

# Band-Gap Structure of Spectra of Periodic Dielectric and Acoustic Media. II. 2D Photonic Crystals

A. Figotin\*

Department of Mathematics  
University of North Carolina at Charlotte  
Charlotte, NC 28223

P. Kuchment†

Department of Mathematics and Statistics  
Wichita State University  
Wichita, KS 67260-0033

## Abstract

We consider the two-component dielectric medium consisting of a periodic array of parallel air columns of square cross section embedded into a lossless optically dense host material with the dielectric constant  $\zeta > 1$ . We show that if  $\zeta$  is large enough and the relative distance  $\delta$  between the air columns is such that  $\zeta\delta \gg 1$  and  $\zeta\delta^2 \ll 1$ , then the corresponding Maxwell operator has a series of gaps in the spectrum. We also provide some analytic formulas that enable one to detect location of bands and gaps in the spectrum. In particular, the typical wavelength exhibiting a photonic band gap is  $2\pi L\sqrt{\zeta\delta}$ , where  $L$  is the distance between the axes of adjacent air columns. We also give some estimates on the space distribution of electric field energy for different eigenmodes.

**Key words:** propagation of electromagnetic and acoustic waves, band-gap structure of the spectrum, periodic dielectrics, periodic acoustic media.

**AMS subject classification:** 35B27, 73D25, 78A45.

## Contents

<b>1</b>	<b>Introduction</b>	<b>2</b>
<b>2</b>	<b>Statement of Results</b>	<b>4</b>
<b>3</b>	<b>An Outline of the Main Arguments</b>	<b>9</b>
<b>4</b>	<b>1D Schrödinger Operator with a Periodic Point Potential</b>	<b>13</b>
4.1	Eigenvalues and spectra . . . . .	13
4.2	Negative eigenvalues . . . . .	17
4.3	Positive eigenvalues . . . . .	18
4.4	Perturbations of the spectrum of the Schrödinger operator with point potential . . . . .	20

---

\*This work was supported by the U.S. Air Force Grant F49620-94-1-0172DEF

†This work was partially supported by the NSF Grant DMS 910211 and by NSF EPSCOR Grant

4.5	Auxiliary spectra . . . . .	23
4.6	Eigenfunctions . . . . .	25
<b>5</b>	<b>Relations Between Schrödinger Operators with Point and Well Potentials</b>	<b>26</b>
5.1	Positive eigenvalues . . . . .	28
5.2	Negative eigenvalues . . . . .	30
5.3	Eigenfunctions . . . . .	31
<b>6</b>	<b>Scalar Models</b>	<b>35</b>
6.1	Separated variables case . . . . .	36
6.2	2D case with separated variables . . . . .	39
6.2.1	Preliminary analysis of the spectra . . . . .	39
6.2.2	$E$ -subspectrum . . . . .	40
6.2.3	$H$ -subspectrum . . . . .	41
6.3	General scalar 2D case. . . . .	42
<b>7</b>	<b>Spectrum of the Maxwell Operator</b>	<b>46</b>
7.1	General properties and Floquet-Bloch theory . . . . .	46
7.2	Proof of the main results . . . . .	56
7.3	Space distribution of the electric field energy . . . . .	56

## 1 Introduction

Periodic dielectrics, often referred to as photonic crystals, have attracted much attention in recent years. These crystals as conducting media for electromagnetic waves are expected to exhibit properties similar to those of solid crystals as conducting media for electronic waves. It is well known from the quantum theory of solids that the energy spectrum of an electron in a solid consists of bands separated by gaps (see, for instance, [AM]). This band-gap structure arises due to periodicity of the underlying crystal, and it is common for many periodic differential operators (see the so called Floquet-Bloch theory in [E], [K93], [RS]). It has been expected that the Maxwell operators that govern propagation of electromagnetic waves through photonic crystals must exhibit similar properties. This is certainly a sound idea, but proof of existence of gaps for a specific periodic medium, not to mention more complete investigation of geometry of the spectrum as a function of parameters of the media, turns out to be a hard mathematical problem. The goal of our series of papers (the first part was [FK], and subsequent parts are planned) is to provide some basic mathematical theory that describes how the band gaps arise in periodic dielectric and acoustic media. We also plan to consider problems of numerical estimates of the spectrum in a separate publication.

The idea of designing periodic dielectric materials that exhibit gaps in the spectrum was introduced in papers [Y], [J87]. The basic physical reason for the rise of gaps lies in the coherent multiple scattering and interference of waves (see, for instance [J91] and references therein). The tremendous number of applications that are expected in optics and electronics (including high efficiency lasers, laser diodes, etc.) warrant thorough investigation of this matter. So, one is not surprised by the persistent attention that this problem has attracted. The most recent theoretical and experimental results on the photonic band-gap structures are published in the series of papers [DE] and in the book [JMW]. The experimental results (see [vAL], [DG], [YG]) for periodic and disordered dielectrics indicate that photonic gap regime can be achieved for some nonhomogeneous materials. Fabrication of 2D photonic crystals in the nanoscale was recently reported in [WVG].

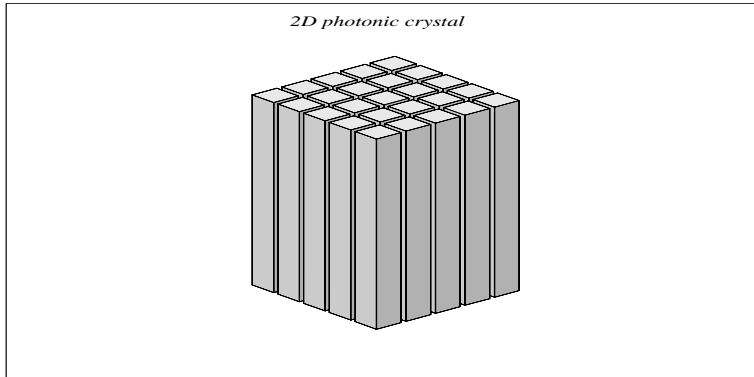


Fig. 1 The dielectric constant equals 1 in the vertical columns and it equals  $\epsilon \gg 1$  in the rest of the media. The distance between the centers of adjacent columns equals  $L$  and the spacing between them equals  $\delta L$ . We shall assume that  $L = 1$  for simplicity.

Theory of 2D photonic crystals reduces to investigation of two scalar equations associated with the so called  $E$ -polarized and  $H$ -polarized electromagnetic fields. Some of these equations have the same form as the equations for nonhomogeneous acoustic media, which makes the development of theory of 2D photonic crystals even more important. Various theoretical methods for 2D periodic dielectrics were developed in [VP] for sinusoidally and rectangularly modulated dielectric constants, and in [PM], [MM] for a periodic array of parallel dielectric rods of circular cross-section, whose intersections with a perpendicular plane form a triangular or square lattice. Similar structures were studied theoretically and experimentally in [MBRJ] and [MPD]. All these results (see also [EZ], [LL], [ZS], [HCS], [SSE]) indicate the possibility of a gap (or pseudogap) regime for some two-component periodic dielectrics. Our analysis of the spectral attributes of 2D photonic crystals is based on a thorough analysis of the relevant one-dimensional equations. These equations are similar to ones arisen in diffraction problems associated with dielectric and conducting lamellar gratings and which have been proven to be valuable and efficient tools in the analysis of the diffraction patterns, [1B], [2B], [M], [PSS], [RMP]. The list of publications on the subject is already rather lengthy, and we do not pretend to present the complete bibliography.

In this paper we consider the two-component dielectric medium that consists of a periodic array of parallel air columns with square cross section imbedded into an optically dense host material. We assume that the dielectric constant contrast (the mass density, or the elasticity contrast in the acoustic case) tends to infinity, and the distance between the air columns tends to zero. We show that if the rates of these two convergencies are properly related to each other, then one can guarantee existence of gaps in some prescribed parts of the spectrum. If there is no such coordination between the two rates, then one should expect the rise of pseudogaps rather than of real gaps [F94]. We also show that the spectrum associated with that medium splits into two subspectra, which we refer to as  $E$ -subspectrum and  $H$ -subspectrum. Both of them have band gap structure, but the typical sizes of the bands and gaps for the  $E$ -subspectrum are asymptotically much smaller, than those for the  $H$ -subspectrum. The spatial energy distribution of the corresponding eigenmodes is also different for these subspectra. We have discovered recently that the statement on the spectral structure of the Maxwell operator that we made in our paper [FK94] apparently requires some modifications, since we overlooked there the possibility of a subspectrum analogous to the  $E$ -subspectrum for 2D photonic crystals.

This is a long paper, filled with plenty of technical details (mostly related to a thorough analysis of some auxiliary one-dimensional problems). Unfortunately, there is no natural way of splitting this work into smaller pieces. We hope that an outline of main results and arguments provided below will

help the reader to survive through a mess of approximations, asymptotic formulas, and estimates. Some additional technical details omitted in the paper can be found in the preprint [FK95].

We are very grateful to the reviewers of our paper for their valuable suggestions.

## 2 Statement of Results

Our consideration of dielectric media is based on the Maxwell equations

$$\nabla \cdot \mathbf{D} = 0, \nabla \times \mathbf{E} = -\frac{1}{c} \frac{\partial \mathbf{B}}{\partial t}, \mathbf{D} = \varepsilon \mathbf{E}, \quad (1)$$

$$\nabla \cdot \mathbf{B} = 0, \nabla \times \mathbf{H} = \frac{1}{c} \frac{\partial \mathbf{D}}{\partial t}, \mathbf{B} = \mu \mathbf{H}, \quad (2)$$

where  $\mathbf{E}$  and  $\mathbf{D}$  are respectively the electric field and electric induction,  $\mathbf{H}$  and  $\mathbf{B}$  are respectively the magnetic field and magnetic induction, and  $c$  is the velocity of light. We shall assume that  $\mu \equiv 1$  (this condition holds for many dielectric materials of interest). The dielectric constant  $\varepsilon$  is assumed to be position-dependent, i.e.  $\varepsilon = \varepsilon(\mathbf{x}) \geq 1$ .

Let us introduce the standard basis vectors  $\mathbf{e}_j, 1 \leq j \leq 3$  in the space  $\mathbf{R}^3$  and the domains in  $\mathbf{R}^2$ :

$$X = [0, 1] \times [0, 1], \quad O_\delta = [\delta, 1] \times [\delta, 1], \quad (3)$$

where  $\delta \in (0, 1)$ . We will also need the domain

$$X' = [\delta/2, 1 + \delta/2] \times [\delta/2, 1 + \delta/2]. \quad (4)$$

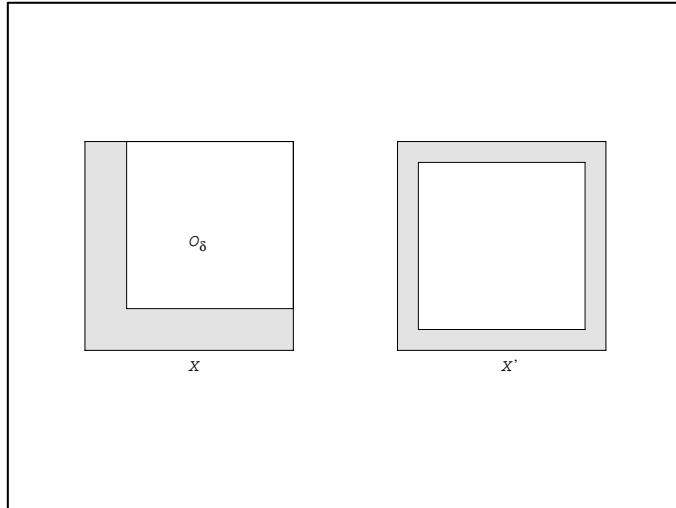


Fig. 2 Domains  $X$  and  $X'$ . The darker area indicates the location of the optically dense component where the dielectric constant equals  $\zeta > 1$ . The light area corresponds to the air component.

Since we are going to consider two-dimensional periodic media, we impose the following conditions

on the dielectric constant  $\varepsilon(\mathbf{x})$ ,  $\mathbf{x} = (x_1, x_2, x_3)$  :

$$\varepsilon(\mathbf{x}) = \varepsilon(x_1, x_2) = \begin{cases} 1 & \text{if } (x_1, x_2) \in O_\delta \\ \zeta & \text{if } (x_1, x_2) \in X - O_\delta \end{cases}, \quad \zeta > 1 \quad (5)$$

with the periodicity condition

$$\varepsilon(\mathbf{x} + n_1 \mathbf{e}_1 + n_2 \mathbf{e}_2) = \varepsilon(\mathbf{x}), \quad \mathbf{x} \in \mathbf{R}^3, n_1, n_2 \in \mathbf{Z}, \quad (6)$$

where  $\mathbf{Z}$  is the set of integers. For this kind of periodic media we will be interested in the waves propagating along the plane  $\langle \mathbf{e}_1, \mathbf{e}_2 \rangle$ , which leads to the condition that the magnetic and electric fields  $\mathbf{H}$  and  $\mathbf{E}$  depend on coordinates  $x_1, x_2$  only. That is, from now on we shall assume that

$$\mathbf{H} = \mathbf{H}(x_1, x_2), \quad \nabla \cdot \mathbf{H} = 0; \quad \mathbf{E} = \mathbf{E}(x_1, x_2), \quad \nabla \cdot \varepsilon \mathbf{E} = 0. \quad (7)$$

Let us describe first the relevant operators without rigorous technical details which will be provided in Section 7. We define the Maxwell operator as acting on an appropriate space of pairs  $\mathbf{E}(\mathbf{x}), \mathbf{H}(\mathbf{x})$  as follows:

$$M \begin{bmatrix} \mathbf{E}(\mathbf{x}) \\ \mathbf{H}(\mathbf{x}) \end{bmatrix} = ci \begin{bmatrix} \varepsilon(\mathbf{x})^{-1} \nabla \times \mathbf{H}(\mathbf{x}) \\ -\nabla \times \mathbf{E}(\mathbf{x}) \end{bmatrix}. \quad (8)$$

The operator  $M$  is self-adjoint. If  $\omega$ , which can be viewed as the frequency of a harmonic eigenmode, is a point in the spectrum  $\sigma(M)$ , and the pair  $\{\mathbf{E}_\omega, \mathbf{H}_\omega\}$  is the corresponding generalized eigenfunction, then we have

$$\varepsilon(\mathbf{x})^{-1} \nabla \times \mathbf{H}_\omega(\mathbf{x}) = -i \frac{\omega}{c} \mathbf{E}_\omega(\mathbf{x}), \quad (9)$$

$$\nabla \times \mathbf{E}_\omega(\mathbf{x}) = i \frac{\omega}{c} \mathbf{H}_\omega(\mathbf{x}). \quad (10)$$

These relations imply

$$M_H \mathbf{H}_\omega(\mathbf{x}) = \nabla \times (\varepsilon(\mathbf{x})^{-1} \nabla \times \mathbf{H}_\omega(\mathbf{x})) = \left(\frac{\omega}{c}\right)^2 \mathbf{H}_\omega(\mathbf{x}), \quad (11)$$

$$M_E \mathbf{E}_\omega(\mathbf{x}) = \varepsilon(\mathbf{x})^{-1} \nabla \times (\nabla \times \mathbf{E}_\omega(\mathbf{x})) = \left(\frac{\omega}{c}\right)^2 \mathbf{E}_\omega(\mathbf{x}). \quad (12)$$

The operators  $M_H$  and  $M_E$  can be viewed as self-adjoint, nonnegative, unbounded operators on appropriate subspaces (which incorporate the zero divergence conditions from (1) and (2)) of the Hilbert spaces  $L_2(\mathbf{R}^3, \mathbf{C}^3)$  and  $L_2(\mathbf{R}^3, \mathbf{C}^3, \varepsilon dx)$  respectively. We denote here by  $L_2(\mathbf{R}^3, \mathbf{C}^3)$  the space of  $\mathbf{C}^3$ -valued square integrable vector functions with the scalar product  $\int \Psi^* \Phi dx$ , and by  $L_2(\mathbf{R}^3, \mathbf{C}^3, \varepsilon dx)$  the analogous space, where the scalar product is defined as  $\int \Psi^* \Phi \varepsilon dx$ . We notice that the spaces  $L_2(\mathbf{R}^3, \mathbf{C}^3)$  and  $L_2(\mathbf{R}^3, \mathbf{C}^3, \varepsilon dx)$  consist of the same functions, and their norms are equivalent.

It will be shown in the section 7.1 that for the case of two-dimensional photonic crystals when the waves propagate in the crystal's plane the following decomposition of spectra holds:

$$\omega \in \sigma(M) \Leftrightarrow \left(\frac{\omega}{c}\right)^2 \in \sigma(\Gamma_\varepsilon) \cup \sigma(\Theta_\varepsilon), \quad (13)$$

where operators  $\Gamma_\varepsilon$  and  $\Theta_\varepsilon$  are defined as

$$\Gamma_\varepsilon H_3 = -(\partial_1 \varepsilon^{-1} \partial_1 + \partial_2 \varepsilon^{-1} \partial_2) H_3, \quad (14)$$

$$\Theta_\varepsilon E_3 = -\varepsilon^{-1} (\partial_1^2 + \partial_2^2) E_3 \quad (15)$$

on appropriate domains in  $L_2(\mathbf{R}^3, \mathbf{C}^3)$  and  $L_2(\mathbf{R}^3, \mathbf{C}^3, \varepsilon dx)$  respectively. Here  $\sigma(\Gamma_\varepsilon)$  and  $\sigma(\Theta_\varepsilon)$  represent the spectra for  $H$ -polarized and  $E$ -polarized fields. *Abusing the notation we will sometimes mean by  $\sigma(M)$  the set of values  $(\omega/c)^2$  instead of values  $\omega \in \sigma(M)$ .*

The relations between two parameters  $\zeta$  and  $\delta$  that lead to gaps in the spectrum roughly speaking are as follows:

$$\zeta\delta^{3/2} \ll 1, \quad \zeta\delta \gg 1, \quad (16)$$

which, in particular, imply that

$$\zeta \gg 1, \quad \delta \ll 1. \quad (17)$$

In other words, our main results are of asymptotic nature. We shall also need the auxiliary parameters:

$$\beta = (\zeta\delta^2)^{-1} > \beta_1 = (\zeta\delta^{3/2})^{-1} > \beta_2 = (\zeta\delta^{4/3})^{-1} > w = (\zeta\delta)^{-1}. \quad (18)$$

In particular, the original parameters  $\zeta$  and  $\delta$  can be expressed as

$$\zeta = \beta w^{-2} = \beta_1^2 w^{-3} = \beta_2^3 w^{-4}, \quad \delta = w\beta^{-1} = (w\beta_1^{-1})^2 = (w\beta_2^{-1})^3. \quad (19)$$

The following trivial statement follows readily from the equalities (19):

**Lemma 1** *Suppose that  $\beta > C$  (or  $\beta_1 > C$ , or  $\beta_2 > C$ ) for some positive constant  $C$ . Then  $w \rightarrow 0$  implies  $\zeta \rightarrow \infty$  and  $\delta \rightarrow 0$ .*

For instance, the conditions (16) are met if

$$\zeta = C\delta^{-(1+\eta)}, \quad 0 < \eta < 1/2 \quad (20)$$

The spectrum  $\sigma(M)$  we are interested in naturally splits into two subspectra  $\sigma_E(M)$  and  $\sigma_H(M)$ , which we shall call respectively  $E$ -subspectrum and  $H$ -subspectrum. They can be described as follows. Let  $\tilde{w}$  be defined as

$$\tilde{w} = \frac{w}{1-w\delta} = \frac{w}{1-\zeta^{-1}}. \quad (21)$$

(in particular, under the conditions of the Lemma 1 we have  $\tilde{w} \sim w$ ). Then

$$\sigma_E(M) = \bigcup_{n \geq 0} [\tilde{w}D_n^-(\zeta, \delta), \tilde{w}D_n^+(\zeta, \delta)], \quad (22)$$

where the intervals  $[D_n^-(\zeta, \delta), D_n^+(\zeta, \delta)]$  are disjoint for different values of  $n$ , and their endpoints can be described as follows:

$$D_n^\pm(\zeta, \delta) = 2\pi n(1 + \chi_n^\pm), \quad n \geq 1; \quad D_0^-(\zeta, \delta) = 0, \quad D_0^+(\zeta, \delta) = 4 + \chi_0^+ \quad (23)$$

$$D_n^+(\zeta, \delta) - D_n^-(\zeta, \delta) = \pi + \eta_n^+, \quad D_{n+1}^-(\zeta, \delta) - D_n^-(\zeta, \delta) = 2\pi + \eta_n^- \quad (24)$$

The sub-spectrum  $\sigma_H(M)$  can be represented as

$$\sigma_H(M) = \bigcup_{\mathbf{n} \geq 0} [(\pi\mathbf{n})^2 + \rho_{\mathbf{n}}^-, (\pi\mathbf{n})^2 + \rho_{\mathbf{n}}^+]. \quad (25)$$

Under appropriate conditions on  $\zeta$  and  $\delta$  the quantities  $\chi_n^\pm$ ,  $\eta_n^\pm$  and  $\rho_{\mathbf{n}}^\pm$  are small.

It turns out, that under some conditions on  $\zeta$  and  $\delta$  any finite number of the first bands and gaps in the spectrum can be found very accurately in terms of some absolute set:

$$\sigma_E = \bigcup_{n \geq 0} [D_n^-, D_n^+] \approx [0, 4] \bigcup \left\{ \bigcup_{n > 0} [2\pi n, 2\pi n + \pi] \right\}, \quad (26)$$

where the intervals  $[D_n^-, D_n^+]$  do not intersect and their endpoints  $D_n^\pm$  do not depend on any parameters of the problem. Properties of these endpoints are described in the Lemmas 15 and 16.

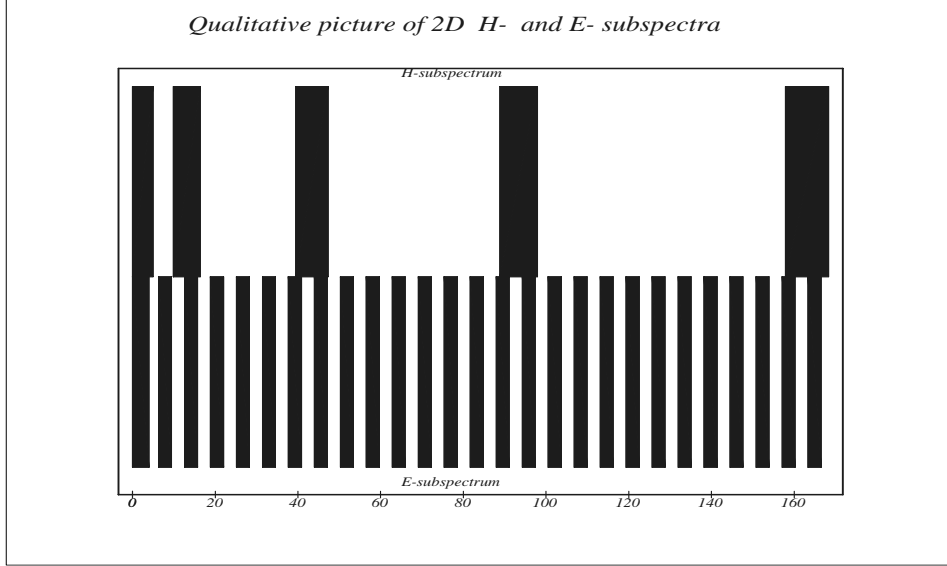


Fig. 3 The horizontal axis is the spectral axis corresponding to  $(\omega/c)^2$ . The black columns above the axis display the location of the  $H$ -subspectrum whereas the columns below the axis display the location of the  $E$ -subspectrum.

Our main results are:

**Theorem 2** For any natural number  $N_0 > 1$  and any positive constant  $C$  there exists a positive constant  $c$  such that for any  $\beta_1 > C$  and for any  $w < c$  the following is true:

$$\sigma(\Theta_\varepsilon) \cap I = \left[ \bigcup_{0 \leq n \leq N_0} [wD_n^-(\zeta, \delta), wD_n^+(\zeta, \delta)] \right] \cap I, \quad \text{where } I = [0, 2\pi w(N_0 - 1)], \quad (27)$$

$$\sigma(\Gamma_\varepsilon) \cap I \subseteq [0, 8w + O(w^2)], \quad (28)$$

and the endpoints  $D_n^\pm(\zeta, \delta)$  can be approximated by the numbers  $D_n^\pm$  from (26) as follows:

$$|D_n^\pm(\zeta, \delta) - D_n^\pm| \leq 2(4w + 10^3 N_0^3 \beta^{-1}). \quad (29)$$

Under somewhat stronger conditions we can describe the location of the spectrum in any finite interval of the spectral axis.

**Theorem 3** For any positive constant  $N$  there exist positive constants  $C$  and  $c$  such that for any  $\beta_2 > C$  and for any  $w < c$  the following is true:

$$\omega \in \sigma(M) \cap [0, N] \Leftrightarrow \left(\frac{\omega}{c}\right)^2 \in [\sigma_E(M) \cup \sigma_H(M)] \cap [0, N], \quad (30)$$

where  $\sigma_E(M)$  and  $\sigma_H(M)$  satisfy (22)-(25), and the quantities  $\chi_n^\pm$ ,  $\eta_n^\pm$  and  $\rho_{\mathbf{n}}^\pm$  satisfy the relations:

$$|\chi_n^\pm| \leq 100N\beta^{-1} + 6e^{-0.3n} + 10N^2\beta_2^{-3}wn^{-1}, 1 \leq n \leq N(\pi w)^{-1}, \quad (31)$$

$$|\eta_n^\pm| \leq 5 \cdot 10^3 N\beta^{-1} + 2 \cdot 10^3 e^{-0.3n} + 3n^{-1} + 301w, 1 \leq n \leq N(\pi w)^{-1}, \quad (32)$$

and for some constant  $C_1$

$$|\rho_{\mathbf{n}}^\pm| \leq C_1 w, |\mathbf{n}| \leq \sqrt{N}\pi^{-1}. \quad (33)$$

In particular, the spectrum of values of  $(\omega/c)^2$  has adjacent bands and gaps of approximately same size (of order  $w$ ).

