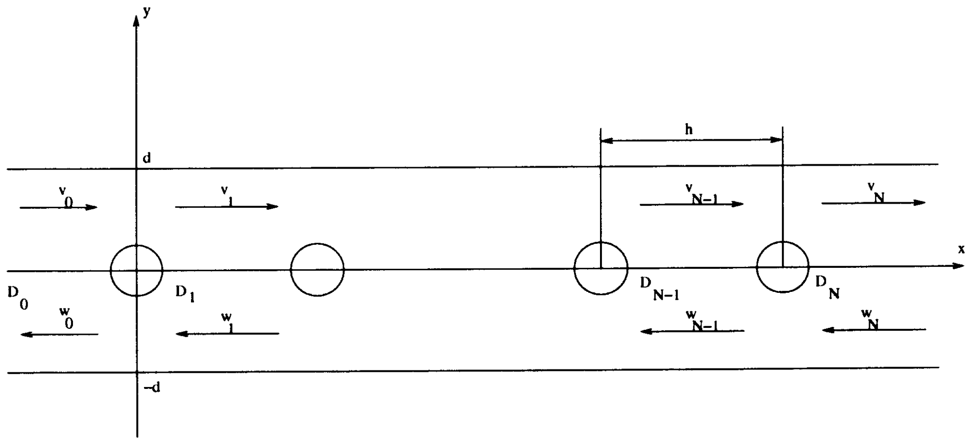

Figure 2.3 Fundamental waveguide with N scatterers.

$$D_m = \{t_m < x < x_{m+1}, -d < y < d\}, \quad m = 1, ..., N-1,$$

and define the regions D_0 and D_N by

$$D_0 = \{-\infty < x < x_1, -d < y < d\},$$

$$D_N = \{t_N < x < \infty, -d < y < d\}.$$

Here

$$x_m = -1 + (m-1)h, \quad t_m = 1 + (m-1)h, \quad m = 1, ..., N.$$

We can rewrite the incident plane wave (2.2) in the form

$$u_i(x,y) = e^{i(\gamma_J x + \beta_J y)}, \tag{2.22}$$

where J and β are such that

$$k \sin\theta = \frac{J\pi}{d} + \beta, \quad -\frac{\pi}{2d} < \beta < \frac{\pi}{2d},$$

and β_J and γ_J are defined in Eqs. (2.13) and (2.14) with $n = J$. We shall seek the scattered field in the form of a linear combination of propagating and evanescent plane waves

$$w_0(x,y) = \sum_{n=-\infty}^{\infty} b_{0n} e^{-i\gamma_n(x-x_1)+i\beta_n y}, \quad (x,y) \in D_0, \tag{2.23}$$

and the transmitted field by

$$v_N(x,y) = \sum_{n=-\infty}^{\infty} a_{Nn} e^{i\gamma_n(x-t_N)+i\beta_n y}, \quad (x,y) \in D_N. \tag{2.24}$$

In the region D_m the field is given by $v_m + w_m$, where

$$v_m(x,y) = \sum_{n=-\infty}^{\infty} b_{mn} e^{i\gamma_n(x-t_m)+i\beta_n y}, \quad (x,y) \in D_m, \tag{2.25}$$

$$w_m(x,y) = \sum_{n=-\infty}^{\infty} a_{mn} e^{-i\gamma_n(x-x_{m+1})+i\beta_n y}, \quad (x,y) \in D_m. \tag{2.26}$$

Here a_{mn} and b_{mn} are unknown complex amplitudes, $v_m(x,y)$ is the sum of plane waves propagating in direction $+x$ ($n = -L, ..., M$) and evanescent waves (for the other n) in the positive x direction. Similarly, $w_m(x,y)$ is the sum of plane waves propagating in the opposite direction.

We can describe the field in the region D_m by infinite vectors

$$\begin{aligned} \mathbf{a}_m &= (..., a_{m(-L)}, a_{m(-L+1)}, ..., a_{m0}, ..., a_{mM}, a_{m(M+1)}, ...)^\top, \\ \mathbf{b}_m &= (..., b_{m(-L)}, b_{m(-L+1)}, ..., b_{m0}, ..., b_{mM}, b_{m(M+1)}, ...)^\top. \end{aligned} \tag{2.27}$$

Incident, scattered, and transmitted fields are also described by infinite vectors:

$$\mathbf{a}_0 = (..., a_{0(-L)}, a_{0(-L+1)}, ..., a_{00}, ..., a_{0M}, a_{0(M+1)}, ...)^{\top},$$

$$\mathbf{b}_0 = (..., b_{0(-L)}, b_{0(-L+1)}, ..., b_{00}, ..., b_{0M}, b_{0(M+1)}, ...)^{\top}, \tag{2.28}$$

$$\mathbf{a}_N = (..., a_{N(-L)}, a_{N(-L+1)}, ..., a_{N0}, ..., a_{NM}, a_{N(M+1)}, ...)^{\top},$$

respectively.

Consider the cylinder at $y = 0$. If

$$S = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \tag{2.29}$$

is the generalized scattering matrix for one cylinder, we can write

$$\mathbf{b}_0 = S_{11} D \mathbf{a}_0 + S_{12} D \mathbf{b}_1,$$

$$\mathbf{a}_1 = S_{21} D \mathbf{a}_0 + S_{22} D \mathbf{b}_1, \tag{2.30}$$

where the diagonal matrix D is defined by

$$D_{mn} = e^{i\gamma_m (h-2)} \delta_{mn} \tag{2.31}$$

and δ_{mn} is the Kronecker delta function.

By translating the cylinder to $x = mh$ and introducing a suitable change of variables,i.e., $X = x - mh$, we can deduce

$$\mathbf{b}_m = S_{11} D \mathbf{a}_m + S_{12} D \mathbf{b}_{m+1},$$

$$\mathbf{a}_{m+1} = S_{21} D \mathbf{a}_m + S_{22} D \mathbf{b}_{m+1}. \tag{2.32}$$

We then seek a solution of the these equations in the form

$$\mathbf{a}_m = e^{\mu m} \alpha, \quad \mathbf{b}_m = e^{\mu m} \beta. \tag{2.33}$$

Substitution of these representations into (4.10) yields

$$S_{11}D\alpha + e^{\mu}S_{12}D\beta = \beta,$$
$$(2.34)$$
$$e^{-\mu}S_{21}D\alpha + S_{22}D\beta = \alpha.$$

This is a generalized eigenvalue problem for e^{μ}. By solving it, we can find the characteristic numbers e^{μ} and eigenvectors α and β. Eq. (2.34) is similar to the equations obtained in Ref. [1] except now the S_{ij} are infinite matrixes. We note here one important property this generalized eigenvalue problem: if e^{μ} is an eigenvalue with eigenvector $(\alpha,\, \beta)^{\top}$ then $e^{-\mu}$ is an eigenvalue with eigenvector $(\beta,\, \alpha)^{\top}$.

For numerical computation we need to decide how many evanescent modes we should take into account, i.e., where we should truncate matrixes S_{ij}. To obtain some insight into this truncation process we first consider the problem with only two columns of cylinders. In the following section we derive a formula for the amplitudes of the waves, both propagating and evanescent in the region to the right of this structure. This formula involves the S_{ij} described above. We then describe a numerical method which determines the S_{ij} and the amplitudes of the transmitted waves. These amplitudes are then compared to those obtained from an accurate boundary integral equation method which takes into account both cylinders.

2.5 Computation of Transmission Coefficient for Two Arrays

In this section we find an approximation for the transmission coefficients for two cylinders in the waveguide by applying the above theory which uses the generalized scattering matrix for a single cylinder. Let vectors $\mathbf{a}_0$ and $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{b}_0$, $\mathbf{b}_1$ describe an incident wave and the scattered field (see Fig. 2.4). The vectors $\mathbf{a}_0$, $\mathbf{b}_0$, $\mathbf{a}_1$, and $\mathbf{b}_1$ are related by Eq. (2.30)

$$\begin{pmatrix} \mathbf{b}_0 \\ \mathbf{a}_1 \end{pmatrix} = \begin{pmatrix} S_{11}D & S_{12}D \\ S_{21}D & S_{22}D \end{pmatrix} \begin{pmatrix} \mathbf{a}_0 \\ \mathbf{b}_1 \end{pmatrix}. \tag{2.35}$$

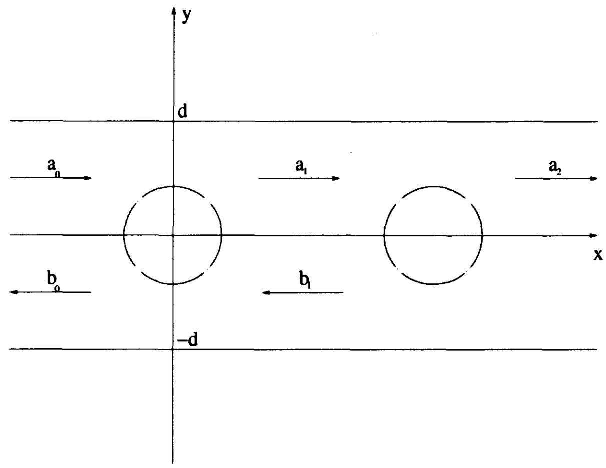

Figure 2.4 Two scatterers in the waveguide.

Similarly, $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{b}_1$ are related by Eq. (2.32) with $m = 1$

$$\begin{pmatrix} \mathbf{b}_1 \\ \mathbf{a}_2 \end{pmatrix} = \begin{pmatrix} S_{11}D & S_{12}D \\ S_{21}D & S_{22}D \end{pmatrix} \begin{pmatrix} \mathbf{a}_1 \\ \mathbf{0} \end{pmatrix}, \tag{2.36}$$

where the diagonal matrix D is defined by Eq. (2.31). This is the system of four linear equations with four unknowns $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{b}_0$ and $\mathbf{b}_1$. Solving it we get expression for the vector $\mathbf{a}_2$ whose elements are the transmission coefficients for both propagation and evanescent modes

$$\mathbf{a}_2 = S_{21}D(I - S_{22}DS_{11}D)^{-1}S_{21}D\mathbf{a}_0. \tag{2.37}$$

2.6 Numerical Results for Two Arrays

We consider a particular width of the waveguide $d = 2.5$, the radius of cylinders $r = 1$, normal incidence $\beta = 0$, and $k = 1$. For these particular parameters there is only one propagating mode in the fundamental waveguide. In Fig. 2.5 we show the amplitude and phase of the transmission coefficient of this mode as a function of h the distance between the cylinders.

The solid line corresponds to the solution obtained from a boundary integral equation method applied to both cylinders and the dashed lines to the solution obtained from Eq. (2.37) without evanescent waves. We consider the former results to be exact, as we choose our discretization to produce very accurate computations. Thus, from Fig. 2.5 we see that neglecting evanescent modes produces for the above set of parameters a very good results unless $h < 4$.

In Fig. 2.6 we show the dependence of the amplitude and phase error on h for two, four, and zero evanescent modes. These errors are obtained by subtracting our exact and approximate transmission coefficients. Again when $h > 0$ the inclusion of the evanescent modes offers only marginal improvement. However, when $h < 4$ then inclusion increases the accuracy significantly.

In Fig. 2.7 we fix the distance between the cylinders at $h = 3$ and show of the transmission coefficient on k. Again the solid lines represent the exact solution and the dashed our approximation with no evanescent modes. The omission of these modes produces very good results for $0.2 < k < 0.6$. However, for larger k the results are poor, especially near $k = 1.2$. This point is close to $k = \pi/d \approx 1.26$, where a second mode becomes propagating. The inclussion of four evanescent modes, as in the previous examples, yields a result which is almost indistinguishable from the exact solution.

2.7 Computation of Transmission Coefficient for the N Arrays

The calculations described in Section 2.5 allow us to decide where to truncate the infinite matrix **S**. Let S_{11}, S_{12}, S_{21}, and S_{22} denote the $n \times n$ matrixes obtained after truncation of S_{11}, S_{12}, S_{21}, and S_{22}. Assume that we have found the characteristic numbers e^{μ_1}, e^{μ_2},...,$e^{\mu_{2n}}$ and the corresponding eigenvectors

$$\begin{pmatrix} \alpha_1 \\ \beta_1 \end{pmatrix}, \begin{pmatrix} \alpha_2 \\ \beta_2 \end{pmatrix}, \quad \cdots \quad, \begin{pmatrix} \alpha_{2n} \\ \beta_{2n} \end{pmatrix}$$

for generalized eigenvalue problem (2.34). These can be obtained numerically by employing standard methods for finding generalized eigenvalues and egenvectors. As it was mentioned in Section 2.5 if e^{μ} is an eigenvalue with eigenvector α, β then $e^{-\mu}$ is an eigenvalue with eigenvector β, α. Using this property we can divide eigenvalues into two groups each consisting of n elements. In the first group μ is real and less then zero or μ is complex and $Re\,\mu > 0$ and in the second group μ is real and greater then zero or μ is complex and $Re\,\mu < 0$. We renumber $\mu_1,...,\mu_{2n}$ so that $\mu_1,...,\mu_n$ are from the first group and $\mu_{n+1},...,\mu_{2n}$ are from the second. We can say that the eigenvalues from the first group correspond to the wave propagating in direction $+x$ and the eigenvalues from the second group correspond to the wave propagating in direction $-x$.

We will seek the solution of the system (2.32) of the form

$$\begin{pmatrix} \mathbf{a}_m \\ \mathbf{b}_m \end{pmatrix} = \sum_{j=1}^{n} C_j e^{\mu_j m} \begin{pmatrix} \alpha_j \\ \beta_j \end{pmatrix} + \sum_{j=n+1}^{2n} C_j e^{\mu_j (m-N)} \begin{pmatrix} \alpha_j \\ \beta_j \end{pmatrix}, \tag{2.38}$$

$$m = 0, 1, ..., N.$$

It follows from the form of the incident waves, that

$$\mathbf{a}_0 = (0, ..., e^{-ik}, ..., 0)^{\top}, \quad \mathbf{b}_N = (0, ..., 0, ..., 0)^{\top}, \tag{2.39}$$

where in the vector $\mathbf{a}_0$ the coordinate corresponding to the propagating mode is equal to e^{-ik}. Setting $m = 0$ and $m = N$ into Eq. (2.38) we obtain

$$\mathbf{a}_0 = \sum_{j=1}^{n} C_j \alpha_j + \sum_{j=n+1}^{2n} C_j e^{-\mu_j N} \alpha_j, \tag{2.40}$$

$$\mathbf{b}_N = \sum_{j=1}^{n} C_j e^{\mu_j N} \beta_j + \sum_{j=n+1}^{2n} C_j \beta_j. \tag{2.41}$$

Eqs. (2.39)-(2.41) give us $2n$ linear equations with $2n$ unknowns C_1, C_2,...,C_{2n}. Solving them we can compute the remaining $\mathbf{a}_m$ and $\mathbf{b}_m$ and thus the electromagnetic field in each region D_m. The coordinates of the vectors $\mathbf{b}_0$, $\mathbf{a}_N$ corresponding to propagating waves are the reflection and transmission coefficients, respectively, for N cylinders in the waveguide.

2.8 Numerical Results for 10 Arrays

We consider the periodic structure made of $N = 10$ columns and take the same parameters as in section 2.6: $d = 2.5$, $r = 1$, $\beta = 0$, and $k = 1$.

In Fig. 2.8 we show the dependence of the modulus of the transmission coefficient on h, the distance between the cylinder centers. The dashed line corresponds to modulus obtained without evanescent waves and the solid line to the modulus with two evanescent modes. Increasing the number of evanescent modes further does not significantly alter the results. Thus, from Fig. 2.8 we see that neglecting evanescent modes produces a very good results unless $h < 4$.

In Fig. 2.9 we fix the distance between the cylinders at $h = 3$ and show the dependence of modulus of the transmission coefficient on k. The dashed line corresponds to the modulus obtained without evanescent modes and the solid line corresponds to the modulus obtained with two evanescent modes. Again, increasing the number of evanescent modes does not significantly alter the results. Thus, from Fig. 2.9 we see that the omission of these modes produces very good results for $0.2 < k < 0.6$. However, for larger k the results are poor, especially near $k = 1.2$ which is close to $k = \pi/d \approx 1.26$, where a second mode becomes propagating.

It should be noted that once the scattering matrix for a single cylinder is calculated we can plot similar graphs, almost instantly, for any number of cylinders. Boundary integral equation methods such as these developed in Ref. [2,3] take significantly more time to produce such curves, especially Fig. 2.8. Because for this their codes must be applied for each value of distance between cylinders and for each number of cylinder.

2.9 Conclusions

Without making any assumptions about normal incidence, single mode propagation, and sufficient inter-scatterer separation in the direction of propagation, we have developed a generalized scattering matrix approach to compute the transmission and reflection coefficients of periodic structures. Our approach only requires the generalized scattering matrix for a single element. This is computed by applying a boundary integral equation method which is described in the appendix. The generalized scattering matrix takes into account the effect of evanescent modes. Results obtained from a numerical study of a structure with two columns gives us insight into the estimation of the number evanescent modes we should take into account to obtain numerical solution with prescribed accuracy.

We then find the solution with N columns. Using the generalized matrix for a single scatterer we derived a matrix difference equation whose solution gives the amplitude of propagating and evanescent waves in the region between the elements. Associated with this matrix difference equation is an associated eigenvalue problem. We have shown how the eigenvalues of this related problem contain the essence of wave propagation in two dimensional periodic structures; they determine the location of pass and stop bands. The solution of this eigenvalue problem is then used to efficiently determine the transmission and reflection coefficients for this photonic structure. Finally, we have shown the effect of evanescent modes on the transmission and reflection coefficients of propagating modes. Generally speaking, they are important when the inter-column spacing, h, is reduced.

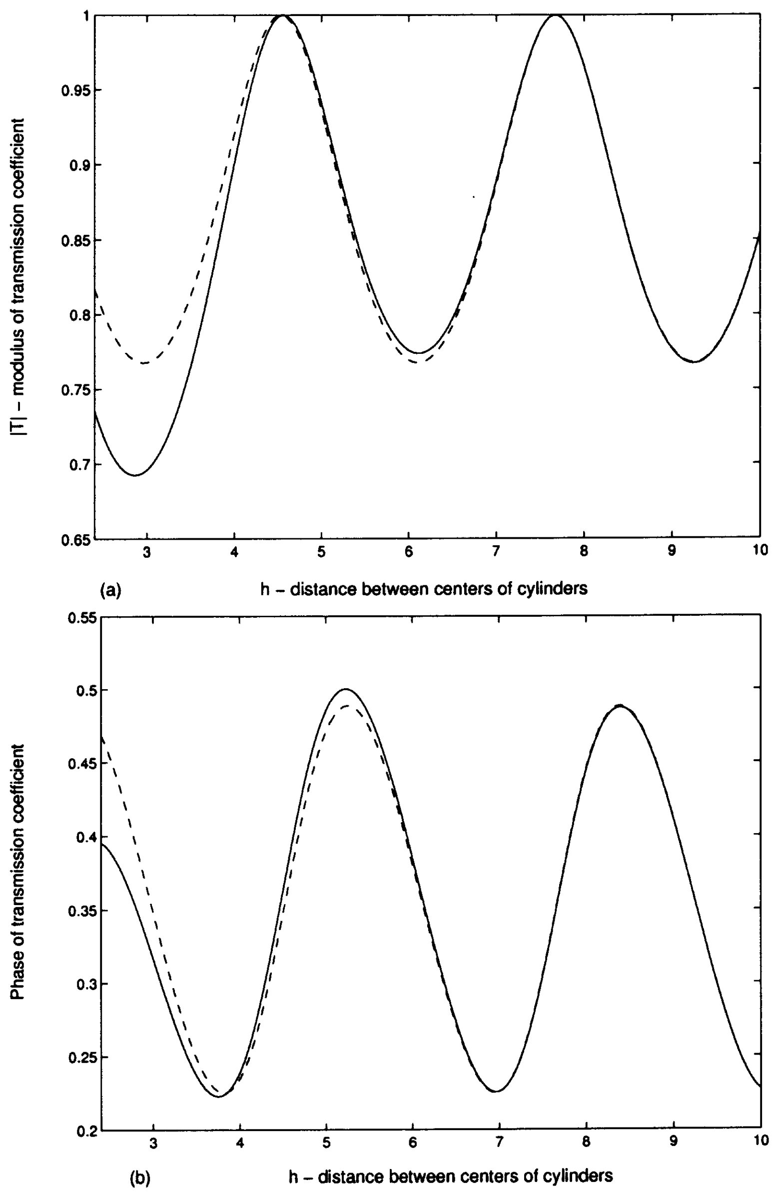

Figure 2.5 Dependence of modulus (a) and phase (b) of transmission coefficient on distance between cylinders (for fixed wave number $k = 1$). Solid line corresponds to results obtained from integral equation and dashed line corresponds to results obtained from scattering matrix approach without evanescent modes.