Specific estimates for the quantities  $D_n^\pm$ ,  $\chi_n^\pm$ ,  $\eta_n^\pm$  and  $\rho_{\mathbf{n}}^\pm$ , as well as structure of eigenmodes are discussed in the subsequent sections.

### Summary of the results.

1. The spectrum  $\sigma(M)$  of the Maxwell operator consists of two subspectra of different structure which we shall refer to as  $E$ -subspectrum and  $H$ -subspectrum.
2. The  $E$ -subspectrum is generated exclusively by  $E$ -polarized fields. It consists of almost equal bands and gaps of the approximate width  $\pi w$ . The typical dimension of the wavelength exhibiting a photonic band gap is  $2\pi L\sqrt{\zeta\delta}$ , where  $L$  is the distance between the centers of adjacent air columns.
3. The  $H$ -subspectrum arises due to both polarizations.  $H$ -subspectra for both polarizations are about the same and consist of bands of width of order  $w$  which are located approximately at the points  $(\pi\mathbf{n})^2$ . The only difference is that  $H$ -subspectrum for  $E$ -polarization starts approximately at the point  $\pi^2$  whereas  $H$ -subspectrum for  $H$ -polarization starts at 0.
4.  $E$ -subspectrum and  $H$ -subspectrum differ also in the way the energy of the corresponding eigenmodes is distributed in the space. The eigenmodes associated with the  $E$ -subspectrum have most of the electric field energy residing in the areas where the dielectric constant is large (i.e. in the optically dense component), though the relative area occupied by this component is small. On the contrary, most of the electric field energy for the eigenmodes associated with the  $H$ -subspectrum for  $E$ -polarized fields resides in the air columns, where the dielectric constant is 1. The eigenmodes associated with  $E$ -subspectrum are exponentially confined to the dielectric and can be viewed as a manifestation of the total reflection phenomenon.

We finish this section by adopting the notation:

$$L_2^3(X) = [L_2(X)]^3 = L_2(X, d\mathbf{x}, \mathbf{C}^3);$$

$$L_{2,\varepsilon}^3(\mathbf{X}) = [L_2(\mathbf{X}, \varepsilon(\mathbf{x}) d\mathbf{x})]^3 = L_2(\mathbf{X}, \varepsilon(\mathbf{x}) d\mathbf{x}, \mathbf{C}^3);$$

$l_2^3 = l_2(\mathbf{Z}^3, \mathbf{C}^3)$  is the Hilbert space of  $\mathbf{C}^3$ -valued functions  $\Phi(m)$ ,  $m \in \mathbf{Z}^3$  such that  $\|\Phi\|^2 = \sum_m |\Phi(m)|^2 < \infty$ ;

$h_1^3$  is the Hilbert space of  $\mathbf{C}^3$ -valued functions  $\Phi(m)$ ,  $m \in \mathbf{Z}^3$  such that  $\|\Phi\|^2 = \sum_m (1+m^2)|\Phi(m)|^2 < \infty$ ;

$\delta_{m,n}$  is the Kronecker symbol;

$\mathbf{Z}_+$  is the set of nonnegative integers;

$\mathbf{Z}_+^d$  is the Cartesian product of  $d$  copies of  $\mathbf{Z}_+$ .

For a vector  $\mathbf{n} = (n_1, \dots, n_d) \in \mathbf{R}^d$ ,  $\mathbf{n} > 0$  means that all components of the vector  $\mathbf{n}$  are strictly positive, and  $|\mathbf{n}| = |n_1| + \dots + |n_d|$ .



### 3 An Outline of the Main Arguments

The proofs of the main statements are lengthy. In this section we give an outline of the basic arguments that lead to the Theorem 3. We believe that this will be a reader's guide to the rest of the text. The proof of the Theorem 2 is similar, and in fact simpler.

The problem of finding the spectrum  $\sigma(M)$  reduces to the two eigenvalue problems for a scalar function  $\varphi(\mathbf{x})$ ,  $\mathbf{x} = (x_1, x_2) \in \mathbf{R}^2$ :

$$\begin{aligned}\Gamma_\varepsilon \varphi(\mathbf{x}) &= -[\partial_1 \varepsilon^{-1}(\mathbf{x}) \partial_1 + \partial_2 \varepsilon^{-1}(\mathbf{x}) \partial_2] \varphi(\mathbf{x}) = \lambda \varphi(\mathbf{x}), \\ \Theta_\varepsilon \varphi(\mathbf{x}) &= -\varepsilon(\mathbf{x})^{-1} \Delta \varphi(\mathbf{x}) = \lambda \varphi(\mathbf{x}),\end{aligned}$$

where operators  $\Gamma_\varepsilon$  and  $\Theta_\varepsilon$  act respectively in the Hilbert spaces  $L_2(\mathbf{R}^2)$  and  $L_2(\mathbf{R}^2, \varepsilon(\mathbf{x}) d\mathbf{x})$  (see section 7.1 for details). We have investigated the spectrum of the operator  $\Gamma_\varepsilon$  in the first part [FK] of the paper. Hence, here we need to investigate the spectrum of the operator  $\Theta_\varepsilon$  only. It differs significantly from the spectrum of the operator  $\Gamma_\varepsilon$ .

Since the dielectric constant  $\varepsilon(\mathbf{x})$  is a periodic function, the standard Floquet-Bloch theory (see, for instance, [E], [RS], [K82], [K93]) says that we need to consider the eigenvalue problem on the fundamental cell  $X$ :

$$\Theta_{\mathbf{k}, \varepsilon} \varphi(\mathbf{x}) = -\varepsilon(\mathbf{x})^{-1} \Delta \varphi(\mathbf{x}) = \lambda \varphi(\mathbf{x}), \quad \mathbf{x} \in X,$$

where  $\varphi$  satisfies the boundary conditions

$$\begin{aligned}\varphi(1, x_2) &= e^{ik_1} \varphi(0, x_2), \quad \varphi(x_1, 1) = e^{ik_2} \varphi(x_1, 0), \\ \nabla \varphi(1, x_2) &= e^{ik_1} \nabla \varphi(0, x_2), \quad \nabla \varphi(x_1, 1) = e^{ik_2} \nabla \varphi(x_1, 0)\end{aligned}\tag{34}$$

for  $\mathbf{k} = (k_1, k_2)$ ,  $k_j \in [0, 2\pi]$ . The spectrum of the operator  $\Theta_\varepsilon$  coincides with the union (for all  $\mathbf{k}$ ) of spectra of these problems.

It turns out that the spectrum of the operator  $\Theta_\varepsilon$  will remain almost the same, if we replace the original periodic function  $\varepsilon(\mathbf{x})$  defined in (5) by

$$\varepsilon(\rho, \mathbf{x}) = \varepsilon(\rho_{\zeta, \delta}, \mathbf{x}) = \rho_{\zeta, \delta}(x_1) + \rho_{\zeta, \delta}(x_2),$$

where the auxiliary function  $\rho_{\zeta, \delta}(y)$ ,  $y \in \mathbf{R}$  is defined as

$$\rho_{\zeta, \delta}(y) = \begin{cases} \zeta - 1/2 & \text{if } 0 \leq y < \delta \\ 1/2 & \text{if } \delta \leq y < 1 \end{cases}, \quad \rho(y) = \rho(y + n), n \in \mathbf{Z}, y \in \mathbf{R}.$$

It is easy to see that the functions  $\varepsilon(\rho, \mathbf{x})$  and  $\varepsilon(\mathbf{x})$  coincide all over the space  $\mathbf{R}^2$  except for small squares with sides of length  $\delta$ . The advantage of the new eigenvalue problem is that it has separable variables. This, in turn, will enable us to reduce the problem to a one-dimensional one. Thus, let us consider now the following eigenvalue problem

$$\overset{\circ}{\Theta}_{\zeta, \delta} \varphi(\mathbf{x}) \equiv -\varepsilon^{-1}(\rho, \mathbf{x}) \Delta \varphi(\mathbf{x}) = \lambda \varphi(\mathbf{x}), \quad \mathbf{x} \in X.\tag{35}$$

The circle on the top of an operator will indicate that we deal with a separate variables case. Let us rewrite the problem (35) as

$$S_{\mathbf{k}, \lambda} \varphi = -\Delta \varphi - \lambda v(\rho, \mathbf{x}) \varphi = \lambda \varphi, \quad v(\rho, \mathbf{x}) = \sum_{j=1,2} (\rho_{\zeta, \delta}(x_j) - 1/2).\tag{36}$$

This problem can be viewed as the spectral problem for the Schrödinger operator with the potential  $\lambda v$  (i.e., the potential depends on the spectral parameter). To reduce that to a standard spectral problem we

consider the eigenvalues of the following Schrödinger operator satisfying the cyclic boundary conditions (34)

$$S_{\mathbf{k},\lambda}\varphi = \xi(\mathbf{m}, \mathbf{k}, \lambda)\varphi, \quad \mathbf{x} \in X, \quad S_{\mathbf{k},\lambda}\varphi = -\Delta\varphi - \lambda v(\rho, \mathbf{x})\varphi, \quad (37)$$

where  $\mathbf{m}$  is an index which counts the eigenvalues  $\xi(\mathbf{m}, \mathbf{k}, \lambda)$  of the Schrödinger operator  $S_{\mathbf{k},\lambda}$ . This operator involves a new independent parameter  $\lambda \geq 0$ . Hence, the eigenvalues of the problem (35) are the solutions for  $\lambda \geq 0$  the equations

$$\xi(\mathbf{m}, \mathbf{k}, \lambda) = \lambda \quad (38)$$

with the index  $\mathbf{m}$  counting these eigenvalues.

**The equation (38) is our key equation.** To understand its solutions we need to analyze the eigenvalues of the Schrödinger operator  $S_{\mathbf{k},\lambda}$  as functions of all the variables  $\zeta, \delta, \lambda$ , and  $\mathbf{k}$ . At this point we observe that the potential  $\lambda v$  is the sum of two one-dimensional ones, and therefore

$$\xi(\mathbf{m}, \mathbf{k}, \lambda) = \xi_{m_1}(k_1, \lambda) + \xi_{m_2}(k_2, \lambda); \quad \mathbf{k} = (k_1, k_2), \quad \mathbf{m} = (m_1, m_2), \quad (39)$$

where  $\xi_m(k, \lambda), m = 0, 1, \dots$  are the eigenvalues of the Floquet-Bloch component  $Q_{\kappa,\lambda}$  of the one-dimensional Schrödinger operator:

$$Q_\lambda = -\frac{\partial^2}{\partial y^2} - \lambda(\rho_{\zeta,\delta}(y) - 1/2). \quad (40)$$

Hence, the key equation (38) can be rewritten as follows:

$$\xi_{m_1}(k_1, \lambda) + \xi_{m_2}(k_2, \lambda) = \lambda, \quad \text{where } m_1, m_2 = 0, 1, \dots \quad (41)$$

We notice now that  $\rho_{\zeta,\delta}(y) - 1/2$  is a well potential which equals zero everywhere except for an interval of the length  $\delta$ , where it is equal to  $\zeta - 1 \gg 1$  (in view of the conditions (16)). It is important that this potential appears in the operator  $Q_{\kappa,\lambda}$  with the *negative* amplitude  $-\lambda$ .

We will use the following parameterization of the operator  $Q_{\kappa,\lambda}$

$$Q(D, \delta)\psi(y) = -\psi''(y) - q_{D,\delta}(y)\psi(y), \quad y \in \mathbf{R}, \quad (42)$$

where  $q$  is the periodic potential that depends on two parameters  $D \geq 0$  and  $\delta > 0$  as

$$q_{D,\delta}(y) = \begin{cases} D\delta^{-1} & \text{if } 0 \leq y < \delta \\ 0 & \text{if } \delta \leq y < 1 \end{cases}, \quad q(y) = q(y+n), \quad n \in \mathbf{Z}, \quad y \in \mathbf{R}. \quad (43)$$

The idea behind introducing the parameter  $D$  is that the potential  $q_{1,\delta}$  approximates the Dirac's  $\delta$ -function when  $\delta$  is small. Comparing the values of the potentials  $\lambda(\rho - 1/2)$ , and  $q_{D,\delta}$  in the area  $0 \leq y < \delta$ , we get the relations:

$$\begin{aligned} \lambda(\zeta - 1) &= D\delta^{-1}, \quad D = \lambda(\delta\zeta - \delta), \quad \text{or} \\ \lambda &= Dw(1 - \zeta^{-1})^{-1} = D\tilde{w}. \end{aligned} \quad (44)$$

Let us denote by  $Q(\kappa, D, \delta)$  the Floquet-Bloch component of the operator  $Q(D, \delta)$  that corresponds to the quasi-momentum  $\kappa$  (i.e., the operator  $Q(D, \delta)$  with the boundary conditions (34)). Then the following simple relation holds:

$$Q_{\kappa,\lambda} = Q(\kappa, \lambda \tilde{w}^{-1}, \delta), \quad \tilde{w}^{-1} = w^{-1} - \delta.$$

When

$$\beta^{-1} = \zeta\delta^2 \rightarrow 0, \quad w = (\zeta\delta)^{-1} \rightarrow 0, \quad (45)$$

the next limit operator naturally arises

$$Q(D) = -\frac{\partial^2}{\partial y^2} - D \sum_{n \in \mathbf{Z}} \delta(y - n),$$

where  $\delta(y)$  is the Dirac delta-function. The eigenvalues of the operators  $Q(D, \delta)$  and  $Q(D)$  are denoted respectively by  $\xi_n(\kappa, D, \delta)$ ,  $\xi_n(\kappa, D)$ ,  $n = 0, 1, \dots$ . These eigenvalues are positive for  $n \geq 1$ . It is convenient to introduce the quantities

$$\mu_n(\kappa, D, \delta) = \sqrt{\xi_n(\kappa, D, \delta)}, \quad \mu_n(\kappa, D) = \sqrt{\xi_n(\kappa, D)}, \quad n \geq 1 \quad (46)$$

It is well known from the spectral theory of one-dimensional periodic operators (see, for instance, [E], [RS]) that in order to find the endpoints of bands of the spectrum it is sufficient to consider just the values  $\kappa = 0, \pi$ . We introduce the quantities:

$$\mu_n^+(D, \delta) = \max_{\kappa=0, \pi} \mu_n(\kappa, D, \delta), \quad \mu_n^-(D, \delta) = \min_{\kappa=0, \pi} \mu_n(\kappa, D, \delta), \quad (47)$$

which correspond to the endpoints of bands of the spectrum of the periodic Schrödinger operators  $Q(D, \delta)$ . Both eigenvalues  $\xi_0(\kappa, D, \delta)$  and  $\xi_0(\kappa, D)$  are negative for  $D > 4$ . They play a significant role in all further analysis. We also introduce the real-valued functions:

$$\nu_0(D, \delta) = \sqrt{-\xi_0(0, D, \delta)} > \nu_1(D, \delta) = \sqrt{-\xi_0(\pi, D, \delta)}, \quad (48)$$

and the corresponding functions  $\nu_0(D)$  and  $\nu_1(D)$  for the operator  $Q(D)$ . The function  $\nu_1$  is defined when  $\xi_0(\pi, D, \delta) < 0$  (i.e., for  $D > 4$ ).

Analysis shows that structure of equations (41) significantly depends on whether one of the indices  $m_j$  is zero. Thus, we should investigate separately two series of equations depending on this circumstance. *These two sets of equations produce correspondingly two series of bands in the spectrum of the operator  $\mathring{\Theta}_{\zeta, \delta}$ .* The first series of bands which we call *E-subspectrum* is associated with the equations where at least one of the indices  $m_j$  is zero. The *H-subspectrum* corresponds to the equations where both  $m_j$  are positive. The first subset of equations (41), when at least one  $m_j$  is zero, after switching to the parameter  $D = \lambda \tilde{w}^{-1}$  can be rewritten as

$$\xi_0(k_1, D, \delta) + \xi_n(k_2, D, \delta) = D\tilde{w}, \quad \tilde{w} = w(1 - w\delta)^{-1}; n \geq 0. \quad (49)$$

For a fixed  $n \geq 0$  the set of values  $D\tilde{w}$  for all solutions  $D$  to this equation (when both  $k_j$  run over the interval  $[0, \pi]$ ) yields the  $n$ -th band of the *E*-subspectrum. We denote this band, which is an interval, by

$$[\tilde{w}D_n^-(\zeta, \delta), \tilde{w}D_n^+(\zeta, \delta)].$$

The second set of equations takes the form

$$\xi_{n_1}(k_1, \lambda\tilde{w}^{-1}, \delta) + \xi_{n_2}(k_2, \lambda\tilde{w}^{-1}, \delta) = \lambda, \quad n_1, n_2 > 0. \quad (50)$$

For a fixed  $\mathbf{n} = (n_1, n_2) > 0$  the set of solutions  $\lambda$  to this equation (when both  $k_j$  run over the interval  $[0, \pi]$ ) yields the  $\mathbf{n}$ -th band of the *H*-subspectrum. We show that

$$\mu_n^-(D, \delta) \cong \pi n, \quad \mu_n^+(D, \delta) \cong \pi(n + \gamma_n(D)), \quad n \geq 1, \quad \text{where} \quad (51)$$

$$\gamma_n(D) \cong 1 - \frac{2}{\pi} \arctan \frac{D}{2\pi n}, \quad D \geq 0, \quad n \geq 1, \quad (52)$$

and

$$\nu_0(D, \delta) = (1 + O(\beta^{-1}))D/2; \nu_0(D, \delta) - \nu_1(D, \delta) \sim e^{-D/2}. \quad (53)$$

Using (46), (47) and (48), we can rewrite the equations (49) for the endpoints  $D_n^\pm(\zeta, \delta)$  of the  $n$ -th band as

$$\mu_n^-(D, \delta) = \sqrt{\nu_0^2(D, \delta) + D\tilde{w}} = \nu_0(D, \delta)(1 + O(w)) : \text{for } D_n^-(\zeta, \delta) \quad (54)$$

$$\mu_n^+(D, \delta) = \sqrt{\nu_1^2(D, \delta) + D\tilde{w}} = \nu_1(D, \delta)(1 + O(w)) : \text{for } D_n^+(\zeta, \delta). \quad (55)$$

Based on these relationships it may be shown that the following approximations to equations (54) and (55) hold:

$$\pi n \cong (1 + O(\beta^{-1}))D/2 : \text{for } D_n^-(\zeta, \delta) \quad (56)$$

$$\pi(n + 1 - \frac{2}{\pi} \arctan \frac{D}{2\pi n}) \cong (1 + O(\beta^{-1}))D/2 : \text{for } D_n^+(\zeta, \delta). \quad (57)$$

Solutions to these equations can be found in the form of asymptotic formulas (23) and (24), which give our description of the  $E$ -subspectrum. (All these considerations will be made precise later on in the paper).

As far as the equations (50) are concerned, we notice that under the condition (45) we obtain for  $n \geq 1$  from (51) and (52) the approximate formula

$$\xi_n(\kappa, \lambda\tilde{w}^{-1}, \delta) \cong (\pi n)^2 + O(w) \quad (58)$$

This immediately implies that the solution  $\lambda_{\mathbf{n}}$  to the equation (50) is approximately equal to  $(\pi \mathbf{n})^2 + O(w)$ . This observation leads directly to the formula (25) for the  $H$ -subspectrum. Now we see that the  $H$ -subspectrum has structure similar to the spectrum of the operator  $\Gamma_\varepsilon$ , and hence the spectrum of the Maxwell operator  $M$  satisfies the statement of the main Theorem 3.

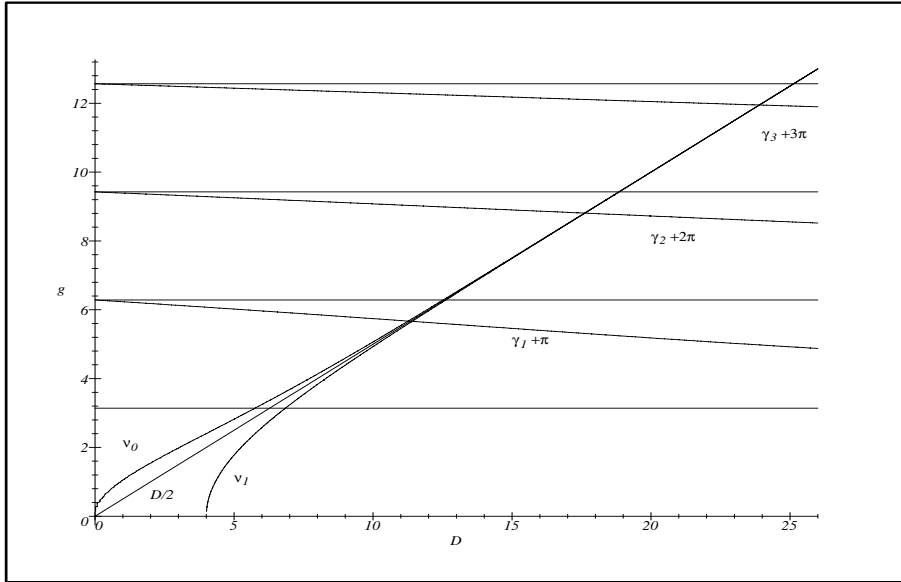


Fig. 4 The graphs of the functions  $\mu_n^\pm(D) = \lim_{\delta \rightarrow 0} \mu_n^\pm(D, \delta)$ ,  $\nu_j(D) = \lim_{\delta \rightarrow 0} \nu_j(D, \delta)$ ,  $j = 0, 1$ . The limit functions equal:  $\mu_n^+(D) = \pi n + \gamma_n(D)$ ,  $\mu_n^-(D) = \pi n$ ,  $\nu_j(D) \cong D/2$ .

The rest of the paper contains thorough spectral analysis of the Schrödinger operators  $Q(D, \delta)$ ,  $Q(D)$ , analysis of functions  $\mu_n^\pm(D, \delta)$ ,  $\nu_0(D, \delta)$ ,  $\nu_1(D, \delta)$ , justifications of all approximations, precise definitions of the Maxwell operators, and the corresponding version of the Floquet theory.

## 4 1D Schrödinger Operator with a Periodic Point Potential

We consider in this section some auxiliary 1D problems. Based on this study we will be able to obtain necessary estimates for location of the spectrum of the relevant 2D and 3D scalar models.

Let us consider the one-dimensional Schrödinger operator  $Q(D, \delta)$  with the well potential defined in (42)-(43). Let  $D \geq 0$ , and  $\delta \rightarrow 0$ . Then the potential converges (in the distributional sense) to the function  $D \sum_{n \in \mathbf{Z}} \delta(y - n)$ , where  $\delta(y)$  is the Dirac delta function. The "limit" operator (and we will not make the meaning of the word "limit" precise) should be

$$Q(D) = -\frac{d^2}{dy^2} - D \sum_{n \in \mathbf{Z}} \delta(y - n). \quad (59)$$

Note that this operator can be considered as a periodic version of Kronig-Penny model. We have to describe the domain and the action of this operator. Its natural domain consists of functions  $\psi(x) \in L_2(\mathbf{R})$  such that  $\psi$  belongs to the Sobolev space  $H^2[n, n+1]$  for any integer  $n$ , and satisfies the conditions:

$$\sum_n \|\psi''\|_{L^2[n, n+1]}^2 < \infty, \quad (60)$$

$$\psi(n+0) = \psi(n-0), \quad \psi'(n+0) - \psi'(n-0) = -D\psi(n), \quad n \in \mathbf{Z}. \quad (61)$$

The operator acts on functions from the domain as  $-d^2/dy^2$  away from the integer points. The condition (61) can be explained as follows. Let us have  $Q(D, \delta)\psi = f$  for some function  $f$  in  $L_2$ . Then, solving this ordinary differential equation on the interval  $[n, n+\delta]$  with the initial data  $\psi(n)$  and  $\psi'(n)$ , and taking the limit in  $\psi'(n+\delta)$  when  $\delta \rightarrow 0$ , one easily gets (61). It can be shown that the operator  $Q(D)$  is self-adjoint and can be also defined by the quadratic form  $Q_D[\psi] = \int |\psi'|^2 - D \sum_{n \in \mathbf{Z}} |\psi(n)|^2$  with the domain  $H^1(\mathbf{R})$ .