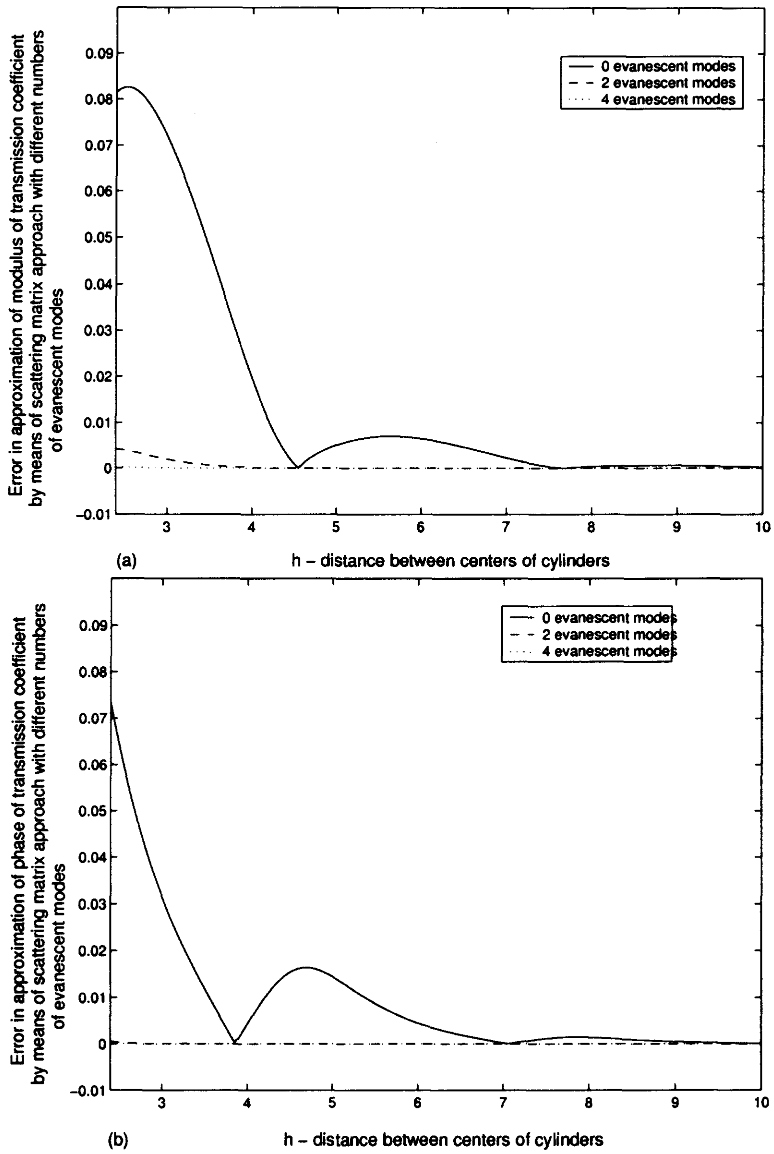

Figure 2.6 Dependence of error in approximation of modulus (a) and phase (b) of transmission coefficient on distance between cylinders (for fixed wave number $k = 1$). Solid line corresponds to results obtained from scattering matrix approach without evanescent modes, dashed, and dotted line corresponds to results obtained from scattering matrix approach with 2 and 4 evanescent modes.

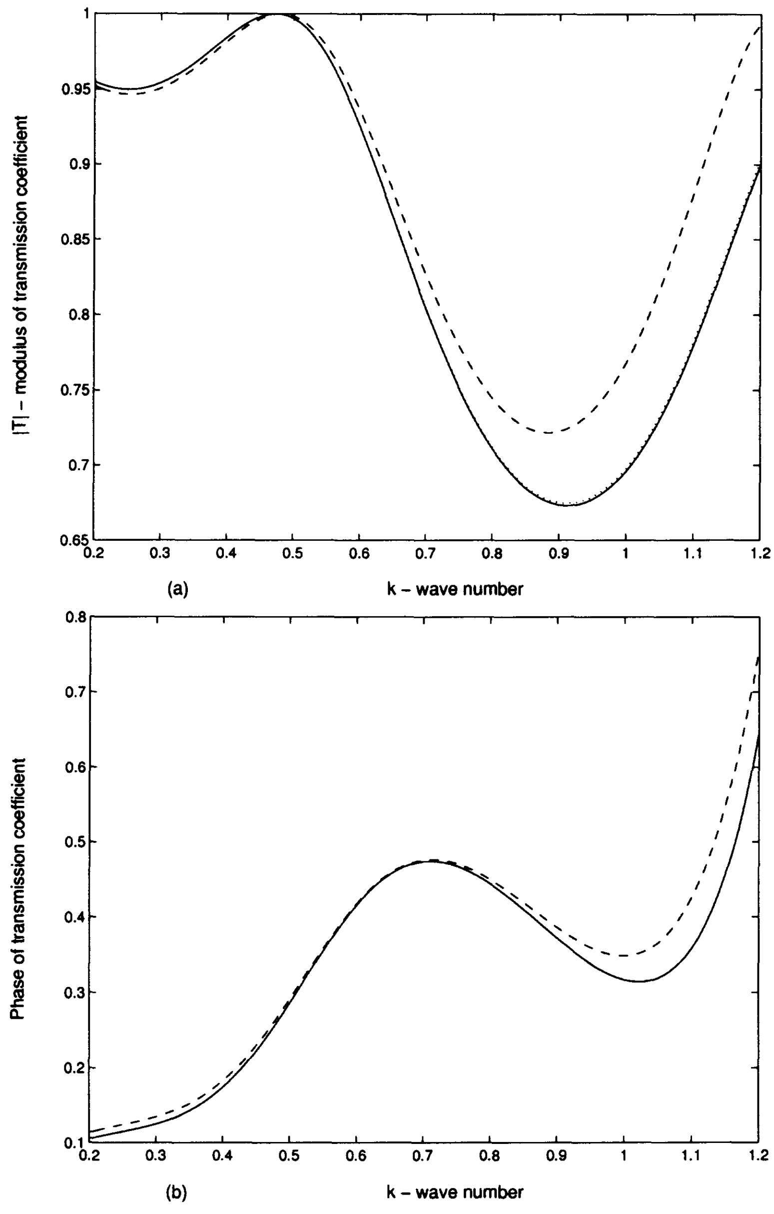

Figure 2.7 Dependence of modulus (a) and phase (b) of transmission coefficient on wave number k (for fixed distance between cylinders $h = 3$). Solid line corresponds to results obtained from integral equation and dashed line corresponds to results obtained from scattering matrix approach without evanescent modes.

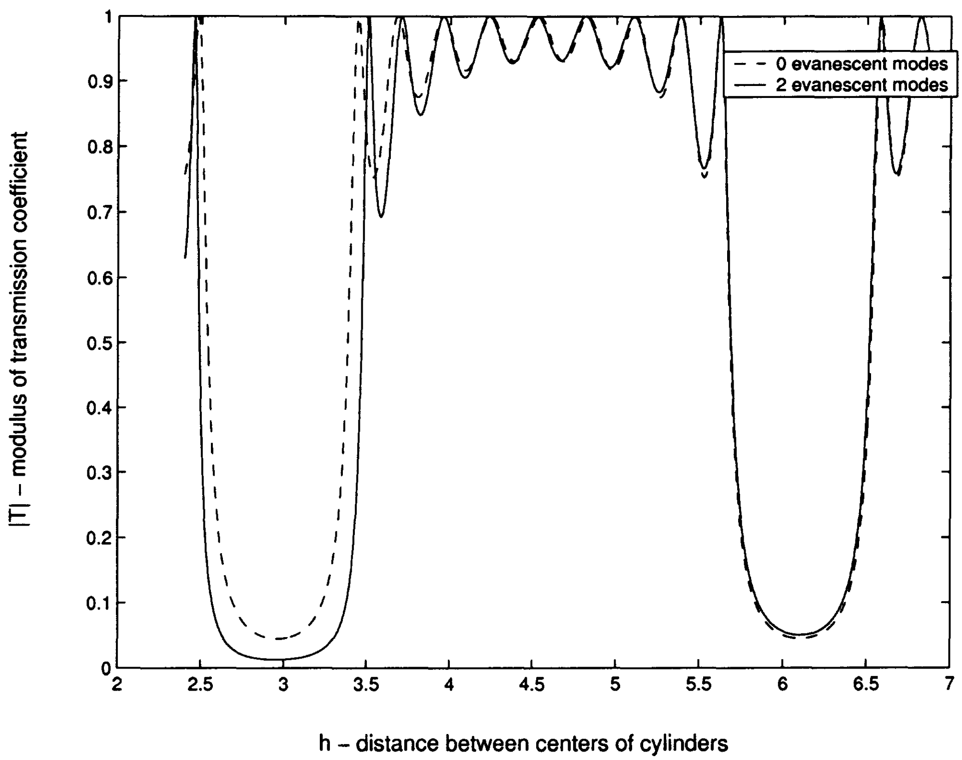

Figure 2.8 Dependance of modulus of transmission coefficient on distance between cylinders for 10 cylinders (for fixed wave number $k = 1$).

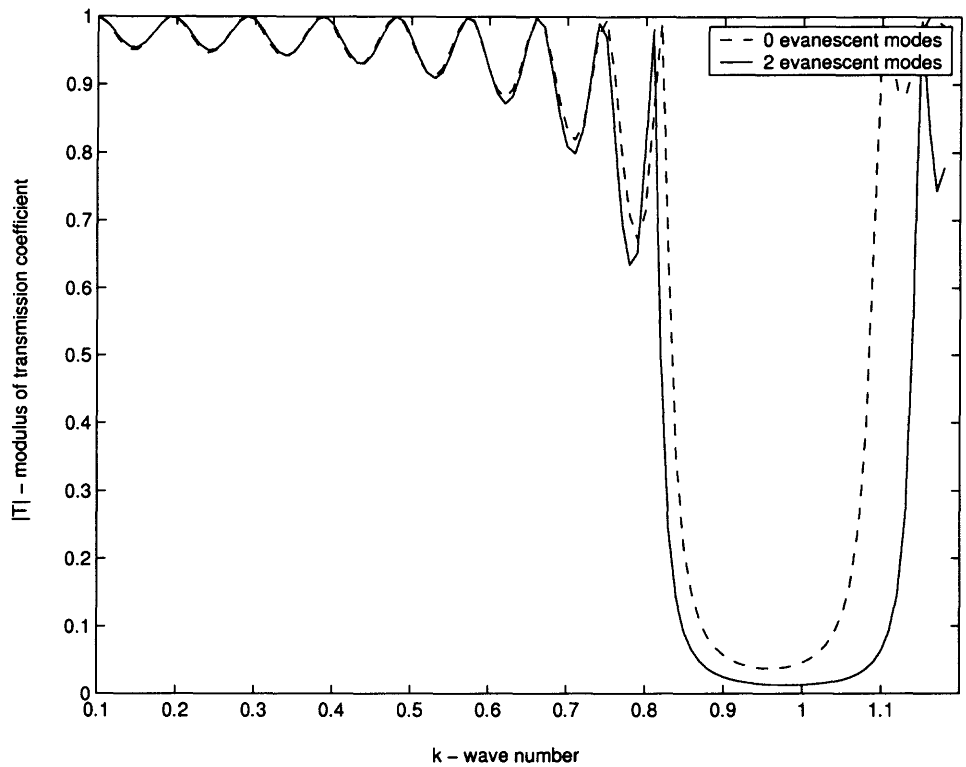

Figure 2.9 Dependance of modulus of transmission coefficient on wave number for 10 cylinders (for fixed distance between centers of cylinders $d = 3$).

CHAPTER 3

COMPUTATION OF THE GENERALIZED SCATTERING MATRICES FOR METALLIC AND DIELECTRIC OBSTACLES

3.1 Introduction

In this chapter, we show how to solve the problem on diffraction of plane wave by one column of cylinders. In Sections 3.2 and 3.3 we consider the cases of metallic and dielectric cylinders. As mentioned in Section 2.3, it allows us to compute the generalized scattering matrices for one column of metallic and dielectric cylinders.

We use the boundary integral equation technique to solve the problem. To reduce the problem to the boundary integral equation we represent the field in terms of single and double layer potentials with periodic Green's function. In the case of metallic cylinders we obtain the Fredholm integral equation of the second kind and in the case of dielectric cylinders we obtain the system of Fredholm integral equations of the second kind. In order to discretize them we apply the quadrature formulae based on Legandre polynomials [9-11].

3.2 Computation of the Generalized Scattering Matrix for Metallic Obstacle

In this Section, we apply the boundary integral technique to solve the problem on diffraction of plane wave by one column of metallic cylinders (2.1)-(2.3). In order to reduce this problem to the boundary integral equation we introduce periodic Green's function, i.e., function G which satisfies the following equation

$$\Delta G + k^2 G = -\delta(X) \sum_{m=-\infty}^{\infty} \delta(Y - 2\pi m) e^{2imd\beta}. \tag{3.1}$$

Using separation of variables it is not difficult to show that

$$G(x, y) = \frac{1}{4d} \sum_{m=-\infty}^{\infty} \frac{e^{-\gamma_m |X|} e^{i\beta_m Y}}{\gamma_m}, \tag{3.2}$$

where

$$x = (x_1, x_2), \quad y = (y_1, y_2),$$

$$X = x_1 - y_1, \quad Y = x_2 - y_2,$$

$$\beta_m = \beta + \frac{m\pi}{d}, \tag{3.3}$$

$$\gamma_m = \left(\beta_m^2 - k^2\right)^{1/2} = -i\left(k^2 - \beta_m^2\right)^{1/2}. \tag{3.4}$$

If points $x = (x_1, x_2)$ and $y = (y_1, y_2)$ are close, this formula is not suitable for calculating G because in this case $e^{-\gamma_m|X|}$ is small and the series in Eq. (3.2) converges slowly. To calculate G in this case, we use the Ewald representation of G [8]

$$\begin{aligned} G(x,y) = &\frac{1}{4\pi} \sum_{m=-\infty}^{\infty} e^{i2\beta m d} \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{kd}{a}\right)^{2n} E_{n+1}\left(\frac{a^2 r_m^2}{4d^2}\right) \\ &+ \frac{1}{4\sqrt{\pi} d} \sum_{m=-\infty}^{\infty} e^{i\beta_m Y} \sum_{n=0}^{\infty} \frac{E_{n+1/2}\left((\gamma_m d/a)^2\right)}{(-4)^n n! (d/a)^{2n-1}} X^{2n}, \end{aligned} \tag{3.5}$$

where a is any positive number,

$$r_m^2 = X^2 + (Y - 2md)^2,$$

$$E_n(z) = \int_1^{\infty} \frac{e^{-zt}}{t^n}\, dt.$$

Further we will use the derivatives of the Green's function. If points $x = (x_1, x_2)$ and $y = (y_1, y_2)$ are far apart ($|x_1 - y_1| > 0.2$) we use the following formulae for derivatives

$$\frac{\partial G}{\partial y_1} = \frac{\operatorname{sign}(X)}{4d} \sum_{m=-\infty}^{\infty} e^{-\gamma_m|X|} e^{i\beta_m Y}, \tag{3.6}$$

$$\frac{\partial G}{\partial y_2} = -\frac{i}{4d} \sum_{m=-\infty}^{\infty} \frac{\beta_m e^{-\gamma_m|X|} e^{i\beta_m Y}}{\gamma_m} \tag{3.7}$$

and otherwise we use Ewald's representation for derivatives

$$\frac{\partial G}{\partial y_1} = \frac{X}{8\pi}\frac{a^2}{d^2}\sum_{m=-\infty}^{\infty} e^{i2\beta md}\sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{kd}{a}\right)^{2n} E_n\left(\frac{a^2 r_m^2}{4d^2}\right)$$

$$-\frac{1}{2\sqrt{\pi}d}\sum_{m=-\infty}^{\infty} e^{i\beta_m Y}\sum_{n=1}^{\infty}\frac{E_{n+1/2}\left((\gamma_m d/a)^2\right)}{(-4)^n(n-1)!(d/a)^{2n-1}}X^{2n-1}, \tag{3.8}$$

$$\frac{\partial G}{\partial y_2} = \frac{1}{8\pi}\frac{a^2}{d^2}\sum_{m=-\infty}^{\infty} e^{i2\beta md}\left(Y-2md\right)\sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{kd}{a}\right)^{2n} E_n\left(\frac{a^2 r_m^2}{4d^2}\right)$$

$$-\frac{i}{4\sqrt{\pi}d}\sum_{m=-\infty}^{\infty}\beta_m e^{i\beta_m Y}\sum_{n=0}^{\infty}\frac{E_{n+1/2}\left((\gamma_m d/a)^2\right)}{(-4)^n n!(d/a)^{2n-1}}X^{2n}. \tag{3.9}$$

Using properties of single and double layer potentials we can reduce the scattering problem (2.1)-(2.3) with one row of cylinders to the boundary integral equation of the second kind

$$-\psi(x) + 2\int_S \frac{\partial G(x,y)}{\partial n(y)}\psi(y)dS_y = 2\int_S G(x,y)g(y)dS_y, \tag{3.10}$$

where G is periodic Green's function, S is the boundary of the cylinder in the fundamental waveguide, $\psi = u_s|_S$, and

$$g = \left.\frac{\partial u_i}{\partial n}\right|_S.$$

To solve it we use technique developed in Ref. [10,11]. We can rewrite the last equation in the form:

$$-\psi(x) + 2\int_S \frac{\partial F(x,y)}{\partial n(y)}\psi(y)dS_y + 2\int_S \frac{\partial (G(x,y)-F(x,y))}{\partial n(y)}\psi(y)dS_y$$

$$= 2\int_S F(x,y)g(y)dS_y + 2\int_S (G(x,y)-F(x,y))g(y)dS_y, \tag{3.11}$$

where

$$F(x,y) = \frac{i}{4}H_0^{(1)}(k|x-y|)$$

is the fundamental solution to the two-dimensional Helmholtz equation.

The integrals

$$\int_S \frac{\partial F(x,y)}{\partial n(y)}\psi(y)dS_y, \quad \int_S F(x,y)g(y)dS_y \tag{3.12}$$

can be discretized by use of quadrature formulae based on Legendre polynomials [10]

$$\int_S \frac{\partial F(x,y)}{\partial n(y)}\psi(y)dS_y$$

$$= \frac{1}{2\pi}\int_0^{2\pi} K(t,\tau)\tilde{\psi}_p(\tau)\,d\tau = \sum_{k=0}^{2n-1}\left(R^{(n)}_{|j-k|}K_1(t_j,t_k) + \frac{1}{2n}K_2(t_j,t_k)\right)\tilde{\phi}_{pk},$$

$$\int_S F(x,y)g(y)dS_y$$

$$= \frac{1}{2\pi}\int_0^{2\pi} L(t,\tau)\tilde{g}_p(\tau)\,d\tau = \sum_{k=0}^{2n-1}\left(R^{(n)}_{|j-k|}L_1(t_j,t_k) + \frac{1}{2n}L_2(t_j,t_k)\right)\tilde{g}_{pk}.$$

Here

$$K(t,\tau) = i\pi\left|\sin\frac{t-\tau}{2}\right| H_1^{(1)}\left(2k\left|\sin\frac{t-\tau}{2}\right|\right),$$

$$K_1(t,\tau) = -k\sin\frac{t-\tau}{2}J_1\left(2k\sin\frac{t-\tau}{2}\right),$$

$$K_2(t,\tau) = K(t,\tau) - K_1(t,\tau)\ln 4\sin^2\frac{t-\tau}{2},$$

$$L(t,\tau) = L_1(t,\tau)\ln\left(4\sin^2\frac{t-\tau}{2}\right) + L_2(t,\tau),$$

$$L_1(t,\tau) = -J_0\left(2k\sin\frac{t-\tau}{2}\right),$$

$$L_2(t,\tau) = L(t,\tau) - L_1(t,\tau)\ln 4\sin^2\frac{t-\tau}{2},$$

$$R_j^{(n)} = -\frac{1}{n}\left(\sum_{m=1}^{n-1}\frac{1}{m}\cos\frac{mj}{n} + \frac{(-1)^j}{2n}\right), \quad j = 0, ..., 2n-1.$$

Note that the kernels K_1, K_2, L_1, and L_2 are analytic and

$$K_2(t,t) = 1,$$

$$L_2(t,t) = -2\ln\frac{k}{2} - 2C + i\pi,$$

where $C = 0.57721...$ is the Euler constant.

For the other two integrals we apply trapezoid rule. The trapezoid approximation for this integrals has exponential rate of convergence because the function $G - F$ is smooth.

3.3 Computation of the Generalized Scattering Matrix for Dielectric Obstacle

In this Section, we apply the boundary integral technique to solve the problem on diffraction of plane wave by one column of dielectric cylinders, i.e., the two dimensional scattering problem the two dimensional scattering problem governed by the Helmholtz equation

$$\Delta u + k^2 n^2 u = 0, \tag{3.13}$$

$$n^2 = \begin{cases} 1 & \text{outside the cylinders,} \\ \epsilon & \text{inside the cylinders,} \end{cases} \tag{3.14}$$

$$u = \begin{cases} u_i + u_s & \text{outside the cylinders,} \\ u_{int} & \text{inside the cylinders,} \end{cases} \tag{3.15}$$

where u_i is an incident plane wave impinging normally upon our structure

$$u_i = e^{ik(\cos\theta x + \sin\theta y)}, \tag{3.16}$$

u_s is the scattered field, and u_{int} is the field inside the cylinders. On the interface of each cylinder, the matching boundary conditions satisfy

$$\begin{aligned} u_i + u_s &= u_{int}, \\ \nu\left(\frac{\partial u_i}{\partial n} + \frac{\partial u_s}{\partial n}\right) &= \frac{\partial u_{int}}{\partial n}, \end{aligned} \tag{3.17}$$

where $\nu = 1$ in the case of E polarization (TM waves) and $\nu = \epsilon$ in the case of H polarization (TE waves).

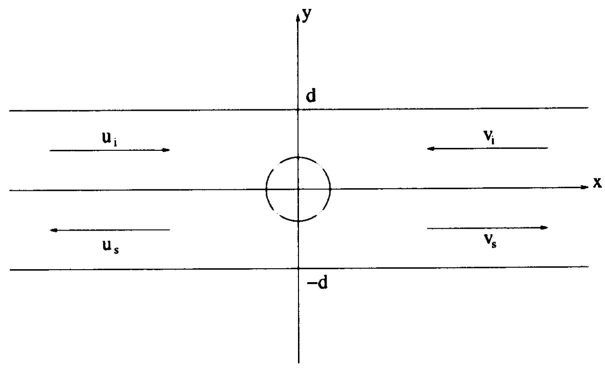

Figure 3.1 Geometry of the problem on scattering by one row of cylinders.

It is known [9] that if

$$\phi = u_s|_S, \quad \psi = \left.\frac{\partial u_s}{\partial n}\right|_S, \quad g = \left.\frac{\partial u_i}{\partial n}\right|_S$$

then the functions ϕ and ψ satisfy the following system of boundary integral equations

$$\begin{aligned} &\phi(x) + \int_S -\frac{\partial(G-F)(x,y)}{\partial n(y)}\phi(y) + (G-\nu F)(x,y)\psi(y)\, dS(y) = 2u_i, \\ &\frac{1+\nu}{2}\psi(x) + \int_S -\frac{\partial^2(G-F)(x,y)}{\partial n(y)\partial n(x)}\phi(y) + \frac{\partial(G-\nu F)(x,y)}{\partial n(x)}\psi(y)\, dS(y) = 2g, \end{aligned} \tag{3.18}$$

where

$$F(x,y) = \frac{i}{4} H_0^{(1)}(\tilde{k}|x-y|),$$

$$\tilde{k} = k\sqrt{\epsilon}.$$

Discretization of integrals

$$\int_S F(x,y)\phi(y)\, dS(y), \quad \int_S \frac{\partial F(x,y)}{\partial n(y)} \phi(y)\, dS(y), \tag{3.19}$$

$$\int_S G(x,y)\phi(y)\, dS(y) = 0, \quad \int_S \frac{\partial G(x,y)}{\partial n(y)} \phi(y)\, dS(y),$$

is described in Section 3.2. Now we show how to discretize integral

$$\int_S \frac{\partial^2 (G-F)(x,y)}{\partial n(y) \partial n(x)} \phi(y)\, dS(y). \tag{3.20}$$

We have

$$\frac{\partial^2 (G-F)}{\partial n(y)\partial n(x)} = \frac{\partial^2 (G-F)}{\partial x_1 \partial y_1} n_1(x) n_1(y) + \frac{\partial^2 (G-F)}{\partial x_1 \partial y_2} n_1(x) n_2(y) +$$

$$+ \frac{\partial^2 (G-F)}{\partial x_2 \partial y_1} n_2(x) n_1(y) + \frac{\partial^2 (G-F)}{\partial x_2 \partial y_2} n_2(x) n_2(y).$$

Here

$$\frac{\partial^2 F}{\partial y_1 \partial x_1} = \frac{i\tilde{k}^2}{4} \frac{X^2}{r_0^2} H_0^{(1)}(\tilde{k} r_0) + \left(\frac{i\tilde{k}}{4} \frac{1}{r_0} - \frac{i\tilde{k}}{2} \frac{X^2}{r_0^3} \right) H_1^{(1)}(\tilde{k} r_0),$$

$$\frac{\partial^2 F}{\partial y_1 \partial x_2} = \frac{i\tilde{k}^2}{4} \frac{XY}{r_0^2} H_0^{(1)}(\tilde{k} r_0) - \frac{i\tilde{k}}{2} \frac{XY}{r_0^3} H_1^{(1)}(\tilde{k} r_0),$$

$$\frac{\partial^2 F}{\partial y_2 \partial x_1} = \frac{\partial^2 F}{\partial y_1 \partial x_2},$$

$$\frac{\partial^2 F}{\partial y_2 \partial x_2} = \frac{i\tilde{k}^2}{4} \frac{Y^2}{r_0^2} H_0^{(1)}(\tilde{k} r_0) + \left(\frac{i\tilde{k}}{4} \frac{1}{r_0} - \frac{i\tilde{k}}{2} \frac{Y^2}{r_0^3} \right) H_1^{(1)}(\tilde{k} r_0).$$

If points $x = (x_1, x_2)$ and $y = (y_1, y_2)$ are far enough ($|x - y| > 0.2$) we use the following formulae for the second-order partial derivatives of G

$$\frac{\partial^2 G}{\partial y_1 \partial x_1} = \frac{1}{4d} \sum_{m=-\infty}^{\infty} \gamma_m e^{-\gamma_m |X|} e^{i\beta_m Y},$$

$$\frac{\partial^2 G}{\partial y_1 \partial x_2} = \frac{\operatorname{sign}(X) i}{4d} \sum_{m=-\infty}^{\infty} \beta_m e^{-\gamma_m |X|} e^{i\beta_m Y},$$

$$\frac{\partial^2 G}{\partial y_1 \partial x_2} = \frac{\partial^2 G}{\partial y_2 \partial x_1},$$

$$\frac{\partial^2 G}{\partial y_2 \partial x_2} = \frac{1}{4d} \sum_{m=-\infty}^{\infty} \frac{\beta_m^2 e^{-\gamma_m |X|} e^{i\beta_m Y}}{\gamma_m}.$$

If points $x = (x_1, x_2)$ and $y = (y_1, y_2)$ are close to each other ($|x - y| < 0.2$) we use Ewald representation for the second-order partial derivatives of G

$$\frac{\partial^2 G}{\partial y_1 \partial x_1} = \frac{a^2}{2d^2} \sum_{m=-\infty}^{\infty} \frac{1}{4\pi} e^{i2\beta md} \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{kd}{a}\right)^{2n} E_n \left(\frac{a^2 r_m^2}{4d^2}\right) +$$

$$+ \frac{a^4 X^2}{4d^4} \sum_{m=-\infty}^{\infty} \frac{1}{4\pi} e^{i2\beta md} \left(f \left(\frac{a^2 r_m^2}{4d^2}\right) - \sum_{n=1}^{\infty} \frac{1}{n!} \left(\frac{kd}{a}\right)^{2n} E_{n-1} \left(\frac{a^2 r_m^2}{4d^2}\right)\right) -$$

$$- \sum_{m=-\infty}^{\infty} e^{i\beta_m Y} \sum_{n=1}^{\infty} \frac{1}{4\sqrt{\pi} d} \frac{E_{n+1/2}\left((\gamma_m d/a)^2\right)}{(-4)^n n! (d/a)^{2n-1}} (4n^2 - 2n) X^{2n-2},$$

$$\frac{\partial^2 G}{\partial y_1 \partial x_2} = \frac{a^4 X}{4d^4} \sum_{m=-\infty}^{\infty} \frac{1}{4\pi} e^{i2\beta md} (Y - 2md) \left(f \left(\frac{a^2 r_m^2}{4d^2}\right) - \sum_{n=1}^{\infty} \frac{1}{n!} \left(\frac{kd}{a}\right)^{2n} E_{n-1} \left(\frac{a^2 r_m^2}{4d^2}\right)\right) -$$

$$-2i \sum_{m=-\infty}^{\infty} \beta_m e^{i\beta_m Y} \sum_{n=1}^{\infty} n \frac{1}{4\sqrt{\pi} d} \frac{E_{n+1/2}\left((\gamma_m d/a)^2\right)}{(-4)^n n! (d/a)^{2n-1}} X^{2n-1},$$

$$\frac{\partial^2 G}{\partial y_2 \partial x_2} = \frac{a^2}{2d^2} \sum_{m=-\infty}^{\infty} \frac{1}{4\pi} e^{i2\beta md} \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{kd}{a}\right)^{2n} E_n \left(\frac{a^2 r_m^2}{4d^2}\right) +$$

$$+\frac{a^4}{4d^4}\sum_{m=-\infty}^{\infty}\frac{1}{4\pi}e^{i2\beta md}(Y-2md)^2\left(f\left(\frac{a^2r_m^2}{4d^2}\right)-\sum_{n=1}^{\infty}\frac{1}{n!}\left(\frac{kd}{a}\right)^{2n}E_{n-1}\left(\frac{a^2r_m^2}{4d^2}\right)\right)+$$

$$+\sum_{m=-\infty}^{\infty}\beta_m^2e^{i\beta_mY}\sum_{n=0}^{\infty}\frac{1}{4\sqrt{\pi}d}\frac{E_{n+1/2}\left((\gamma_md/a)^2\right)}{(-4)^nn!(d/a)^{2n-1}}X^{2n}.$$

Here

$$f(z)=E'(z)=-e^{-z}\frac{(1+z)}{z^2}.$$

Show that

$$\frac{\partial^2(G-F)(x,y)}{\partial n(y)\partial n(x)}=const_1\ln r_0+const_2+o(|r_0|),\quad r_0=|x-y|^2,$$

i.e.,it has "log" singularity. For that we extract singularities from the second-order partial derivatives of G

$$\frac{\partial^2G}{\partial y_1\partial x_1}=\frac{1}{2\pi r_0^2}-\frac{k^2}{4\pi}\ln r_0-\frac{X^2}{\pi r_0^4}-\frac{k^2}{4\pi}\frac{X^2}{r_0^2}-\frac{k^2}{8\pi}\left(\ln\left(\frac{a^2}{4d^2}\right)+C\right)-\frac{a^2}{8\pi d^2}+P+o(|r_0|),$$

$$\frac{\partial^2G}{\partial y_1\partial x_2}=-\frac{XY}{\pi r_0^4}-\frac{k^2}{4\pi}\frac{XY}{r_0^2}+Q+o(|r_0|),$$

$$\frac{\partial^2G}{\partial y_2\partial x_2}=\frac{1}{2\pi r_0^2}-\frac{k^2}{4\pi}\ln r_0-\frac{Y^2}{\pi r_0^4}-\frac{k^2}{4\pi}\frac{Y^2}{r_0^2}-\frac{k^2}{8\pi}\left(\ln\left(\frac{a^2}{4d^2}\right)+C\right)-\frac{a^2}{8\pi d^2}+R+o(|r_0|).$$

(3.21)

To extract singularity from the second-order partial derivatives of F we use asymptotic expansion of F

$$F(kr_0)=\frac{i}{4}H_0^{(1)}(kr_0)=-\frac{1}{2\pi}\ln r_0+q_1+q_2r_0^2\ln r_0+q_3r_0^2+O(r_0^4\ln r_0),$$

where

$$q_1=\frac{i}{4}-\frac{1}{2\pi}(C-\ln 2)-\frac{1}{2\pi}\ln\tilde{k},$$

$$q_2 = \frac{1}{8\pi}\tilde{k}^2,$$

$$q_3 = \left(\frac{1}{8\pi}(C - \ln 2) - \frac{1}{8\pi} - \frac{i}{16}\right)\tilde{k}^2 + \frac{1}{8\pi}\tilde{k}^2 \ln \tilde{k}.$$

Here C is the Euler constant. It follows from this formula that

$$\frac{\partial^2 F(\tilde{k}r_0)}{\partial y_1 \partial x_1} = \frac{1}{2\pi r_0^2} - \frac{X^2}{\pi r_0^4} - \frac{\tilde{k}^2}{4\pi}\ln r_0 - \frac{\tilde{k}^2}{4\pi}\frac{X^2}{r_0^2} - (q_2 + 2q_3) + O(r_0^2 \ln r_0),$$

$$\frac{\partial^2 F(\tilde{k}r_0)}{\partial y_1 \partial x_2} = -\frac{XY}{\pi r_0^4} - \frac{\tilde{k}^2}{4\pi}\frac{XY}{r_0^2} + O(r_0^2 \ln r_0),$$

$$\frac{\partial^2 F(\tilde{k}r_0)}{\partial y_2 \partial x_2} = \frac{1}{2\pi r_0^2} - \frac{X^2}{\pi r_0^4} - \frac{\tilde{k}^2}{4\pi}\ln r_0 - \frac{\tilde{k}^2}{4\pi}\frac{X^2}{r_0^2} - (q_2 + 2q_3) + O(r_0^2 \ln r_0).$$

(3.22)

It follows from Eqs. (3.21)-(3.22) that

$$\frac{\partial^2 G}{\partial n(y)\partial n(x)} - \frac{\partial^2 F}{\partial n(y)\partial n(x)} \sim \frac{\tilde{k}^2 - k^2}{4\pi}\ln r_0 + P + Q + R + C_1 - C_2, \tag{3.23}$$

where

$$C_1 = -\frac{k^2}{4\pi}\frac{X^2}{r_0^2} - \frac{k^2}{8\pi}(\ln v + C) - \frac{a^2}{8\pi d^2},$$

$$C_2 = -(q_2 + 2q_3).$$

We have that

$$F(\tilde{k}r) \sim -\frac{1}{2\pi}\ln r_0 + q_1.$$

It follows from this equality and Eq. (3.23) that

$$\frac{\partial^2 G}{\partial n(y)\partial n(x)} - \frac{\partial^2 F}{\partial n(y)\partial n(x)} - \frac{k^2 - \tilde{k}^2}{2}F \sim$$

where

$$\sim P + Q + R + C_1 - C_2 - C_3,$$

$$C_3 = \frac{k^2 - \tilde{k}^2}{2} q_1.$$

Thus, we prove that function

$$\frac{\partial^2 G}{\partial n(y)\partial n(x)} - \frac{\partial^2 F}{\partial n(y)\partial n(x)} - \frac{k^2 - \tilde{k}^2}{2} F$$

is continuous and

$$\left. \frac{\partial^2 G}{\partial n(y)\partial n(x)} - \frac{\partial^2 F}{\partial n(y)\partial n(x)} - \frac{k^2 - \tilde{k}^2}{2} F \right|_{x=y} = D,$$

where

$$D = P + Q + R + C_1 - C_2 - C_3.$$

To discretize the integral (3.20) we represent it in the form

$$\int_S \frac{\partial^2 (G - F)(x, y)}{\partial n(y)\partial n(x)} \phi(y) \, dS(y) =$$

$$\frac{k^2 - \tilde{k}^2}{2} \int_S F(x, y)\phi(y) \, dS(y) + \int_S \left(\frac{\partial^2 (G - F)(x, y)}{\partial n(y)\partial n(x)} - \frac{k^2 - \tilde{k}^2}{2} F(x, y) \right) \phi(y) \, dS(y).$$

The first integral can be descretize by technique described in Section 3.2. For the second integral we can apply trapezoid rule. Trapezoid approximation for this integral has exponential rate of convergence because the kernel is smooth.

We apply the developed method to the particular set of parameters: $d = 2.5$, $k = 1$, $\theta = 0$. In Fig. 3.2, we show the dependence of the modulus of the transmission coefficient on $\tilde{k}$.

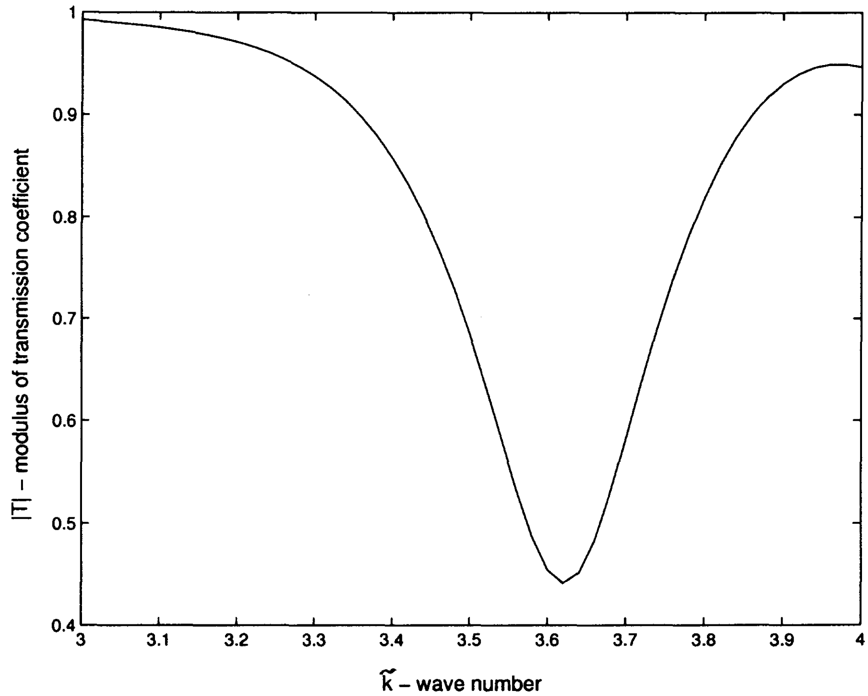

Figure 3.2 Dependence of the modulus of the transmission coefficient on $\tilde{k}$

CHAPTER 4

ANALYTICAL MODELING OF PHOTONIC CRYSTALS

4.1 Introduction

In recent years, a great deal of effort has been devoted to the study of photonic crystals. Photonic crystals are artificial structures composed of dielectric or metallic materials which are designed to control the propagation of light. Usually, the properties of photonic crystals are investigated numerically or experimentally. Only a few papers have been devoted to the investigation of photonic crystals using approximate analytical methods [1-5]. In Ref. [5], the governing equation was slightly modified in such a way that separation of variables can be used. The eigenfunctions and the spectra of the modified operators are then used to obtain Rayleigh-Ritz-type estimates of the spectrum of the governing operator. In this paper, we develop an approximate method which can be applied to the investigation of the scattering and reflection of waves through a two-dimensional photonic crystal which consists of a periodic array of parallel rods of a rectangular cross section. For this particular geometry we find an analytical formula which turns out to be a good approximation to the exact solution.

The reminder of the paper proceeds as follows. We formulate the scattering problem in Section 4.2. In order to solve this problem we consider three auxiliary problems in Sections 4.3-4.5. In Sections 4.3 and 4.4 we develop an analytical method for computing the generalized scattering matrix for a stepped waveguide (see Fig. 4.3) and for a single gap (see Fig. 4.4). The method is based upon mode matching. In general, mode matching for such problems produces a coupled, infinite system of linear equations of the first kind. By taking into account only a finite number of propagating and evanescent modes in a specific part of the periodic structure we show how the truncated infinite system can be solved. This requires inverting a $2M \times 2M$ matrix where M is the number of modes taken into account. In the particular case

$M = 1$, this matrix can be inverted explicitly, i.e, in this case we can derive an explicit formula for the elements of the generalized scattering matrices. We show numerically that these explicit formulas give a good approximation of the solution, if the thin part of the waveguide is small (see Fig. 4.3 and 4.4) and the wave number is not close to the point where the second mode becomes propagating.

In Section 4.4, we apply our scattering matrix approach to find the generalized scattering matrix for $N-1$ gaps (see Fig. 4.5). We derive matrix difference equations for the amplitudes of the propagating and evanescent modes in the thin part of the waveguide. In order to solve these equations we need to find eigenvalues and eigenvectors of a generalized $2M \times 2M$ eigenvalue problem. This can be done numerically. In the particular case $M = 1$, we solve it explicitly, i.e, in this case we derive an explicit formula for the elements of the generalized scattering matrix.

Combining the results from Sections 4.3-4.5 we find the formulas for the transmission and reflection coefficients for the two-dimensional photonic crystal in Sections 4.6. In particular for the case $M = 1$, we derive explicit formulas for these coefficients.

4.2 Governing Equations

The infinite array we wish to study made up of N columns of identical rectangle metallic cylinders. The centers of the rectangular cylinders are located at points $(2(L+d)m,\ H+2Hn)$, $m = 1, ..., N$, $n = 0, \pm 1, \pm 2, \dots$, where $2L$ is the spacing between cylinders in the x-direction and $2h$ is the spacing in the y (see Fig. 4.1). The projection of cylinder on plane $0xy$ is a rectangle with length $2d$ and width $2(H-h)$.