### 4.1 Eigenvalues and spectra

Let us consider the standard cyclic (Floquet) boundary value problems related to the operator  $Q(D)$ :

$$Q(\kappa, D)\psi(y) = \xi\psi(y), \quad 0 \leq y \leq 1, \quad (62)$$

where the operator  $Q(\kappa, D)$  is defined as

$$Q(\kappa, D) = -\psi''(y) - D\delta(y)\psi(y)$$

on functions  $\psi(x) \in L_{2,loc}(\mathbf{R})$  such that  $\psi \in H^2[n, n+1]$  for any integer  $n$ ,  $\psi$  satisfies the conditions (61), and the Floquet conditions

$$\psi(y+1) = e^{i\kappa}\psi(y). \quad (63)$$

Due to (63), the function  $\psi$  is completely defined by its restriction to the interval  $[0, 1]$ . The operator  $Q(\kappa, D)$  can now be described as follows:

$$\begin{aligned} Q(\kappa, D)\psi(y) &= -\psi''(y), \quad 0 \leq y \leq 1, \\ \psi(1) &= e^{i\kappa}\psi(0), \quad \psi'(1) = e^{i\kappa}[\psi'(0) + D\psi(0)], \quad -\pi \leq \kappa \leq \pi, \end{aligned} \quad (64)$$

where the last condition for the derivative of  $\psi$  combines (63) with (61). Considering the equation conjugate to (62), we find that the spectra of the operators  $Q(\kappa, D)$  and  $Q(-\kappa, D)$  are identical and the corresponding eigenfunctions are conjugate. Thus from now on we shall consider just the values  $0 \leq \kappa \leq \pi$ . Let  $\xi_0(\kappa, D) \leq \xi_1(\kappa, D) \leq \dots$  be the set of eigenvalues of the problem (62) counted with their multiplicity. Our equation (62) can be rewritten as a system with respect to the vector  $U_p(x) = (\psi(x), \psi'(x))$ . The corresponding monodromy matrix is:

$$W_p = \begin{bmatrix} \cos \sqrt{\xi} - D\xi^{-1/2} \sin \sqrt{\xi} & \xi^{-1/2} \sin \sqrt{\xi} \\ -D \cos \sqrt{\xi} - \sqrt{\xi} \sin \sqrt{\xi} & \cos \sqrt{\xi} \end{bmatrix}. \quad (65)$$

For a given  $k$  the sequence of eigenvalues  $\xi_l$ ,  $l \geq 0$  can be found as solutions of the discriminant equation (see [E], [RS])

$$\begin{aligned} \text{Tr} W_p &= 2 \cos \kappa, \quad \text{or} \\ \cos \sqrt{\xi} - \frac{D}{2\sqrt{\xi}} \sin \sqrt{\xi} &= \cos \kappa \end{aligned} \quad (66)$$

If  $\psi(x)$  is an eigenfunction of the problem (62), then  $W_p U_p(0) = e^{i\kappa} U_p(0)$ . It is not hard to find the corresponding eigenvector  $U_p$ :

$$\begin{aligned} U_p(-0) &= \begin{bmatrix} \psi(-0) \\ \psi'(-0) \end{bmatrix} = \begin{bmatrix} \xi^{-1/2} \sin \xi^{1/2} \\ -\cos \xi^{1/2} + e^{i\kappa} + D\xi^{-1/2} \sin \xi^{1/2} \end{bmatrix} \\ &= \begin{bmatrix} \xi^{-1/2} \sin \xi^{1/2} \\ (D/2)\xi^{-1/2} \sin \xi^{1/2} + i \sin \kappa \end{bmatrix} \end{aligned} \quad (67)$$

(where the last equality follows using (66)). It also follows from (61) and (63) that

$$\psi(+0) = \psi(-0), \quad \psi'(+0) = \psi'(-0) - D\psi(-0), \quad (68)$$

$$\psi(1) = e^{i\kappa}\psi(-0), \quad \psi'(1) = e^{i\kappa}\psi'(-0), \quad (69)$$

$$U_p(+0) = \begin{bmatrix} \psi(+0) \\ \psi'(+0) \end{bmatrix} = \begin{bmatrix} \xi^{-1/2} \sin \xi^{1/2} \\ -(D/2)\xi^{-1/2} \sin \xi^{1/2} + i \sin \kappa \end{bmatrix}. \quad (70)$$

The left side  $\Delta_D(\xi) = \cos \sqrt{\xi} - (D/2\sqrt{\xi}) \sin \sqrt{\xi}$  of the equation (66) is an entire function of the parameter  $\xi$ . In particular, it is well defined for all  $\xi \in \mathbf{R}$ . For positive and negative values of  $\xi$  the equation (66) can be rewritten respectively as

$$\cos \mu - \frac{D}{2\mu} \sin \mu = \cos \kappa, \quad \text{where } \xi = \mu^2 \quad (71)$$

$$\cosh \nu - \frac{D}{2\nu} \sinh \nu = \cos \kappa, \quad \text{where } \xi = -\nu^2. \quad (72)$$

The function  $\cos \mu - (D/2\mu) \sin \mu$ , which is an entire function with respect to  $\mu$ , will be denoted by  $A(D, \mu)$  and will be frequently used later on.

For  $D = 0$  the eigenvalues  $\xi_l$  can be easily found, namely

$$\begin{aligned}\xi_l|_{D=0} &= \mu_l^2|_{D=0}, \text{ where} \\ \mu_0|_{D=0} &= \kappa, \mu_{2m-1}|_{D=0} = -\kappa + 2\pi m, \\ \mu_{2m}|_{D=0} &= \kappa + 2\pi m, m = 1, 2, \dots\end{aligned}\tag{73}$$

We will need some properties of the function  $\Delta_D(\xi)$  for  $\xi \in \mathbf{R}$  that we will collect in the next lemma.

**Lemma 4** *The function  $\Delta_D(\xi)$  possesses the following properties:*

- (i) *It is monotonic in any interval where  $|\Delta_D(\xi)| < 1$ .*
- (ii) *It has infinitely many oscillations for positive values of  $\xi$  (according to i), all peaks must happen outside of the horizontal strip  $|\Delta| < 1$ .*
- (iii) *If we denote by  $\xi_0(k, D) \leq \xi_1(k, D) \leq \dots$  the sequence of solutions (counted with multiplicities) of the equation  $\Delta_D(\xi) = \cos k, k \in [0, \pi]$ , then  $\xi_0(0, D) < 0$ , and for  $D > 4$  also  $\xi_0(\pi, D) < 0$ . For all other values of  $l$  the solutions  $\xi_l$  are positive.*
- (iv) *For any  $D \geq 0$  we have*

$$\xi_{2m-1}(\pi, D) = [(2m-1)\pi]^2, \xi_{2m}(0, D) = [2m\pi]^2, m = 1, 2, \dots\tag{74}$$

(v) *All functions  $\xi_l(k, D)$  are monotonically increasing functions of  $k$  for even values of  $l$ , and decreasing ones for odd values of  $l$ .*

(vi) *All functions  $\xi_l(k, D)$  are decreasing functions of  $D$ .*

(vii)  *$\xi_l(k, D) \neq \xi_m(k, D)$  for  $l \neq m$ .*

**Proof.** A standard proof from the Floquet theory (see, for instance, Theorem XII.89 in [RS]) can be applied to show (i).

The statement (ii) follows from the fact that the graph of  $\Delta_D(\xi)$  hits infinitely many times both lines  $\Delta_D = \pm 1$ :

$$\Delta_D([2m\pi]^2) = 1, \Delta_D([(2m-1)\pi]^2) = -1, m = 1, 2, \dots\tag{75}$$

This equality can be checked by direct substitution into the definition of  $\Delta_D(\xi)$ .

To prove (iii) we introduce as before a new positive parameter  $\nu$  such that  $\xi = -\nu^2$  and the function

$$\Lambda_D(\nu) = \cosh \nu - \frac{D}{2\nu} \sinh \nu.$$

Considering  $k = 0$ , we get the equation  $\Lambda_D(\nu) = 1$ , which can be rewritten as

$$\begin{aligned}\nu &= \frac{D \tanh \nu}{2(1 - (\cosh \nu)^{-1})}, \text{ or} \\ \nu &= \frac{D}{2} \coth \frac{\nu}{2}, \text{ or } \nu = \frac{D(1 + e^{-\nu})}{2(1 - e^{-\nu})}\end{aligned}$$

The function in the right side of the last equality decreases from infinity to (asymptotically)  $D/2$ . This shows existence of a unique solution  $\nu_0$ , or  $\xi_0(0, D) = -(\nu_0)^2$ . Consider now the case  $k = \pi$ , i.e. the case of the equation  $\nu = \frac{D(1 - e^{-\nu})}{2(1 + e^{-\nu})}$ . Here the function on the right side starts with the zero value at  $\nu = 0$ , and increases (being convex) to  $D/2$ . Then the existence of a negative solution is governed by  $D$ : for large values of  $D$  (namely, for  $D > 4$ ) the tangent line at the origin to the graph will make the angle more than  $\pi/4$  with the  $\nu$  axis, so there will be a unique intersection of two graphs. When  $D < 4$ , there is no intersection beyond the origin. This proves (iii).

Let us turn to the proof of (iv) now. First of all, the equalities (75) show that the numbers  $[2m\pi]^2$  are among the members of the sequence  $\xi_l(0, D)$ , and the numbers  $[(2m-1)\pi]^2$  are among the members of the sequence  $\xi_l(\pi, D)$ . The only problem is to check the correspondence between the values of  $m$  and  $l$ , which amounts to checking the locations of other solutions of the equations  $\Delta_D(\xi) = \pm 1$ . We already know the situation for negative values of  $\xi$ , so we assume now that  $\xi \geq 0$ . Consider first the case of  $k = 0$  (or of the equation  $\Delta_D(\xi) = 1$ ). We introduce here an important auxiliary function of the argument  $\mu = \sqrt{\xi}$ , which we will use rather often:

$$\varphi_D(\mu) = \arctan[D/(2\mu)], \quad \mu \geq 0; \quad 0 \leq \varphi_D(\mu) \leq \pi/2. \quad (76)$$

In terms of this function we can express  $\Delta_D(\xi)$  as follows:

$$\Delta_D(\xi) = \frac{\cos(\mu + \varphi_D(\mu))}{\cos(\varphi_D(\mu))}. \quad (77)$$

Then the equation  $\Delta_D(\xi) = 1$  reduces to

$$\begin{aligned} \cos(\mu + \varphi_D(\mu)) &= \cos(\varphi_D(\mu)), \quad \text{or} \\ \mu + \varphi_D(\mu) &= \pm \varphi_D(\mu) + 2\pi m. \end{aligned}$$

Choosing different signs in the right side, we get two equations:  $\mu = 2\pi m$ , which provides exactly the points  $\xi = [2m\pi]^2$  that we already know, and

$$\mu + 2\varphi_D(\mu) = 2\pi m, \quad \text{or} \quad 2\pi m - \mu = 2\varphi_D(\mu). \quad (78)$$

The graphs of the functions  $\Delta_D = 2\pi m - \mu$  provide a set of parallel lines in the  $(\Delta_D, \mu)$ -plane. Consider the graph of the function  $2\varphi_D(\mu)$ . First of all,  $2\varphi_D(\mu) > 0$ , and  $2\varphi_D(0) = \pi$ . Therefore, it can intersect only the lines for  $m = 1, 2, \dots$ . The lowest of these lines starts for  $\mu = 0$  at the height  $2\pi$ . Now, differentiation shows that the function  $2\varphi_D(\mu)$  is decreasing, and convex downward. Then the first intersection can happen not earlier than at  $\mu = \pi$ . Direct calculation shows that the absolute value of the derivative of  $2\varphi_D(\mu)$  for  $\mu > \pi$  is less than one. This means that the equation (78) has exactly one solution in each interval  $(2\pi m, 2\pi(m+1))$ . Hence, the numbers  $(2\pi m)^2$  for  $m = 1, 2, \dots$  provide all roots  $\xi_{2m}(0, D)$ . A similar consideration works for the case  $k = \pi$ , or for the equation  $\Delta_D(\xi) = -1$ .

The statement (v) is an obvious consequence of (i)-(iii).

The statement (vi) follows from the following inequality between the corresponding quadratic forms:  $Q_{D_1} \leq Q_{D_2}$  for  $D_1 > D_2$ . Validity of (vii) follows from the fact that  $\partial_\mu A(D, \mu)$  (where, as before  $A(D, \mu) = \Delta_D(\mu^2)$ ) is not equal to zero at the points  $\pi m$  ( $m = 1, 2, \dots$ ), and from (iv). This finishes the proof.  $\square$

We conclude that for any positive  $D$

$$\begin{aligned} \xi_{2m-2}(0, D) &\leq \xi_{2m-2}(\kappa, D) \leq \xi_{2m-2}(\pi, D) < \\ \xi_{2m-1}(\pi, D) &\leq \xi_{2m-1}(\kappa, D) \leq \xi_{2m-1}(0, D) < \\ \xi_{2m}(0, D) &\leq \xi_{2m}(\kappa, D) \leq \xi_{2m}(\pi, D), \quad m = 1, 2, \dots \end{aligned} \quad (79)$$

We also notice from the equation (66) that according to the standard scheme of Floquet theory (which can be easily implemented in our situation), the spectrum  $\sigma(Q(D))$  coincides with the set of the eigenvalues  $\xi_n(\kappa, D)$  for all  $n \geq 0, 0 \leq \kappa \leq \pi$ . Therefore, this spectrum can be described as follows:



**Lemma 5** For any  $D > 0$  the spectrum  $\sigma(Q(D))$  consists of nonoverlapping intervals  $I_n(Q(D))$  such that

$$\sigma(Q(D)) = \bigcup_{n \geq 0} I_n(Q(D)), \quad I_0(Q(D)) = [-(\nu_0(D))^2, \xi_0(D)], \quad (80)$$

$$I_n(Q(D)) = [(\pi n)^2, \{\pi(n + \gamma_n(D))\}^2], \quad n = 1, 2, \dots, \quad (81)$$

where

$$\nu_0(D) = \sqrt{-\xi_0(0, D)}, \quad \xi_0(D) = \xi_0(\pi, D), \quad (82)$$

$$\pi(n + \gamma_n(D)) = \begin{cases} \sqrt{\xi_n(0, D)} & \text{if } n \text{ is odd} \\ \sqrt{\xi_n(\pi, D)} & \text{if } n \text{ is even} \end{cases}, \quad n = 1, 2, \dots, \quad (83)$$

$$\xi_0(0, D) < 0, \quad \xi_0(\pi, D) < \pi^2, \quad 0 < \gamma_n(D) < 1. \quad (84)$$

In particular,

$$\pi n \leq \mu_n(\kappa, D) = \sqrt{\xi_n(\kappa, D)} \leq \pi(n + \gamma_n(D)), \quad n = 1, 2, \dots \quad (85)$$

**Proof.** The statements of the lemma follow readily from the Lemma 4.  $\square$

We shall study dependence of the spectrum  $\sigma(Q(D))$  on  $D$ . To do this we rewrite the basic equations (71) and (72) for the spectra for  $\kappa = 0$ , and for  $\kappa = \pi$  as

$$\cos(\mu + \varphi_D(\mu)) = \mp \cos \varphi_D(\mu), \quad (86)$$

$$\nu = \frac{D \tanh \nu}{2(1 \mp (\cosh \nu)^{-1})}, \quad \nu \geq 0, \quad (87)$$

respectively. Here '-' and '+' correspond to  $\kappa = 0$  and to  $\kappa = \pi$ . We also remind that the equations (86) and (87) define the endpoints of bands of the spectrum.

## 4.2 Negative eigenvalues

Let us consider the lowest band  $I_0(Q(D)) = [-(\nu_0(D))^2, \xi_0(\pi, D)]$  of  $\sigma(Q(D))$ .

**Lemma 6** The functions  $\nu_0(D)$  and  $\xi_0(\pi, D)$  possess the following properties for  $D \geq 0$ :

(i)  $\nu_0(D)$  is the unique solution of the equation

$$\nu = \frac{D(1 + e^{-\nu})}{2(1 - e^{-\nu})}, \quad \nu \geq 0 \quad (88)$$

and is a strictly increasing function of  $D$ ;

(ii)  $\xi_0(\pi, D)$  is a continuous strictly decreasing function of  $D$  such that

$$\begin{aligned} \xi_0(\pi, 4) = 0; \quad 0 \leq \xi_0(\pi, D) \leq \pi^2 \text{ for } 0 \leq D \leq 4, \\ \xi_0(\pi, D) < 0 \text{ for } D > 4. \end{aligned} \quad (89)$$

Besides, for  $D > 4$  we have  $\xi_0(\pi, D) = -(\nu_1(D))^2$ , where  $\nu_1(D) (< \nu_0(D))$  is the unique positive solution of the equation

$$\nu = \frac{D(1 - e^{-\nu})}{2(1 + e^{-\nu})}, \quad \nu > 0, \quad D > 4. \quad (90)$$

$\nu_1(D)$  is a strictly increasing function of  $D$ ;

(iii) the functions  $\nu_j(D), j = 0, 1$  satisfy the inequalities

$$\frac{D}{2} < \nu_0(D) < \frac{D}{2} \coth \frac{D}{4} = \frac{D(1+e^{-D/2})}{2(1-e^{-D/2})}, \quad D > 0, \quad (91)$$

$$\frac{D}{2} \left\{ 1 - \frac{2e^{-D/2}}{1+e^{-D/2}} \right\} = \frac{D}{2} \tanh \frac{D}{4} < \nu_1(D) < \frac{D}{2} \text{ for } D > 4. \quad (92)$$

**Proof.** (i): The equation (88) has been discussed already in the proof of the Lemma 4. Monotonicity of  $\nu_0$  follows from the decreasing character of the function  $(e^\nu + 1)/(e^\nu - 1)$ .

(ii): It was mentioned in the proof of the Lemma 4 that  $\xi_0(\pi, 4) = 0, \xi_0(\pi, D) \geq 0$  for  $D \in [0, 4]$ , and  $\xi_0(\pi, D) < 0$  for  $D > 4$ . Besides,  $\xi_0(\pi, D) < \xi_1(\pi, D) = \pi^2$ . The equation (90) has also been established earlier. Increasing behavior of  $\nu_1(D)$  follows from (90) and from convexity and monotonicity of  $(e^\nu - 1)/(e^\nu + 1)$ .

(iii): Since  $\frac{D(1+e^{-\nu})}{2(1-e^{-\nu})} > \frac{D}{2}$ , the equation (88) implies that  $\nu_0(D) > D/2$ . This inequality and monotonicity of  $(1+e^{-\nu})/(1-e^{-\nu})$  together with (88) imply that  $\nu_0(D) < \frac{D(1+e^{-D/2})}{2(1-e^{-D/2})}$ . In the similar manner, since  $\frac{D(1-e^{-\nu})}{2(1+e^{-\nu})} < \frac{D}{2}$ , we get  $\nu_1(D) < D/2$ , and then from (90)  $\nu_1(D) > \frac{D}{2} \tanh \frac{D}{4}$ . This finishes the proof.  $\square$

**Lemma 7** *The following relationships hold:*

$$\partial_D \nu_j(D) \geq 0.3, \quad j = 0, 1, \quad \text{for } D \geq 4 \quad (93)$$

$$\partial_D \xi_0(\pi, D)|_{D=4} = -3. \quad (94)$$

**Proof.** Differentiating the equations (88) and (90) with respect to  $D$ , and using then the inequalities (91) and (92), we easily obtain

$$\begin{aligned} \partial_D \nu_0(D) &= \frac{1}{2} \frac{\coth(\nu_0(D)/2)}{1 + (D/4) \sinh^{-2}(\nu_0(D)/2)} \geq \frac{1}{2} \frac{\coth[(D/4) \coth(D/4)]}{1 + (D/4) \sinh^{-2}(D/4)}, \\ \partial_D \nu_1(D) &= \frac{1}{2} \frac{\tanh(\nu_1(D)/2)}{1 - (D/4) \cosh^{-2}(\nu_1(D)/2)} \geq \frac{1}{2} \frac{\tanh[(D/4) \tanh(D/4)]}{1 - (D/4) \cosh^{-2}(D/4)}. \end{aligned}$$

The function in the right side of the first inequality is increasing for  $D \geq 4$ , and its value at  $D = 4$  is not less than 0.3. The function in the right side of the second inequality decreases to 1/2. This gives (93). To prove (94) we differentiate (66) with respect to  $D$ , and then evaluate the result at  $D = 4$ , taking into account that  $\xi = 0$ .  $\square$

### 4.3 Positive eigenvalues

Let us turn now to the bands  $I_n(Q(D)), n \geq 1$  lying according to the Lemma 5 above  $\pi^2$ . As it follows from that lemma, analysis of these bands amounts to analysis of the functions  $\gamma_n(D)$ . Proof of the Lemma 4 shows that  $\mu = \pi(n + \gamma_n(D))$  satisfies the equation

$$\cos(\mu + \varphi_D(\mu)) = (-1)^n \cos \varphi_D(\mu). \quad (95)$$

**Lemma 8** *The functions  $\gamma_n(D), n \geq 1$  have the following properties:*

(i)  $\gamma_n(D)$  are strictly decreasing functions of  $D > 0$  taking values in the interval  $(0, 1)$ . For each  $n \geq 1$ ,  $\gamma_n(D)$  is the unique solution of the equation

$$\pi\gamma + 2\varphi_D(\pi(n + \gamma)) = \pi. \quad (96)$$

In addition to that,

$$0 < \gamma_n(D) < \gamma_{n+1}(D) < 1, \quad (97)$$

$$\gamma_n(D) = 1 - \frac{2}{\pi} \arctan \frac{D}{2\pi[n + \gamma_n(D)]} \quad (98)$$

In particular,

$$1 - \frac{2}{\pi} \arctan \frac{D}{2\pi n} < \gamma_n(D) < 1 - \frac{2}{\pi} \arctan \frac{D}{2\pi(n+1)} \quad (99)$$

(ii) For any positive constant  $C$

$$\lim_{n \rightarrow \infty} \gamma_n(Cn) = 1 - \frac{2}{\pi} \arctan \frac{C}{2\pi}. \quad (100)$$

$$\gamma_n(D) = \frac{4n}{D} [1 + O(D^{-1})], \quad D \rightarrow \infty \quad (101)$$

**Proof.** The equation (96) follows from (95) and from our analysis of  $\xi_i$  in the Lemma 4. Then we notice that the function  $\varphi_D(\mu)$  is strictly decreasing with respect to  $\mu > 0$ , and increasing with respect to  $D > 0$ . In addition to that,

$$\max_{D>0} \left| \frac{\partial \varphi_D(\mu)}{\partial \mu} \right| \leq \frac{1}{2\mu}. \quad (102)$$

This implies:

$$\frac{\partial}{\partial \gamma} [\pi\gamma + 2\varphi_D(\pi(n + \gamma))] \geq \pi - \frac{1}{n} > 0, \quad n \geq 1,$$

which means that the left side of the equation (96) is a strictly increasing function of the argument  $\gamma$  for any  $n \geq 1$ . We also notice that this left side takes at  $\gamma = 0$  the value  $2\varphi_D(\pi n) < \pi$ , and at  $\gamma = 1$  takes the value  $\pi + 2\varphi_D(\pi(n+1)) > \pi$ . This implies that the equation (96) has unique solution  $\gamma_n(D)$ . The inequalities (97) follow readily from the monotonicity properties of the function  $\varphi$ . The identity (98) is a straight consequence of (96) and (76). The inequalities (99) easily follow from (98) and (97). The relation (100), in turn, follows straightforwardly from (99). Consider now (101). We will show it only for odd values of  $n$ . The considerations for the even ones are similar. Consider the equation (78) that determines  $\xi_{2m-1}$ . From this equation, using Taylor expansion of  $\arctan(1/x)$  at  $\infty$ , we get

$$\mu = \pi(2m-1) + \frac{4\pi(2m-1)}{D} + O(D^{-2}),$$

which finishes the proof.  $\square$

**Lemma 9** Let  $p$  and  $a$  be real numbers such that  $|p| < 1$  and  $|a| \leq 4\pi$ . Then the following inequality holds for  $n \geq 1$ :

$$|\gamma_n((1+p)2\pi n + a) - 1/2| \leq |p| + 3/n. \quad (103)$$

**Proof.** Using the relations (98), (97) and the elementary inequality  $|\arctan(t_1) - \arctan(t_2)| \leq |t_1 - t_2|$ , we easily obtain:

$$\begin{aligned} |\gamma_n((1+p)2\pi n + a) - 1/2| &= \frac{2}{\pi} \left| \arctan \frac{(1+p)2\pi n + a}{2\pi[n + \gamma_n(D)]} - \arctan 1 \right| \leq \\ &|p| + (|a| + 2\pi)/(2\pi n), \end{aligned}$$

which together with  $|a| \leq 4\pi$  leads to (103).  $\square$

It will be convenient to introduce the quantities

$$\begin{aligned}\mu_n^-(D) &= \min_{\kappa=0,\pi} \mu_n(\kappa, D) = \pi n \\ \mu_n^+(D) &= \max_{\kappa=0,\pi} \mu_n(\kappa, D) = \pi(n + \gamma_n(D)), \quad n \geq 1.\end{aligned}\tag{104}$$

Note that (101) implies that for any  $n \geq 1$

$$\mu_n^+(D) = \pi n + \frac{4n}{D} [1 + O(D^{-1})], \quad D \rightarrow \infty.\tag{105}$$

#### 4.4 Perturbations of the spectrum of the Schrödinger operator with point potential

We plan to investigate later on the location of the spectrum of the Schrödinger operator  $Q(\kappa, D, \delta)$  as a perturbation of the operator  $Q(\kappa, D)$ . To do this we need to establish some properties of the equation (71) for  $\kappa = 0, \pi$ , and to study behavior of corresponding solutions under some "small" perturbations of the equation.

Let, as before  $A(D, \mu) = \cos \mu - \frac{D}{2\mu} \sin \mu$ ,  $D \geq 0$ .

**Lemma 10** *Suppose that  $\kappa = 0$ , or  $k = \pi$ . Let us rewrite the equation (71) in the form*

$$A(D, \mu) = \cos \kappa (= \pm 1).\tag{106}$$

Let  $\mu_1(\kappa, D) \leq \mu_2(\kappa, D) \dots$  be its solutions in the interval  $[\pi, \infty)$ , and  $\partial_\mu A(D, \mu)$  is the derivative of the function  $A$  with respect to  $\mu$ . Then  $\partial_\mu A(D, \mu_l) \neq 0$  for  $l = 1, 2, \dots$ . Besides, for  $\mu = \pi n$ , and  $\mu = \pi(n + \gamma_n(D))$ ,  $n \geq 1$  we have:

$$\partial_\mu A(D, \mu) = \frac{D}{2\mu} \left[ (-1)^{n+1} - \frac{\sin \mu}{\mu} \right].\tag{107}$$

In particular,

$$|\partial_\mu A(D, \mu_l(\kappa, D))| \geq \frac{D [1 - \mu_l^{-1}(\kappa, D)]}{2\mu_l(\kappa, D)}.\tag{108}$$

**Proof.** Validity of (107) for  $\mu = \pi n$  is subject of simple direct calculation, so let us prove it for  $\mu = \pi(n + \gamma_n(D))$ . It was established in the proof of the Lemma 4 that

$$A(D, \mu) = \frac{\cos(\mu + \varphi_D(\mu))}{\cos \varphi_D(\mu)}, \quad \mu \in \mathbf{R}.\tag{109}$$

Differentiating, we get:

$$\partial_\mu A(D, \mu) = -\frac{\sin(\mu + \varphi_D(\mu))}{\cos \varphi_D(\mu)} (1 + \partial_\mu \varphi_D(\mu)) + \frac{\sin(\varphi_D(\mu)) \cos(\mu + \varphi_D(\mu))}{\cos^2 \varphi_D(\mu)} \partial_\mu \varphi_D(\mu).$$

Combining terms with  $\partial_\mu \varphi_D(\mu)$ , and performing some simple trigonometric conversion, we get

$$\partial_\mu A(D, \mu) = -\frac{\sin(\mu + \varphi_D(\mu))}{\cos \varphi_D(\mu)} - \frac{\sin \mu}{\cos^2 \varphi_D(\mu)} \partial_\mu \varphi_D(\mu).$$

In the first term we multiply and divide by  $\sin(\varphi_D(\mu))$ , and then use in both terms the equality  $\tan(\varphi_D(\mu)) = D/2\mu$ . This leads to

$$\partial_\mu A(D, \mu) = \frac{D}{2\mu} \left[ -\frac{\sin(\mu + \varphi_D(\mu))}{\sin \varphi_D(\mu)} - \frac{\sin \mu}{\mu} \right]. \quad (110)$$

Since  $k = 0$  or  $k = \pi$ , the equation (106) leads to  $|\cos(\mu + \varphi_D(\mu))| = |\cos \varphi_D(\mu)|$ , which in turn implies  $|\sin(\mu + \varphi_D(\mu))| = |\sin \varphi_D(\mu)|$ . In fact, more precisely

$$\frac{\sin(\mu + \varphi_D(\mu))}{\sin \varphi_D(\mu)} = (-1)^n, \text{ if } \mu = \pi(n + \gamma_n(D)).$$

This gives (107), which implies the inequality (108).  $\square$

We are interested now, what happens if we are "almost" at a solution of the equation (106), i.e. if  $|A(D, \mu)|$  is close to 1.