The field u satisfies the two-dimensional Helmholtz equation

$$\Delta u + k^2 u = 0, \tag{4.1}$$

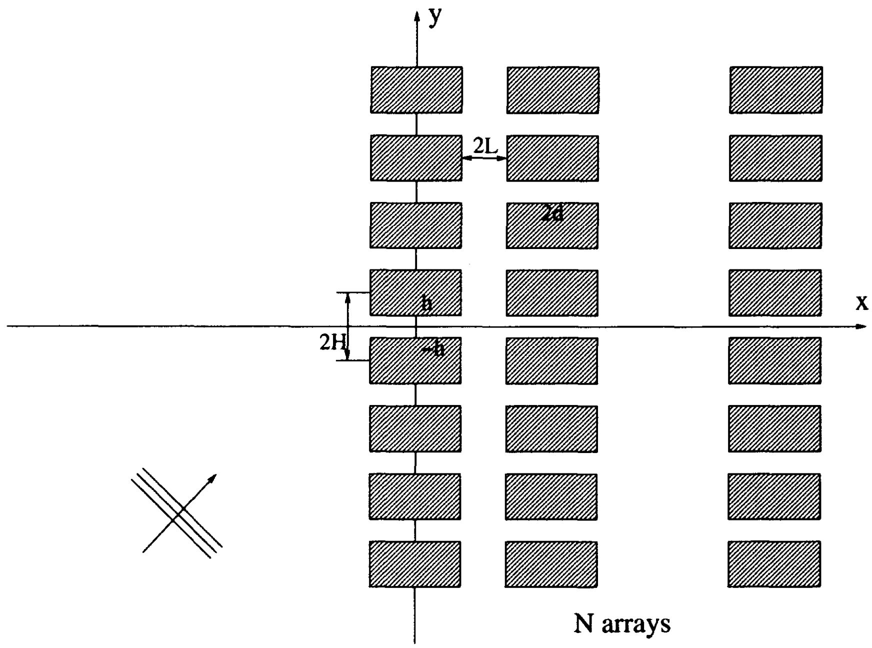

Figure 4.1 Geometry of the problem.

and is represented by

$$u = u_i + u_s,$$

where u_s is unknown scattered field and u_i is an incident plane wave with wave number k impinging upon our structure

$$u_i = e^{ik(\cos\theta x + \sin\theta y)}. \tag{4.2}$$

We assume that on the surface of each cylinder the field satisfies Neumann boundary conditions

$$\frac{\partial u}{\partial n} = 0. \tag{4.3}$$

Because of the periodicity of the problem in the y-direction we can formulate and study the problem in the fundamental waveguide (see Fig. 4.2)

$$R = \{(x,y) : -\infty < x < \infty, -H \le y \le H\}. \tag{4.4}$$

To do this we represent the incident and scattered fields in the form

$$u_i = e^{i\beta y}\tilde{u}_i, \quad u_s = e^{i\beta y}\tilde{u}_s, \tag{4.5}$$

where $\tilde{u}_i$ and $\tilde{u}_e$ are periodic functions with respect to y and β is determined by the form of the incident plane wave. The periodic function u_s satisfies the equation

$$\Delta\tilde{u}_s + 2i\beta\frac{\partial\tilde{u}_s}{\partial y} + \left(k^2 - \beta^2\right)\tilde{u}_s = 0 \tag{4.6}$$

with the periodic boundary conditions

$$\tilde{u}_s\big|_{y=-H} = \tilde{u}_s\big|_{y=H}, \quad \left.\frac{\partial\tilde{u}_s}{\partial y}\right|_{y=-H} = \left.\frac{\partial\tilde{u}_s}{\partial y}\right|_{y=H} \tag{4.7}$$

on the part of the boundary of the fundamental waveguide where $y = \pm H$, and

$$\frac{\partial\tilde{u}_s}{\partial y} = 0$$

on the boundaries of the rectangular cylinders.

Taking into account Eq. (4.5) we can recast the problem (4.1)-(4.3) in the fundamental waveguide R with quasi periodic boundary conditions

$$u_s\big|_{y=-H} = e^{2i\beta H}\, u_s\big|_{y=H}, \quad \left.\frac{\partial u_s}{\partial y}\right|_{y=-H} = e^{2i\beta H}\left.\frac{\partial u_s}{\partial y}\right|_{y=H} \tag{4.8}$$

on the part of the boundary of the fundamental waveguide where $y = \pm H$, and

$$\frac{\partial u_s}{\partial y} = 0 \tag{4.9}$$

on the boundaries of the rectangular cylinders.

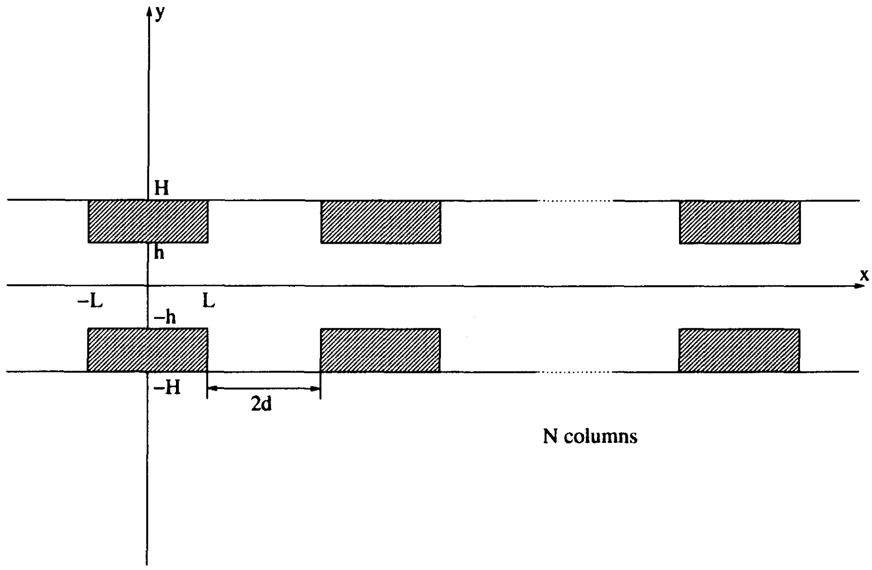

Figure 4.2 Fundamental waveguide.

4.3 Generalized Scattering Matrix for Stepped Waveguide

In this Section, we develop an analytical method for computing the generalized scattering matrix for a stepped waveguide (see Fig. 4.3). This Section consists of 4 subsections. In Subsection 4.3.1, we define the generalized scattering matrix for a stepped waveguide and describe how it can be computed. This involves the solution of the problem of scattering by a stepped waveguide. We solve this problem in Subsection 4.3.2. In Subsection 4.3.3, we consider a particular case in which we can derive an explicit formula for the solution. In Subsection 4.3.4, we examine the accuracy of this explicit formula.

4.3.1 Definition of the Generalized Scattering Matrix and its Computation

In this Subsection, we define and show how to calculate the generalized matrix for a stepped waveguide (see Fig. 4.3). Let u_i and v_i be the incident fields, and u_s and v_s be the scattered fields. We assume that u_i and v_i are given by

$$u_i = \sum_{n=-\infty}^{\infty} a_n \phi_n(y) e^{i\gamma_n x}, \quad x < 0, \quad -H < y < H, \tag{4.10}$$

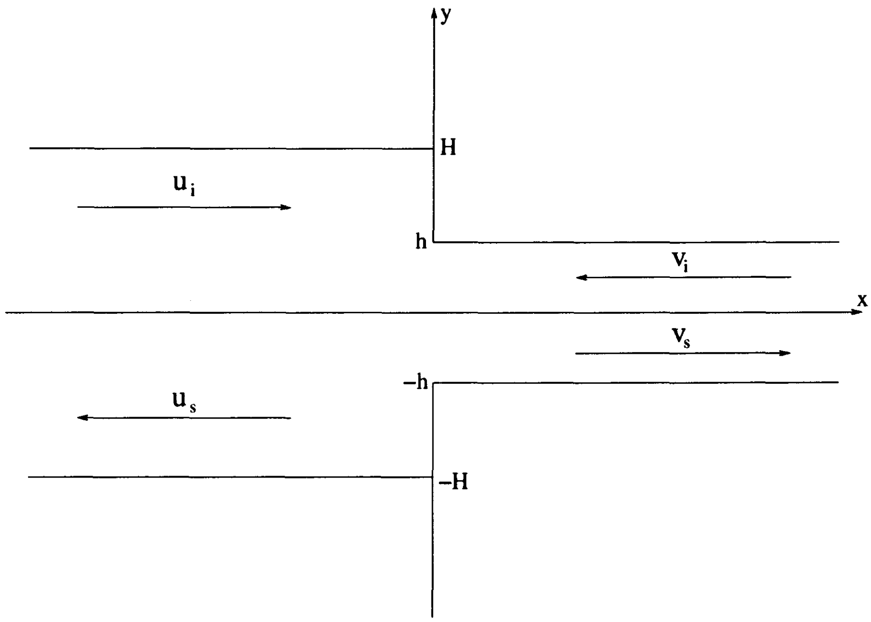

Figure 4.3 Stepped waveguide.

$$v_i = \sum_{n=0}^{M} b_n \psi_n(y) e^{-i\gamma_n x}, \quad x > 0, \quad -h < y < h. \tag{4.11}$$

Here

$$\phi_n(y) = e^{i\beta_n y}, \quad \beta_n = \beta + \frac{\pi n}{H}, \tag{4.12}$$

and

$$\psi_n(y) = \cos \alpha_n (y + h), \quad \alpha_n = \frac{\pi n}{h} \tag{4.13}$$

are transverse eigenfunctions and

$$\gamma_n = \sqrt{k^2 - \beta_n^2} = i\sqrt{\beta_n^2 - k^2}, \tag{4.14}$$

$$\sigma_n = \sqrt{k^2 - \alpha_n^2} = i\sqrt{\alpha_n^2 - k^2} \tag{4.15}$$

are their corresponding propagation constants.

We next expand the scattered fields u_s and v_s into sum of propagating plane and evanescent waves,

$$u_s = \sum_{n=-\infty}^{\infty} c_n \phi_n(y) e^{-i\gamma_n x}, \quad x < 0, \quad -H < y < H, \tag{4.16}$$

$$v_s = \sum_{n=0}^{M} d_n \psi_n(y) e^{i\gamma_n x}, \quad x > 0, \quad -h < y < y. \tag{4.17}$$

We can succinctly describe u_i, v_i, u_s, and v_s by the column vectors

$$\mathbf{a} = (..., a_{-1}, a_0, a_1, ...)^{\top}, \quad \mathbf{b} = (b_0, ..., b_M)^{\top},$$

$$\mathbf{c} = (..., c_{-1}, c_0, c_1, ...)^{\top}, \quad \mathbf{d} = (d_0, ..., d_M)^{\top},$$

respectively. Because of the linearity of the problem there are matrices R_{11}, R_{12}, R_{21}, R_{22}, which relate the amplitudes of the incident waves $\mathbf{a}$, $\mathbf{b}$ and the amplitudes of the scattered waves $\mathbf{c}$, $\mathbf{d}$

$$\begin{pmatrix} \mathbf{c} \\ \mathbf{d} \end{pmatrix} = \begin{pmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{pmatrix} \begin{pmatrix} \mathbf{a} \\ \mathbf{b} \end{pmatrix}. \tag{4.18}$$

Here R_{11}, R_{12}, R_{21}, R_{22} are $\infty \times \infty$, $\infty \times (M+1)$, $(M+1) \times \infty$, $(M+1) \times (M+1)$ matrices respectively. The matrix

$$\mathbf{S} = \begin{pmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{pmatrix} \tag{4.19}$$

is called generalized scattering matrix. The difference between generalized scattering matrix and standard scattering matrix is the former takes into account both propagating and evanescent modes, while the latter only handles the propagating modes.

To calculate R_{11} and R_{12} we consider the incident field described by

$$\mathbf{a} = (..., 0, 1, 0, ...)^\top, \quad \mathbf{b} = (0, ..., 0)^\top, \tag{4.20}$$

where the m-th coordinate of the vector $\mathbf{a}$ is equal to 1 $(-\infty < m < \infty)$. We assume that we know the scattered field

$$\mathbf{c} = (..., c_{-1}, c_0, c_1, ...)^\top, \quad \mathbf{d} = (d_0, ..., d_M)^\top.$$

It follows from Eq. (4.18) that

$$(R_{11})_{nm} = c_n, \quad (R_{21})_{nm} = d_n.$$

In order to compute R_{21} and R_{22} we consider incident field described by

$$\mathbf{a} = (0, ..., 0, ..., 0)^\top, \quad \mathbf{b} = (0, ..., 1, ..., 0)^\top, \tag{4.21}$$

where the m-th coordinate of a vector $\mathbf{b}$ is equal to 1 $(0 \leq m \leq M)$. We assume that we know scattered field

$$\mathbf{c} = (..., c_{-1}, c_0, c_1, ...)^\top, \quad \mathbf{d} = (d_0, ..., d_M)^\top.$$

It follows from Eq. (4.18) that

$$(R_{12})_{nm} = c_n, \quad (R_{22})_{nm} = d_n.$$

In the next Subsection, we show how to find the two sets of scattered fields.

4.3.2 Scattering by Stepped Waveguide

In this subsection, we show how to find the scattered field if the incident waves are given by

$$u_i = ae^{i\gamma_p x}\phi_p(y), \quad -\infty < p < \infty, \quad x < 0, \quad -H < y < H, \tag{4.22}$$

$$v_i = be^{-i\gamma_q x}\psi_q(y), \quad 0 \le q \le M, \quad x > 0, \quad -h < y < h, \tag{4.23}$$

where $\phi_n(y)$, $\psi_n(y)$, β_n, α_n, γ_n, σ_n are defined by Eqs. (4.12)-(4.15). Let u_s and v_s be the scattered field in thick and thin parts of stepped waveguide respectively (see Fig. 4.3). We expand them into the sum of propagating plane and evanescent waves

$$u_s = \sum_{n=-\infty}^{\infty} d_n\phi_n(y)e^{-i\gamma_n x}, \quad x < 0, \quad -H < y < H, \tag{4.24}$$

$$v_s = \sum_{n=0}^{M} c_n\psi_n(y)e^{i\gamma_n x}, \quad x > 0, \quad -h < y < y. \tag{4.25}$$

Here the coefficients c_n and d_n are unknown and we now describe a method to find them.

It follows from the continuity of the field and its derivative with respect to y at $x = 0$ $-h < y < h$ and the Neumann boundary condition at $x = 0$, $y \in [-H, -h] \cup [h, H]$ that

$$a\phi_p(y) + \sum_{n=-\infty}^{\infty} c_n\phi_n(y) = b\psi_q(y) + \sum_{n=0}^{M} d_n\psi_n(y), \quad -h < y < h, \tag{4.26}$$

$$a\gamma_p\phi_p(y) - \sum_{n=-\infty}^{\infty} c_n\gamma_n\phi_n(y) = -b\gamma_q\psi_q(y) + \sum_{n=0}^{M} d_n\sigma_n\psi_n(y), \quad -h < y < h, \tag{4.27}$$

$$a\gamma_p\phi_p(y) - \sum_{n=-\infty}^{\infty} c_n\gamma_n\phi_n(y) = 0, \quad y \in [-H, -h] \cup [h, H]. \tag{4.28}$$

We first multiply Eq. (4.27) by $\overline{\phi_m(y)}$ and integrate the result from $-h$ to h. We next multiply Eq. (4.28) by $\overline{\phi_m(y)}$ and integrate this expression from $-H$ to $-h$ and from h to H. Adding these two results we obtain

$$\delta_{pm}a\gamma_p\|\phi_m\|^2 - c_m\gamma_m\|\phi_m\|^2 = -b\gamma_q(\psi_q, \phi_m) + \sum_{n=0}^{M} d_n\sigma_n(\psi_n, \phi_m). \tag{4.29}$$

Here the inner products are defined by

$$(\psi_m, \phi_n) = \overline{(\phi_n, \psi_m)}, \tag{4.30}$$

$$(\phi_n, \psi_m) = \int_{-h}^{h} \phi_m(y)\overline{\psi_n(y)}\, dy = \tag{4.31}$$

$$\frac{\sin(\beta_n + \alpha_m)h}{(\beta_n + \alpha_m)} e^{i\alpha_m h} + \frac{\sin(\beta_n - \alpha_m)h}{(\beta_n - \alpha_m)} e^{-i\alpha_m h},$$

and

$$\|\phi_m\|^2 = (\phi_m, \phi_m) = 2H. \tag{4.32}$$

We can express the coefficients c_m in terms of d_m from Eq. (4.29) by

$$c_m = \delta_{pm} a + \frac{b\gamma_q(\psi_q, \phi_m)}{\gamma_m \|\phi_m\|^2} - \frac{1}{\gamma_m \|\phi_m\|^2} \sum_{n=0}^{M} d_n \sigma_n (\psi_n, \phi_m). \tag{4.33}$$

Substituting this expression for c_m into Eq. (4.26) we obtain

$$2a\phi_p(y) + \sum_{n=-\infty}^{\infty} \left(\frac{b\gamma_q(\psi_q, \phi_n)}{\gamma_n \|\phi_n\|^2} - \frac{1}{\gamma_n \|\phi_n\|^2} \sum_{j=0}^{M} d_j \sigma_j (\psi_j, \phi_n) \right) \phi_n(y) =$$

$$= b\psi_q(y) + \sum_{n=0}^{M} d_n \psi_n(y), \quad -h < y < h. \tag{4.34}$$

Multiplying this equation by $\overline{\psi_m(y)}$ and integrating from $-h$ to h we deduce the $(M+1) \times (M+1)$ system of linear equations for the $(M+1)$ unknowns $d_0,...,d_M$

$$\mathbf{A}\mathbf{d} = \mathbf{e}, \tag{4.35}$$

$$A_{mj} = \sigma_j \sum_{n=-\infty}^{\infty} \frac{(\psi_j, \phi_n)(\phi_n, \psi_m)}{\gamma_n \|\phi_n\|^2} + \|\psi_m\|^2 \delta_{mj}, \quad m, j = 0, ..., M, \tag{4.36}$$

$$e_m = 2a(\phi_p, \psi_m) + \sum_{n=-\infty}^{\infty} \frac{b\gamma_q(\psi_q, \phi_n)(\phi_n, \psi_m)}{\gamma_n \|\phi_n\|^2} - \delta_{qm} \|\psi_m\|^2, \quad m = 0, ..., M, \tag{4.37}$$

where

$$\|\psi_m\|^2 = \begin{cases} h & m = 1, ..., M, \\ 2h & m = 0. \end{cases}$$

By solving this system of linear equations we obtain amplitudes d_0, d_1,..., d_M describing of the scattered field in the thin part of the waveguide. Amplitudes c_0, c_1,... of the scattered field in the thick part of the waveguide can be found from Eq. (4.33). Note that our approximation of the scattered field takes into account all the modes in the thick part of the waveguide.

4.3.3 Explicit Formula for the Case $M = 0$

In the case $M = 0$, we can solve system (4.35) explicitly. The final formulas for the scattering matrix are as follows

$$(R_{11})_{pm} = \delta_{pm} - \frac{2k(\phi_p, \psi_0)(\psi_0, \phi_m)}{\gamma_m(Z+1)\|\psi_0\|^2\|\phi_m\|^2}, \quad -\infty < p, m < \infty, \tag{4.38}$$

$$(R_{12})_m = \frac{2k(\psi_0, \phi_m)}{(Z+1)\gamma_m\|\phi_m\|^2}, \quad -\infty < m < \infty, \tag{4.39}$$

$$(R_{21})_p = \frac{2(\phi_p, \psi_0)}{(Z+1)\|\psi_0\|^2}, \quad -\infty < p < \infty, \tag{4.40}$$

$$R_{22} = \frac{Z-1}{Z+1}, \tag{4.41}$$

where

$$Z = \frac{k}{\|\psi_0\|^2} \sum_{n=-\infty}^{\infty} \frac{|(\psi_0, \phi_n)|^2}{\gamma_n\|\phi_n\|^2}. \tag{4.42}$$

4.3.4 Numerical Results

In this Subsection, we demonstrate that the explicit formulas, from the previous Section give good results if the thin part of the waveguide is small and the wave number is not close to the point where the second mode becomes propagating. To do this we consider the problem with two sets of parameters. At first we consider the problem with $h = 0.05$ and $H = 0.5$. This corresponds to a relatively small, thin part of the waveguide. For these particular parameters there is only one propagating mode both in the thin and the thick regions of the waveguide. For this problem, $(R_{11})_{00}$ is the reflection coefficient. In Fig. 4.7 we show the modulus and phase of this reflection coefficient as a function of the wave number k of the normally incident plane wave. The modulus and phase of the reflection coefficient are computed using the explicit formula (4.38). To examine the accuracy of this graph we have computed the modulus and phase of the reflection coefficient by taking into account 8 evanescent waves in the thin part of the waveguide, using the method developed in Subsection 4.3.2. We have found that the difference between the results is of order 10^{-3}. Increasing M further produces results that differ by increasingly smaller amounts. This result shows that the explicit formulas (4.38)-(4.40) give good results for this set of parameters.

Now we consider the problem with a relatively big, thin part of the waveguide: $h = 0.35$ and $H = 0.5$. In Fig. 4.8 we show the modulus and phase of this reflection coefficient as a function of k. The modulus and phase are computed using the explicit formula (4.38). To examine the accuracy of this result we have computed the modulus and phase of the reflection coefficient by again taking into account 8 evanescent waves in the thin part of the waveguide. In Fig. 4.9 we show the dependence of the modulus and phase of the difference between these results. This graph shows that as M increases the error decreases. Thus, we infer that the $M = 0$ formula produces small error if k is not close to $\pi/2H = 6.28$ where the second mode becomes propagating.

4.4 Scattering Matrix for One Gap

In this Section, we develop an analytical method for computing the generalized scattering matrix for two discontinuity in the waveguide (see Fig. 4.4). We will refer to this structure as one gap. This section consists of four subsections. In Subsection 4.4.1, we define the generalized scattering matrix for one gap and describe how it can be computed. This involves the solution of the problem of scattering by one gap. We solve this problem in Subsection 4.4.2. In Subsection 4.4.3, we consider particular case in which we can derive an explicit formula for the solution. In Subsection 4.4.4, we examine the accuracy of this explicit formula.