**Lemma 11** *Let us assume that for some  $\mu \geq 2$*

$$\left| |A(D, \mu)| - 1 \right| \leq a < 1, \quad (111)$$

$$\tan \varphi_D(\mu) = D/(2\mu) \geq \alpha. \quad (112)$$

Then

$$|\partial_\mu A(D, \mu)| \geq \left[ (1-a)(1-a(2+a)(1+\alpha^{-2})) - \frac{1}{2} \right] (D/2\mu). \quad (113)$$

If  $\alpha$  and  $a$  satisfy the condition

$$6\sqrt{a} \leq \alpha < 1, \quad (114)$$

In particular, if

$$\mu \geq 2, \quad D \geq 12\sqrt{a}\mu, \quad (115)$$

then

$$|\partial_\mu A(D, \mu)| > D/(7\mu). \quad (116)$$

**Proof.** We notice first that based on the representation (109) we can rewrite (111) as

$$\left| \left| \frac{\cos(\mu + \varphi_D(\mu))}{\cos \varphi_D(\mu)} \right| - 1 \right| \leq a. \quad (117)$$

Then formula (110) together with the condition  $\mu \geq 2$  gives

$$|\partial_\mu A| = \frac{D}{2\mu} \left| \frac{\sin(\mu + \varphi_D(\mu))}{\sin \varphi_D(\mu)} + \frac{\sin \mu}{\mu} \right| \geq \frac{D}{2\mu} \left( \left| \frac{\sin(\mu + \varphi_D(\mu))}{\sin \varphi_D(\mu)} \right| - \frac{1}{2} \right).$$

Representing

$$\left| \frac{\sin(\mu + \varphi_D(\mu))}{\sin \varphi_D(\mu)} \right| = \left| \frac{\cos(\mu + \varphi_D(\mu))}{\cos \varphi_D(\mu)} \right| \cdot \left| \frac{\tan(\mu + \varphi_D(\mu))}{\tan \varphi_D(\mu)} \right|,$$

and using (117), we get:

$$|\partial_\mu A| \geq \frac{D}{2\mu} \left( (1-a) \left| \frac{\tan(\mu + \varphi_D(\mu))}{\tan \varphi_D(\mu)} \right| - \frac{1}{2} \right).$$

Now,

$$\begin{aligned}
(1-a) \left| \frac{\tan(\mu + \varphi_D(\mu))}{\tan \varphi_D(\mu)} \right| &= (1-a) \sqrt{\left( \frac{\tan^2(\mu + \varphi_D(\mu))}{\tan^2 \varphi_D(\mu)} - 1 \right)} + 1 \geq \\
&\geq (1-a) \left( 1 - \left| \frac{\tan^2(\mu + \varphi_D(\mu))}{\tan^2 \varphi_D(\mu)} - 1 \right| \right) \\
&= (1-a) \left( 1 - \left| \frac{\cos^2(\mu + \varphi_D(\mu))}{\cos^2 \varphi_D(\mu)} - 1 \right| \frac{1}{\sin^2 \varphi_D(\mu)} \right) \\
&\geq (1-a) (1 - a(2+a)(1 + \alpha^{-2}))
\end{aligned}$$

We used here the elementary inequality  $|\sqrt{1+u} - 1| \leq |u|$ , for  $|u| \leq 1$ , and the estimate

$$\sin^{-2} \varphi_D(\mu) = 1 + \cot^2 \varphi_D(\mu) = 1 + (D/2\mu)^{-2} \leq 1 + \alpha^{-2}.$$

This gives (113). The inequality (116) follows straightforwardly from (113) and (114).  $\square$

Given a positive  $a$  we introduce the set

$$\mathcal{A} = \{\mu \geq 2 : ||A(D, \mu)| - 1| \leq a\}, \quad (118)$$

and represent it as  $\mathcal{A} = \bigcup_{i \geq 1} J_i$ , where  $J_i$  are some disjoint intervals.

**Lemma 12** *Suppose that numbers  $a, N$ , and  $D$  satisfy the following condition:*

$$\min(D/(7N), 1) > 6\sqrt{a}. \quad (119)$$

*Then there exist only a finite number  $L$  of intervals  $J_i = [\eta_i^-, \eta_i^+]$  such that  $J_i \cap [0, N] \neq \emptyset$ , and each of them contains exactly one solution  $\eta_i$  of exactly one of the equations (106). In addition to that,*

$$|\eta_i - \eta_i^\pm| \leq a / \min(D/(7N), 1) \leq (1/6)\sqrt{a}. \quad (120)$$

**Proof.** We notice first of all that finiteness of the set of the intervals  $J_i$  such that  $J_i \cap [0, N] \neq \emptyset$  follows from analyticity of the function  $A(D, \mu)$ . Due to (119), there exists a number  $\alpha \in (0, 1)$  such that  $D/(7N) > \alpha$ , and  $6\sqrt{a} < \alpha < 1$  (and so (114) is satisfied). It is easy to see that in view of Lemma 11 and the conditions (119) the derivative  $\partial_\mu A(D, \mu)$ , being a continuous function, satisfies exactly one of the next inequalities

$$\partial_\mu A(D, \mu) \geq D/7\eta_i^+ \geq \alpha, \text{ or } \partial_\mu A(D, \mu) \leq -D/7\eta_i^- \leq -\alpha, \mu \in J_i. \quad (121)$$

This implies monotonicity of the function  $A(D, \mu)$  on each of the intervals  $J_i$ . Therefore, each interval  $J_i = [\eta_i^-, \eta_i^+]$  contains exactly one solution  $\eta_i$  to exactly one of the equations (106). Besides,

$$A(D, \eta_i^\pm) = \omega_{1,i} \pm \omega_{2,i}a, \quad |\omega_{j,i}| = 1, \quad j = 1, 2. \quad (122)$$

The relations (121) and (122) imply now that the solution  $\eta_i$  satisfies the inequalities (120).  $\square$

We consider now a perturbation

$$\tilde{A}(D, \mu) = A(Ds_\mu, \mu) + v_\mu$$

of the function  $A(D, \mu)$ , where  $s_\mu$  and  $v_\mu$  are functions of  $\mu$  that will be assumed to be close in a smooth sense to 1 and 0 correspondingly (see details in the next lemma). We need to investigate solutions (for  $k = 0$  or  $\pi$ ) of the equation

$$\tilde{A}(D, \mu) = \cos k (= \pm 1). \quad (123)$$

**Lemma 13** Suppose that the functions  $s_\mu$  and  $v_\mu$  are continuously differentiable with respect to  $\mu$ , and satisfy (together with parameters  $D$  and  $N$ ) the conditions:

$$|s_\mu - 1| \leq v, |v_\mu| \leq v, \text{ for } 2 \leq \mu \leq N + 1, \quad (124)$$

$$18\sqrt{v} < \min\{D/(7(N + 1)), 1\}, \quad (125)$$

$$|\partial_\mu s_\mu| \leq 1/8, |\partial_\mu v_\mu| \leq D/(16\mu) \text{ for } 2 \leq \mu \leq N + 1. \quad (126)$$

Then there exists a finite system of disjoint intervals  $J_j$  that satisfies the following conditions:

- (i) The length of each of these intervals is less than  $8v/\min\{D/(7N), 1\}$
- (ii) Every solution  $\mu \in [3, N]$  of the equation

$$A(D, \mu) = \cos k (= \pm 1) \quad (127)$$

belongs to only one of the intervals.

- (iii) Each of these intervals contains exactly one solution  $\tilde{\eta}$  of the equation (123).
- (iv) Every solution  $\tilde{v} \in [2, N]$  of the equation (123) belongs to some of these intervals.

**Proof.** The estimates can be derived based on Lemmas 11 and 12.  $\square$

The last lemma implies the following statement that we shall use later on.

**Theorem 14** Let  $2 \leq \mu_1(D) \leq \dots \leq \mu_L(D) \leq N$  be all the solutions of the equations (106) in the interval  $[2, N]$ . Suppose also that  $\eta_1(D) \leq \dots \leq \eta_L(D)$  are the first  $L$  solutions in the interval  $[2, \infty]$  of the equations:

$$A(Ds_\mu, \mu) + v_\mu = \pm 1.$$

If the numbers  $D$  and  $N$ , and the functions  $s_\mu$  and  $v_\mu$  satisfy the conditions (124), (124), and (126), then

$$|\eta_l(D) - \mu_l(D)| \leq 8v/\min\{D/(7(N + 1)), 1\}, \quad 1 \leq l \leq L$$

## 4.5 Auxiliary spectra.

In this section we introduce and investigate properties of some auxiliary sets in terms of which the spectrum of the Maxwell operator can be described. We use here some previously defined functions. Let us introduce for any non-negative integer  $n$  the set:

$$\mathcal{B}_n(D) = \{\xi_0(k_1, D) + \xi_n(k_2, D) \mid k_1, k_2 \in [0, \pi]\}. \quad (128)$$

Due to continuity of the functions  $\xi_n(k, D)$ , these sets are in fact closed intervals of the real line. Consider also the sets

$$B_n = \{D \geq 0 : \mathcal{B}_n(D) \ni 0\}, \quad n \geq 0. \quad (129)$$

**Lemma 15** For any integer  $n \geq 0$  the following statements hold:

- (i) The interval  $\mathcal{B}_n(D)$  can be represented as

$$\mathcal{B}_0(D) = [-2(\nu_0(D))^2, 2\xi_0(\pi, D)], \quad (130)$$

$$\mathcal{B}_n(D) = [-(\nu_0(D))^2 + (\pi n)^2, \xi_0(\pi, D) + [\pi(n + \gamma_n(D))]^2], \quad n > 0, \quad (131)$$

and its endpoints are continuous strictly decreasing functions of the argument  $D$ ;

- (ii) The set  $B_n$  coincides with the set of values of  $D$  such that for some  $k_1, k_2 \in [0, \pi]$  the following equality holds

$$\xi_0(k_1, D) + \xi_n(k_2, D) = 0 \quad (132)$$

- (iii) The set  $B_n$  is an interval, i.e.  $B_n = [D_n^-, D_n^+]$ ,  $D_n^- \leq D_n^+$ ;  
(iv) The endpoints of the interval  $B_0$  are

$$D_0^- = 0, \quad D_0^+ = 4, \quad (133)$$

and  $D_0^+$  is the unique solution of the equation  $\xi_0(\pi, D) = 0$ ;

- (v) For  $n \geq 1$   $D_n^-$  and  $D_n^+$  are the unique solutions of the equations

$$\nu_0(D) = \pi n, \quad \text{and} \quad \nu_1(D) = \pi(n + \gamma_n(D)) \quad (134)$$

- (vi) the next inequalities are true

$$D_n^- < D_{n+1}^-; \quad D_n^+ < D_{n+1}^+, \quad n \geq 0. \quad (135)$$

**Proof.**

(i) The left and right endpoints of the interval  $\mathcal{B}_n(D)$  coincide correspondingly with the sum of the left and right endpoints of the intervals  $I_0(Q(D))$  and  $I_n(Q(D))$ . This along with the Lemmas 5, and 6 imply the statement (i).

The statement (ii) is just a rephrasing of the definition of the sets.

Since the endpoints of the interval  $\mathcal{B}_n(D)$  are continuous strictly decreasing functions of  $D$ , we get (iii). The rest of the statements follows from the properties of the functions  $\nu_0(D)$ ,  $\nu_1(D)$ ,  $\xi_0(\pi, D)$ , and  $\gamma_n(D)$  described in the Lemmas 5, 6, 8.  $\square$

The intervals  $B_n$  do not depend on any parameters and can be found once and forever. They are closely related to the spectra of interest. The next lemma provides a rather accurate description of the location of the intervals  $B_n$ .

**Lemma 16** *The endpoints  $D_n^-$  and  $D_n^+$  satisfy the estimates:*

$$D_0^- = 0, \quad D_0^+ = 4, \quad (136)$$

$$2\pi n - 4t \frac{e^{-t}}{1 - e^{-\tau}} \Big|_{t=\pi n-1} < D_n^- < 2\pi n, \quad n \geq 1 \quad (137)$$

$$D_n^+ > 2\pi \left[ n + 1 - \frac{2}{\pi} \arctan \frac{n+1 - \pi^{-1}}{n} \right], \quad (138)$$

$$D_n^+ < 2\pi \left[ n + 1 - \frac{2}{\pi} \arctan \frac{n}{n+1} \right] + 2\tau \frac{e^{-\tau}}{1 + e^{-\tau}} \Big|_{\tau=\pi n}, \quad n \geq 1 \quad (139)$$

In particular, when  $n \rightarrow \infty$  we get the asymptotic formulas

$$D_n^- = 2\pi n + O(ne^{-\pi n}); \quad D_n^+ = 2\pi \left( n + \frac{1}{2} \right) + O(n^{-1}). \quad (140)$$

The intervals  $B_n = [D_n^-, D_n^+]$ ,  $n \geq 0$  are disjoint, i.e.  $B_n \cap B_m = \emptyset$  for  $n \neq m$ .

**Proof.** The statements of the lemma can be derived from Lemmas 6, 8 and 15.  $\square$

The numbers  $D_n^\pm$  are the absolute constants that are involved into the description of the set  $\sigma_E$  (see (26)). This set plays an important role in our description of the structure of any finite number of bands and gaps in the spectra of the Maxwell operators  $M$ ,  $M_E$  and  $M_H$ , as well as of the operator  $\Theta_\varepsilon$ .

We also notice that the Lemma 16 justifies the approximation of the set  $\sigma_E$  indicated in (26).



## 4.6 Eigenfunctions

We shall denote the eigenfunction of the operator  $Q(\kappa, D)$  associated with the eigenvalue  $\xi_l(\kappa, D)$  by  $f_l(\kappa, D; y)$ .

Let us consider the Cauchy problem for the operator  $Q(\kappa, D)$  :

$$-P''(y) - D\delta(y)P(y) = \xi P(y), \quad \psi(-0) = \psi_0, \psi'(-0) = \psi_1; y \geq 0. \quad (141)$$

Taking into account (68), we can represent the solution to this problem in the form

$$P(y) = \psi_0 \cos \xi^{1/2} y + (\psi_1 - D\psi_0) \xi^{-1/2} \sin \xi^{1/2} y. \quad (142)$$

The choice of the parameters  $\psi_0$  and  $\psi_1$  in (141) will be convenient when we treat later the operators  $Q(\kappa, D)$  as limits of the operators  $Q(\kappa, D, \delta)$  with well potentials. Assume now that  $\psi$  is an eigenfunction of the operator  $Q(k, D)$  defined by (62)-(63). Then we have the representation (67) for the vector  $(\psi_0, \psi_1)$ :

$$\psi_0 = \xi^{-1/2} \sin \xi^{1/2}, \quad \psi_1 = -\cos \xi^{1/2} + e^{ik} + D\xi^{-1/2} \sin \xi^{1/2}.$$

The equality (142) gives:

$$\begin{aligned} \psi(\kappa, \mu, y) &= \xi^{-1/2} \sin \xi^{1/2} \cos \xi^{1/2} y + (-\cos \xi^{1/2} + e^{ik}) \xi^{-1/2} \sin \xi^{1/2} y \\ &= \mu^{-1} [e^{ik} \sin \mu y + \sin \mu(1-y)], \quad \text{where } \mu = \xi^{1/2}. \end{aligned} \quad (143)$$

For  $k = 0$  or  $k = \pi$  we get correspondingly:

$$\psi(0, \mu, y) = \mu^{-1} [\sin \mu y + \sin \mu(1-y)] = 2\mu^{-1} \sin(\mu/2) \cos(\mu(y-1/2)), \quad (144)$$

$$\begin{aligned} \psi(\pi, \mu, y) &= \mu^{-1} [-\sin \mu y + \sin \mu(1-y)] \\ &= -2\mu^{-1} \cos(\mu/2) \sin(\mu(y-1/2)). \end{aligned} \quad (145)$$

Now we calculate the normalization factor for  $\psi(x)$  :

$$\begin{aligned} I(\kappa, \mu) &= \int_0^1 |e^{ik} \sin \mu y + \sin \mu(1-y)|^2 dy = \\ &= 1 + \cos \kappa [\mu^{-1} \sin \mu - \cos \mu] - \mu^{-1} \sin \mu \cos \mu \end{aligned} \quad (146)$$

for  $\xi \geq 0$ . For instance, for  $k = 0$  and  $k = \pi$  we get:

$$\begin{aligned} I(0, \mu) &= 1 + \mu^{-1} \sin \mu - \cos \mu - \mu^{-1} \sin \mu \cos \mu \\ &= (1 - \cos \mu)(1 + \mu^{-1} \sin \mu) = 2 \sin^2(\mu/2)(1 + \mu^{-1} \sin \mu), \end{aligned} \quad (147)$$

$$\begin{aligned} I(\pi, \mu) &= 1 - (\mu^{-1} \sin \mu - \cos \mu) - \mu^{-1} \sin \mu \cos \mu \\ &= (1 + \cos \mu)(1 - \mu^{-1} \sin \mu) = 2 \cos^2(\mu/2)(1 - \mu^{-1} \sin \mu). \end{aligned} \quad (148)$$

For  $\xi = -v^2 < 0$  we have

$$I(\kappa, \nu) = -1 - \cos \kappa [\nu^{-1} \sinh \nu - \cosh \nu] + \nu^{-1} \sinh \nu \cosh \nu, \quad (149)$$

which can be transformed for  $k = 0, \pi$  analogously to the previous case.

Now the normalized eigenfunctions can be represented as

$$f_l(\kappa, D; y) = V(\kappa, \xi_l(\kappa, D), y), \quad 0 \leq y \leq 1; \quad l = 0, 1, \dots, \quad \text{where} \quad (150)$$

$$V(\kappa, \mu, y) = I(\kappa, \mu)^{-1/2} [e^{i\kappa} \sin \mu y + \sin \mu(1 - y)]. \quad (151)$$

In particular, we get from (144), (145), (147) and (148):

$$V(0, \mu, y) = \frac{\sqrt{2} \cos[\mu(y - (1/2))]}{\sqrt{1 + \mu^{-1} \sin \mu}}, \quad V(\pi, \mu, y) = \frac{\sqrt{2} \sin[\mu(y - (1/2))]}{\sqrt{1 - \mu^{-1} \sin \mu}}, \quad (152)$$

$$V(0, \nu, y) = \frac{\sqrt{2} \cosh[\nu(y - (1/2))]}{\sqrt{\nu^{-1} \sinh \nu + 1}}, \quad V(\pi, \nu, y) = \frac{\sqrt{2} \sinh[\nu(y - (1/2))]}{\sqrt{\nu^{-1} \sinh \nu - 1}} \quad (153)$$

**Remark 17** Note that in the formula (67) the vector  $U_p(0)$  degenerates to 0 if  $\xi^{1/2}$  is a multiple of  $\pi$  and  $\kappa = 0$  or  $\pi$ . Under these conditions  $I(\kappa, \xi)$  is equal to 0. The formulas (152) show that after the normalization this degeneration disappears, and we can define

$$f_l(\kappa, D; x)|_{\kappa=0, \pi} = \lim_{\kappa \rightarrow 0, \pi} f_l(\kappa, D; x). \quad (154)$$

In particular, using (152), (71), and (74) we easily obtain:

$$f_{2m-1}(\pi, D; y) = \sqrt{2} \sin(2m-1)\pi y, \quad 0 \leq y \leq 1; \quad (155)$$

$$f_{2m}(0, D; y) = \sqrt{2} \sin 2m\pi y, \quad 0 \leq y \leq 1; \quad m = 1, 2, \dots \quad (156)$$

## 5 Relations Between Schrödinger Operators with Point and Well Potentials

We are interested now in the following eigenvalue problems related to the periodic Schrödinger operator  $Q(D, \delta)$ :

$$\begin{aligned} Q(\kappa, D, \delta)\psi(y) &= -\psi''(y) - q_{D, \delta}(y)\psi(y) = \xi\psi(y), \quad 0 \leq y \leq 1 \\ \psi(1) &= e^{i\kappa}\psi(0), \quad \psi'(1) = e^{i\kappa}\psi'(0), \quad -\pi \leq \kappa \leq \pi \end{aligned} \quad (157)$$

The main objective of this section is to show that for  $\delta \rightarrow 0$  the operators  $Q(\kappa, D, \delta)$ , their eigenvalues and eigenfunction are small perturbation of the operators  $Q(\kappa, D)$  (see (62)) and of their eigenvalues and eigenfunctions correspondingly.

Let  $\xi_0(\kappa, D, \delta) \leq \xi_1(\kappa, D, \delta) \leq \dots$  be the eigenvalues of the problem (157) counted with their multiplicity. Consider the vector  $U(x) = (\psi(x), \psi'(x))$ . Solving the equation (157) on the interval  $[0, \delta]$ , we get

$$U(y) = \begin{bmatrix} \psi(0) \cos P_1 y + \psi'(0) P_1^{-1} \sin P_1 y \\ -\psi(0) P_1 \sin P_1 y + \psi'(0) \cos P_1 y \end{bmatrix}, \quad 0 \leq y \leq \delta, \quad (158)$$

where  $P_1 = \sqrt{D\delta^{-1} + \xi}$ . Solving the problem on the whole interval  $[0, 1]$ , we find the monodromy matrix

$$W = \begin{bmatrix} a_1 a_2 - p b_1 b_2 & P_2^{-1} a_1 b_2 + P_1^{-1} a_2 b_1 \\ -P_2 a_1 b_2 - P_1 a_2 b_1 & a_1 a_2 - p^{-1} b_1 b_2 \end{bmatrix}, \quad \text{where} \quad (159)$$

$$P_1 = \sqrt{D\delta^{-1} + \xi}, \quad P_2 = \sqrt{\xi}, \quad p = P_1 P_2^{-1} \quad (160)$$

$$a_1 = \cos(P_1 \delta), \quad b_1 = \sin(P_1 \delta) \quad (161)$$

$$a_2 = \cos(P_2(1 - \delta)), \quad b_2 = \sin(P_2(1 - \delta)) \quad (162)$$

The eigenvalues of the problem (157) can be found from the equation  $\text{Tr}W = 2 \cos \kappa$ , i.e.

$$a_1 a_2 - \frac{1}{2}(p + p^{-1})b_1 b_2 = \cos \kappa, \text{ or} \quad (163)$$

$$\cos(P_1 \delta) \cos(P_2(1 - \delta)) - \frac{p + p^{-1}}{2} \sin(P_1 \delta) \sin(P_2(1 - \delta)) = \cos \kappa \quad (164)$$

If  $\psi(x)$  is an eigenfunction of the problem (157), then  $WU(0) = e^{i\kappa}U(0)$ , and using (163) one can easily obtain

$$U(0) = \begin{bmatrix} \psi(0) \\ \psi'(0) \end{bmatrix} = \begin{bmatrix} P_2^{-1}a_1 b_2 + P_1^{-1}a_2 b_1 \\ (p - p^{-1})b_1 b_2 / 2 + i \sin \kappa \end{bmatrix}. \quad (165)$$

Note that (158) and (165) imply

$$U(\delta) = \begin{bmatrix} \psi(\delta) \\ \psi'(\delta) \end{bmatrix} = \begin{bmatrix} P_2^{-1}b_2 + P_1^{-1}b_1 e^{i\kappa} \\ e^{i\kappa} a_1 - a_2 \end{bmatrix}. \quad (166)$$

Using (160), we can rewrite the equation (164) in the form

$$\cos T_\xi \cos(\sqrt{\xi}(1 - \delta)) - \left(\frac{D}{2} + \xi\delta\right) \frac{\sin T_\xi}{T_\xi} \frac{\sin(\sqrt{\xi}(1 - \delta))}{\sqrt{\xi}} = \cos \kappa, \quad (167)$$

$$T_\xi = \sqrt{D\delta + \xi\delta^2}.$$

We introduce now the function

$$Y(\xi, D, \delta) = \cos T_\xi \cos(\sqrt{\xi}(1 - \delta)) - \left(\frac{D}{2} + \xi\delta\right) \frac{\sin T_\xi}{T_\xi} \frac{\sin(\sqrt{\xi}(1 - \delta))}{\sqrt{\xi}}.$$

Then the equation (167) can be rewritten as  $Y(\xi, D, \delta) = \cos \kappa$ . Note that  $Y(\xi, D, \delta)$  is an entire function of variable  $\xi$  which takes on real values for all real  $\xi$ . The set of eigenvalues  $\xi_0(\kappa, D, \delta) \leq \xi_1(\kappa, D, \delta) \leq \dots$  coincides with the set of solutions of the equation (167) for  $\xi \in \mathbf{R}$ . For  $D = 0$  the functions  $\xi_l(\kappa, D, \delta)$  do not depend on  $\delta$  and thus the formulas (73) are applicable to them. Besides,  $\xi_l(\kappa, D, \delta)$  are decreasing functions of  $D$  (which follows from an obvious inequality for the corresponding quadratic forms, compare with the proof of the Lemma 4). From the last observation we obtain a priori estimates:

$$\xi_l(\kappa, D, \delta) \leq [\pi(l + 1)]^2, \quad l \geq 0. \quad (168)$$

The elementary but rather lengthy analysis shows the validity of the following estimates.

**Lemma 18** *If  $D = 5$  and  $0 < \delta \leq 0.1$ , then the equation (167) has a unique negative solution which coincides with  $\xi_0(\kappa, D, \delta)$ . If*

$$D \geq 5, D\delta \leq 1/4, \quad (169)$$

then

$$\xi_0(\kappa, D, \delta) < 0; \quad \xi_1(\kappa, D, \delta) > 2 \quad (170)$$

Using the substitution  $\xi = \mu^2$  we can represent equation (164) in the form

$$\cos \tau_\mu \cos(\mu(1 - \delta)) - \left(\frac{D}{2} + \mu^2\delta\right) \frac{\sin \tau_\mu}{\tau_\mu} \frac{\sin(\mu(1 - \delta))}{\mu} = \cos \kappa, \quad \tau_\mu = \sqrt{D\delta + \mu^2\delta^2}. \quad (171)$$

In particular, if  $\mu = i\nu, \nu > 0$ , then (171) takes the form

$$\cos \tau_\nu \cosh(\nu(1-\delta)) - \left(\frac{D}{2} - \nu^2\delta\right) \frac{\sin \tau_\nu}{\tau_\nu} \frac{\sinh(\nu(1-\delta))}{\nu} = \cos \kappa, \quad (172)$$

$$\tau_\nu = \sqrt{D\delta - \nu^2\delta^2}$$

To view the equations (171) and (172) as perturbations of the equations (71) and (72) (or (87)) we rewrite them as follows:

$$\cos \tilde{\mu} - \frac{Ds_\mu}{2} \frac{\sin \tilde{\mu}}{\tilde{\mu}} + h_\mu = \cos \kappa, \quad \tilde{\mu} = \mu(1-\delta), \quad (173)$$

$$h_\mu = -(1 - \cos \tau_\mu) \cos \tilde{\mu} - \mu\delta (\tau_\mu^{-1} \sin \tau_\mu) \sin \tilde{\mu}, \quad (174)$$

$$s_\mu = (1-\delta)\tau_\mu^{-1} \sin \tau_\mu. \quad (175)$$

Correspondingly, (172) will look like

$$\nu = \frac{(D - 2\nu^2\delta)\tau_\nu^{-1} \tan \tau_\nu \tanh \tilde{\nu}}{2 \left\{ 1 - \cos \kappa [\cos \tau_\nu \cosh \tilde{\nu}]^{-1} \right\}}, \quad \tilde{\nu} = \nu(1-\delta). \quad (176)$$

## 5.1 Positive eigenvalues

To estimate the solutions of the equation (173) we will need the following inequalities for  $h_\mu$  and  $s_\mu$  which can be derived elementary from the definitions of those quantities.

**Lemma 19** *Suppose that*

$$\tau_\mu^2 = D\delta + \mu^2\delta^2 \leq 1; \quad \mu \geq 2 \quad (177)$$

*and  $h_\mu$  and  $s_\mu$  are defined respectively by (174) and (175). Then*

$$|h_\mu| \leq (1/2)D\delta + 2\mu\delta, \quad |\partial_\mu h_\mu| \leq (1/2)D\delta + 3\mu\delta \quad (178)$$

$$|1 - s_\mu| \leq (1/6)D\delta + \mu\delta, \quad |\partial_\mu s_\mu| \leq (1/2)\mu\delta^2 \quad (179)$$

We notice now that using the notation from Lemma 10 we can rewrite the equations (173) (and hence (171)) as follows:

$$A(Ds_\mu, \tilde{\mu}) + h_\mu = \cos \kappa, \quad s_\mu = (1-\delta)\tau_\mu^{-1} \sin \tau_\mu, \quad \tilde{\mu} = \mu(1-\delta) \quad (180)$$

The following lemma is the key tool in the approximations of the eigenvalues  $\mu_n(\kappa, D, \delta)$  by  $\mu_n(\kappa, D)$ .

**Lemma 20** *Let  $L$  be a natural number and  $\alpha$  and  $C_0$  be positives constants such that*

$$0 < \alpha < 1, \quad C_0 \geq 1. \quad (181)$$

*Suppose that  $\kappa = 0, \pi$  and  $\mu_1(\kappa, D, \delta) \leq \dots \leq \mu_L(\kappa, D, \delta)$  are the first  $L$  solutions of the equation (180) (and hence of (171)), and  $\mu_1(\kappa, D) \leq \dots \leq \mu_L(\kappa, D)$  are the first  $L$  solutions of the equation (106). Suppose that the parameter  $\delta$  satisfies the inequality*

$$18\sqrt{(4C_0 + 3)\pi(L+1)\delta} \leq \alpha < \min(4C_0/11, 1), \quad (182)$$

and that the parameter  $D$  varies in the range

$$11\alpha\pi(L+1) \leq D \leq 4C_0\pi(L+1). \quad (183)$$

Then

$$|\mu_l(\kappa, D, \delta) - \mu_l(\kappa, D)| \leq (33C_0 + 26)\pi(L+2)\delta/\alpha. \quad (184)$$

In particular,

$$|\mu_l(\kappa, D, \delta) - \mu_l(\kappa, D)| \leq 0.041\alpha \leq 0.041. \quad (185)$$

**Proof.** The proof of this lemma is based on the results of Lemma 13, Theorem 14, and Lemma 19. Hence, we have to check the conditions (124)-(126), and (177). Note first of all that (85) yields

$$2 \leq \mu_L(\kappa, D) \leq \pi(L+1). \quad (186)$$

Let us denote  $v = (4C_0 + 3)\pi(L+1)\delta$  and  $N = \pi(L+1)$ . Using (182) and (183) we obtain for any  $\mu \in [2, N]$

$$\tau_\mu^2 = D\delta + \mu^2\delta^2 \leq 4C_0\pi(L+1)\delta + [\pi(L+2)\delta]^2 \leq (\alpha/18)^2 + \alpha^2/(9 \cdot 18) < 1.$$

This enables us to apply Lemma 19 for  $\mu \in [2, N+1]$ . From (178) and (179) it easily follows that

$$|h_\mu|, |1 - s_\mu| \leq v, \mu \in [2, N+1]. \quad (187)$$

This gives (124) in Lemma 13. Then from (178), (179), (182) and (183) we obtain

$$\begin{aligned} |\partial_\mu h_\mu| &\leq \frac{D}{\mu} \left( (1/2) + \frac{3}{D/\mu} \right) \mu\delta \leq \frac{D}{\mu} \left( (1/2) + (9/8)\alpha^{-1} \right) \pi(L+2)\delta \\ &\leq \frac{D}{2\mu} \left( (1/2) + (9/8)\alpha^{-1} \right) \left( \frac{\alpha}{18} \right)^2 = \frac{D}{2(18)^2\mu} \left( \frac{\alpha^2}{2} + \frac{9\alpha}{8} \right) \\ &\leq \frac{D}{(18)^2\mu} < \frac{D}{16\mu}, \end{aligned} \quad (188)$$

$$|\partial_\mu s_\mu| \leq \frac{1}{\mu} [\pi(L+1)\delta]^2 \leq \frac{1}{\mu} \left( \frac{\alpha}{18} \right)^2 \leq \frac{1}{(18)^2\mu}. \quad (189)$$

Now we have to make some little adjustments since the equation (180) involves variable  $\tilde{\mu}$ . Namely, (189) easily yields

$$|\partial_{\tilde{\mu}} (s_\mu)_{\mu=\tilde{\mu}(1-\delta)^{-1}}| \leq \frac{(1-\delta)^2}{(18)^2\tilde{\mu}} \leq \frac{1}{18\tilde{\mu}} \quad (190)$$

One can check now the inequality (126). The inequalities (187), (188) and (190) along with (182) and (183) allow us to apply here Theorem 14, which implies the inequality

$$|(\mu_L(\kappa, D, \delta) - (1-\delta)^{-1}\mu_L(\kappa, D))| \leq 8(1-\delta)^{-1}(4C_0 + 3)\pi(L+1)\delta/\alpha, \quad (191)$$

which along with (186) easily yields the desired inequality (184). The inequality (185) follows from (184) and (182).  $\square$

We will also need the following corollaries of Lemma 20.

**Lemma 21** Let  $N_0$  be a natural number and suppose that the parameter  $\delta$  is small enough to satisfy the inequality

$$18\sqrt{7\pi(N_0+1)}\delta \leq [11\pi(N_0+1)]^{-1}. \quad (192)$$

Then for any  $1 \leq l \leq N_0$  and any  $D$  such that  $1 \leq D \leq 4\pi(N_0+1)$

$$|\mu_l(\kappa, D, \delta) - \mu_l(\kappa, D)| \leq 1300\pi^2(N_0+2)^2\delta. \quad (193)$$

**Proof.** The statement of this lemma follows immediately from the Lemma 20 if we pick  $\alpha = [11\pi(N_0+1)]^{-1}$  and  $C_0 = 1$ .  $\square$

**Lemma 22** Let  $N_0$  be a natural number,  $C_0 \geq 1$  be a constant and suppose that the parameter  $\delta$  is small enough to satisfy the inequality

$$18\sqrt{(4C_0+3)(N_0+1)}\delta \leq [11\pi(N_0+1)]^{-1}. \quad (194)$$

Then for any  $1 \leq l \leq N_0$  and any  $D$  such that  $1 \leq D \leq 4\pi C_0$

$$|\mu_l(\kappa, D, \delta) - \mu_l(\kappa, D)| \leq 2600\pi^2 C_0(N_0+2)^2\delta. \quad (195)$$

In particular, for any  $1 \leq l \leq N_0$  and for any  $0 \leq D \leq 4\pi C_0$

$$\mu_l(\kappa, D, \delta) \geq \pi l - 2600\pi^2 C_0(N_0+2)^2\delta. \quad (196)$$

**Proof.** The estimates (195) follow from the Lemma 20 if we pick  $\alpha = [4\pi(N_0+1)]^{-1}$ . The inequalities (196) follow easily from (195) and (85). Note that we may extend the range of values of  $D$  to 0 since  $\mu_l(\kappa, D, \delta)$  are decreasing functions of the argument  $D$ .  $\square$

**Lemma 23** Suppose that all conditions of the Lemma 20 are satisfied. Then for any  $0 \leq D \leq 4C_0\pi(L+1)$

$$\pi l - (33C_0 + 26)\pi(L+2)\delta/\alpha \leq \mu_l(\kappa, D, \delta) \leq \pi(L+1). \quad (197)$$

In particular,

$$\mu_l(\kappa, D, \delta) \geq \pi l - 0.041\alpha \geq \pi l - 0.041. \quad (198)$$

**Proof.** The right-hand inequality in (197) is a consequence of (168). The left-hand inequality in (197) follows from (184) and (85). It is true for any  $D \leq 4C_0\pi(L+1)$  since  $\mu_L(\kappa, D, \delta)$  is a decreasing function of the argument  $D$ . The inequalities (198) follow in similar fashion from (185) and (85).  $\square$

## 5.2 Negative eigenvalues

Now, in order to complete our comparison of eigenvalues of the operators  $Q(\kappa, D, \delta)$  with the ones of the operators  $Q(\kappa, D)$ , it remains to analyze the lowest eigenvalue  $\xi_0(\kappa, D, \delta)$ , which becomes negative for large  $D$ . Based Lemmas 6 and 18 the following properties  $\xi_0(\kappa, D, \delta)$  can be established.

**Lemma 24** The next statements are true:

(i)  $\xi_0(\kappa, D, \delta)$  is a decreasing function of  $D \geq 0$  and increasing function of  $\kappa$  such that  $\xi_0(\kappa, 0, \delta) = \kappa$ , and  $\xi_0(\kappa, D, \delta) \geq -D\delta^{-1}$ ;

(ii) if  $\xi_0(\kappa, D, \delta) \leq 0$  and we define  $\nu_0(D, \delta) = \sqrt{-\xi_0(0, D, \delta)}$ ,  $\nu_1(D, \delta) = \sqrt{-\xi_0(\pi, D, \delta)}$  then  $\nu_0(D, \delta) \geq \nu_1(D, \delta)$ ;

(iii) if  $C$  and  $c$  are positive constants then the following limits hold uniformly for  $0 \leq D \leq C$  and  $0 \leq \kappa \leq \pi$

$$\lim_{\delta \rightarrow 0} \xi_0(\kappa, D, \delta) = \xi_0(\kappa, D); \quad (199)$$

If  $c \leq D \leq C$ , then

$$\xi_0(\kappa, D, \delta) = \xi_0(\kappa, D) + O(\delta), \quad \delta \rightarrow 0 \quad (200)$$

(iv) suppose that  $D \geq 5, D\delta \leq 1/4$ , then for  $\delta \leq 0.02$  and  $j = 0, 1$  the following representations hold

$$\nu_j(D, \delta) = \frac{u_j D}{1 + \sqrt{1 + 2u_j^2 D\delta}}, \quad 0 \leq u_j - 1 \leq (1/2)D\delta + 5e^{-D/8} \quad (201)$$

In particular,

$$\nu_j(D, \delta) = (1 + p_j)D/2, \quad |p_j| \leq 9D\delta + 5e^{-D/8} \quad (202)$$

**Lemma 25** Suppose that  $D \geq 40, D\delta \leq 10^{-2}$ , then

$$0.3D \leq \nu_j(D, \delta) \leq 0.7D, \quad j = 0, 1 \quad (203)$$

$$|\partial_D \nu_j(D, \delta) - (1/2)| \leq 4D\delta + 30e^{-0.3D} \quad (204)$$

In addition to that, for  $D \geq 30, D\delta \leq 10^{-2}$  we have

$$0 \leq \nu_0(D, \delta) - \nu_1(D, \delta) \leq 4e^{-0.59D} \quad (205)$$

### 5.3 Eigenfunctions

In this section we establish some properties of eigenfunctions of the operators  $Q(\kappa, D, \delta)$ . We shall need these properties in order to estimate the deviation of the spectrum of the operator  $\Theta_\epsilon$  from the spectrum of the operator  $\mathring{\Theta}_{\zeta, \delta}$  with separate variables.

**Lemma 26** Let  $f(y)$  be a complex-valued function with square integrable derivative on the interval  $[0, 1]$ . Then for any positive  $\alpha \leq 1/2$

$$|f(y)|^2 \leq 2\alpha^{-1} \int_0^1 |f(t)|^2 dt + \alpha \int_0^1 |f'(t)|^2 dt, \quad 0 \leq y \leq 1 \quad (206)$$

**Proof.** Without loss of generality we shall assume that  $y \in [0, 1/2]$ . We notice that

$$|f(y) - f(z)|^2 \leq |y - z| \int_0^1 |f'(t)|^2 dt, \quad 0 \leq y, z \leq 1. \quad (207)$$

Integrating the inequality  $|f(y)|^2 \leq 2[|f(z)|^2 + |f(y) - f(z)|^2]$  with respect to  $z \in [y, y + \alpha]$  and using the inequality (207) we obtain (206).  $\square$

**Lemma 27** Let  $\theta \geq -D^2$  and  $\psi_\theta(\kappa, D, \delta; y) = \psi(y)$  be respectively an eigenvalue and the corresponding eigenfunction of the operator  $Q(\kappa, D, \delta)$ . Then

$$|\psi(y)|^2 \leq \sqrt{8C_{D, \theta}} \int_0^1 |\psi(t)|^2 dt, \quad 0 \leq y \leq 1, \quad (208)$$

$$\int_0^\delta |\psi(y)|^2 dy \leq \delta \sqrt{8C_{D, \theta}} \int_0^1 |\psi(t)|^2 dt, \quad \text{where} \quad (209)$$

$$C_{D, \theta} = 4 \begin{cases} 2D_1^2 & \text{if } \theta < 0 \\ 2D_1^2 + \theta & \text{if } \theta \geq 0 \end{cases}, \quad D_1 = \max\{D, 1\}. \quad (210)$$

For  $\theta$  negative we also have

$$\int_0^\delta |\psi(y)|^2 dy > -D^{-1} \delta \theta \int_0^1 |\psi(y)|^2 dy \quad (211)$$

**Proof.** The function  $\psi$  satisfies the equation

$$\begin{aligned} -\psi''(y) &= (q_{D,\delta}(y) + \theta)\psi(y), \quad 0 \leq y \leq 1 \\ \psi(1) &= e^{ik}\psi(0), \quad \psi'(1) = e^{ik}\psi'(0). \end{aligned}$$

Multiplying both sides of the equation by  $\overline{\psi(y)}$  and integrating the result with respect to  $y \in [0, 1]$ , we get the identity

$$\int_0^1 |\psi'(y)|^2 dy = D\delta^{-1} \int_0^\delta |\psi(y)|^2 dy + \theta \int_0^1 |\psi(y)|^2 dy.$$

Since the left side of this inequality is positive, we obtain (211). This and the following corollary of the inequality (206)

$$\int_0^\delta |f(y)|^2 dy \leq 2\alpha^{-1}\delta \int_0^1 |f(t)|^2 dt + \alpha\delta \int_0^1 |f'(t)|^2 dt,$$

imply

$$\int_0^1 |\psi'(y)|^2 dy \leq (2D\alpha^{-1} + \theta) \int_0^1 |\psi(y)|^2 dy + D\alpha \int_0^1 |\psi'(y)|^2 dy.$$

This, in turn, implies for any  $\alpha < D^{-1}$

$$\int_0^1 |\psi'(y)|^2 dy \leq d_\alpha \int_0^1 |\psi(y)|^2 dy, \quad d_\alpha = \frac{2D\alpha^{-1} + \theta}{1 - D\alpha}. \quad (212)$$

Now we can estimate the coefficient  $d_\alpha$  as follows. We observe first that the coefficient  $d_\alpha$  is an increasing function of  $D$  when  $\theta \geq -D^2$  and  $\alpha < D^{-1}$ . Using this and denoting  $D_1 = \max\{D, 1\}$ ,  $D_1\alpha = u < 1$  and then using the condition  $\theta \geq -D^2$  we obtain

$$d_\alpha = \frac{2D_1^2 + u\theta}{u(1-u)} \leq \frac{1}{u(1-u)} \times \begin{cases} 2D_1^2 & \text{if } \theta < 0 \\ 2D_1^2 + \theta & \text{if } \theta \geq 0 \end{cases}$$

This combined with (210) yields  $d_\alpha|_{\alpha=D_1^{-1}/2} \leq C_{D,\theta}$ . This inequality and (210) imply

$$\int_0^1 |\psi'(y)|^2 dy \leq C_{D,\theta} \int_0^1 |\psi(y)|^2 dy. \quad (213)$$

Finally, combining the inequalities (206) and (213) we obtain

$$|\psi(y)|^2 \leq (2\alpha^{-1} + \alpha C_{D,\theta}) \int_0^1 |\psi(t)|^2 dt, \quad 0 \leq y \leq 1.$$

Now we take  $\alpha = \sqrt{2/C_{D,\theta}}$ . One can check that  $\alpha < D^{-1}$ . Since  $C_{D,\theta} \geq 8$ ,  $\alpha$  is less than 1/2. We conclude that (208) is true. The inequality (209) follows from (208).  $\square$

The next two lemmas are devoted to some properties of the eigenfunctions  $f_l(\kappa, D, \delta; y)$ ,  $l \geq 0$ , of the operators  $Q(\kappa, D, \delta)$ . We shall need them later on when we consider space distribution of the electric field energy.

**Lemma 28** *Suppose that  $D \rightarrow \infty$ ,  $D\delta \rightarrow 0$  (and hence  $\delta \rightarrow 0$ ). Then the eigenfunctions  $f_l(\kappa, D, \delta; y)$ ,  $l \geq 1$  satisfy the estimates:*



$$\int_0^\delta |f_l(\kappa, D, \delta; y)|^2 dx \leq \delta [O(D^{-2}) + O(D\delta)], \quad (214)$$

$$\int_\delta^1 |f_l(\kappa, D, \delta; y)|^2 dx = (\pi l)^2 (1 - \cos \kappa) + o(1) \quad (215)$$

**Proof.** Let us fix any natural  $l \geq 1$  and recall that the initial values  $f_l(\cdot, 0), f_l'(\cdot, 0)$  of the eigenfunction  $f_l$  associated with the eigenvalue  $\xi_l$  are given by the formula (165) where  $\xi = \xi_l = \mu_l^2$ . We shall use the notation  $U(y) = (f_l(\cdot; y), f_l'(\cdot; y))$ . Using the inequality (195) for  $C_0 = D$  and equality (105), we get the estimate

$$\mu_l(\kappa, D, \delta) = \pi l + 4lD^{-1} + O(D^{-2} + D\delta). \quad (216)$$

Let us now denote  $\tau = \sqrt{D\delta + \mu^2\delta^2}$ . We notice that  $\tau \rightarrow 0$  under the conditions of the lemma. Using (165), (160) we obtain for  $l \geq 1$  and  $\mu = \mu_l$

$$U(0) = \begin{bmatrix} f_l(\kappa, D, \delta; 0) \\ f_l'(\kappa, D, \delta; 0) \end{bmatrix} = \begin{bmatrix} \mu^{-1} \sin(1 - \delta)\mu \cos \tau + \delta\tau^{-1} \cos(1 - \delta)\mu \sin \tau \\ -D(2\mu)^{-1}(\tau^{-1} \sin \tau) \sin(1 - \delta)\mu + i \sin \kappa \end{bmatrix}. \quad (217)$$

Using the fact that  $\tau, \delta \ll 1$ , we conclude that this vector can be represented as

$$\left[ \begin{array}{c} \mu^{-1} \sin \mu + O(\delta + \tau^2) \\ -(2\mu)^{-1} D \sin \mu + O(D\delta + \tau^2 D \mu^{-1} \sin \mu + \mu\delta) \end{array} \right] \Big|_{\mu=\mu_l}.$$

From (217) and (158) we conclude that for  $0 \leq y \leq \delta$

$$\begin{aligned} f_l(y) &= f_l(0) \cos(\tau\delta^{-1}y) + f_l'(0)(D\delta^{-1} + \mu^2)^{-1/2} \sin(y(D\delta^{-1} + \mu^2)^{1/2}) \\ &= f_l(0) \cos(\tau\delta^{-1}y) + f_l'(0)\delta\tau^{-1} \sin(y(D\delta^{-1} + \mu^2)^{1/2}), \quad \mu = \mu_l \end{aligned}$$

Now, according to (216), we have for a fixed  $l \geq 1$ :  $\sin \mu_l = O(D^{-1} + D\delta)$ . Together with the previous inequalities, this gives for  $0 \leq y \leq \delta$ :  $f_l(k, D, \delta; y) = O(D^{-1}) + O(\delta + \tau^2)$ . This yields the estimate (214).

To verify (215) we consider first  $U(\delta)$ . Based on (166) together with (160) we obtain

$$\begin{aligned} U(\delta) &= \begin{bmatrix} f_l(\kappa, D, \delta; \delta) \\ f_l'(\kappa, D, \delta; \delta) \end{bmatrix} = \\ &= \left[ \begin{array}{c} \mu^{-1} \sin \mu(1 - \delta) + P_1 e^{i\kappa} \sin P_1 \delta \\ e^{i\kappa} \cos P_1 \delta - \cos \mu(1 - \delta) \end{array} \right] \Big|_{\mu=\mu_l}, \quad P_1 = (D\delta^{-1} + \mu^2)^{-1/2}. \end{aligned}$$

Using the parameter  $\tau$  ( $\tau \rightarrow 0$ , as it has been noted earlier), we come to the representation:

$$U(\delta) = \left[ \begin{array}{c} \mu^{-1} \sin \mu + O(\delta) \\ e^{i\kappa} - \cos \mu + O(\tau^2) \end{array} \right] \Big|_{\mu=\mu_l}. \quad (218)$$

Note now that the vector function  $U(y + \delta)$  and the vector function  $U_p(y)$  (which is associated with the problem (64)) on the interval  $[0, 1 - \delta]$  correspond to the same differential equation

$$-\psi''(y) = \mu^2 \psi(y), \quad 0 \leq y \leq 1 - \delta,$$

but to different initial conditions. Namely, using (218) and (70) we may conclude that

$$U(y + \delta)|_{y=0} = \left[ \begin{array}{c} \psi(y) \\ \psi'(y) \end{array} \right] \Big|_{y=0} = \left[ \begin{array}{c} \mu^{-1} \sin \mu + O(\delta) \\ e^{i\kappa} - \cos \mu + O(\tau^2) \end{array} \right] \Big|_{\mu=\mu_l(\kappa, D, \delta)},$$

$$U_p(y)|_{\xi=\pi^2 l^2} = \left[ \begin{array}{c} \psi(y) \\ \psi'(y) \end{array} \right] \Big|_{y=0} = \left[ \begin{array}{c} \mu^{-1} \sin \mu \\ e^{i\kappa} - \cos \mu \end{array} \right] \Big|_{\mu=\mu_l(\kappa, D)}.$$

From these observations and (216) we easily get that

$$\max_{0 \leq y \leq 1-\delta} |f_l(\kappa, D, \delta; y + \delta) - f_l(\kappa, D; y)| = o(1).$$

This implies

$$\int_{\delta}^1 |f_l(\kappa, D, \delta; y)|^2 dx = \int_0^{1-\delta} |f_l(\kappa, D; y)|^2 dx + o(1). \quad (219)$$

We recall now (see (143)) that

$$f_l(\kappa, D; y) = \mu^{-1} [e^{i\kappa} \sin \mu y + \sin \mu(1-y)], \quad \mu = \mu_l(\kappa, D). \quad (220)$$

We obtain from (143) and (105):

$$\int_0^1 |f_l(\kappa, D; y)|^2 dx = \mu^{-2} I(\kappa, \mu)|_{\mu=\mu_l(\kappa, D)} = (\pi l)^{-2} (1 - \cos \kappa) + o(1).$$

The last formula along with (220) (which implies that  $f_l(\kappa, D; y)$  is bounded) leads to the representation:

$$\int_0^{1-\delta} |f_l(\kappa, D; y)|^2 dx = (\pi l)^{-2} (1 - \cos \kappa) + o(1).$$

This equality and (219) imply the estimate (215).  $\square$

**Lemma 29** *Suppose that  $0 \leq D \leq C$  for some constant  $C$  and that  $\delta \rightarrow 0$ . Then the eigenfunctions  $f_0(\kappa, D, \delta; y)$  satisfy the estimates*

$$\int_0^{\delta} |f_0(\kappa, D, \delta; y)|^2 dx = \delta [\nu^{-2} \sinh \nu^2 + o(1)], \quad (221)$$

$$\int_{\delta}^1 |f_0(\kappa, D, \delta; y)|^2 dx = I(\kappa, \nu) + o(1), \quad (222)$$

where  $I(\kappa, \nu)$  is defined by (149) and  $\nu = \sqrt{-\xi(\kappa, D)}$ .