4.4.1 Definition of Generalized Scattering Matrix for One Gap and its Calculation

Now show how to find the scattering matrix for one gap. Let u_i and v_i be the incident fields, and u_s and v_s be the scattered field (see Fig. 4.4). Assume that u_i and v_i are given by

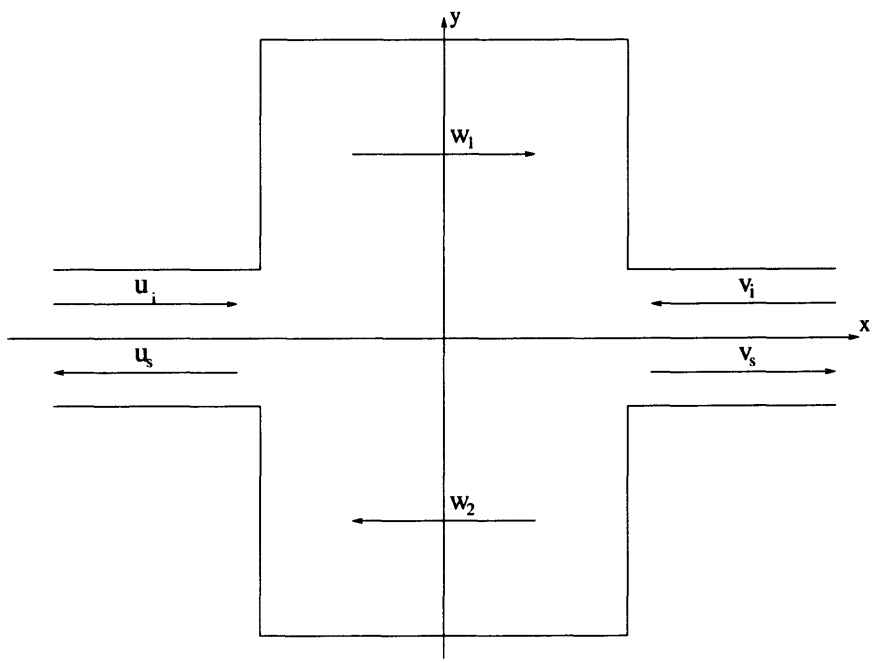

Figure 4.4 One gap.

$$u_i = \sum_{n=0}^{M} a_n \phi_n(y) e^{i\gamma_n(x+L)}, \quad x < -L, \quad -h < y < h, \tag{4.43}$$

$$v_i = \sum_{n=0}^{M} b_n \psi_n(y) e^{-i\gamma_n(x-L)}, \quad x > L, \quad -h < y < h. \tag{4.44}$$

We next expand the scattered fields into sum of propagating and evanescent modes.

$$u_s = \sum_{n=0}^{M} c_n \phi_n(y) e^{-i\gamma_n(x+L)}, \quad x < -L, \quad -h < y < h, \tag{4.45}$$

$$v_s = \sum_{n=0}^{M} d_n \psi_n(y) e^{i\gamma_n(x-L)}, \quad x > L, \quad -h < y < h. \tag{4.46}$$

We can succinctly describe u_i, v_i, u_s, and v_s by the column vectors

$$\mathbf{a} = (a_0, ..., a_M)^\top, \quad \mathbf{b} = (b_0, ..., b_M)^\top,$$

$$\mathbf{c} = (c_0, ..., c_M)^\top, \quad \mathbf{d} = (d_0, ..., d_M)^\top,$$

respectively. Because of the linearity of the problem there are matrices S_{11}, S_{12}, S_{21}, S_{22}, which relate the amplitudes of the incident waves $\mathbf{a}$, $\mathbf{b}$ and the amplitudes of the scattered waves $\mathbf{c}$, $\mathbf{d}$

$$\begin{pmatrix} \mathbf{c} \\ \mathbf{d} \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} \mathbf{a} \\ \mathbf{b} \end{pmatrix}. \tag{4.47}$$

To calculate S_{11} and S_{12} we consider the incident field described by

$$\mathbf{a} = (0, ..., 1, ..., 0)^\top, \quad \mathbf{b} = (0, ..., 0)^\top, \tag{4.48}$$

where the m-th coordinate of the vector $\mathbf{a}$ is equal to 1 ($0 \le m \le M$). In the Subsection (4.42), we describe how to find the scattered fields

$$\mathbf{c} = (c_0, ..., c_M)^\top, \quad \mathbf{d} = (d_0, ..., d_M)^\top.$$

It follows from Eq. (4.5) that

$$(S_{11})_{nm} = c_n, \quad (S_{21})_{nm} = d_n.$$

Because of symmetry we have

$$S_{12} = S_{21}, \quad S_{11} = S_{22}.$$

4.4.2 Scattering by One Gap

In this Subsection, we show how to find the scattered field if the incident waves are given by

$$u_i = e^{i\sigma_l(x+L)}\psi_l(y), \quad x < -L, \quad -h < y < h, \tag{4.49}$$

$$u_i = 0, \quad x > L, \quad -h < y < h \tag{4.50}$$

(see Fig. 4.4). Let u_s and v_s be the scattered fields and w_1 and w_2 be the fields in the thick region of the waveguide. We expand them into the sum of propagating and evanescent waves

$$u_s = \sum_{n=0}^{M} c_n e^{-i\sigma_n(x+L)}\psi_n(y), \quad x < L, \quad -h < y < h, \tag{4.51}$$

$$v_s = \sum_{n=0}^{M} d_n e^{i\sigma_n(x-L)}\psi_n(y), \quad x > L, \quad -h < y < h, \tag{4.52}$$

$$w_1 = \sum_{n=-\infty}^{\infty} f_n e^{i\gamma_n(x+L)}\phi_n(y), \quad -L < x < L, \quad -H < y < H, \tag{4.53}$$

$$w_2 = \sum_{n=-\infty}^{\infty} g_n e^{-i\gamma_n(x-L)}\phi_n(y), \quad -L < x < L, \quad -H < y < H. \tag{4.54}$$

Here the functions $\phi_n(y)$ and $\psi_m(y)$ are defined by Eqs. (4.12)-(4.15). It follows from the continuity of the field and its derivative with respect to x at $x = L\ -h < y < h$ and Neumann boundary condition on $x = L$, $y \in [-H, -h] \cup [h, H]$ that

$$\sum_{n=-\infty}^{\infty} f_n\phi_n(y) + \sum_{n=-\infty}^{\infty} g_n e^{2i\gamma_n L}\phi_n(y) = \psi_l(y) + \sum_{n=0}^{M} c_n\psi_n(y), -h < y < h, \tag{4.55}$$

$$\sum_{n=-\infty}^{\infty} f_n e^{2i\gamma_n L}\phi_n(y) + \sum_{n=-\infty}^{\infty} g_n\phi_n(y) = \sum_{n=0}^{M} d_n\psi_n(y), \quad -h < y < h, \tag{4.56}$$

$$\sum_{n=-\infty}^{\infty} f_n\gamma_n\phi_n(y) - \sum_{n=-\infty}^{\infty} g_n\gamma_n e^{2i\gamma_n L}\phi_n(y) =$$

$$= \sigma_l\psi_l(y) - \sum_{n=0}^{M} c_n\sigma_n\psi_n(y). \quad -h < y < h. \tag{4.57}$$

We first multiply Eq. (4.56) by $\overline{\phi_m(y)}$ and integrate the result from $-h$ to h. We next multiply Eq. (4.57) by $\overline{\phi_m(y)}$ and integrate this expression from $-H$ to $-h$ and from h to H. Adding these two results we obtain

$$f_m\gamma_m\|\phi_m\|^2 - g_m\gamma_m e^{2i\gamma_m L}\|\phi_m\|^2 =$$

$$= \sigma_l(\psi_l, \phi_m) - \sum_{n=0}^{M} c_n\sigma_n(\psi_n, \phi_m). \tag{4.58}$$

It follows from the continuity of the field and its derivative with respect to x at $x = -L\ -h < y < h$ and the Neumann boundary condition on $x = -L$, $y \in [-H, -h] \cup [h, H]$ that

$$\sum_{n=-\infty}^{\infty} f_n\gamma_n\phi_n(y) - \sum_{n=-\infty}^{\infty} g_n\gamma_n e^{2i\gamma_n L}\phi_n(y) = 0, \quad y \in [-H, -h] \cup [h, H], \tag{4.59}$$

$$\sum_{n=-\infty}^{\infty} f_n \gamma_n e^{2i\gamma_n L} \phi_n(y) - \sum_{n=-\infty}^{\infty} g_n \gamma_n \phi_n(y) =$$

$$= \sum_{n=0}^{M} d_n \sigma_n \psi_n(y), \quad -h < y < h, \tag{4.60}$$

$$\sum_{n=-\infty}^{\infty} f_n \gamma_n e^{2i\gamma_n L} \phi_n(y) - \sum_{n=-\infty}^{\infty} g_n \gamma_n \phi_n(y) = 0, \quad y \in [-H, -h] \cup [h, H]. \tag{4.61}$$

We first multiply Eq. (4.59) by $\overline{\phi_m(y)}$ and integrate the result from $-h$ to h. We next multiply Eq. (4.60) by $\overline{\phi_m(y)}$ and integrate this expression from $-H$ to $-h$ and from h to H. Adding these two results we obtain

$$f_m \gamma_m e^{2i\gamma_m L} ||\phi_m||^2 - g_m \gamma_m ||\phi_m||^2 = \sum_{n=0}^{M} d_n \sigma_n (\psi_n, \phi_m). \tag{4.62}$$

This is a 2×2 system of linear equations for f_m and g_m. By solving it we can express the coefficients f_m and g_m in terms of c_n and d_n

$$f_m = \sum_{n=0}^{M} s_{mn}^{(1)} c_n + \sum_{n=0}^{M} s_{mn}^{(2)} d_n + s_{ml}^{(3)}, \tag{4.63}$$

$$s_{mn}^{(1)} = \frac{1}{(e^{4i\gamma_m L} - 1)} \frac{1}{\gamma_m ||\phi_m||^2} \sigma_n (\psi_n, \phi_m), \tag{4.64}$$

$$s_{mn}^{(2)} = \frac{1}{(e^{4i\gamma_m L} - 1)} \frac{e^{2i\gamma_m L}}{\gamma_m ||\phi_m||^2} \sigma_n (\psi_n, \phi_m), \tag{4.65}$$

$$s_{ml}^{(3)} = -\frac{1}{(e^{4i\gamma_m L} - 1)} \frac{1}{\gamma_m ||\phi_m||^2} \sigma_l (\psi_l, \phi_m), \tag{4.66}$$

$$g_m = \sum_{n=0}^{M} s_{mn}^{(4)} c_n + \sum_{n=0}^{M} s_{mn}^{(5)} d_n + s_{ml}^{(6)}, \tag{4.67}$$

$$s_{mn}^{(4)} = \frac{1}{(e^{4i\gamma_m L} - 1)} \frac{e^{2i\gamma_m L}}{\gamma_m ||\phi_m||^2} \sigma_n (\psi_n, \phi_m), \tag{4.68}$$

$$s_{mn}^{(5)} = \frac{1}{\left(e^{4i\gamma_m L} - 1\right)} \frac{1}{\gamma_m \|\phi_m\|^2} \sigma_n(\psi_n, \phi_m), \tag{4.69}$$

$$s_{ml}^{(6)} = -\frac{1}{\left(e^{4i\gamma_m L} - 1\right)} \frac{e^{2i\gamma_m L}}{\gamma_m \|\phi_m\|^2} \sigma_l(\psi_l, \phi_m). \tag{4.70}$$

Substituting these expressions for f_m and g_m into boundary conditions (4.55) and (4.59), multiplying this equation by $\overline{\psi_m(y)}$, and integrating from $-h$ to h we obtain the $(2M+2) \times (2M+2)$ system of linear equations for the $(2M+2)$ unknowns c_j and d_j

$$\begin{aligned}
&\sum_{j=0}^{M} c_j \left(\sum_{n=-\infty}^{\infty} s_{nj}^{(1)} (\phi_n, \psi_m) + \sum_{n=-\infty}^{\infty} s_{nj}^{(4)} e^{2i\gamma_n L} (\phi_n, \psi_m) - \delta_{mj} \|\psi_m\|^2 \right) + \\
&+ \sum_{j=0}^{M} d_j \left(\sum_{n=-\infty}^{\infty} s_{nj}^{(2)} (\phi_n, \psi_m) + \sum_{n=-\infty}^{\infty} s_{nj}^{(5)} e^{2i\gamma_n L} (\phi_n, \psi_m) \right) = \\
&= \delta_{ml} \|\psi_m\|^2 - \sum_{n=-\infty}^{\infty} s_{nl}^{(3)} (\phi_n, \psi_m) - \sum_{n=-\infty}^{\infty} s_{nl}^{(6)} e^{2i\gamma_n L} (\phi_n, \psi_m),
\end{aligned} \tag{4.71}$$

$$\begin{aligned}
&\sum_{j=0}^{M} c_j \left(\sum_{n=-\infty}^{\infty} s_{nj}^{(1)} e^{2i\gamma_n L} (\phi_n, \psi_m) + \sum_{n=-\infty}^{\infty} s_{nj}^{(4)} (\phi_n, \psi_m) \right) + \\
&+ \sum_{j=0}^{M} d_j \left(\sum_{n=-\infty}^{\infty} s_{nj}^{(2)} e^{2i\gamma_n L} (\phi_n, \psi_m) + \sum_{n=-\infty}^{\infty} s_{nj}^{(5)} (\phi_n, \psi_m) - \delta_{mj} \|\psi_m\|^2 \right) = \\
&= - \sum_{n=-\infty}^{\infty} s_{nl}^{(3)} e^{2i\gamma_n L} (\phi_n, \psi_m) - \sum_{n=-\infty}^{\infty} s_{nl}^{(6)} (\phi_n, \psi_m).
\end{aligned} \tag{4.72}$$

4.4.3 Explicit Formula

In the case $M = 0$, we can explicitly solve the 2×2 system (4.71)-(4.72) using the definitions (4.64)-(4.66) and (4.68)-(4.70). In this case, the matrix elements S_{ij} are just numbers and are given by

$$S_{11} = S_{22} = \frac{r^2 - s^2 - 1}{(r-1)^2 - s^2}, \tag{4.73}$$

$$S_{12} = S_{21} = \frac{-2s}{(r-1)^2 - s^2}, \tag{4.74}$$

where

$$r = \sum_{n=-\infty}^{\infty} \frac{\left(e^{4i\gamma_n L} + 1\right) k|(\psi_0, \phi_n)|^2}{\left(e^{4i\gamma_n L} - 1\right) \gamma_n \|\phi_n\|^2 \|\phi_0\|^2}, \tag{4.75}$$

$$s = \sum_{n=-\infty}^{\infty} \frac{2e^{2i\gamma_n L} k|(\psi_0, \phi_n)|^2}{\left(e^{4i\gamma_n L} - 1\right) \gamma_n \|\phi_n\|^2 \|\phi_0\|^2}. \tag{4.76}$$

4.4.4 Numerical Results

In this Subsection, we demonstrate that the explicit formulas (4.73) and (4.74) give good results if the thin part of the waveguide is small and the wave number is not close to the point where the second mode becomes propagating. To do this we consider the problem with two sets of parameters. At first we consider the problem with $h = 0.05$, $H = 0.5$, and $L = 0.75$. This corresponds to a relatively small thin part of the waveguide. For these particular parameters, there is only one propagating mode both in the thin and the thick regions of the waveguide. For this problem, S_{11} is the reflection coefficient. In Fig. 4.10 we show the modulus and phase of this reflection coefficient as a function of the wave number k of the normal incident plane wave. The modulus and phase of the reflection coefficient are computed using the explicit formula (4.73). To examine the accuracy of this graph we have computed the modulus and phase of the reflection coefficient by taking into account 8 evanescent waves in the thin part of the waveguide using the method developed in Subsection 4.4.2. We have found that the difference between the results is of the order 10^{-2}. This result shows that the explicit formulas (4.73)-(4.74) give good results for this set of parameters.

Now we consider the problem with a relatively big, thin part of the waveguide: $h = 0.35$, $H = 0.5$, and $L = 0.5$. In Fig. 4.11 a) we show the modulus of the reflection coefficient as a function of k. The modulus and phase are computed using explicit formula (4.73). To examine the accuracy of this graph we have computed the modulus and phase of the reflection coefficient by again taking into account 8 evanescent waves in the thin part of the waveguide using the method developed in Subsection 4.3.2. In Fig. 4.11 b) we show the dependence the modulus and phase of the difference between these results. This graph shows that the error is small if k is not close to $\pi/2H = 6.14$ which corresponds to the point where the second mode becomes propagating.

4.5 Scattering Matrix for $N-1$ Gaps

In this Section, we show how to find the generalized scattering matrix for $N-1$ gaps (see Fig. 4.5). This section consists of three subsections. In Subsection 4.5.1, we define the generalized scattering matrix for $N-1$ gaps and describe how it can be computed. This involves the solution of the problem of scattering by $N-1$ gaps. We solve this problem in Subsection 4.5.2. In Subsection 4.5.3, we consider a particular case in which we can derive an explicit formula for the elements of the generalized scattering matrix.

4.5.1 Definition of generalized scattering matrix for $N-1$ gaps and its computation

In this Subsection we define and show how to compute the scattering matrix for $N-1$ gaps (see Fig. 4.5). We begin by defining the regions D_m $(1 \leq m \leq N)$ by

$$D_1 = \{-\infty < x < t_1, -h < y < h\}, \tag{4.77}$$

$$D_m = \{t_m < x < x_{m+1}, -h < y < h\}, \quad m = 2, ..., N-1, \tag{4.78}$$

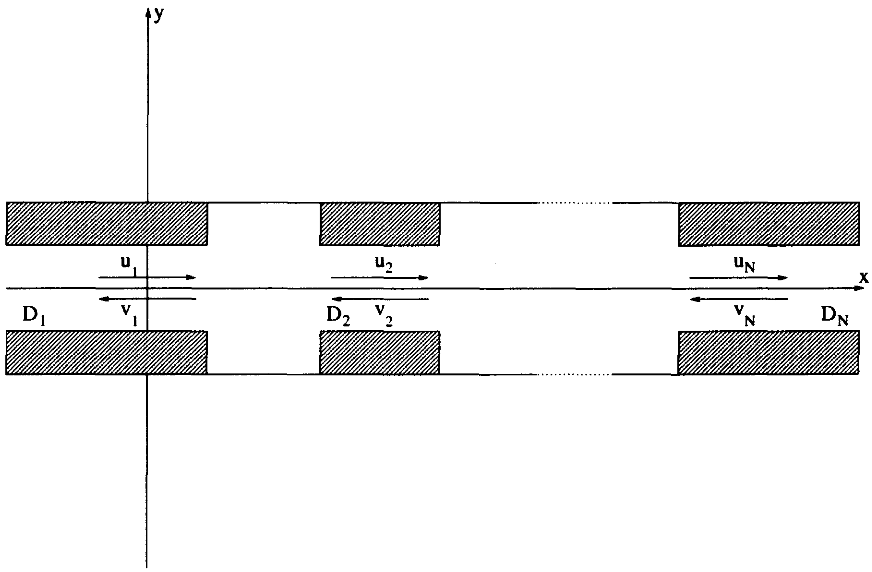

Figure 4.5 $N-1$ gaps.

$$D_N = \{x_N < x < \infty, -h < y < h\}, \tag{4.79}$$

where

$$x_m = d + 2L + 2(d+L)(m-2), \quad m = 2, ..., N, \tag{4.80}$$

$$t_m = d + 2(d+L)(m-1), \quad m = 1, ..., N-1. \tag{4.81}$$

Let u_1 and v_N be the incident fields, and v_1 and u_N be the scattered fields. Assume that u_1 and v_N are given by

$$u_1 = \sum_{n=0}^{M} a_n \phi_n(y) e^{i\gamma_n(x+t_1)}, \quad x < t_1, \quad -h < y < h, \tag{4.82}$$

$$v_N = \sum_{n=0}^{M} b_n \psi_n(y) e^{-i\gamma_n(x-x_N)}, \quad x > x_N, \quad -h < y < h. \tag{4.83}$$

We next expand the scattered field into sum of propagating and evanescent waves.

$$v_1 = \sum_{n=0}^{M} c_n \phi_n(y) e^{-i\gamma_n(x+t_1)}, \quad x < t_1, \quad -h < y < h, \tag{4.84}$$

$$u_N = \sum_{n=0}^{M} d_n \psi_n(y) e^{i\gamma_n(x-x_N)}, \quad x > x_N, \quad -h < y < h. \tag{4.85}$$

We can succinctly describe u_i, v_i, u_s, and v_s by column vectors

$$\mathbf{a} = (a_0, ..., a_M)^\top, \quad \mathbf{b} = (b_0, ..., b_M)^\top,$$

$$\mathbf{c} = (c_0, ..., c_M)^\top, \quad \mathbf{d} = (d_0, ..., d_M)^\top.$$

Because of the linearity of the problem there are matrices S_{11}, S_{12}, S_{21}, S_{22}, which relate the amplitudes of the incident waves **a**, **b** and the amplitudes of the scattered waves **c**, **d**

$$\begin{pmatrix} \mathbf{c} \\ \mathbf{d} \end{pmatrix} = \begin{pmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{pmatrix} \begin{pmatrix} \mathbf{a} \\ \mathbf{b} \end{pmatrix}. \tag{4.86}$$

To compute Q_{11} and Q_{12} we consider the incident field described by

$$\mathbf{a} = (0, ..., 1, ..., 0)^\top, \quad \mathbf{b} = (0, ..., 0)^\top, \tag{4.87}$$

where the m-th coordinate of the vector **a** is equal to 1 ($0 \leq m \leq M$). We assume that we know the scattered field

$$\mathbf{c} = (c_0, ..., c_M)^\top, \quad \mathbf{d} = (d_0, ..., d_M)^\top.$$

It follows from Eq. (4.86) that

$$(Q_{11})_{nm} = c_n, \quad (Q_{21})_{nm} = d_n.$$

To compute Q_{12} and Q_{22} consider incident field described by

$$\mathbf{a} = (0, ..., 0)^\top, \quad \mathbf{b} = (0, ..., 1, ..., 0)^\top, \tag{4.88}$$

where m-th coordinate of vector $\mathbf{b}$ is equal to 1 $(0 \leq m \leq M)$. Assume that we know how to find the scattered fields

$$\mathbf{c} = (c_0, ..., c_M)^\top, \quad \mathbf{d} = (d_0, ..., d_M)^\top.$$

It follows from Eq. (4.86) that

$$(Q_{12})_{nm} = c_n, \quad (Q_{22})_{nm} = d_n.$$

In the next Subsection, we show how to find the two sets of scattered fields.