**Proof.** Proof of this lemma is similar to the proof of the previous one. Let us consider first  $D > 4$ . In this case  $\xi_0(\kappa, D)$  and  $\xi_0(\kappa, D, \delta)$  are negative for small  $\delta$ . We remind the notation  $\xi = -\nu^2$ . Using (165) and (160) again, we get

$$U(0) = \left[ \begin{array}{c} f_0(\kappa, D, \delta; y) \\ f_0'(\kappa, D, \delta; y) \end{array} \right] = \left[ \begin{array}{c} \nu^{-1} \sinh \nu + o(1) \\ e^{i\kappa} - \cosh \nu \end{array} \right]$$

From this representation we obtain for  $0 \leq y \leq \delta$ :  $f_0(\kappa, D, \delta; y) = \nu^{-1} \sinh \nu + o(1)$ , which implies the estimate (221). Reasoning similar to the one used to justify (215) leads to the equality (222).

If  $D < 4$ , then one can check that the statements of the lemma still hold, but in this case  $\sqrt{-\xi(\kappa, D)}$  will be purely imaginary. Of course, all functions and integrals of interest for this case are still real-valued.

$\square$

## 6 Scalar Models

In this section we consider some general properties of the spectra of scalar operators associated with the Maxwell operator (similar operators arise for acoustic waves).

As it will be shown in the section 7.1, in order to estimate the spectral bands of the Maxwell operator, we need to consider, in particular, the following scalar operator:

$$\Theta_{d,\varepsilon} \varphi = -\varepsilon(\mathbf{x})^{-1} \Delta \varphi, \quad \varphi \in L_2(\mathbf{R}^d, \varepsilon(\mathbf{x}) d\mathbf{x}, \mathbf{C}), \quad \mathbf{x} \in \mathbf{R}^d$$

Here we are interested only in the values  $d = 3$  and  $d = 2$ .

Along with the operator  $\Theta_\varepsilon$  acting in the space  $L_2(\mathbf{R}^d, \varepsilon(\mathbf{x}) d\mathbf{x}, \mathbf{C})$ , we will consider its Floquet components

$$\Theta_{\mathbf{k},\varepsilon} \varphi = -\varepsilon(\mathbf{x})^{-1} \Delta \varphi, \quad \varphi \in L_{2,\varepsilon}^1 = L_2(X, \varepsilon(\mathbf{x}) d\mathbf{x}, \mathbf{C}), \quad \mathbf{k} = (k_1, \dots, k_d) \quad (223)$$

with the boundary conditions

$$\varphi(\mathbf{x})|_{x_j=1} = e^{ik_j} \varphi(\mathbf{x})|_{x_j=1}, \quad (224)$$

$$\frac{\partial \varphi}{\partial x_j} \Big|_{x_j=1} = e^{ik_j} \frac{\partial \varphi}{\partial x_j} \Big|_{x_j=1}, \quad j = 1, \dots, d. \quad (225)$$

The main results of this section are the following statements.

**Theorem 30** *For any natural number  $N_0$  and any positive constant  $C$  there exists a positive constant  $c$  such that for any  $\beta > C$  and for any  $w < c$*

$$\sigma(\Theta_\varepsilon) \cap I = \left[ \bigcup_{0 \leq n \leq N_0} [wD_n^-(\zeta, \delta), wD_n^+(\zeta, \delta)] \right] \cap I, \quad (226)$$

$$I = [0, 2\pi w(N_0 - 1)],$$

where the endpoints  $D_n^\pm(\zeta, \delta)$  can be approximated by the numbers  $D_n^\pm$  (defined in (133), (134)) as follows:

$$|D_n^\pm(\zeta, \delta) - D_n^\pm| \leq 2(4w + 10^3 N_0^3 \beta^{-1}). \quad (227)$$

In fact, we can describe the asymptotic location of the spectrum in any finite interval of the spectral axis.

**Theorem 31** *For any constant  $N \geq \pi$  there exist positive constants  $C$  and  $c$  such that for any  $\beta_2 > C$  and for any  $w < c$*

$$\sigma(\Theta_\varepsilon) \cap [0, N] = \left[ \sigma_E(\Theta_\varepsilon) \cup \sigma_H(\Theta_\varepsilon) \right] \cap [0, N], \quad (228)$$

where the sets  $\sigma_E(\Theta_\varepsilon)$  and  $\sigma_H(\Theta_\varepsilon)$  are respectively of the form (22), (23), (25):

$$\sigma_E(M) = \bigcup_{n \geq 0} [\tilde{w}D_n^-(\zeta, \delta), \tilde{w}D_n^+(\zeta, \delta)], \quad \text{where}$$

$$D_n^\pm(\zeta, \delta) = 2\pi n(1 + \chi_n^\pm), \quad n \geq 1; \quad D_0^-(\zeta, \delta) = 0, \quad D_0^+(\zeta, \delta) = 4 + \chi_0^+,$$

$$\sigma_H(M) = \bigcup_{\mathbf{n} \geq 0} [(\pi \mathbf{n})^2 + \rho_{\mathbf{n}}^-, (\pi \mathbf{n})^2 + \rho_{\mathbf{n}}^+],$$

and the quantities  $\chi_n^\pm, \eta_n^\pm$  and  $\rho_{\mathbf{n}}^\pm$  satisfy the estimates

$$|\chi_n^\pm| \leq 100N\beta^{-1} + 6e^{-0.3n} + 10N^2\beta_2^{-3}wn^{-1}, 1 \leq n \leq N(\pi w)^{-1}, \quad (229)$$

$$|\eta_n^\pm| \leq 5 \cdot 10^3 N\beta^{-1} + 2 \cdot 10^3 e^{-0.3n} + 3n^{-1} + 301w, 1 \leq n \leq N(\pi w)^{-1}, \quad (230)$$

and for some constant  $C_1$

$$|\rho_{\mathbf{n}}^\pm| \leq C_1 w \text{ for } |\mathbf{n}| \leq \sqrt{N}\pi^{-1}. \quad (231)$$

In particular, the spectrum  $\sigma(\Theta_\varepsilon)$  has adjacent bands and gaps of order  $w$ .

The proof of these theorems is based upon an approximation of the operator  $\Theta_{\mathbf{k},\varepsilon}$  by an operator with separable variables. Such an operator can be analyzed on the basis of our results for one-dimensional models.

## 6.1 Separated variables case

It turns out that asymptotic behavior of spectra of the operators  $\Theta_{\mathbf{k},\varepsilon}$  when  $\delta$  and  $\zeta^{-1}$  approach 0 in a suitable manner can be analyzed in terms of spectra of similar operators with separable variables. In this subsection we consider the case of separated variables when the dielectric constant  $\varepsilon(\mathbf{x})$  has the following special form:

$$\overset{\circ}{\varepsilon}(\mathbf{x}) = \sum_{1 \leq j \leq d} \rho_{\zeta,\delta}(x_j), \quad \mathbf{x} = (x_1, \dots, x_d). \quad (232)$$

Here the auxiliary function  $\rho_{\zeta,\delta}(y), y \in \mathbf{R}$  is defined by the formula

$$\rho_{\zeta,\delta}(y) = \begin{cases} \zeta - (d-1)d^{-1} & \text{if } 0 \leq y < \delta \\ d^{-1} & \text{if } \delta \leq y < 1 \end{cases}, \quad (233)$$

where  $\rho(y) = \rho(y+n)$  for  $n \in \mathbf{Z}, y \in \mathbf{R}$ . We introduce now the notation

$$\overset{\circ}{\Theta}_{\zeta,\delta} = -\left(\overset{\circ}{\varepsilon}(\mathbf{x})\right)^{-1} \Delta,$$

and  $\overset{\circ}{\Theta}_{\mathbf{k},\zeta,\delta}$  is the respective Floquet-Bloch component of the operator  $\overset{\circ}{\Theta}_{\zeta,\delta}$ . We will use the "circle" symbol  $\circ$  in order to indicate quantities associated with the separate variables case. As before, we are interested primarily in the cases  $d = 2, 3$ . We now notice that the eigenvalue problem

$$-\left(\overset{\circ}{\varepsilon}(\mathbf{x})\right)^{-1} \Delta \varphi = \lambda \varphi \quad (234)$$

with the boundary conditions (224), (225) can be rewritten as

$$S_{\mathbf{k},\lambda} \varphi = -\Delta \varphi - \lambda v(\mathbf{x}) \varphi = \lambda \varphi, \quad v(\mathbf{x}) = \sum_{1 \leq j \leq d} (\rho_{\zeta,\delta}(x_j) - d^{-1}). \quad (235)$$

Thus, to find the eigenvalues of the problem (234) we can do the following. First, we find the eigenvalues  $\xi(\mathbf{m}, \mathbf{k}, g)$  of the Schrödinger operator satisfying the boundary conditions (224), (225) and depending on the parameter  $g \geq 0$ :

$$S_{\mathbf{k},g} \varphi = -\Delta \varphi - gv(\mathbf{x}) \varphi, \quad (236)$$

where  $\mathbf{m}$  is an index which counts the eigenvalues  $\xi$ . We solve then for  $g \geq 0$  the equations

$$\xi(\mathbf{m}, \mathbf{k}, g) = g \quad (237)$$

for all values of the index  $\mathbf{m}$ . This gives us the set of eigenvalues of the eigenvalue problem (234), (224), (225).

We also notice here that the dielectric constant  $\overset{\circ}{\varepsilon}(\mathbf{x})$  does not differ much from the original dielectric constant  $\varepsilon(\mathbf{x})$ . Namely, for  $d = 2$  and  $\Gamma_{11} = [0, \delta] \times [0, \delta]$  we have

$$\overset{\circ}{\varepsilon}(\mathbf{x}) - \varepsilon(\mathbf{x}) = \begin{cases} 0 & \text{if } \mathbf{x} \in X - \Gamma_{11} \\ 2\zeta - 1 & \text{if } \mathbf{x} \in \Gamma_{11} \end{cases}. \quad (238)$$

A similar formula holds for  $d = 3$ .

To proceed with the Schrödinger operator  $S_{g,\mathbf{k}}$  with separable variables we introduce the one-dimensional Schrödinger operator:

$$Q_g = -\frac{\partial^2}{\partial y^2} - g(\rho_{\zeta,\delta}(y) - d^{-1}).$$

Then the standard Floquet expansion holds:

$$Q_g = \int^{\oplus} Q_{\kappa,g} d\kappa, \quad Q_{\kappa,g} = Q(\kappa, g(w^{-1} - \delta d^{-1}), \delta), \quad g \geq 0, \quad (239)$$

and the operator in the right side is defined in (157) (this includes boundary conditions as well). Let now  $\xi_m(\kappa, g, \zeta, \delta)$  and  $f_m(\kappa, g, \zeta, \delta, y)$  be respectively the eigenvalues and normalized eigenfunctions of  $Q_{\kappa,g}$ , i.e.

$$Q_{\kappa,g} f_m = \xi_m f_m; \quad \int_0^1 |f_m(y)|^2 dy = 1, \quad m = 0, 1, \dots \quad (240)$$

Thus, if  $I$  is the identity operator in  $L_2(\mathbf{R})$ , then we have

$$S_{\mathbf{k},g} = Q_{\kappa,g} \otimes I + I \otimes Q_{\kappa,g} \text{ for } d = 2, \quad (241)$$

$$S_{\mathbf{k},g} = Q_{\kappa,g} \otimes I \otimes I + I \otimes Q_{\kappa,g} \otimes I + I \otimes I \otimes Q_{\kappa,g} \text{ for } d = 3. \quad (242)$$

We can now represent the eigenfunctions and the eigenvalues of the Schrödinger operator  $S_{\mathbf{k},g}$  as

$$F_{\mathbf{m}}(\mathbf{x}) = F_{\mathbf{m}}(\mathbf{k}, g, \zeta, \delta, \mathbf{x}) = \prod_{1 \leq j \leq d} f_{m_j}(k_j, x_j), \quad (243)$$

$$\xi(\mathbf{m}) = \xi(\mathbf{m}, \mathbf{k}, g, \zeta, \delta) = \sum_{1 \leq j \leq d} \xi_{m_j}(k_j), \quad \mathbf{m} = (m_1, \dots, m_d) \in \mathbf{Z}_+^d. \quad (244)$$

To analyze the equations (237) we need the following lemmas.

**Lemma 32** *The eigenvalues  $\xi(\mathbf{m}, \mathbf{k}, g)$  are decreasing functions of the parameter  $g \geq 0$ . Each equation*

$$\xi(\mathbf{m}, \mathbf{k}, g) = g, \quad \mathbf{m} \in \mathbf{Z}_+^d \quad (245)$$

*has a unique solution  $g = \overset{\circ}{\lambda}(\mathbf{m}, \mathbf{k}, \zeta, \delta)$ .*

**Proof.** As it easily follows from the definition (239) of the operator  $Q_g$  and from (157), we have  $Q_{\kappa, g_1} \leq Q_{\kappa, g_2}$ , for  $g_1 \geq g_2$ . This together with (244) imply that  $\xi(\mathbf{m}, \mathbf{k}, g)$  are decreasing functions of the parameter  $g$ . Then we notice that  $\xi_l|_{g=0} = \xi_l|_{D=0}$ . The last statement along with (73) and monotonicity of the functions  $\xi(\mathbf{m}, \mathbf{k}, g)$  imply that each of the equations (245) has a unique solution  $\overset{\circ}{\lambda}(\mathbf{m}, \mathbf{k}, \zeta, \delta) \geq 0$ .  $\square$

The following statement is standard for operators with separable variables.

**Lemma 33** The numbers  $\overset{\circ}{\lambda}(\mathbf{m}, \mathbf{k}, \zeta, \delta)$ ,  $\mathbf{m} \in \mathbf{Z}_+^d$  form the set of all eigenvalues of the operator  $\overset{\circ}{\Theta}_{\mathbf{k}, \zeta, \delta}$ , taking into account their multiplicity. Moreover, the functions

$$\overset{\circ}{\Psi}_{\mathbf{m}}(\mathbf{k}, \zeta, \delta, \mathbf{x}) = F_{\mathbf{m}}(\mathbf{k}, g, \zeta, \delta, \mathbf{x})|_{g=\overset{\circ}{\lambda}(\mathbf{m}, \mathbf{k}, \zeta, \delta)}, \quad \mathbf{m} \in \mathbf{Z}_+^d \quad (246)$$

form the complete set of eigenfunctions of the operator  $\overset{\circ}{\Theta}_{\mathbf{k}, \zeta, \delta}$  such that

$$\overset{\circ}{\Theta}_{\mathbf{k}, \zeta, \delta} \overset{\circ}{\Psi}_{\mathbf{m}}(\zeta, \delta, \mathbf{k}, \mathbf{x}) = \overset{\circ}{\lambda}(\mathbf{m}, \mathbf{k}, \zeta, \delta) \overset{\circ}{\Psi}_{\mathbf{m}}(\zeta, \delta, \mathbf{k}, \mathbf{x}), \quad \mathbf{m} \in \mathbf{Z}_+^d. \quad (247)$$

**Proof.** The proof readily follows from the definition of the operators  $\overset{\circ}{\Theta}_{\mathbf{k}, \zeta, \delta}$  and (232).  $\square$

The main results of this section are the next two statements for the case  $d = 2$ .

**Theorem 34** Let  $d = 2$ . For any natural number  $N_0$  and any positive constant  $C$  there exists a positive constant  $c$  such that for any  $\beta > C$  and for any  $w < c$

$$\sigma(\overset{\circ}{\Theta}_{\zeta, \delta}) \cap I = \left[ \bigcup_{0 \leq n \leq N_0} [wD_n^-(\zeta, \delta), wD_n^+(\zeta, \delta)] \right] \cap I, \quad (248)$$

$$I = [0, 2\pi w(N_0 - 1)],$$

and the endpoints  $D_n^\pm(\zeta, \delta)$  can be approximated by the numbers  $D_n^\pm$  (which are defined in (133), (134)) as

$$|D_n^\pm(\zeta, \delta) - D_n^\pm| \leq 7w \quad (249)$$

In fact, we can describe location of the spectrum in any bounded portion of the spectral axis as it is formulated in the next statement.

**Theorem 35** Let  $d = 2$ . For any constant  $N \geq \pi$  there exist positive constants  $C$  and  $c$  such that for any  $\beta > C$  and for any  $w < c$

$$\sigma(\overset{\circ}{\Theta}_{\zeta, \delta}) \cap [0, N] = [\sigma_E(\overset{\circ}{\Theta}_{\zeta, \delta}) \cup \sigma_H(\overset{\circ}{\Theta}_{\zeta, \delta})] \cap [0, N], \quad (250)$$

where the sets  $\sigma_E(\overset{\circ}{\Theta}_{\zeta, \delta})$  and  $\sigma_H(\overset{\circ}{\Theta}_{\zeta, \delta})$  are respectively of the form (22), (23), (25):

$$\sigma_E(\overset{\circ}{\Theta}_{\zeta, \delta}) = \bigcup_{n \geq 0} [\tilde{w}D_n^-(\zeta, \delta), \tilde{w}D_n^+(\zeta, \delta)], \quad \text{where}$$

$$D_n^\pm(\zeta, \delta) = 2\pi n(1 + \chi_n^\pm), \quad n \geq 1; \quad D_0^-(\zeta, \delta) = 0, \quad D_0^+(\zeta, \delta) = 4 + \chi_0^+,$$

$$\sigma_H(\overset{\circ}{\Theta}_{\zeta, \delta}) = \bigcup_{\mathbf{n} \geq 0} [(\pi \mathbf{n})^2 + \rho_{\mathbf{n}}^-, (\pi \mathbf{n})^2 + \rho_{\mathbf{n}}^+],$$

and the quantities  $\chi_n^\pm$ ,  $\eta_n^\pm$  and  $\rho_{\mathbf{n}}^\pm$  satisfy the estimates

$$|\chi_n^\pm| \leq 100N\beta^{-1} + 6e^{-0.3n}, \quad 1 \leq n \leq N(\pi w)^{-1}, \quad (251)$$

$$|\eta_n^\pm| \leq 5 \cdot 10^3 N\beta^{-1} + 2 \cdot 10^3 e^{-0.3n} + 3n^{-1} + 300w, \quad 1 \leq n \leq N(\pi w)^{-1}, \quad (252)$$

and for some constant  $C_1$

$$|\rho_{\mathbf{n}}^\pm| \leq C_1(w + \beta^{-1}), \quad |\mathbf{n}| \leq \sqrt{N}\pi^{-1}. \quad (253)$$

In particular, the spectrum  $\sigma(\overset{\circ}{\Theta}_{\zeta, \delta})$  has adjacent bands and gaps of order  $w$ .

The proofs of the theorems are provided below; they are based on the results that we obtained for one-dimensional operators and on appropriate estimates for the eigenvalues of the operator  $\Theta_{\mathbf{k}, \varepsilon}$ .

## 6.2 2D case with separated variables

From now on we shall assume that  $d = 2$ . The relationships (237), (239), (244) and Lemmas 32, 33 imply the next statement.

**Corollary 36** *For  $d = 2$  the spectrum  $\sigma(\mathring{\Theta}_{\zeta, \delta})$  of the operator  $\mathring{\Theta}_{\zeta, \delta}$  can be represented as*

$$\sigma(\mathring{\Theta}_{\zeta, \delta}) = \bigcup_{\mathbf{n} \in \mathbf{Z}_+^2} B_{\mathbf{n}}(\zeta, \delta), \quad \mathbf{n} = (n_1, n_2), \quad (254)$$

where each band  $B_{\mathbf{n}}(\zeta, \delta)$  is the set:

$$B_{\mathbf{n}}(\zeta, \delta) = \{g(\mathbf{n}, \mathbf{k}, \zeta, \delta) : \mathbf{k} = (k_1, k_2), 0 \leq k_1, k_2 \leq \pi\}. \quad (255)$$

Here  $g(\mathbf{n}, \mathbf{k}, \zeta, \delta)$  is the unique solution of the equation

$$\xi_{n_1}(k_1, g\tilde{w}^{-1}, \delta) + \xi_{n_2}(k_2, g\tilde{w}^{-1}, \delta) = g. \quad (256)$$

The bands  $B_{\mathbf{n}}(\zeta, \delta)$  can overlap, but this possibility is limited by the following statements.

**Lemma 37** *Each band  $B_{\mathbf{n}}(\zeta, \delta)$ ,  $\mathbf{n} \in \mathbf{Z}_+^2$  is an interval, i.e.  $B_{\mathbf{n}}(\zeta, \delta) = [G_{\mathbf{n}}^-(\zeta, \delta), G_{\mathbf{n}}^+(\zeta, \delta)]$ . The endpoints  $G_{\mathbf{n}}^-(\zeta, \delta) < G_{\mathbf{n}}^+(\zeta, \delta)$  of the interval  $B_{\mathbf{n}}(\zeta, \delta)$  can be found from the equations:*

$$\xi_{n_1}(\kappa, g\tilde{w}^{-1}, \delta) + \xi_{n_2}(\kappa, g\tilde{w}^{-1}, \delta) = g, \quad \text{for } \kappa = 0, \pi. \quad (257)$$

In addition to that,

$$G_{\mathbf{n}}^-(\zeta, \delta) \leq G_{\mathbf{m}}^-(\zeta, \delta), \quad G_{\mathbf{n}}^+(\zeta, \delta) \leq G_{\mathbf{m}}^+(\zeta, \delta), \quad \text{if } m_j \geq n_j, \quad j = 1, 2. \quad (258)$$

In particular, if for some natural  $N$  the set  $\bigcup_{|\mathbf{n}|_1 \leq N} B_{\mathbf{n}}(\zeta, \delta)$  has an interior gap, then the entire set  $\bigcup B_{\mathbf{n}}(\zeta, \delta)$  has this gap. (Here  $|\mathbf{n}|_1 = n_1 + n_2$ .)

**Proof.** We notice first that  $\xi_n(\kappa, D, \delta)$ , being the eigenvalues of the Schrödinger operator  $Q(\kappa, D, \delta)$ , are monotonic functions of the argument  $\kappa$  (see [RS]), and according to our definition  $\xi_n(\kappa, D, \delta) \geq \xi_m(\kappa, D, \delta)$  if  $n \geq m$ . These observations along with (256) imply all the statements of the lemma.  $\square$

In particular, Lemma 37 enables us to consider just a finite number of bands  $B_{\mathbf{n}}(\zeta, \delta)$  in order to prove existence of a gap in the spectrum.

### 6.2.1 Preliminary analysis of the spectra

Analysis of the spectrum  $\sigma(\mathring{\Theta}_{\zeta, \delta})$  is based on Corollary 36 and on our results for the Schrödinger operators with point potential. It shows that the spectrum naturally splits into two subspectra. Both of these subspectra have band gap structure, but the typical sizes of bands and gaps for these spectra are different. Moreover, the eigenmodes associated with these subspectra have different spatial energy distribution. We will call these subspectra  $E$ -subspectrum and  $H$ -subspectrum. They can be defined in terms of the intervals  $B_{\mathbf{n}}$  from Corollary 36 as follows:

$$\sigma(\mathring{\Theta}_{\zeta, \delta}) = \sigma_E(\mathring{\Theta}_{\zeta, \delta}) \bigcup \sigma_H(\mathring{\Theta}_{\zeta, \delta}), \quad \text{where} \quad (259)$$

$$\sigma_E(\mathring{\Theta}_{\zeta, \delta}) = \bigcup_{n \in \mathbf{Z}_+} B_{(0, n)}(\zeta, \delta); \quad \sigma_H(\mathring{\Theta}_{\zeta, \delta}) = \bigcup_{n_1, n_2 > 0} B_{(n_1, n_2)}(\zeta, \delta). \quad (260)$$

Thus, the  $E$ -subspectrum can be associated with the equations (256) where at least one index  $n_j$  is zero, while the  $H$ -subspectrum can be associated with these equations when both indices  $n_j$  are positive. To analyze the equations for the  $E$ -subspectrum we substitute  $D = g\tilde{w}^{-1}$  and rewrite these equations as

$$\xi_0(k_1, D, \delta) + \xi_n(k_2, D, \delta) = D\tilde{w}. \quad (261)$$

Correspondingly, the spectrum  $\sigma_E(\mathring{\Theta}_{\zeta, \delta})$  can be rewritten as

$$\sigma_E(\mathring{\Theta}_{\zeta, \delta}) = \bigcup_{n \in \mathbf{Z}_+} \tilde{w} \tilde{B}_{(0, n)}(\zeta, \delta), \quad (262)$$

where the band  $\tilde{B}_{(0, n)}, n \geq 0$  is the set described as

$$\tilde{B}_{(0, n)}(\zeta, \delta) = \{D(n, \mathbf{k}, \zeta, \delta) : \mathbf{k} = (k_1, k_2), 0 \leq k_1, k_2 \leq \pi\}. \quad (263)$$

Here  $D(n, \mathbf{k}, \zeta, \delta)$  is the unique solution of the equation (261).

We notice now that if  $w$  is small, then the equations (256) can be viewed as perturbations of the equations (132), hence

$$\sigma_E(\mathring{\Theta}_{\zeta, \delta}) \approx \tilde{w} \sigma_E = \left\{ [0, 4\tilde{w}] \bigcup \left[ \bigcup_{n > 0} [2\pi n \tilde{w}, (2\pi n + 1)\tilde{w}] \right] \right\}. \quad (264)$$

Here  $\sigma_E$  is the absolute spectrum described by (26) and by the Lemma 16. As far as the intervals  $B_{\mathbf{n}}, \mathbf{n} > 0$  are concerned, we notice that for small  $w$  and  $n > 0$

$$\xi_n(\kappa, g\tilde{w}^{-1}, \delta) \approx (\pi n)^2 \approx g,$$

therefore

$$\sigma_H(\mathring{\Theta}_{\zeta, \delta}) \approx \bigcup_{\mathbf{n} > 0} [(\pi \mathbf{n})^2 - c_{\mathbf{n}} w, (\pi \mathbf{n})^2 + c_{\mathbf{n}} w], \quad (265)$$

where  $c_{\mathbf{n}}$  are some constants.

### 6.2.2 $E$ -subspectrum

This subsection is devoted to precise formulation of the approximate formula (264). Analysis of this subspectrum amounts to investigating the equations (261). These equations can be viewed as perturbations of the equation (132). This analysis is based on the results of the Lemmas 20, 23, 24, 25, and, in particular, on the relationships (184), (202), (204) and (205).

We start with the  $E$ -subspectrum  $\sigma_E(\mathring{\Theta}_{\zeta, \delta})$  and with the equations (261). It is sufficient to consider the case when  $\{k_1, k_2\} = \{0, \pi\}$ . If  $\kappa = 0, \pi$ , then the equations (261) can be rewritten as

$$\mu_n(\kappa, D, \delta) = \sqrt{\nu_j^2(D, \delta) + D\tilde{w}}, \quad j = 0, 1; \kappa = 0, \pi; n > 0 \quad (266)$$

If  $w$  (and hence  $\delta$ ) is small, this is a perturbation of the equation

$$\mu_n(\kappa, D) = \nu_j(D), \quad j = 0, 1; \kappa = 0, \pi; n > 0 \quad (267)$$

This is just the equation (132), which has already been studied well. As it follows from the general theory ([RS]), depending on parity of  $n$ , either  $\mu_n(0, D) > \mu_n(\pi, D)$ , or  $\mu_n(0, D) < \mu_n(\pi, D)$ . It is convenient to introduce the quantities

$$\mu_n^+(D, \delta) = \max_{\kappa=0, \pi} \mu_n(\kappa, D, \delta), \quad \mu_n^-(D, \delta) = \min_{\kappa=0, \pi} \mu_n(\kappa, D, \delta). \quad (268)$$



In particular, for  $\delta = 0$  these are the previously defined quantities  $\mu_n^\pm(D)$  (see (104)). The endpoints  $D_n^\pm(\zeta, \delta)$  of the bands  $B_{(0,n)}(\zeta, \delta)$ ,  $n \geq 0$  (see notation in Lemma 37) are the unique solutions of the equations:

$$\mu_n^-(D, \delta) = \sqrt{\nu_0^2(D, \delta) + D\tilde{w}} \text{ for } D_n^-(\zeta, \delta). \quad (269)$$

$$\mu_n^+(D, \delta) = \sqrt{\nu_1^2(D, \delta) + D\tilde{w}} \text{ for } D_n^+(\zeta, \delta). \quad (270)$$

Here the dependence of these endpoints on the parameter  $\zeta$  is hidden in the parameter  $w$ . If  $\tilde{w}$  (and hence  $\delta$ ) is small, these equation can be viewed as perturbations of the equations (134).

Two lemmas below are the key statements in describing the  $E$ -subspectrum which can be established based on Lemmas 6, 7, 25, 9, 20, 21, 24.

**Lemma 38** *Suppose that  $\beta > C$  for some positive constant  $C$ . Then for any integer  $n \geq 0$*

$$\lim_{w \rightarrow 0} D_n^\pm(\zeta, \delta) = D_n^\pm. \quad (271)$$

Moreover, for any natural number  $N_0$

$$|D_n^\pm(\zeta, \delta) - D_n^\pm| \leq 6w, \quad 0 \leq n \leq N_0 \quad (272)$$

for sufficiently small  $w$ .

**Lemma 39** *For any constant  $N \geq \pi$  there exist constants  $C$  and  $c$  such that for any  $\beta > C$  and  $w < c$ , and for any integer  $n \in [1, Nw^{-1}]$  the following representations hold:*

$$D_n^\pm(\zeta, \delta) = 2\pi n(1 + \chi_n^\pm), \quad |\chi_n^\pm| \leq 100N\beta^{-1} + 6e^{-0.3n} \quad (273)$$

$$D_n^+(\zeta, \delta) - D_n^-(\zeta, \delta) = \pi + \eta_n^+; \quad D_{n+1}^-(\zeta, \delta) - D_n^-(\zeta, \delta) = 2\pi + \eta_n^- \quad (274)$$

$$|\eta_n^+| \leq 5 \cdot 10^3 N\beta^{-1} + 2 \cdot 10^3 e^{-0.3n} + 3n^{-1} + 300w \quad (275)$$

$$|\eta_n^-| \leq 2 \cdot 10^3 N\beta^{-1} + 800e^{-0.6n} + 80w \quad (276)$$

### 6.2.3 $H$ -subspectrum

In this section we investigate the portion of spectrum associated with the equations (256) for  $\mathbf{n} = (n_1, n_2) > 0$ . If we fix the multiindex  $\mathbf{n}$  then according to Lemma 37 the endpoints  $G_{\mathbf{n}}^-(\zeta, \delta), G_{\mathbf{n}}^+(\zeta, \delta)$  of the band  $B_{\mathbf{n}}(\zeta, \delta)$  are the solutions to the equations

$$[\mu_{n_1}^-(g\tilde{w}^{-1}, \delta)]^2 + [\mu_{n_2}^-(g\tilde{w}^{-1}, \delta)]^2 = g \quad \text{for } g_{\mathbf{n}}^-(\zeta, \delta), \quad (277)$$

$$[\mu_{n_1}^+(g\tilde{w}^{-1}, \delta)]^2 + [\mu_{n_2}^+(g\tilde{w}^{-1}, \delta)]^2 = g \quad \text{for } g_{\mathbf{n}}^+(\zeta, \delta), \quad (278)$$

where  $\mu_n^\pm$  are defined by (268) and (104).

We start with the following preliminary statement.

**Lemma 40** *For any constant  $N \geq \pi$  there exist constants  $C$  and  $c$  such that for any  $\beta > C$  and  $w < c$  and for any  $\mathbf{n} = (n_1, n_2)$  such that  $n_1, n_2 \in [1, \sqrt{N}/\pi]$  the following inequalities hold:*

$$0.99(\pi\mathbf{n})^2 \leq g_{\mathbf{n}}^\pm(\zeta, \delta) \leq 4(\pi\mathbf{n})^2. \quad (279)$$

**Proof.** Let us denote the left sides of the equations (277) and (278) respectively by  $L_{\mathbf{n}}^-(g)$  and  $L_{\mathbf{n}}^+(g)$ . Under the conditions of the lemma we may use the inequalities (196) and (195) from Lemma 22, where  $C_0 = 2Nw^{-1}$ . Those inequalities hold for any  $0 \leq D \leq 7\pi N\tilde{w}^{-1}$ . Together with (85), (97), they imply for sufficiently big  $C$  and small  $c$

$$0.99(\pi\mathbf{n})^2 \leq L_{\mathbf{n}}^{\pm}(g) \leq 4(\pi\mathbf{n})^2, \quad 0 \leq g \leq 7\pi N.$$

These inequalities along with (277) and (278) imply the inequalities (279) in the indicated range of the index  $\mathbf{n}$ .  $\square$

Now we can get some more precise estimates for the endpoints  $g_{\mathbf{n}}^{\pm}(\zeta, \delta)$ .

**Lemma 41** *For any constant  $N \geq \pi$  there exist constants  $C, L$  and  $c$  such that for any  $\beta > C$  and  $w < c$  and for any  $\mathbf{n} = (n_1, n_2)$  such that  $n_1, n_2 \in [1, \sqrt{N}/\pi]$  the following inequalities hold:*

$$\left| g_{\mathbf{n}}^{\pm}(\zeta, \delta) - (\pi\mathbf{n})^2 \right| \leq L(w + \beta^{-1}) \quad (280)$$

**Proof.** Due to of the Lemma 40, we can use again the inequalities (195) in order to estimate  $g_{\mathbf{n}}^{\pm}(\zeta, \delta)$  more precisely. Setting in (195)  $N_0$  equal to the smallest natural number grater than  $\sqrt{N}/\pi$  and  $C_0 = 2Nw^{-1}$ , and using (279), we consequently arrive at the next inequalities for sufficiently small  $w$ :

$$\left| \mu_{n_j}^{\pm} (g_{\mathbf{n}}^{\pm}(\zeta, \delta)\tilde{w}^{-1}, \delta) - \mu_{n_j}^{\pm} (g_{\mathbf{n}}^{\pm}(\zeta, \delta)\tilde{w}^{-1}) \right| \leq L_1\beta^{-1}, \quad (281)$$

$$\left| L_{\mathbf{n}}^{\pm} (g_{\mathbf{n}}^{\pm}(\zeta, \delta)\tilde{w}^{-1}) - \sum_{j=1,2} \left[ \mu_{n_j}^{\pm} (g_{\mathbf{n}}^{\pm}(\zeta, \delta)\tilde{w}^{-1}) \right]^2 \right| \leq L_2\beta^{-1}, \quad (282)$$

where  $L_1$  and  $L_2$  are some constants. Then using (104), (101) and (279), we obtain

$$\mu_{n_j}^{\pm} (g_{\mathbf{n}}^{\pm}(\zeta, \delta)\tilde{w}^{-1}) = \pi n_j, \quad \left| \mu_{n_j}^{\pm} (g_{\mathbf{n}}^{\pm}(\zeta, \delta)\tilde{w}^{-1}) - \pi n_j \right| \leq L_3 w \quad (283)$$

for some constant  $L_3$ . The last inequalities together with (282) imply the desired inequalities (280).  $\square$

**Proof of Theorems 34 and 35.** To prove Theorem 34 we use the representation of the spectrum  $\sigma_E \left( \overset{\circ}{\Theta}_{\zeta, \delta} \right)$  as the union of intervals provided by the formulas (260), (262), (263) and notice that  $D_n^-(\zeta, \delta) \leq D(n, \mathbf{k}, \zeta, \delta) \leq D_n^+(\zeta, \delta)$ . This along with Lemma 38 and (21) implies the statement of Theorem 34.

The proof of Theorem 35 is also based on formulas (260), (262), (263) for  $E$ -subspectrum and, in addition to that, on the formulas (255), (256) (where  $\mathbf{n} > 0$ ) for  $H$ -subspectrum. Then we notice that  $g_{\mathbf{n}}^{\pm}(\zeta, \delta) \leq g(n, \mathbf{k}, \zeta, \delta) \leq g_{\mathbf{n}}^{\pm}(\zeta, \delta)$ . This observation along with the asymptotic relationships from Lemmas 39 and 41 imply the statement of Theorem 35.  $\square$ .

### 6.3 General scalar 2D case.

In this section we deal only with the case  $d = 2$ . We show that under some appropriate condition on  $\zeta$  and  $\delta$ , the difference between the function  $\overset{\circ}{\varepsilon}(\mathbf{x})$  (for which variables separate) and  $\varepsilon(\mathbf{x})$  is sufficiently small, which ensures closeness of the corresponding spectra.

We denote the eigenvalues of a self-adjoint operator  $\mathcal{A}$  by  $\lambda_0(\mathcal{A}) \leq \lambda_1(\mathcal{A}) \leq \dots$ . We also denote the eigenfunctions of the operator  $\Theta_{\mathbf{k}, \varepsilon(\mathbf{x})}$  by  $e_l(\varepsilon, \mathbf{k}, \mathbf{x}), l = 0, 1, \dots$

**Lemma 42** *Suppose that  $\varepsilon(\mathbf{x}) \leq \varepsilon_1(\mathbf{x})$  and the eigenfunctions  $e_l(\varepsilon_1, \mathbf{k}, \mathbf{x})$  are normalized as*

$$\int_X \varepsilon_1(\mathbf{x}) e_m^*(\varepsilon_1, \mathbf{k}, \mathbf{x}) e_l(\varepsilon_1, \mathbf{k}, \mathbf{x}) d\mathbf{x} = \delta_{m,l}. \quad (284)$$

Then

$$\lambda_n (\Theta_{\mathbf{k}, \varepsilon(\mathbf{x})}) \geq \lambda_n (\Theta_{\mathbf{k}, \varepsilon_1(\mathbf{x})}), \quad n = 0, 1, \dots \quad (285)$$

Let the matrix  $A_n$  with the entries

$$A_n(m, l) = \int_X [\varepsilon_1(\mathbf{x}) - \varepsilon(\mathbf{x})] e_m^*(\varepsilon_1, \mathbf{k}, \mathbf{x}) e_l(\varepsilon_1, \mathbf{k}, \mathbf{x}) d\mathbf{x}, \quad (286)$$

$$0 \leq m, l \leq n$$

have the  $l_2$ -norm  $\|A_n\| < 1$ . Then

$$\lambda_m (\Theta_{\mathbf{k}, \varepsilon(\mathbf{x})}) \leq \lambda_m (\Theta_{\mathbf{k}, \varepsilon_1(\mathbf{x})}) (1 - \|A_n\|)^{-1}, \quad 0 \leq m \leq n. \quad (287)$$

In particular,

$$\lambda_m (\Theta_{\mathbf{k}, \varepsilon(\mathbf{x})}) \leq \lambda_m (\Theta_{\mathbf{k}, \varepsilon_1(\mathbf{x})}) + \lambda_m (\Theta_{\mathbf{k}, \varepsilon_1(\mathbf{x})}) \|A_n\| (1 - \|A_n\|)^{-1}, \quad 0 \leq m \leq n. \quad (288)$$

**Proof.** From the min-max principle we have for  $m = 0, 1, \dots$

$$\lambda_m (\Theta_{\mathbf{k}, \varepsilon(\mathbf{x})}) = \min_{V^m \subset \mathcal{D}} \max_{\varphi \in V^m} \left( \int_X |\nabla \varphi(\mathbf{x})|^2 d\mathbf{x} \right) \left( \int_X |\varphi(\mathbf{x})|^2 \varepsilon(\mathbf{x}) d\mathbf{x} \right)^{-1}, \quad (289)$$

where  $\mathcal{D}$  is the domain of the quadratic form of the operator  $\Theta_{\mathbf{k}, \varepsilon(\mathbf{x})}$  and  $V^m$  is a subspace of the dimension  $m + 1$ . Since the domain does not depend on  $\varepsilon$ , this representation implies the inequality (285). To prove (287) we pick the subspace  $W^{n+1}$  to be equal to the linear span of the vectors  $e_l = e_l(\varepsilon_1, \mathbf{k}, \mathbf{x})$ ,  $0 \leq l \leq n$ . Then (289) leads to

$$\lambda_m (\Theta_{\mathbf{k}, \varepsilon(\mathbf{x})}) \leq \min_{V^m \subset W^{n+1}} \max_{\varphi \in V^m} \left( \int_X |\nabla \varphi(\mathbf{x})|^2 d\mathbf{x} \right) \left( \int_X |\varphi(\mathbf{x})|^2 \varepsilon(\mathbf{x}) d\mathbf{x} \right)^{-1}. \quad (290)$$

Introducing notation  $t = (t_0, \dots, t_n) \in \mathbf{C}^{n+1}$  and  $\varphi_t = \sum t_j e_j$ , we obtain from (289)

$$\lambda_m (\Theta_{\mathbf{k}, \varepsilon(\mathbf{x})}) \leq \min_{V^m \subset W^{n+1}} \max_{t \in V^m} \left( \int_X |\nabla \varphi_t(\mathbf{x})|^2 d\mathbf{x} \right) \left( \int_X |\varphi_t(\mathbf{x})|^2 \varepsilon(\mathbf{x}) d\mathbf{x} \right)^{-1}. \quad (291)$$

Let us introduce the matrix  $L_n$  with the entries

$$L_n(m, l) = \lambda_l (\Theta_{\mathbf{k}, \varepsilon_1(\mathbf{x})}) \delta_{l, m}, \quad 0 \leq m, l \leq n,$$

and the identity matrix  $I_n$  acting in the space  $\mathbf{C}^{n+1}$ . Then, since  $e_l$  are the normalized eigenfunctions of the operator  $\Theta_{\mathbf{k}, \varepsilon_1(\mathbf{x})}$ , we can rewrite (291) as

$$\lambda_m (\Theta_{\mathbf{k}, \varepsilon(\mathbf{x})}) \leq \min_{V^m \subset W^{n+1}} \max_{t \in V^m} \frac{(L_n t, t)}{((I_n - A_n)t, t)}. \quad (292)$$

Since  $|((I_n - A_n)t, t)| \geq (1 - \|A\|)(t, t)$ , where  $(\cdot, \cdot)$  is the Hermitian scalar product in  $\mathbf{C}^{n+1}$ , the inequality (292) implies (287).  $\square$

To estimate the norm  $\|A_n\|$  we use the following simple statement which is the consequence of the inequality

$$\|A\| = \max \lambda_j(A) \leq \text{Tr} \{A\} \leq (n + 1) \max_{0 \leq m \leq n} \{|A_{m, m}|\}.$$

**Proposition 43** Let  $A = \{A_{m,l}\}, 0 \leq m, l \leq n$  be a positive definite matrix and  $\|A\|$  be its  $l_2$ -norm. Then

$$\|A\| \leq (n+1) \max_{0 \leq m \leq n} \{|A_{m,m}|\}. \quad (293)$$

We now apply Lemma 42 for  $\varepsilon_1(\mathbf{x}) = \overset{\circ}{\varepsilon}(\mathbf{x}) = \varepsilon_\rho$ . In this case  $\Theta_{\mathbf{k}, \overset{\circ}{\varepsilon}} \equiv \overset{\circ}{\Theta}_{\mathbf{k}, \zeta, \delta}$ . To use the lemma we need to normalize the eigenfunctions  $e_q(\varepsilon_\rho, \mathbf{k}, \mathbf{x})$  according to (284). We recall that these eigenfunctions can be represented, due to separation of variables, by means of the formulas (243) and (246). Thus, taking in account that the eigenfunctions  $f_m(\kappa, y)$  are normalized according to (240), we define now the normalized eigenfunctions  $\overset{\circ}{\Psi}_{\mathbf{m}}(\mathbf{k}, \zeta, \delta, \mathbf{x})$ :

$$\begin{aligned} \overset{\circ}{\Psi}_{\mathbf{m}}(\mathbf{k}, \zeta, \delta, \mathbf{x}) &= \overset{\circ}{\Psi}_{\mathbf{m}}(\mathbf{k}, \mathbf{x}) \\ &= \left( \sum_{1 \leq j \leq d} \int_0^1 \rho_{\zeta, \delta}(y) |f_{m_j}(k_j, y)|^2 dy \right)^{-1/2} \prod_{1 \leq j \leq d} f_{m_j}(k_j, x_j). \end{aligned} \quad (294)$$

It is clear now that

$$\int_X \overset{\circ}{\varepsilon}(\mathbf{x}) \overset{\circ}{\Psi}_{\mathbf{m}}^*(\mathbf{k}, \mathbf{x}) \overset{\circ}{\Psi}_{\mathbf{n}}(\mathbf{k}, \mathbf{x}) d\mathbf{x} = \delta_{\mathbf{m}\mathbf{n}}.$$

To apply Lemma 42 we need to estimate the integrals (286). This is the subject of the next lemma.

**Lemma 44** For any constant  $N \geq \pi$  there exist positive constants  $C$  and  $c$  such that for any  $\beta > C$  and  $w < c$  and for any integer  $n \in [0, Nw^{-1}]$  the following estimates hold:

$$\int_{\Gamma_{1,1}} |\overset{\circ}{\Psi}_{(0,n)}(\mathbf{x})|^2 d\mathbf{x} \leq 8\zeta^{-1} \delta D_n^+(\zeta, \delta) \leq 9\zeta^{-1} \delta \max\{2\pi n, 5\}. \quad (295)$$

If  $\mathbf{n} > 0$  and  $(\pi\mathbf{n})^2 \leq N$ , then

$$\int_{\Gamma_{1,1}} |\overset{\circ}{\Psi}_{\mathbf{n}}(\mathbf{x})|^2 d\mathbf{x} \leq 8\zeta^{-1} \delta w^{-1} g_{\mathbf{n}}^+(\zeta, \delta) \leq 9\zeta^{-1} \delta w^{-1} (\pi\mathbf{n})^2 \leq 9\zeta^{-1} \delta w^{-1} N. \quad (296)$$

**Proof.** Using the notation of the Lemma 27 we normalize the functions  $\psi_\theta(\kappa, D, \delta; y)$  by the condition

$$\int_0^1 |\psi_\theta(\kappa, D, \delta; y)|^2 dy = 1.$$

Consider now two of these functions  $\psi_j = \psi_{\theta_j}(\kappa, D_j, \delta; y)$  and the constants  $C_j = \sqrt{C_{D_j, \theta_j}}$  for  $j = 1, 2$  (see (210)). Then we have

$$\begin{aligned} |\psi_j(y)|^2 &\leq C_j, \quad 0 \leq y \leq \delta; \quad \int_0^1 |\psi_j(y)|^2 dy = 1; \\ L_j &= \int_0^\delta |\psi_j(y)|^2 dy \leq C_j \delta = c_j. \end{aligned} \quad (297)$$

Now we consider the function

$$\begin{aligned} \Psi(\mathbf{x}) &= \Psi(x_1, x_2) = \left( \sum_{1 \leq j \leq 2} \int_0^1 \rho_{\zeta, \delta}(y) |\psi_j(y)|^2 dy \right)^{-1/2} \prod_{1 \leq j \leq 2} \psi_j(x_j) \\ &= \frac{\psi_1(x_1) \psi_2(x_2)}{\sqrt{(\zeta-1)(L_1 + L_2) + 2}} \end{aligned}$$

From (297) it follows that

$$\int_{\Gamma_{1,1}} |\Psi(\mathbf{x})|^2 d\mathbf{x} \leq \frac{L_1 L_2}{(\zeta - 1)(L_1 + L_2) + 2} \leq \frac{c_1 c_2}{(\zeta - 1)(c_1 + c_2) + 2}.$$

(We used here that the middle term in these inequalities is an increasing function of both arguments  $L_1$  and  $L_2$ ). In addition to that, the right-hand side of the last inequality can be estimated as

$$\frac{c_1 c_2}{(\zeta - 1)(c_1 + c_2) + 2} \leq \frac{c_1 c_2}{(\zeta - 1) \max\{c_1, c_2\}} \leq (\zeta - 1)^{-1} \min\{c_1, c_2\}.$$

Hence,

$$\int_{\Gamma_{1,1}} |\Psi(\mathbf{x})|^2 d\mathbf{x} \leq (\zeta - 1)^{-1} \delta \min_{j=1,2} \{ \sqrt{C_{D_j, \theta_j}} \}. \quad (298)$$

Let us consider

$$\Psi(\mathbf{x}) = \overset{\circ}{\Psi}_{(0,n)}(\mathbf{x}) = f_0(k_1, D, \delta; x_1) f_n(k_2, D, \zeta, \delta; x_2) \Big|_{D=D(n, \mathbf{k}, \zeta, \delta)}, \quad (299)$$

where  $f_n$  are the eigenfunctions of the operator  $Q(\kappa, D, \delta)$  and  $D(n, \mathbf{k}, \zeta, \delta)$  is defined by (263). Then  $D_n^-(\zeta, \delta) \leq D(n, \mathbf{k}, \zeta, \delta) \leq D_n^+(\zeta, \delta)$ . Let us apply now the inequality (298) for  $\Psi = \overset{\circ}{\Psi}_{(0,n)}$ . We may use in this inequality  $C_{D_j, \theta_j}$  corresponding to  $f_0$ . This allows us to take the top line in the representation (210) and to set there  $D_1 = D_n^+(\zeta, \delta)$  if  $n > 0$  and  $D_1 = 5$  for  $n = 0$ . Using now (271), (273), (133) and (139) to estimate  $D_n^+(\zeta, \delta)$  and plugging the results consequently in (210) and then in (298), we arrive at the desired inequality (295). We also use Lemma 1 in order to replace  $\zeta - 1$  by  $\zeta$ .

The arguments needed to establish (296) are similar to the ones we used for (295). The only difference is that in the formula (299) we set now  $\Psi = \overset{\circ}{\Psi}_{\mathbf{n}} = f_{n_1} f_{n_2}$ , and  $D(\mathbf{n}, \mathbf{k}, \zeta, \delta) = g(\mathbf{n}, \mathbf{k}, \zeta, \delta) \tilde{w}^{-1}$ . Here  $g(\mathbf{n}, \mathbf{k}, \zeta, \delta)$  is defined after (255). Then we use again the representation (210), where

$$D_1 = g(\mathbf{n}, \mathbf{k}, \zeta, \delta) \tilde{w}^{-1}; \quad \theta_j = \mu_{n_j}(k_j, D, \delta) \Big|_{D=g(\mathbf{n}, \mathbf{k}, \zeta, \delta) \tilde{w}^{-1}}.$$

Then we notice that  $g_{\mathbf{n}}^-(\zeta, \delta) \leq g(\mathbf{n}, \mathbf{k}, \zeta, \delta) \leq g_{\mathbf{n}}^+(\zeta, \delta)$  and use the estimates (280) for  $g_{\mathbf{n}}^{\pm}(\zeta, \delta)$  and the estimates (281) and (283) for  $\mu_{n_j}^{\pm}(D, \delta)$ . Plugging the relevant estimates in the representation (210) and then using the inequality (298), we obtain the inequality (296).  $\square$

Lemmas 44 and 42 imply the following important statements.