4.5.2 Scattering by $N-1$ Gaps

In this Subsection, we show how to find the scattered field if the incident waves are given by Eqs. (4.82)-(4.83) (see Fig. 4.5). Let u_s and v_s be the scattered fields. We shall seek them in the form of a linear combination of propagating and evanescent plane waves

$$v_1 = \sum_{n=0}^{M} b_{1n}\psi_n(y)e^{-i\gamma_n(x-t_1)}, \quad (x, y) \in D_1 \tag{4.89}$$

and the transmitted field by

$$u_N = \sum_{n=0}^{M} a_{Nn}\psi_n(y)e^{i\gamma_n(x-x_N)}, \quad (x, y) \in D_N. \tag{4.90}$$

In the region D_m $(2 \leq m \leq N-1)$, the field is given by $u_m + v_m$, where

$$u_m(x, y) = \sum_{n=0}^{M} a_{mn}\psi_n(y)e^{-i\gamma_n(x-x_m)}, \quad (x, y) \in D_m, \tag{4.91}$$

$$v_m(x, y) = \sum_{n=0}^{M} b_{mn}\psi_n(y)e^{i\gamma_n(x-t_m)}, \quad (x, y) \in D_m. \tag{4.92}$$

Here a_{mn} and b_{mn} are unknown complex amplitudes, $v_m(x, y)$ is the sum of propagating and evanescent waves propagating in direction $-x$. Similarly, $v_m(x, y)$ is the sum of plane waves propagating in the opposite direction.

We can describe the field in the region D_m $(m = 1, ..., N)$ by the column vectors

$$\mathbf{a}_m = (a_{m0}, ..., a_{mM})^\top, \quad \mathbf{b}_m = (b_{m0}, ..., b_{mM})^\top. \tag{4.93}$$

The incident, scattered, and transmitted fields are described by

$$\mathbf{a}_1 = (a_{10}, ..., a_{1M})^\top, \quad \mathbf{b}_1 = (b_{10}, ..., b_{1M})^\top,$$

$$\mathbf{a}_N = (a_{N0}, ..., a_{NM})^\top, \quad \mathbf{b}_N = (b_{N0}, ..., b_{NM})^\top,$$

respectively.

Now we consider the gap between region D_1 and D_2. If

$$S = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \tag{4.94}$$

is the generalized scattering matrix for one gap, we can write

$$\begin{aligned} \mathbf{b}_1 &= S_{11}D\mathbf{a}_1 + S_{12}D\mathbf{b}_2, \\ \mathbf{a}_2 &= S_{21}D\mathbf{a}_1 + S_{22}D\mathbf{b}_2, \end{aligned} \tag{4.95}$$

where the diagonal matrix D is defined by

$$D_{mn} = e^{i\gamma_m h}\delta_{mn} \tag{4.96}$$

and δ_{mn} is the Kronecker delta function.

By translating the gap and introducing a suitable change of variables, we can deduce

$$\begin{aligned} \mathbf{b}_m &= S_{11}D\mathbf{a}_m + S_{12}D\mathbf{b}_{m+1}, \\ \mathbf{a}_{m+1} &= S_{12}D\mathbf{a}_m + S_{22}D\mathbf{b}_{m+1}. \end{aligned} \tag{4.97}$$

We then seek a solution of the matrix difference equation (4.97) of the form

$$\mathbf{a}_m = e^{\mu m}\alpha, \quad \mathbf{b}_m = e^{\mu m}\beta. \tag{4.98}$$

Substitution of these representations into (4.97) yields

$$\begin{aligned} S_{11}D\alpha + e^{\mu}S_{12}D\beta &= \beta, \\ e^{-\mu}S_{21}D\alpha + S_{22}D\beta &= \alpha. \end{aligned} \tag{4.99}$$

This is a generalized eigenvalue problem for e^{μ}. By solving it, we can find the characteristic numbers e^{μ} and eigenvectors α and β. We note here one important property of eigenvalues of this generalized eigenvalue problem. If e^{μ} is an eigenvalue with eigenvector $(\alpha,\ \beta)$ then $e^{-\mu}$ is an eigenvalue with eigenvector $(\beta,\ \alpha)$.

Assume that we have found the characteristic numbers e^{μ_1}, e^{μ_2},...,$e^{\mu_{2(M+1)}}$ and the corresponding eigenvectors

$$\begin{pmatrix} \alpha_1 \\ \beta_1 \end{pmatrix}, \begin{pmatrix} \alpha_2 \\ \beta_2 \end{pmatrix}, \cdots, \begin{pmatrix} \alpha_{2(M+1)} \\ \beta_{2(M+1)} \end{pmatrix}$$

for generalized eigenvalue problem (4.99). These can be obtained numerically by employing standard methods for finding generalized eigenvalues and eigenvectors. We can divide eigenvalues into two groups each consisting of n elements. In the first group μ is real and less then zero or μ is complex and $Re\,\mu > 0$ and in the second group μ is real and greater then zero or μ is complex and $Re\,\mu < 0$. We renumber $\mu_1,...,\mu_{2(M+1)}$ so that $\mu_1,...,\mu_{M+1}$ are from the first group and $\mu_{M+2},...,\mu_{2(M+1)}$ are from the second. We can say that the eigenvalues from the first group correspond to the wave propagating in direction $+x$ and the eigenvalues from the second group correspond to the wave propagating in direction $-x$.

We will seek the solution of the system (4.97) of the form

$$\begin{pmatrix} \mathbf{a}_m \\ \\ \mathbf{b}_m \end{pmatrix} = \sum_{j=1}^{M+1} C_j e^{\mu_j m} \begin{pmatrix} \alpha_j \\ \\ \beta_j \end{pmatrix} + \sum_{j=M+2}^{2(M+1)} C_j e^{\mu_j (m-N)} \begin{pmatrix} \alpha_j \\ \\ \beta_j \end{pmatrix}, \tag{4.100}$$

$$m = 1, ..., N.$$

It follows from the form of the incident waves, that

$$\mathbf{a}_1 = (0, ..., e^{-ik}, ..., 0)^\top, \quad \mathbf{b}_N = (0, ..., 0, ..., 0)^\top, \tag{4.101}$$

where in the vector $\mathbf{a}_0$ the coordinate corresponding to the propagating mode is equal to e^{-ik}. Setting $m = 1$ and $m = N$ into Eq. (4.100) we obtain

$$\mathbf{a}_1 = \sum_{j=1}^{M+1} C_j \alpha_j + \sum_{j=M+2}^{2(M+1)} C_j e^{-\mu_j N} \alpha_j, \tag{4.102}$$

$$\mathbf{b}_N = \sum_{j=1}^{M+1} C_j e^{\mu_j N} \beta_j + \sum_{j=M+2}^{2(M+1)} C_j \beta_j. \tag{4.103}$$

Eqs. (4.101)-(4.102) give us $2(M+1)$ linear equations with $2(M+1)$ unknowns C_1, $C_2,...,C_{2(M+1)}$. Solving them we can compute the remaining $\mathbf{a}_m$ and $\mathbf{b}_m$ and thus the electromagnetic field in each region D_m. The coordinates of the vectors $\mathbf{b}_1$, $\mathbf{a}_N$ corresponding to propagating waves are the reflection and transmission coefficients, respectively, for $N-1$ gaps in the waveguide.

4.5.3 Explicit Formula

In the case $M = 0$, we can solve difference equations (4.91)) explicitly. In this case, the matrix elements Q_{ij} are just numbers and are given by

The final formulas for the scattering matrix are as follows:

$$Q_{11} = \frac{\mu_2^{N-1} - \mu_1^{N-1}}{P} S_{11}, \tag{4.104}$$

$$Q_{12} = \frac{\mu_2 - \mu_1}{P} S_{12}, \tag{4.105}$$

$$Q_{21} = \frac{\mu_1^{N-1}\mu_2^{N-1}(\mu_2 - \mu_1)}{P} S_{21}, \tag{4.106}$$

$$Q_{22} = \frac{(1 - S_{12}e^{2ikd}\mu_1)(1 - S_{12}e^{2ikd}\mu_2)(\mu_2^{N-1} - \mu_1^{N-1})}{R_{11}e^{4ikd}P} S_{21}, \tag{4.107}$$

where the S_{ij} are defined by Eqs. (4.73)-(4.74) and

$$P = \mu_2^{N-1} - \mu_1^{N-1} + R_{12}e^{2ikd}(\mu_2\mu_1^{N-1} - \mu_1\mu_2^{N-1}). \tag{4.108}$$

4.6 Scattering by N Columns of Rectangular Cylinders

In this section, using two auxiliary problems from Sections 4.3 and 4.5 we find the solution for the problem described in Section 4.2. As mentioned in Section 4.2 we can consider the problem in the fundamental waveguide with incident wave given by Eq. (4.2) (see Fig. 4.6).

In this Section, we use the same definitions (4.77)-(4.79) for regions D_m ($2 \leq m \leq N-1$) and representation of the fields in them as in Subsection 4.5.3. We define the regions D_0 and D_{N+1} by

$$D_0 = \{-\infty < x < x_1, -h < y < h\},$$

$$D_{N+1} = \{t_N < x < \infty, -h < y < h\},$$

and redefine the regions D_1 and D_N by

$$D_1 = \{x_1 < x < t_1, -h < y < h\},$$

$$D_N = \{x_N < x < t_N, -h < y < h\}$$

(see Fig. 4.6). Let u_0 be incident field and v_0 and u_{N+1} be the scattered fields in regions D_0 and D_{N+1}. Let these field be characterized by the infinite column vectors $\mathbf{a}_0$, $\mathbf{b}_0$, and $\mathbf{a}_{N+1}$. We can rewrite the incident plane wave (4.2) in the form

$$u_0(x,y) = e^{i(\gamma_J x + \beta_J y)}, \tag{4.109}$$

where J is an integer such that

$$k \sin\theta = \frac{J\pi}{d} + \beta, \quad -\frac{\pi}{2d} < \beta < \frac{\pi}{2d},$$

and β_J and γ_J are defined by Eqs. (4.14) and (4.15) with $n = J$. According to Eq. (4.109) the vector $\mathbf{a}_0$ has the following form:

$$\mathbf{a}_0 = (..., 0, e^{-i\gamma_J d}, 0, ...)^\top,$$

where the coordinate corresponding the J propagating mode is equal to $e^{-i\gamma_J d}$.

It follows from the definition of generalized scattering matrices that

$$\begin{pmatrix} \mathbf{b}_0 \\ \mathbf{a}_1 \end{pmatrix} = \begin{pmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{pmatrix} \begin{pmatrix} \mathbf{a}_0 \\ \mathbf{b}_1 \end{pmatrix}, \tag{4.110}$$

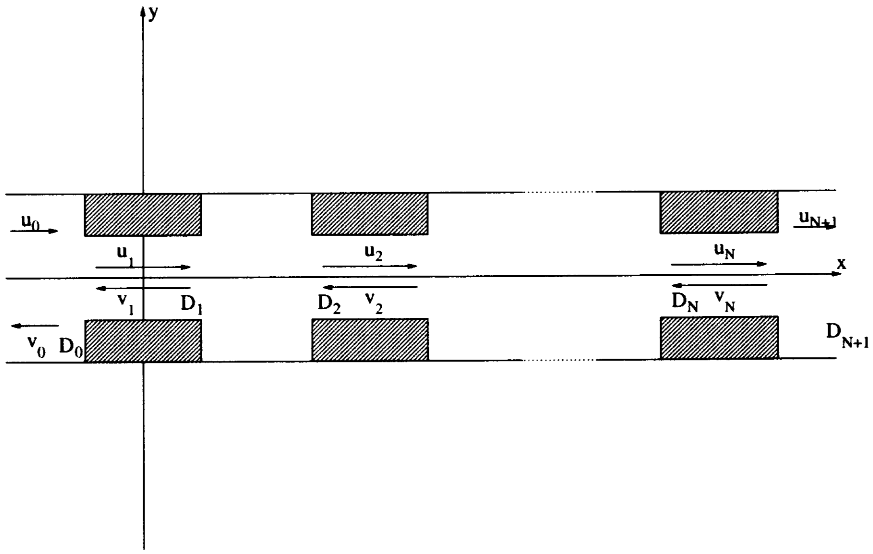

Figure 4.6 Geometry of the problem.

$$\begin{pmatrix} \mathbf{b}_1 \\ \mathbf{a}_N \end{pmatrix} = \begin{pmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{pmatrix} \begin{pmatrix} D\mathbf{a}_1 \\ D\mathbf{b}_N \end{pmatrix}, \tag{4.111}$$

$$\begin{pmatrix} \mathbf{a}_{N+1} \\ \mathbf{b}_N \end{pmatrix} = \begin{pmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{pmatrix} \begin{pmatrix} \mathbf{0} \\ \mathbf{a}_N \end{pmatrix}. \tag{4.112}$$

Eqs. (4.110)-(4.112) are system of six linear equations with six unknowns $\mathbf{b}_0$, $\mathbf{a}_1$, $\mathbf{b}_1$, $\mathbf{a}_N$, $\mathbf{b}_N$, and $\mathbf{a}_{N+1}$. Solving it we obtain

$$\mathbf{b}_0 = (R_{11} + R_{12}A(I - R_{22}A)^{-1}R_{21})\mathbf{a}_0, \tag{4.113}$$

$$\mathbf{a}_{N+1} = R_{12}(I - Q_{22}DR_{22})^{-1}Q_{21}D(I - R_{22}A)^{-1}R_{21}\mathbf{a}_0, \tag{4.114}$$

where

$$A = Q_{11}D + Q_{12}DR_{22}(I - Q_{22}DR_{22})^{-1}Q_{21}D \tag{4.115}$$

and matrix D is defined by Eq. (4.96).

In the case $M = 0$, we can find the elements of the vectors $\mathbf{b}_0$ and $\mathbf{a}_{N+1}$ explicitly

$$b_{0m} = (R_{11})_{m1} + \frac{A(R_{12})_{m1}(R_{21})_{11}}{1 - AR_{22}}, \tag{4.116}$$

$$a_{(N+1)m} = \frac{DQ_{21}(R_{12})_{m1}(R_{21})_{11}}{(1 - Q_{22}DR_{22})(1 - AR_{22})}, \tag{4.117}$$

$$A = Q_{11}D + \frac{D^2 Q_{12}Q_{21}R_{22}}{1 - Q_{22}DR_{22}}, \tag{4.118}$$

where $D = e^{2ikd}$.

In Fig. 4.12 we show the dependence of modulus of the reflection coefficient as a function of k for particular parameters: $h = 0.05$, $H = 0.5$, $L = 0.75$, $d = 1$, $N = 9$.

4.7 Conclusions

We have developed an analytical method to study the problem on scattering and transmission of waves through a two-dimensional photonic crystal which consists of a periodic array of parallel rods of a rectangular cross section. Without making any assumptions about normal incidence, single mode propagation, and sufficient inter-scatterer separation in the direction of propagation, we have shown how to compute the reflection and transmission coefficients for the structure. The method is based on generalized scattering matrix approach. At first we have computed the generalize scattering matrix for a single element of the periodic structure. To find it we have used mode matching. By taking into account only a finite number of propagating and evanescent modes in a specific part of the periodic structure we have shown how the infinite system can be solved. Solution of this system involves inverting the $M \times M$ matrix, where M is the number of modes taken into accounts. In general, it can be done numerically. In the case $M = 1$, we have derived the explicit formulas

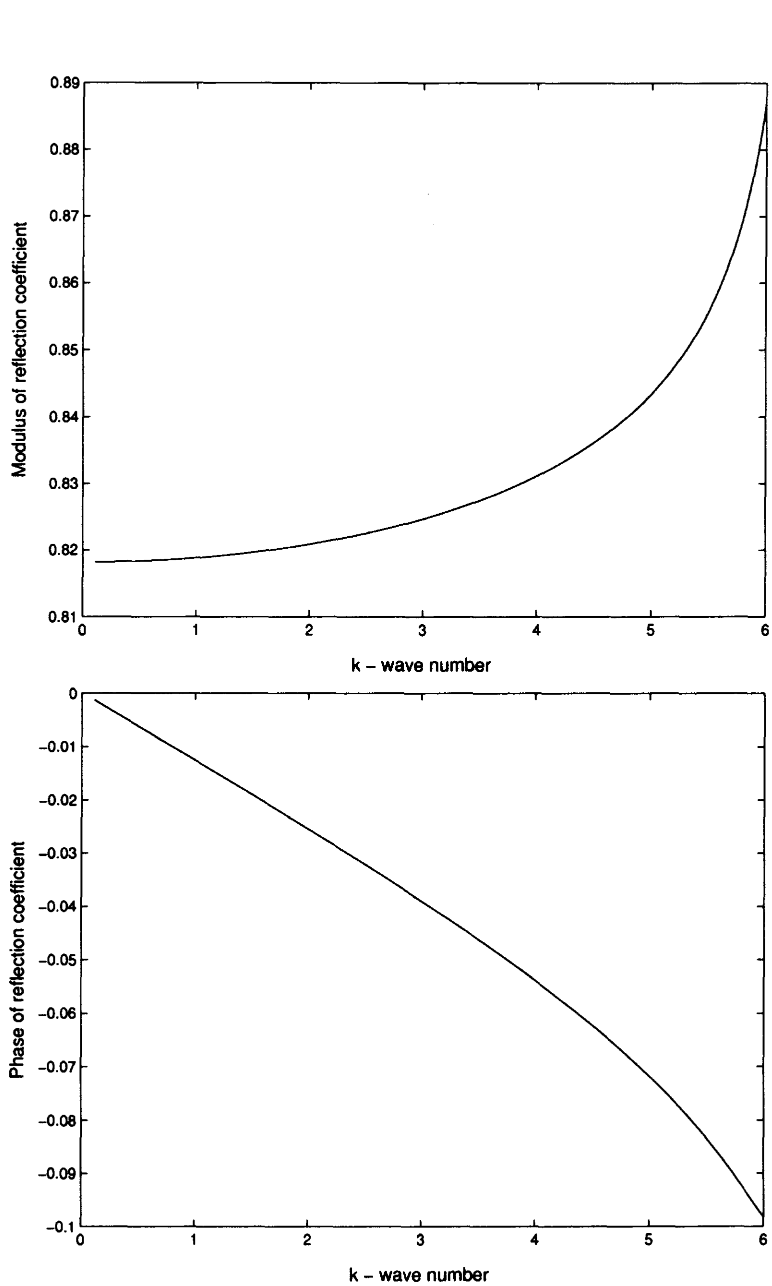

Figure 4.7 Dependence of modulus (a) and phase (b) of the reflection coefficient on wave number k for the scatterer in Fig. 4.3 with $h = 0.05$. It is obtained without taking into account evanescent waves in the thin part of the structure.

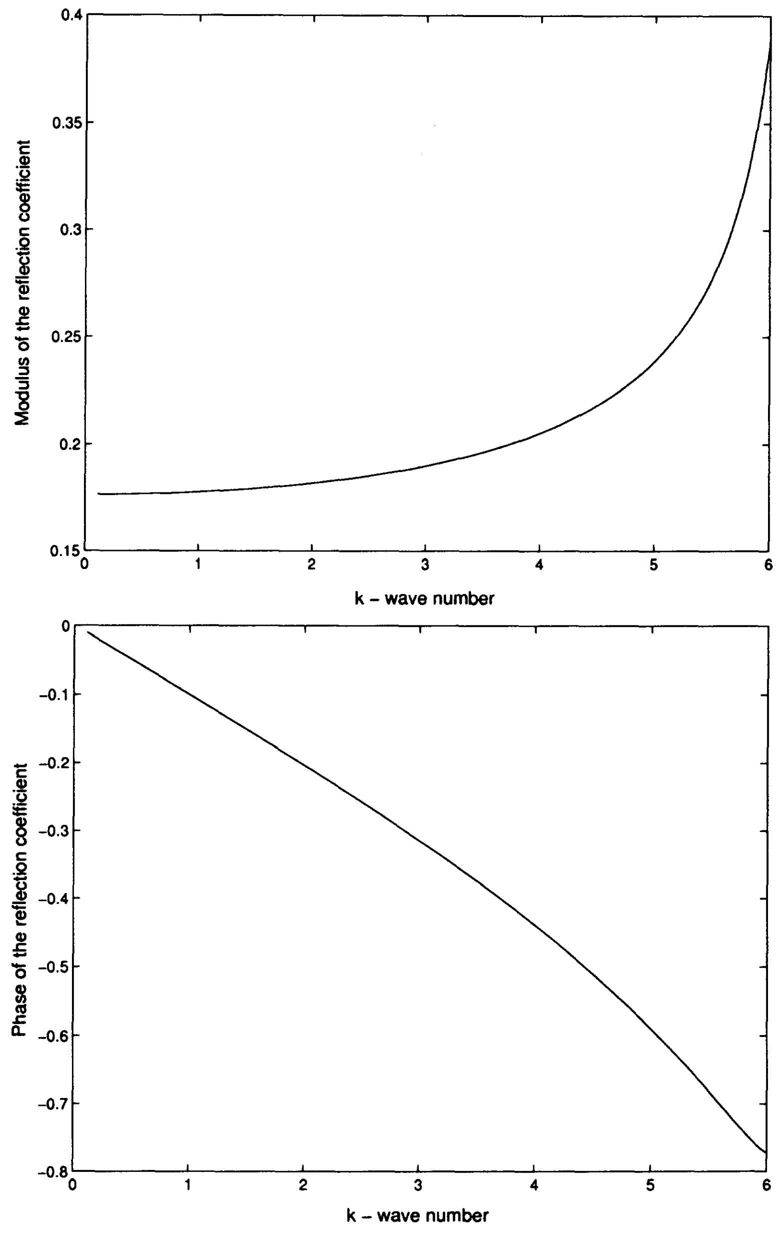

Figure 4.8 Dependence of modulus (a) and phase (b) of the reflection coefficient on wave number k for the scatterer in Fig. 3 with h=0.35. It is obtained without taking into account evanescent waves in the thin part of the structure.

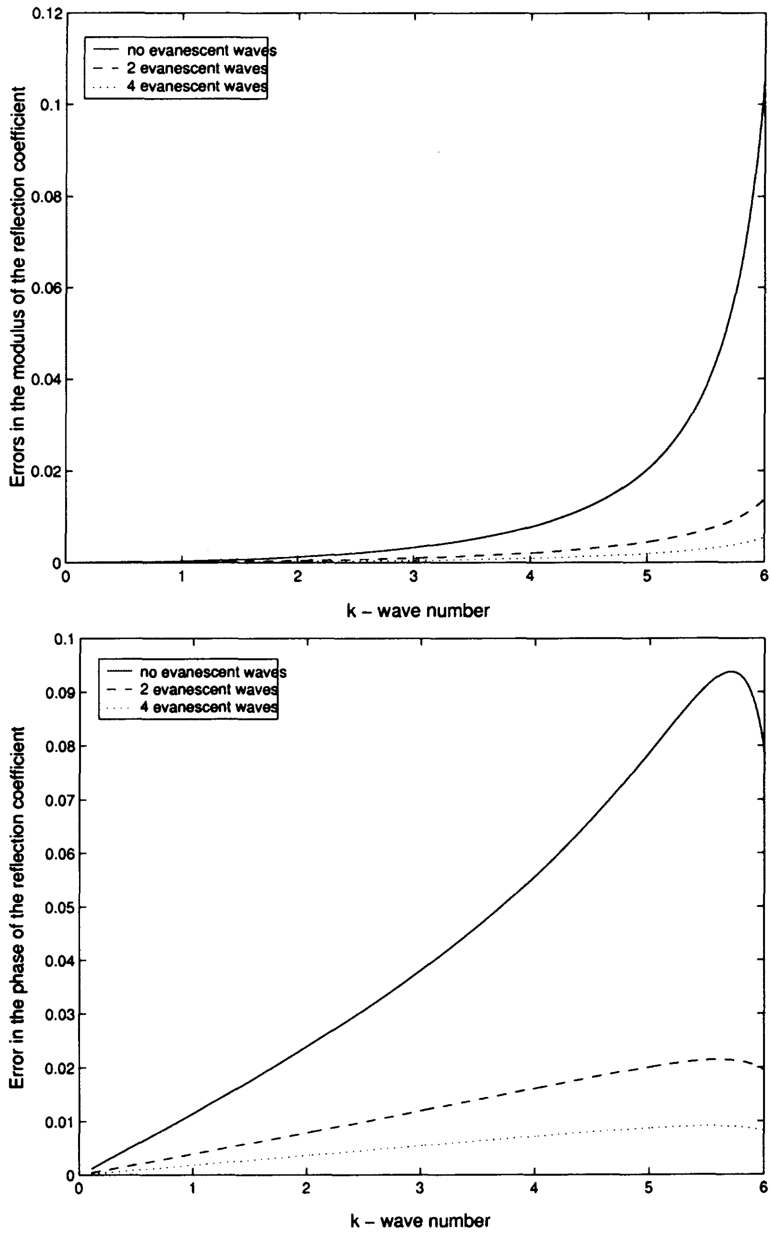

Figure 4.9 Dependence of error in modulus (a) and phase (b) of the reflection coefficient on wave number k obtained with different numbers of evanescent waves for the scatterer in Fig. 4.3 with $h = 0.35$.

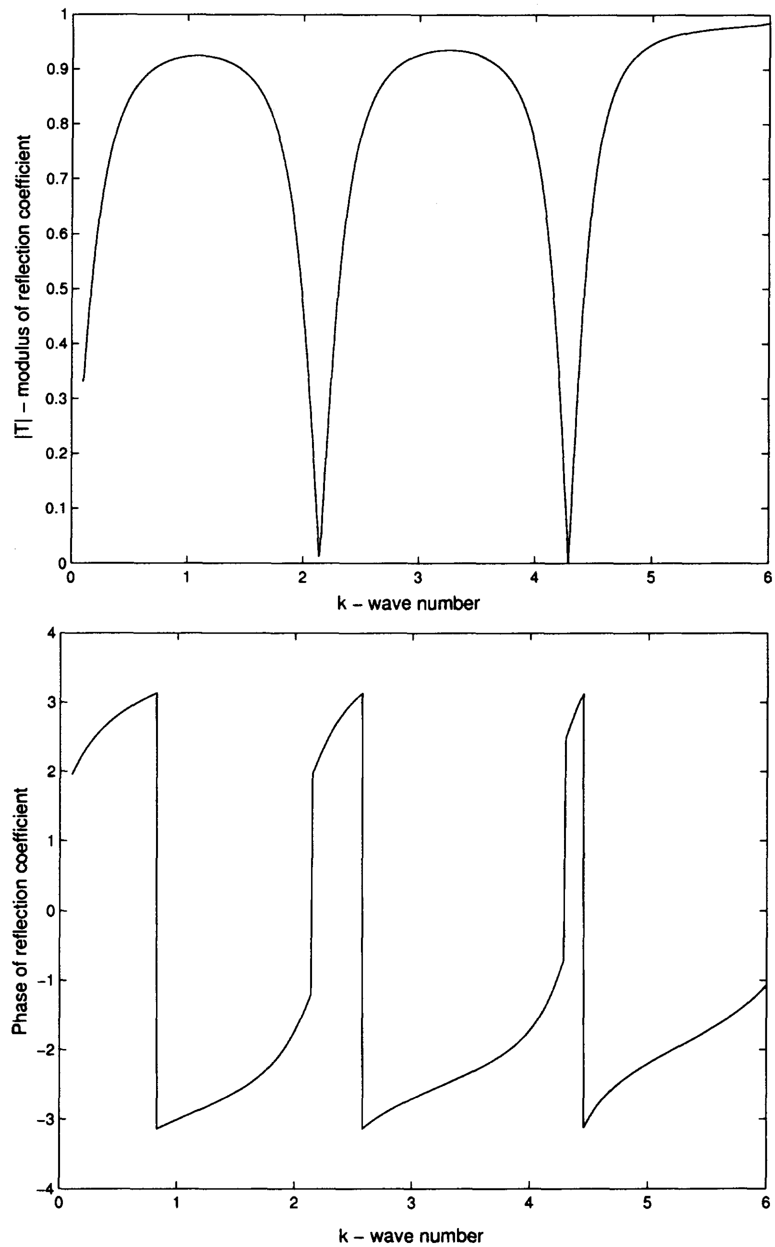

Figure 4.10 Dependence of modulus (a) and phase (b) of the reflection coefficient on wave number k for the scatterer in Fig. 4.4 with $h = 0.05$, $H = 0.5$, and $L = 0.75$. It is obtained without taking into account evanescent waves in the thin part of the structure.

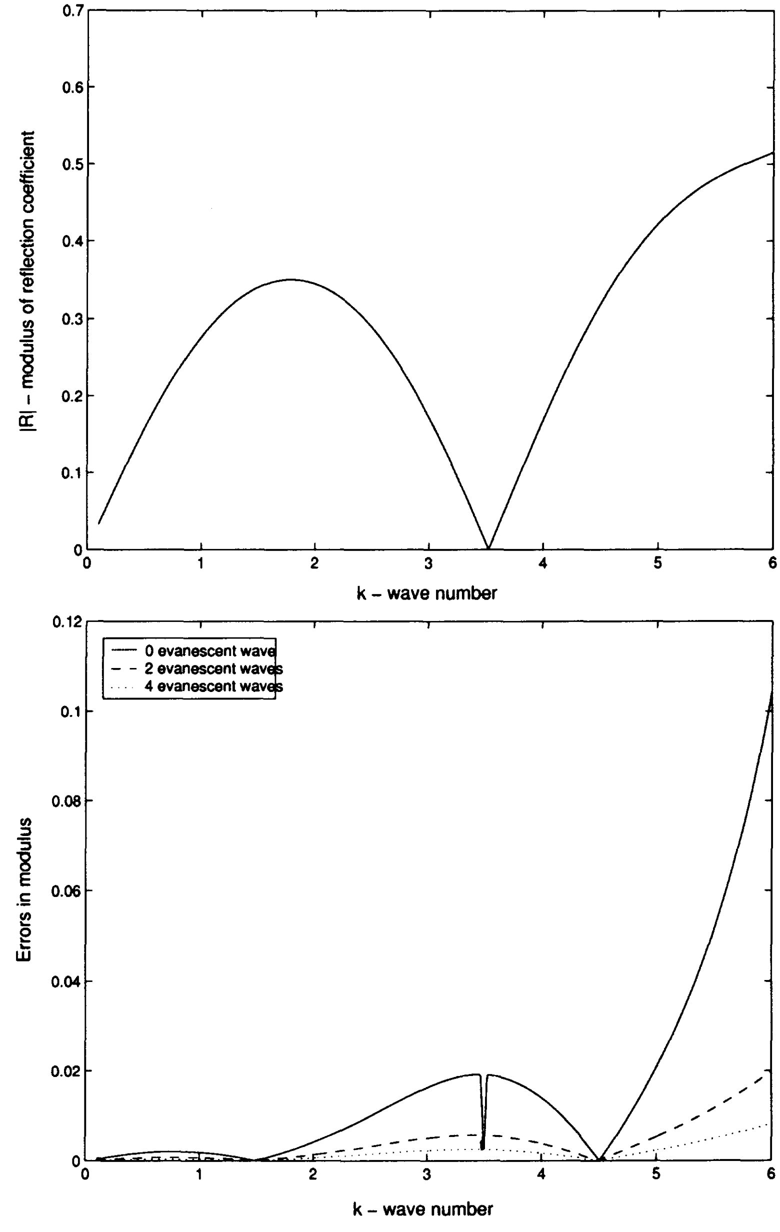

Figure 4.11 Dependence of modulus (a) and error in modulus (b) of the reflection coefficient on wave number k for the scatterer in Fig. 4.4 with $h = 0.35$, $H = 0.5$, and $L = 0.5$.

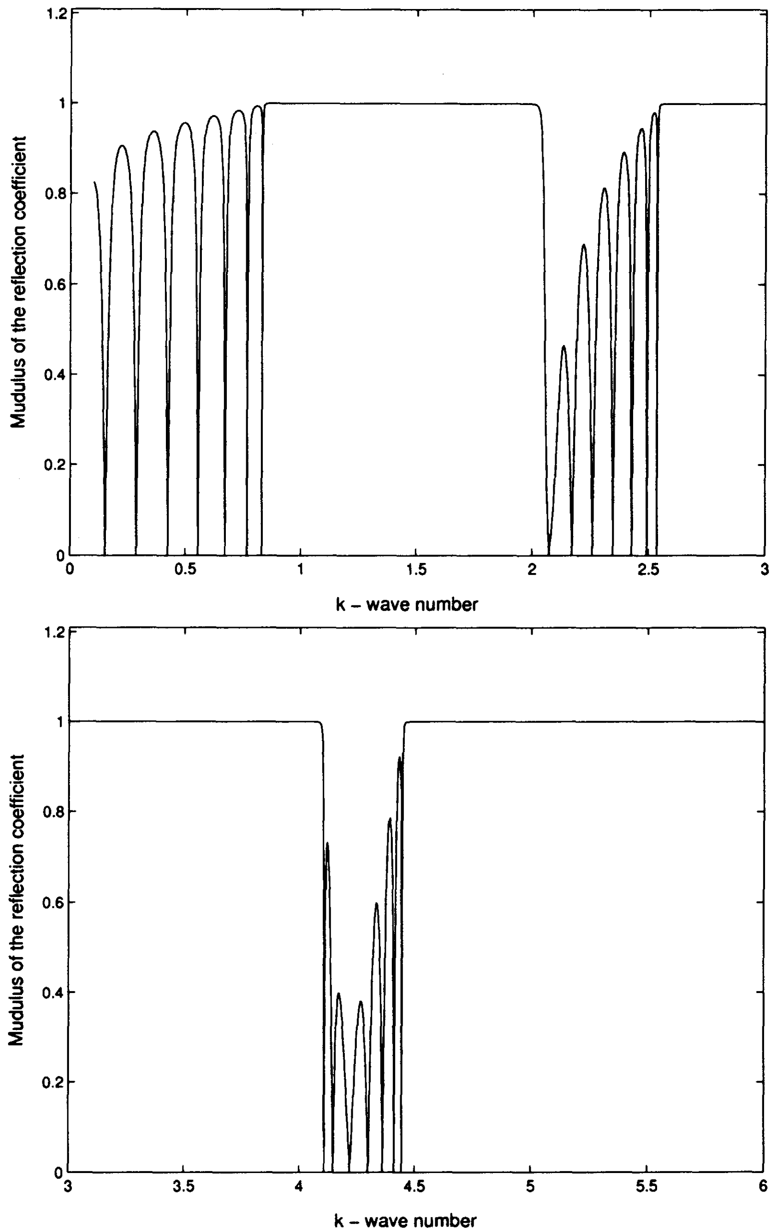

Figure 4.12 Dependence of modulus of the reflection coefficient on wave number k for 9 columns of rods with $h = 0.05$, $H = 0.5$, and $L = 0.75$ computed using the explicit formula.

for the elements of the generalized scattering matrix. We have demonstrated that this explicit formula gives good results under certain conditions on the wave number and the distance between rectangular rods.

To find generalized scattering matrix for $N-1$ elements of the periodic structure we have derived matrix difference equations for the amplitudes of the propagating and evanescent modes in the thin part of the waveguide. We have reduced this difference equation to solution of a generalized $2M \times 2M$ eigenvalue problem. By solving it numerically we have computed the reflection and transmission coefficients of the periodic structure. In the case $M = 1$ we have solved it explicitly and derived an explicit formulas for the elements of the generalized scattering matrix.

CHAPTER 5

ANALYTICAL MODELING OF RAYLEIGH-BLOCH SURFACE WAVES ALONG METALLIC RECTANGULAR RODS

5.1 Introduction

Rayleigh-Bloch surface waves are waves which propagate along two-dimensional diffraction grating which consists of a periodic array of rods and exponentially dump with the distance to the grating. In a recent paper, Porter and Evans [1] developed a boundary integral method for studying the Rayleigh-Bloch surface waves along periodic gratings. They reduced the problem to the boundary integral equation on the surface of one element of the periodic grating and after discretization of it they showed that the surface waves correspond to the zeros of the resulting determinant. They proved that in the case of symmetric elements this determinant is real.

In this Chapter, we develop an analytical method to study propagating surface waves along diffraction grating which consists of a periodic array of rods of a rectangular cross section. For this particular geometry, we use mode matching to show that surface waves correspond to the singularities of a Hermitian matrix. The dependence of the number of surface waves on the length of rectangular cross section is studied.

The reminder of the Chapter proceeds as follows. The problem is formulated in Section 5.2. In Section 5.3, we use mode matching to show that the surface waves correspond to nontrivial solution of homogeneous system of linear equation. In general, mode matching for such problems produces a coupled, infinite system of linear equations of the first kind. By taking into account only a finite number of evanescent modes in a specific part of the periodic structure we show how the truncated infinite system can be solved. We apply our method to the particular set of parameters. We show numerically that the method gives accurate results if we take into account only several evanescent waves.

5.2 Statement of the Problem

Consider an infinite array of identical rectangular metallic cylinders. The cylinders have the length L and the width $2h$ and their centers are located at points $(0,(2m+1)H)$, $m=-\infty,...,+\infty$ where $2H$ is the spacing between centers of rectangular (see Fig. 5.1).

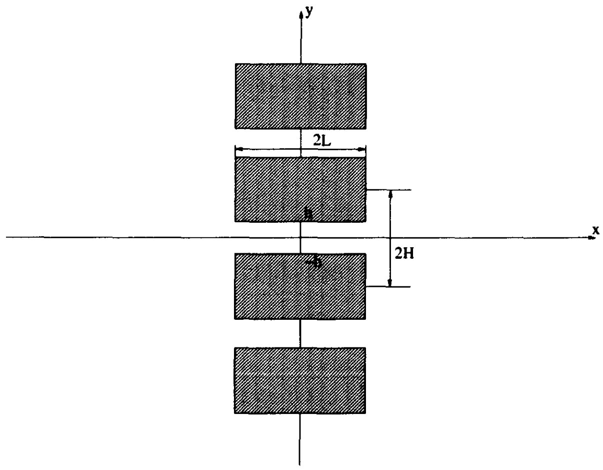

Figure 5.1 Geometry of the problem.

The Rayleigh-Bloch surface wave is a nontrivial solution of the homogeneous Helmholtz equation

$$\Delta u + k^2 u = 0 \tag{5.1}$$

and homogeneous boundary conditions on the interfaces

$$\frac{\partial u}{\partial n} = 0, \tag{5.2}$$

where n is exterior normal to the rods. Rayleigh-Bloch surface waves are damped as $|x| \to 0$:

$$u \to 0 \quad \text{as} \quad |x| \to \infty, \quad -\infty < y < \infty. \tag{5.3}$$

Because of the periodicity of the problem in the y-direction we can formulate and study the problem in the fundamental waveguide (see Fig. 5.2)

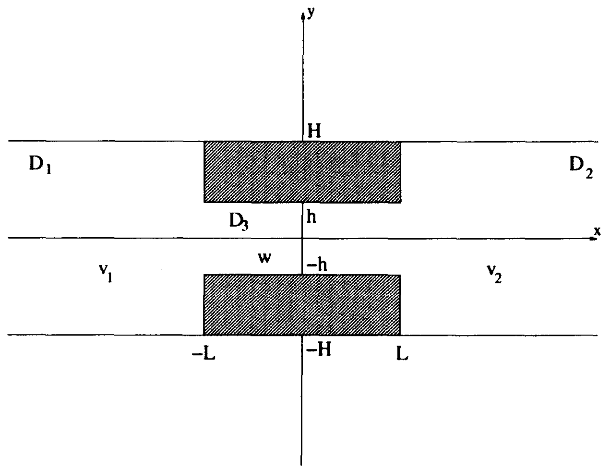

Figure 5.2 Fundamental waveguide

$$R = \{(x, y) : -\infty < x < \infty, -H \leq y \leq H\}. \tag{5.4}$$

To do this we represent the field in the form

$$u = e^{i\beta y}\tilde{u}, \tag{5.5}$$

where $\tilde{u}$ is a periodic function with respect to y and β is to be determined. The periodic function $\tilde{u}$ satisfies the equation

$$\Delta\tilde{u} + 2i\beta\frac{\partial\tilde{u}}{\partial y} + \left(k^2 - \beta^2\right)\tilde{u} = 0 \tag{5.6}$$

with the periodic boundary conditions

$$\tilde{u}\big|_{y=-H} = \tilde{u}\big|_{y=H}, \quad \left.\frac{\partial\tilde{u}}{\partial y}\right|_{y=-H} = \left.\frac{\partial\tilde{u}}{\partial y}\right|_{y=H} \tag{5.7}$$

on the part of the boundary of the fundamental waveguide where $y = \pm H$, and

$$\frac{\partial\tilde{u}}{\partial y} = 0$$

on the boundaries of the rectangular cylinders.

Taking into account Eq. (5.5) we can recast the problem (5.1)-(5.3) in the fundamental waveguide R with quasi periodic boundary conditions

$$u\big|_{y=-H} = e^{2i\beta H}\, u\big|_{y=H}, \quad \left.\frac{\partial u}{\partial y}\right|_{y=-H} = e^{2i\beta H} \left.\frac{\partial u}{\partial y}\right|_{y=H} \tag{5.8}$$

on the part of the boundary of the fundamental waveguide where $y = \pm H$, and

$$\frac{\partial u}{\partial y} = 0 \tag{5.9}$$

on the boundaries of the rectangular cylinders.

5.3 Analytical Approximation to Surface Wave

Let D_1, D_2, and D_3 be the regions defined by

$$D_1 = \{-\infty < x < -L, \quad -H < y < H\}, \tag{5.10}$$

$$D_2 = \{L < x < \infty, \quad -H < y < H\}, \tag{5.11}$$

$$D_3 = \{-L < x < L, \quad -h < y < h\}, \tag{5.12}$$

and v_1, v_2, and v_3 be the functions defined by

$$v_1 = u\big|_{D_1}, \quad v_2 = u\big|_{D_2}, \quad v_3 = u\big|_{D_3}, \tag{5.13}$$

where u is the nontrivial solution of the problem (5.1), (5.8), and (5.9) (see Fig. 5.2). We expand the functions v_1 and v_2 into sum of evanescent modes

$$v_1 = \sum_{n=-\infty}^{\infty} a_n e^{-i\gamma_n(x+L)} \phi_n(y), \tag{5.14}$$

$$v_2 = \sum_{n=-\infty}^{\infty} d_n e^{i\gamma_n(x-L)} \phi_n(y), \tag{5.15}$$

where

$$\phi_n(y) = e^{i\beta_n y}, \quad \beta_n = \beta + \frac{\pi n}{H},$$

$$\psi_n(y) = \cos\alpha_n(y+h), \quad \alpha_n = \frac{\pi n}{h}$$

are transverse eigenfunctions and

$$\gamma_n = \sqrt{k^2 - \beta_n^2} = i\sqrt{\beta_n^2 - k^2},$$

$$\sigma_n = \sqrt{k^2 - \alpha_n^2} = i\sqrt{\alpha_n^2 - k^2}$$

are their corresponding propagation constants. In the region D_3, we seek the unknown field v_3 as the sum of only N propagating and evanescent modes

$$v_3 = \sum_{n=0}^{N} b_n e^{i\sigma_n(x+L)}\psi_n(y) + \sum_{n=0}^{N} c_n e^{-i\sigma_n(x-L)}\psi_n(y). \tag{5.16}$$

For symmetric surface waves we have that

$$d_n = a_n, \quad c_n = b_n, \tag{5.17}$$

and for anti-symmetric surface waves

$$d_n = -a_n, \quad c_n = -b_n. \tag{5.18}$$

At first we consider symmetric case (5.17). It follows from the continuity of the field and its derivative with respect to x at $x = L$, $-h < y < h$ and the Neumann boundary condition at $x = L$, $y \in [-H, -h] \cup [h, H]$ that

$$\sum_{n=-\infty}^{\infty} a_n\phi_n(y) = \sum_{n=0}^{N} b_n \left(e^{2i\sigma_n L} + 1\right)\psi_n(y) \quad -h < y < h, \tag{5.19}$$

$$\sum_{n=-\infty}^{\infty} a_n\gamma_n\phi_n(y) = \sum_{n=0}^{N} b_n\sigma_n \left(e^{2i\sigma_n L} - 1\right)\psi_n(y), \quad -h < y < h, \tag{5.20}$$

$$\sum_{n=-\infty}^{\infty} a_n \gamma_n \phi_n(y) = 0, \quad y \in [-H, -h] \cup [h, H]. \tag{5.21}$$

We first multiply Eq. (5.20) by $\overline{\phi_m(y)}$ and integrate the result from $-h$ to h. We next multiply Eq. (5.21) by $\overline{\phi_m(y)}$ and integrate this expression from $-H$ to $-h$ and from h to H. Adding these two results we obtain

$$a_m \gamma_m \|\phi_m\|^2 = \sum_{n=0}^{N} b_n \sigma_n \left(e^{2i\sigma_n L} - 1\right) (\psi_n, \phi_m). \tag{5.22}$$

Here the inner products are defined by

$$(\psi_m, \phi_n) = \overline{(\phi_n, \psi_m)}, \tag{5.23}$$

$$(\phi_n, \psi_m) = \int_{-h}^{h} \phi_m(y) \overline{\psi_n(y)}\, dy = \tag{5.24}$$

$$\frac{\sin(\beta_n + \alpha_m)h}{(\beta_n + \alpha_m)} e^{i\alpha_m h} + \frac{\sin(\beta_n - \alpha_m)h}{(\beta_n - \alpha_m)} e^{-i\alpha_m h},$$

and

$$\|\phi_m\|^2 = 2H. \tag{5.25}$$

It follows from Eq. (5.22) that

$$a_m = \frac{1}{\gamma_m \|\phi_m\|^2} \sum_{n=0}^{N} b_n \sigma_n \left(e^{2i\sigma_n L} - 1\right) (\psi_n, \phi_m). \tag{5.26}$$

Substitution of this expression for a_m into Eq. (5.19) yields

$$\sum_{j=0}^{N} b_j \left(\sum_{n=-\infty}^{\infty} \frac{\sigma_j (e^{2i\sigma_j L} - 1)(\psi_j, \phi_n) \phi_n(y)}{\gamma_n \|\phi_n\|^2} \right) = \sum_{j=0}^{N} b_j (e^{2i\sigma_j L} + 1) \psi_j(y). \tag{5.27}$$

Multiplying this equation by $\overline{\psi_m(y)}$ and integrating from $-h$ to h we obtain the homogeneous system of linear equations for $b_0,\ldots,b_N$

$$A\mathbf{b} = \mathbf{0}, \tag{5.28}$$

where

$$A_{mj} = \sum_{n=-\infty}^{\infty} \frac{\sigma_j(e^{2i\sigma_j L} - 1)(\psi_j, \phi_n)(\phi_n, \psi_m)}{\gamma_n \|\phi_n\|^2} - \delta_{mj}\left(e^{2i\sigma_m L} + 1\right) |||\psi_m|||^2, \tag{5.29}$$

$$|||\psi_m|||^2 = \begin{cases} h & m = 1, ..., N, \\ 2h & m = 0. \end{cases} \tag{5.30}$$

Rayleigh-Bloch surface waves correspond to these values of β which make the determinant of A vanish. In general, β is complex. We now show how to transform the system (5.28) to an equivalent system with a Hermitian matrix. We rewrite the system (5.28) in the form

$$AGG^{-1}\mathbf{b} = 0, \tag{5.31}$$

where G is $(N+1) \times (N+1)$ matrix with elements defined by

$$G_{mj} = \frac{\delta_{mj}}{\sigma_j(e^{2i\sigma_j L} - 1)}. \tag{5.32}$$

It is equivalent to

$$B\tilde{\mathbf{b}} = \mathbf{0}, \tag{5.33}$$

where

$$B = AG,$$

$$B_{mj} = \sum_{n=-\infty}^{\infty} \frac{i(\psi_j, \phi_n)(\phi_n, \psi_m)}{\gamma_n \|\phi_n\|^2} - \frac{i\delta_{mj}\left(e^{2i\sigma_m L} + 1\right) |||\psi_m|||^2}{\sigma_j(e^{2i\sigma_j L} - 1)}. \tag{5.34}$$

$$\tilde{\mathbf{b}} = G^{-1}\mathbf{b},$$

We consider the case when there are no radiating waves:

$$0 < k < \beta < \frac{\pi}{H} - k.$$

It means that we operate at frequency below the cut-off frequency. In this case all γ_m are complex and we have

$$B_{mj} = \overline{B_{jm}},$$

i.e., matrix B is Hermitian and its determinant is real.

5.4 Numerical Results

In this Section, we apply our method to the particular set of parameters: $L = 1.0$, $h = 0.2$, $H = 1.0$. In Fig. 5.3, we show the dependence of $\det A$ on β for fixed $k = 1.0$. Solid, dashed, and dotted lines correspond to results obtained with 0, 2, and 4 evanescent waves in region D_3. It follows from that graph that for $k = 1.0$ there are two surface waves. In Fig. 5.4, we show dependence of β corresponded to the surface waves on k the wave number.

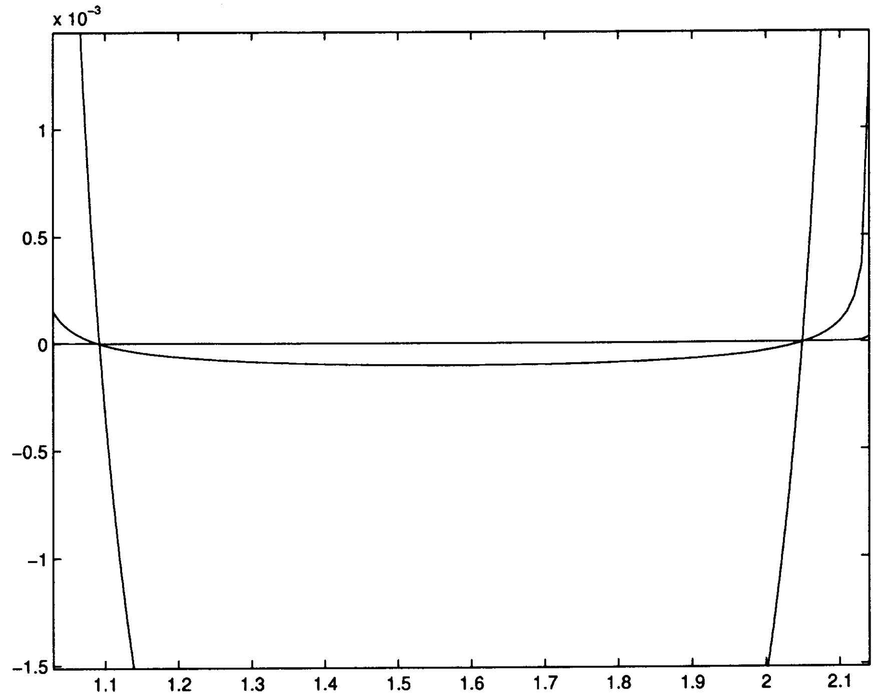

Figure 5.3 Dependence of $\det A$ on β for fixed $k = 1.0$

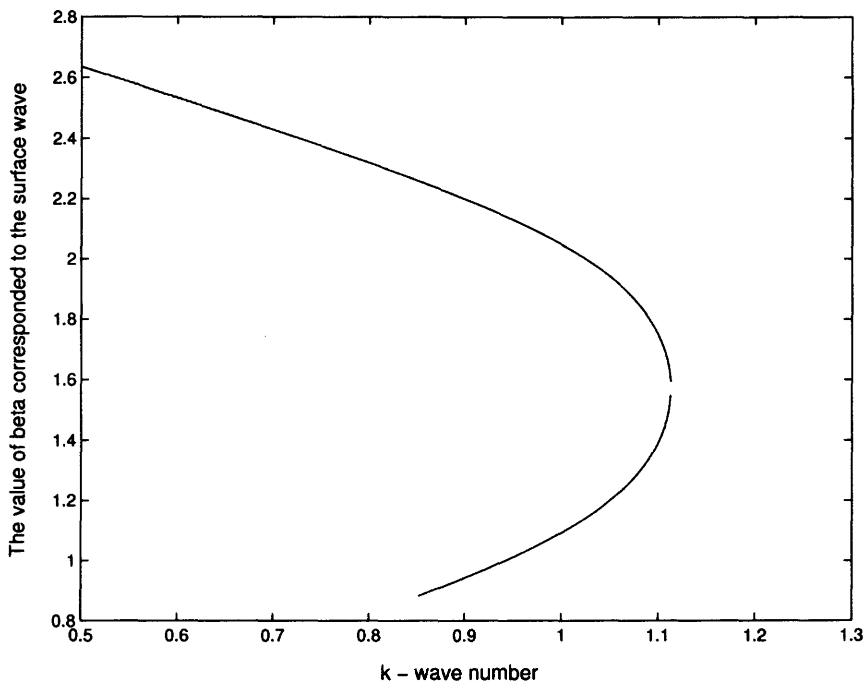

Figure 5.4 The dependence of β corresponded to the surface waves on k the wave number

CHAPTER 6

FUTURE RESEARCH

In Chapter 2 of this dissertation, we have applied the scattering matrix approach to study the scattering and transmission of waves through a two-dimensional photonic crystal. As a topic for future study, it might also be interesting to apply the scattering matrix approach to study the scattering and transmission of waves through a three-dimensional photonic crystal.

In Chapter 4, we have developed an analytical method to analyze and to study the scattering and transmission of waves through a two-dimensional photonic crystal which consists of a periodic array of parallel metallic rods with rectangular cross sections. Similar ideas allow us to develop an analytical method to analyze and to study the scattering and transmission of waves through a three-dimensional photonic crystal which consists of periodic array of metallic cubs. It is also possible to derive an explicit formula for the reflection and transmission coefficients when we take into account only one propagating mode in a specific portion of the periodic structure.

The analytical method developed in Chapter 5 can be applied to analyze and to study the surface waves along three-dimensional structure which consists of periodic array of finite cylinders. It can be showed that the surface waves correspond to the singularity of a Hermitian matrix.

The analytical method developed in Chapter 4 can be applied to study the localized modes along the line defect in two-dimensional periodic structure which consists of a infinite periodic array of parallel metallic rods with rectangular cross sections.

REFERENCES

[1] S. P. Shipman, S. Venakides,"Resonance and Bound States in Photonic Crystal Slabs", *SIAM J. Appl. Math.*, vol. 64, pp. 322-342, 2003.

[2] M. A. Haider, S. P. Shipman, S. Venakides, "Boundary integral calculations of two-dimensional electromagnetic scattering in infinite photonic crystal slab: channel defects and resonances", *SIAM J. Appl. Math.*, vol. 62, pp. 2129-2148, 2002.

[3] G. A. Kriegsmann, "Scattering matrix analysis of a photonic Fabry-Perot resonator" *Wave Motion*, vol. 37, pp. 43–61, 2003.

[4] A. Figotin, Y. A. Godin, " The computation of spectra of some 2D photonic crystals", *Journal of Computational Physics*, vol. 136, pp. 585-598, 1997.

[5] I. Ponomarev, "Separation of variables in the computation of spectra in 2D photonic crystals", *SIAM J. Appl. Math.*, vol. 61, no. 4, pp. 1202-1218, 2000.

[6] S. Venakides, M. A. Haider, V. Papanicolaou, "Boundary integral calculations of two-dimensional electromagnetic scattering by photonic crystal Fabry-Perot structure", *SIAM J. Appl. Math.*, vol. 60, pp. 1686-1706, 2000.

[7] L. F. Canino, J. J. Ottusch, M. A. Stalzer, J. L. Visher, S. M. Wandzura, "Numerical Solution of the Helmholtz equation in 2D and 3D using a high-order Nystrom discretisation", *Journal of Computational Physics*, vol. 148, pp. 627-663, 1998.

[8] P. P. Ewald, "Die Berechnung optischer und elektrostatischer Gitterpotentiale", *Ann. Physik*, vol. 64, pp. 253-287, 1921.

[9] D. Colton and R. Kress, *Inverse Acoustic and Electromagnetic Scattering Theory*, 2nd ed., Springer-Verlag, NY, 1998.

[10] R. Kress, *Linear Integral Equation*, 2nd ed., Springer-Verlag, NY, 1998.

[11] V. Darko, G. A. Kriegsmann, "A discrete unitary S-matrix: a metallic post in a waveguide", Journal of Computational Physics, (submitted).

[12] K. E. Atkinson, *The Numerical Solution of Integral Equations of the Second Kind", Cambridge University Press*, Cambridge, UK, 1997.

[13] C. H. Wilcox, *Scattering Theory for Diffraction Gratings*, Springer-Verlag, NY, 1984.

[14] M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions*, Dover, NY, 1972.

[15] J. T. Londergan, J. P. Carini, D. P. Murdock, *Binding and Scattering in Two-Dimensional Systems*, Springer-Verlag, NY, 1999.

[16] J. D. Joannopoulos, R. D. Meade, J. N. Winn, "Photonic Crystals: Molding the Flow of Light", Princeton University Press, Princeton, NJ, 1995.

[17] K. Sakoda, *Optical Property of Photonic Crystals*, Springer-Verlag, NY, 2001.

[18] F. de Fornel, *Evanescent Waves*, Springer-Verlag, NY, 2000.

[19] E. Yablonovitch, "Photonic bandgap structures", *J. Opt. Soc. Am. B,* vol. 10, pp. 283-295, 1993.

[20] C. A. Kyriazidou, H. F. Contopangos, W. M. Merrill, N. G. Alexopoulos, "Artificial versus natural crystals: effective wave impedance of printed photonic bandgap materials", *IEEE Trans. Antennas Propagation*", vol. 48 , pp. 95-105, 2000.

[21] Y. Qiu, K. M. Leung, L. Carin, D. Kralj, " Dispersion curves and transmission spectra of a two-dimensional photonic band-gap crystal: Theory and experiment", *J. Appl. Phys.*, vol. 77, pp. 3631-3636, 1995.

[22] J. Strain, "Fast potential theory ll. Layer potentials and discrete sums", *Journal of Computational Physics*, vol. 99, pp. 251-270, 1992.

[23] M. M. Sigalas, K. M. Ho, R. Biswas, C. M. Soukoulis, "Theoretical investigation of defects in photonic crystals in the presence of dielectric losses", *Physical Rev. B*, vol. 57, pp.3815-3820, 1998.

[24] M. M. Sigalas, C. M. Soukoulis, E. N. Economou, C. T. Chan, K. M. Ho, " Photonic band gaps and defects in two dimensions: Studies of the transmission coefficient", *Physical Rev. B*, vol. 48, pp.14121-14126, 1993.

[25] C. M. Linton, "The Green's function for the two-dimensional Helmholtz equation in periodic domains", *J. Engng. Mech.*, vol. 33, pp. 377-402, 1998.

[26] R. Porter, D. V. Evans, "Rayleigh-Bloch surface waves along periodic gratings and their connection with trapped modes in waveguides", *J.Fluid Mech.*, vol. 386, pp. 233-258, 1999.

[27] M. Callan, C. M. Linton, D. V. Evans, "Trapped modes in two-dimensional waveguides", *J.Fluid Mech.*, vol. 229, pp. 51-64, 1991.

[28] H. D. Maniar, J. N. Newman, "Wave diffraction by a long array of cylinders", *J.Fluid Mech.*, vol. 339, pp. 309-330, 1997.

[29] C. M. Linton, "The Green's function for the two-dimensional Helmholtz equation in periodic domain", *J. Engng. Mech.*, vol. 33, pp. 377-402, 1998.

[30] E. B. Davies, L. Parnovski, "Trapped modes in acoustic waveguides", *Q. J. Mech. Appl. Maths.*, vol. 51, pp. 477-492, 1998.

[31] P. McIver, C. M. Linton, M. McIver, "Construction of trapped modes for waveguides and diffraction gratings", *Proc. R. Soc. London. A*, vol. 454, pp. 2593-2616, 1998.

[32] C. M. Linton, D. V. Evans, "Integral equations for a class of problems concerning obstacles in waveguides", *J.Fluid Mech.*, vol. 245, pp. 349-365, 1992.

[33] D. V. Evans, R. Porter, "Trapped modes about multiple cylinders in a channel", *J.Fluid Mech.*, vol. 339, pp. 331-356, 1997.

[34] D. V.Evans, M. Livitin, D. Vassiliev, "Existence theorems for trapped modes", *J.Fluid Mech.*, vol. 261, pp. 21-31, 1994.

[35] P. M. Morse, H. Feshbach, *Methods of Theoretical Physics,* McGraw-Hill, NY, 1953.

[36] R. Courant and D. Hilbert, *Methods of Mathematical Physics*, Wiley Classics, 1989.

[37] J. D. Jackson, *Classical Electrodynamics*, John Wiley & Sons, Inc, third Ed., 1998.

[38] D. L. Colton and R. Kress, *Integral Equation Methods in Scattering Theory*, Wiley-Interscience, NY, 1983.

[39] S. G. Johnson, J. D. Joannopoulos, *Photonic Crystals: The Road from Theory to Practice*, Kluwer Academic Publishers, 2002.

[40] S. Fan, P. R. Villeneuve, J. D. Joannopoulos, H. A. Haus "Channel-drop filters in photonic crystals", Optecs Express, vol. 3, pp. 4-11, 1998.

[41] S. G. Tikhodeev, A. L. Yablonskii, E. A. Muljarov, N. A. Gippius, T. Ishihara, "Quasiguided modes and optical properties of photonic crystals slabs", Phys. Rev. B, vol. 66, 2002.

[42] C. Muller, *Foundations of the Mathematical Theory of Electromagnetic Waves*, Springer-Verlag, NY, 1969.

[43] A. Krishnan, T. Thio, T. J. Kim, H. J. Lezec, T. W. Ebbessen, P. A. Wolff, J. Pendry, L. Martin-Moreno, F. J. Garcia-Vidal, "Evanescently coupled resonance in surface plasmon enhanced transmission", *Optics Commun.*, vol. 200, pp, 1-7, 2001.

[44] J. T. Beale, "Scattering frequency of resonators", *Comm. Pure Appl. Math.,* vol. 26, pp. 549-563, 1973.

[45] A. Taflove, S. C. Hagness, *Computational Electrodynamics: The Finite-Difference Time-Domain Method*, Artech House, 2nd ed., 2000.

[46] E. Lidorikis, M. M. Sigalas, E. N. Economou, C. M. Soukoulis, " Gap deformation and classical wave localization in disordered two-dimensional photonic-band-gap materials", *Phys. Rev. B*, vol. 61, pp. 13458-13464, 2000.

[47] S. Fan, P. R. Villeneuve, J. D. Joannopoulos, H. A. Haus "Channel drop tunneling through localized states", *Phys. Rev. Let.,* vol. 80, pp. 960-963, 1998.

[48] S. G. Johnson, S. Fan, P. R. Villeneuve, J. D. Joannopoulos, L. A. Kolodziejski, "Guided modes in photonic crystal slabs", *Phys. Rev. B,* vol. 60, pp. 5751-5758, 1999.

[49] S. G. Johnson, S. Fan, P. R. Villeneuve, J. D. Joannopoulos, "Linear waveguides in photonic-crystal slabs", *Phys. Rev. B,* vol. 62, pp. 8212-8222, 2000.

[50] Photonic Crystals and Light Localization in the 21st Century : Proceedings of the NATO Advanced Study Institute "Photonic Crystals and Light Localization", Crete, Greece, 2000 Edited by C. Soukoulis (NATO ASI Series, Kluwer Academic Publishers, The Netherlands, 2001).

[51] H. S. Sozuer, J. W. Haus, R. Inguva, "Photonic bands: Convergence problems with the plane-wave method", *Phys. Rev. B*, vol. 45, pp. 13962, 1992.