**Lemma 45** *For any natural number  $N_0$  and a positive constant  $C$  there exists a positive constant  $c$  such that for any  $\beta > C$  and for any  $w < c$  and any integer  $m \in [0, N_0 - 1]$  the following is true:*

$$\lambda_m \left( \overset{\circ}{\Theta}_{\mathbf{k}, \zeta, \delta} \right) \leq \lambda_m \left( \Theta_{\mathbf{k}, \varepsilon(\mathbf{x})} \right) \leq \lambda_m \left( \overset{\circ}{\Theta}_{\mathbf{k}, \zeta, \delta} \right) (1 + 64N_0^2 \delta). \quad (300)$$

In particular,

$$\lambda_m \left( \overset{\circ}{\Theta}_{\mathbf{k}, \zeta, \delta} \right) \leq \lambda_m \left( \Theta_{\mathbf{k}, \varepsilon(\mathbf{x})} \right) \leq \lambda_m \left( \overset{\circ}{\Theta}_{\mathbf{k}, \zeta, \delta} \right) + 10^3 N_0^3 \delta. \quad (301)$$

**Proof.** The proof of the lemma is based on Lemmas 42 and 44. Note first of all that in view of Theorem 34 the first  $N_0$  eigenvalues of the operator  $\overset{\circ}{\Theta}_{\mathbf{k}, \zeta, \delta}$  belong to  $E$ -subspectrum and therefore the corresponding eigenfunctions are of the form  $\overset{\circ}{\Psi}_{(0,m)}$ . Now let us apply Lemma 42 and Proposition 43 for  $n = N_0 - 1$ . Then we have

$$A_{m,m} = \zeta \int_{\Gamma_{1,1}} |\overset{\circ}{\Psi}_{(0,m)}(\mathbf{x})|^2 d\mathbf{x}, \quad 0 \leq m \leq N_0 - 1. \quad (302)$$

This identity, inequality (295), and the estimate of the norm  $\|A_{N_0-1}\|$  based on Proposition 43 imply that

$$\lambda_m \left( \overset{\circ}{\Theta}_{\mathbf{k},\zeta,\delta} \right) \leq \lambda_m \left( \Theta_{\mathbf{k},\varepsilon(\mathbf{x})} \right) \leq \lambda_m \left( \overset{\circ}{\Theta}_{\mathbf{k},\zeta,\delta} \right) (1 - 18\pi N_0^2 \delta)^{-1}.$$

The last inequalities under the conditions of Lemma 42 lead to the estimates (300), which, in turn, imply (301).  $\square$

**Lemma 46** *For any constant  $N \geq \pi$  there exist positive constants  $C$  and  $c$  such that for any  $\beta_1 > C$  (see 18), for any  $w < c$ , and for any integer  $m$  such that*

$$\lambda_m \left( \overset{\circ}{\Theta}_{\mathbf{k},\zeta,\delta} \right) \leq N \tag{303}$$

the following inequalities hold:

$$\lambda_m \left( \overset{\circ}{\Theta}_{\mathbf{k},\zeta,\delta} \right) \leq \lambda_m \left( \Theta_{\mathbf{k},\varepsilon(\mathbf{x})} \right) \leq \lambda_m \left( \overset{\circ}{\Theta}_{\mathbf{k},\zeta,\delta} \right) (1 - 64N^2 \delta w^{-2})^{-1}. \tag{304}$$

In particular,

$$\lambda_m \left( \overset{\circ}{\Theta}_{\mathbf{k},\zeta,\delta} \right) \leq \lambda_m \left( \Theta_{\mathbf{k},\varepsilon(\mathbf{x})} \right) \leq \lambda_m \left( \overset{\circ}{\Theta}_{\mathbf{k},\zeta,\delta} \right) + 10^2 N^2 \beta_1^{-2}. \tag{305}$$

**Proof.** The proof of this lemma is similar to the previous one, but it is a little bit more complicated, since now we have to take care of the eigenfunctions associated with both  $E$ -subspectrum and  $H$ -subspectrum. In fact, the condition (303) enables us to treat both cases more or less uniformly.

Let us estimate first the total number  $L$  of the eigenvalues (taking in account their multiplicity) which satisfy the condition (303). We notice that in view of Theorem 35 the total numbers  $L_E$  and  $L_H$  of the eigenvalues from  $E$ -subspectrum and  $H$ -subspectrum respectively satisfying the condition (303) can be roughly estimated as  $L_E \leq Nw^{-1}$ ,  $L_H \leq N$ . These bounds enable us to estimate the maximal permissible indices  $m$  and  $\mathbf{n}$  for both subspectra. These numbers can be used in the estimates (295) and (296). This along with (302) and with the similar identity for index  $\mathbf{n}$  leads to the inequality  $\max A_{l,l} \leq 60N\delta w^{-1}$ . This inequality, in view of the Proposition 43, implies for small  $w$  that  $\|A_L\| \leq 64N^2\delta w^{-2}$ . This bound together with (287) leads immediately to the estimates (304). The estimates (305) follow from (304), if we take into account (18).  $\square$

**Proof of Theorems 30 and 31.** The proof of these theorems is a combination of Theorems 34 and 35 for the operators  $\overset{\circ}{\Theta}_{\zeta,\delta}$  and of the inequalities provided by the Lemmas 45 and 46.

Let us start with the Theorem 30. The inequalities (301), Theorem 34 and trivial observation that  $\delta = \beta^{-1}w$  lead to the statement of Theorem 30.

As far as Theorem 31 is concerned, our intention is to use the inequalities (305) in order to modify the results of the Theorem 35. We observe now using (18) that  $\beta^{-1} = \beta_1^{-2}w < \beta_2^{-2}w$ , which under the condition  $\beta_2 \gg 1$  of Theorem 31 implies  $\beta^{-1} \ll w$ . The last inequality allows us to drop  $\beta^{-1}$  in the estimate (253). In addition to that, we notice that  $\beta_1^{-2} = \beta_2^{-3}w$  which under the condition  $\beta_2 \gg 1$  yields  $\beta_1^{-2} \ll w$ . Combining these observations with the inequalities (305) and Theorem 35, we come to the statement of Theorem 31.  $\square$

## 7 Spectrum of the Maxwell Operator

### 7.1 General properties and Floquet-Bloch theory

We will use the notation introduced in the beginning of the paper, in particular (3), (4) for the domains  $X$  and  $X'$ , standard basis vectors  $\mathbf{e}_j, 1 \leq j \leq 3$  in the space  $\mathbf{R}^3$  and the following domains in  $\mathbf{R}^2$ . The

dielectric constant  $\varepsilon(\mathbf{x})$  satisfies (5) and (6). We remind that for this kind of periodic dielectric media we will be interested in the waves propagating along the plane  $\langle \mathbf{e}_1, \mathbf{e}_2 \rangle$ , which leads to the condition that the fields  $\mathbf{H}$  and  $\mathbf{E}$  depend on coordinates  $x_1, x_2$  only. That is, from now on we shall assume that

$$\mathbf{H} = \mathbf{H}(x_1, x_2), \quad \nabla \cdot \mathbf{H} = 0; \quad \mathbf{E} = \mathbf{E}(x_1, x_2), \quad \nabla \cdot \varepsilon \mathbf{E} = 0.$$

Let us now make the definitions of our operators precise. First of all, due to the two-dimensionality of the problem we will work with the spaces  $L_2(\mathbf{R}^2, \mathbf{C}^3, \varepsilon dx)$  and  $L_2(\mathbf{R}^2, \mathbf{C}^3)$ . Consider in these spaces the linear subspaces

$$J_1 = \{\mathbf{E}(x_1, x_2) \in L_2(\mathbf{R}^2, \mathbf{C}^3, \varepsilon dx) \mid \nabla \cdot \varepsilon \mathbf{E} = 0\} \quad (306)$$

$$J_2 = \{\mathbf{H}(x_1, x_2) \in L_2(\mathbf{R}^2, \mathbf{C}^3) \mid \nabla \cdot \mathbf{H} = 0\} \quad (307)$$

$$J_1 \subset L_2(\mathbf{R}^2, \mathbf{C}^3, \varepsilon dx), \quad J_2 \subset L_2(\mathbf{R}^2, \mathbf{C}^3).$$

In both cases we understand the divergence in the distributional sense. These subspaces are obviously closed in the corresponding spaces. Our main Hilbert space will be the direct sum

$$J = J_1 \oplus J_2. \quad (308)$$

It is well known that for the waves traveling along the  $\langle \mathbf{e}_1, \mathbf{e}_2 \rangle$  plane there are two possible polarizations. Mathematically speaking, they correspond to the splitting of the space  $J$  into the direct sum of two special subspaces:

$$J = S_E \oplus S_H, \quad (309)$$

where the subspace  $S_E$  (of  $E$ -modes) consists of vector fields of the form

$$((0, 0, E), (H_1, H_2, 0)),$$

and  $S_H$  (the space of  $H$ -modes) consists of fields

$$((E_1, E_2, 0), (0, 0, H)).$$

Let us now turn to the operators. We define the curl operator as an operator acting between the spaces  $J_1$  and  $J_2$  in the following way: its domain  $D_1 \subset J_1$ , as of an operator on  $J_1$  is the set

$$D_1 = \{\mathbf{E}(x_1, x_2) \in J_1 \mid \nabla \times \mathbf{E} \in L_2(\mathbf{R}^2, \mathbf{C}^3)\}. \quad (310)$$

Here, as before, the differentiations are understood in the distributional sense. Now  $\text{curl} = \nabla \times$  is naturally defined on  $D_1$ , and maps this domain into  $J_2$  (which is trivial to check). It is convenient to look closely at the conditions that functions from  $D_1$  must satisfy. Let  $\mathbf{E}(x_1, x_2)$  belong to  $D_1$ . Representing  $\mathbf{E} = (E_1, E_2, E_3)$ , and denoting  $\mathbf{E}' = (E_1, E_2)$ , we get:

$$\nabla E_3 \in L_2(\mathbf{R}^2, \mathbf{C}^2) \quad (311)$$

$$\text{div} \varepsilon \mathbf{E}' = 0 \quad (312)$$

$$\frac{\partial E_2}{\partial x_1} - \frac{\partial E_1}{\partial x_2} \in L_2(\mathbf{R}^2). \quad (313)$$

Here we understand "div" in (312) in the two-dimensional sense. Analogously, we define

$$D_2 = \{\mathbf{H}(x_1, x_2) \in J_2 \mid \nabla \times \mathbf{H} \in L_2(\mathbf{R}^2, \mathbf{C}^3; \varepsilon dx) (= L_2(\mathbf{R}^2, \mathbf{C}^3))\}, \quad (314)$$

and for  $\mathbf{H} = (H_1, H_2, H_3) \in D_2$ ,  $\mathbf{H}' = (H_1, H_2)$  we have:

$$\nabla H_3 \in L_2(\mathbf{R}^2, \mathbf{C}^2) \quad (315)$$

$$\nabla \cdot \mathbf{H}' = 0 \quad (316)$$

$$\frac{\partial H_2}{\partial x_1} - \frac{\partial H_1}{\partial x_2} \in L_2(\mathbf{R}^2) \quad (317)$$

The operator  $\varepsilon^{-1}\nabla \times$  maps  $D_2$  into  $J_1$ . We can define now the operator

$$M = \begin{bmatrix} 0 & ci\varepsilon(\mathbf{x})^{-1}\nabla \times \\ -ci\nabla \times & 0 \end{bmatrix},$$

where  $c$  is the velocity of light. The domain of this operator is

$$D = D_1 \oplus D_2. \quad (318)$$

This is our definition of the relevant Maxwell operator. It is easy to check that the operators

$$ci\varepsilon(\mathbf{x})^{-1}\text{curl} : J_2 \rightarrow J_1; \quad -ci\text{curl} : J_1 \rightarrow J_2$$

are adjoint to each other (see, for instance, [BS] for the thorough discussion of such operators in a more general case), so the Maxwell operator  $M$  has the following structure:

$$M = \begin{bmatrix} 0 & A \\ A^* & 0 \end{bmatrix}$$

for some closed operator  $A$ , and hence is self-adjoint. Looking at (311) and (315), one immediately sees that the direct decomposition (309) leads to the corresponding decomposition of the domain  $D$  (since the conditions in (311) and (315) are imposed independently on the third and on the first two components of magnetic and electric fields):

$$D = (D \cap S_E) \oplus (D \cap S_H). \quad (319)$$

Besides, direct computation shows that the operator  $M$  leaves the spaces  $S_E$  and  $S_H$  invariant. Hence,

$$M = \begin{bmatrix} M|_{S_E} & 0 \\ 0 & M|_{S_H} \end{bmatrix},$$

where  $M|_{S_E}$  and  $M|_{S_H}$  are some self-adjoint operators in  $S_E$  and  $S_H$  respectively. We can conclude now that

$$\sigma(M) = \sigma(M|_{S_E}) \cup \sigma(M|_{S_H}). \quad (320)$$

It turns out that the spectrum  $\sigma_H(M) := \sigma(M|_{S_H})$  is exactly the one studied in the first part [FK] of the paper. The other part of the spectrum,  $\sigma_E(M) := \sigma(M|_{S_E})$  is the main subject of our current investigation. Let us collect the relevant facts about the operator  $M|_{S_E}$ :

a) It acts in the space

$$S_E = \{\mathbf{F} = (E, H_1, H_2) \in L_2(\mathbf{R}^2, \mathbf{C}^3) \mid \nabla \cdot \mathbf{H}' = 0\}, \quad (321)$$

where  $\mathbf{H}' = (H_1, H_2)$ , and the divergence is understood in the two-dimensional sense:  $\nabla \cdot \mathbf{H}' = \partial H_1/\partial x_1 + \partial H_2/\partial x_2$ .

b) The domain of the operator is characterized by the conditions

$$\nabla E \in L_2(\mathbf{R}^2, \mathbf{C}^2), \quad \frac{\partial H_2}{\partial x_1} - \frac{\partial H_1}{\partial x_2} \in L_2(\mathbf{R}^2). \quad (322)$$



c) The matrix representation of the operator is:

$$M|_{S_E} = \begin{bmatrix} 0 & -ic\varepsilon^{-1}\frac{\partial}{\partial x_2} & ic\varepsilon^{-1}\frac{\partial}{\partial x_1} \\ -ic\frac{\partial}{\partial x_2} & 0 & 0 \\ ic\frac{\partial}{\partial x_1} & 0 & 0 \end{bmatrix}. \quad (323)$$

We will also need the operator

$$M_E = -\varepsilon^{-1}\Delta = -\varepsilon^{-1}\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2}\right) \quad (324)$$

defined in  $L_2(\mathbf{R}^2, \varepsilon dx)$  with the domain equal to the Sobolev space  $H^2(\mathbf{R}^2)$ .

**Theorem 47** *A real number  $\lambda$  belongs to the spectrum  $\sigma_E(M)$  of the self-adjoint operator  $M|_{S_E}$  if and only if  $\lambda^2$  belongs to  $\sigma(M_E)$ .*

The proof of this theorem will follow from some results about the Floquet expansions of the relevant operators (these results will be described later on in this section).

**Lemma 48** *The domain of the operator  $M|_{S_E}$  can be described as follows: It consists of all vector functions  $\mathbf{F} = (E, H_1, H_2) \in [H^1(\mathbf{R}^2)]^3$  such that*

$$\nabla \cdot \mathbf{H}' = \frac{\partial H_1}{\partial x_1} + \frac{\partial H_2}{\partial x_2} = 0. \quad (325)$$

*The  $H^1$ -norm on the domain is equivalent to the graph norm.*

**Proof.** First of all, any  $\mathbf{F}$  that satisfies the conditions of the lemma obviously belongs to the domain of  $M|_{S_E}$ . So, let us consider the converse statement. Conditions  $E \in L_2$  and  $\nabla E \in L_2$  (see (311) (i)) imply, by the definition of Sobolev spaces, that  $E \in H^1(\mathbf{R}^2)$ , since

$$\|E\|_{H^1}^2 = \|E\|_{L^2}^2 + \|\nabla E\|_{L^2}^2. \quad (326)$$

Now, conditions (325) (which is one of the conditions on elements of the space  $J$ ) and (315) (iii) imply that  $\mathbf{H}'$  satisfies the system of equations:

$$\begin{cases} \partial H_1 / \partial x_1 + \partial H_2 / \partial x_2 = 0 \\ \partial H_2 / \partial x_1 - \partial H_1 / \partial x_2 = f \end{cases} \quad (327)$$

for some  $f \in L_2(\mathbf{R}^2)$ . Ellipticity of this system enables one to gain smoothness of solutions. Namely, let us denote by  $h_j$  (for  $j = 1, 2$ ) the Fourier transform of  $H_j$ . After the Fourier transform the system (327) becomes

$$\begin{cases} \xi_1 h_1(\xi) + \xi_2 h_2(\xi) = 0 \\ -\xi_2 h_1(\xi) + \xi_1 h_2(\xi) = -i\widehat{f}(\xi). \end{cases} \quad (328)$$

Solving (328), we get  $h_1 = i\xi_2 \widehat{f}(\xi) / |\xi|^2$ ,  $h_2 = -i\xi_1 \widehat{f}(\xi) / |\xi|^2$ , and, hence

$$|h|^2 = |h_1|^2 + |h_2|^2 = |\widehat{f}|^2 / |\xi|^2. \quad (329)$$

Expressing now the square of the  $H^1$ -norm of  $\mathbf{H}'$  as

$$\int_{|\xi| \leq 1} |h(\xi)|^2 (1 + |\xi|)^2 d\xi + \int_{|\xi| > 1} |h(\xi)|^2 (1 + |\xi|)^2 d\xi,$$

and using (329) we conclude that the following estimate holds:

$$\|\mathbf{H}'\|_{H^1}^2 \leq 4\|h\|_{L^2}^2 + C \int_{|\xi|>1} |f|^2 \frac{(1+|\xi|)^2}{|\xi|^2} \leq C\{\|\mathbf{H}'\|_{L^2}^2 + \|\operatorname{curl}\mathbf{H}'\|_{L^2}^2\}. \quad (330)$$

The estimates (326) and (330) imply that all components of the field belong to the Sobolev space  $H^1$ , and that the  $H^1$  norm is equivalent to the graph one.  $\square$

Now we remind the reader some basics of the Floquet theory (see details in [RS], [K93]). The operator  $M|_{S_E}$  is invariant with respect to translations on elements of the integer lattice  $\mathbf{Z}^2$ . According to the standard scheme (see [RS], [K93]), this should lead to some direct integral decomposition of our operator:

$$M|_{S_E} = \int_K^\oplus M(k)dk, \quad (331)$$

where  $M(k)$  is some measurable self-adjoint operator function on  $K$ . This will mean, in particular, that

$$\sigma_E(M) = \cup_k \sigma(M(k)).$$

We are going to describe this decomposition in more details. We will also show that the spectra of operators  $M(k)$  are discrete. This will lead to the proof of the Theorem 47.

Let us consider the following Floquet transforms: for  $f \in L_2(\mathbf{R}^2, \mathbf{C}^3)$  we set

$$\widehat{f}(k, x) f(k, x) = \sum_{m \in \mathbf{Z}^2} f(x - m) e^{ik \cdot m} \quad (332)$$

$$\widetilde{f}(k, x) = e^{-ik \cdot x} \widehat{f}(k, x), \quad x \in X', k \in K. \quad (333)$$

Here  $K = [0, 2\pi] \times [0, 2\pi]$ . (We also need the (non-compact) set  $K' = K \setminus 2\pi\mathbf{Z}^2$ .) These transforms are correctly defined, if we consider the sum as a Fourier series in variables  $k$  with values in the Hilbert space  $L_2(X', \mathbf{C}^3)$  (see [K93] for thorough study and history of these transforms). The reason, why we restrict the values of the argument  $x$  only to the set  $X'$  is that the function  $\widehat{f}(k, x)$  satisfies some natural relations with respect to translations:  $\widehat{f}(k, x + n) = e^{ik \cdot n} \widehat{f}(k, x)$  for all  $n \in \mathbf{Z}^2$ . Therefore, its values are determined completely, if they are given on any fundamental domain of the group  $\mathbf{Z}^2$ , in particular, on  $X$  or on  $X'$ . We get the isometry  $\mathcal{F} : f \rightarrow \widehat{f}$  between  $L_2(\mathbf{R}^2, \mathbf{C}^3)$  and  $\int_K^\oplus L_2(X', \mathbf{C}^3)$  (see [K93], [RS]).

We have to study the behavior of the subspace  $S_E$ , and of the domain of the operator  $M|_{S_E}$  with respect to the transform (332). First of all, the images of the spaces  $L_2$  and  $H^1$  under the transform (332) are known (see [K93]). We present these results in the next two lemmas.

**Lemma 49** (see [K93], Theorem 2.2.5) *Transform (332) is an isometry of the space  $L_2(\mathbf{R}^2)$  onto the space  $L_2(K, L_2(X'))$ , where the latter denotes the Hilbert space of square integrable functions on  $K$  with values in the space  $L_2(X')$ .*

**Remark.** It will be convenient for us to identify the space  $L_2(K, L_2(X'))$  with  $L_2(K', L_2(X'))$ , which is obviously possible.

To describe the image of the Sobolev space  $H^1(\mathbf{R}^2)$  we need to define some new objects. Consider the Sobolev space  $H^1(X')$  and its (closed) subspace  $\mathcal{E}_k^1$  (where  $k \in K$ ) that consists of all  $H^1$ -functions that satisfy the cyclic (or Floquet) boundary conditions:

$$\begin{aligned} u(1 + \delta/2, x_2) &= e^{ik_1} u(\delta/2, x_2), \\ u(x_1, 1 + \delta/2) &= e^{ik_2} u(x_1, \delta/2). \end{aligned} \quad (334)$$

This subspace is closed, due to the embedding theorems. It was shown in [K93], Theorem 2.2.1 that  $\mathcal{E}^1 = \cup_{k \in K} \mathcal{E}_k^1$  is an analytic subbundle of the trivial Hilbert bundle  $K \times H^1(X')$  over  $K$ . In fact, the bundle  $\mathcal{E}^1$  is defined over the whole space  $\mathbf{C}^2$  as an analytic (trivial) Hilbert bundle (see [K93]). One of the results of the Theorem 2.2.5 in [K93] can be rephrased as follows:

**Lemma 50** *Transform (332) is an isometry of the space  $H^1(\mathbf{R}^2)$  onto the space  $L_2(K, \mathcal{E}^1)$ , where the latter denotes the Hilbert space of square integrable sections over  $K$  of the bundle  $\mathcal{E}^1$  (i.e., the subspace of the space  $L_2(K, H^1(X'))$ ) that consists of all functions  $g(k)$  such that  $g(k) \in \mathcal{E}_k^1$  for almost all  $k \in K$ .*

**Remark.** As in the previous lemma, we can identify the space  $L_2(K, \mathcal{E}^1)$  with  $L_2(K', \mathcal{E}^1)$ .

Our next task is to describe the image of the space  $S_E$  (which is a subspace of  $[L^2(\mathbf{R}^2)]^3$ ) under the transform  $\mathcal{F}$ . According to (321) and Lemma 49, it reduces to describing the image of the subspace of  $(L_2(\mathbf{R}^2))^2$  that consists of vector-functions  $\mathbf{H} = (H_1, H_2)$  that have zero divergence:  $\text{div} \mathbf{H} = 0$ . The distributional meaning of the zero divergence condition is that

$$(\mathbf{H}, \nabla \varphi) = 0 \quad (335)$$

for all functions  $\varphi \in C_0^\infty(\mathbf{R}^2)$ . The expression in (335) is obviously continuous in  $\varphi \in H^1(\mathbf{R}^2)$ , hence (335) is still valid on the whole space  $H^1(\mathbf{R}^2)$ . We conclude that  $\mathbf{F} = (E, H_1, H_2)$  belongs to  $S_E$  if and only if

$$\begin{aligned} \mathbf{F} &= (E, H_1, H_2) \in [L^2(\mathbf{R}^2)]^3, \text{ and} \\ (\mathbf{H}, \nabla \varphi) &= 0 \text{ for all } \varphi \in H^1(\mathbf{R}^2). \end{aligned} \quad (336)$$

We will rewrite the condition (336) in terms of the transform  $\mathcal{F}$ . Since the operator  $\nabla$  commutes with translations, and due to the Lemma 50, we conclude that (336) is equivalent to:

$$\int_{K'} (\hat{\mathbf{H}}(k, x), \nabla_x g(k, x))_{L^2(X')} dk = 0 \quad (337)$$

for all  $L^2$ -sections  $g$  of the bundle  $\mathcal{E}^1$ . Here  $\nabla_x$  denotes the *gradient* operator with respect to the variable  $x$ . Let us consider the action of this operator for different values of the "quasimomentum"  $k$ . We denote by  $\nabla(k)$  the restriction of the operator  $\nabla$  onto the space  $\mathcal{E}_k^1$ , and consider  $\nabla(k)$  as an operator between the spaces  $\mathcal{E}_k^1$  and  $[L^2(X')]^2$ . We also consider the restriction of the bundle  $\mathcal{E}^1$  to the space  $\mathbf{C}^2 \setminus 2\pi\mathbf{Z}^2$  (in particular, to  $K'$ ). This restriction is certainly an analytic Hilbert bundle by itself.

**Lemma 51** *(i)  $\nabla(k)$  produces an analytic morphism of the bundle  $\mathcal{E}^1$  over  $\mathbf{C}^2$  into the trivial bundle  $\mathbf{C}^2 \times [L^2(X')]^2$ ;*

*(ii) This morphism has zero kernel over  $\mathbf{C}^2 \setminus 2\pi\mathbf{Z}^2$ , and its range is closed in the every fiber over  $\mathbf{C}^2 \setminus 2\pi\mathbf{Z}^2$ .*

**Proof.** Analyticity is standard: using the transform  $f \rightarrow \tilde{f}$  (333) instead of the transform  $\mathcal{F}$  (332), we get the operator family

$$\nabla_x + ik : H^1(\mathbf{T}^2) \rightarrow [L^2(\mathbf{T}^2)]^2,$$

where  $\mathbf{T}^2$  is the two-dimensional torus obtained from the unit cube  $X'$  (see simple details in [K93]). This operator function is obviously analytic (and even linear) with respect to  $k$ . Using the same representation of our operator function we can check the statements about the range and the kernel. Namely, let us expand functions on  $\mathbf{T}^2$  into the Fourier series:

$$g(x) = \sum_{l \in \mathbf{Z}^2} g_l e^{2\pi i l \cdot x}.$$

Then

$$(\nabla_x + ik)g(x) = i \sum_{l \in \mathbf{Z}^2} (2\pi l + k) g_l e^{2\pi i l \cdot x}.$$

If now  $k$  is not in the dual lattice  $2\pi\mathbf{Z}^2$ , then none of the vector coefficients  $(2\pi l + k)$  can vanish, so the kernel of the operator contains only zero (on the dual lattice, however, the kernel is not trivial). Let us notice now that the mapping

$$i \sum_{l \in \mathbf{Z}^2} (2\pi l + k) g_l e^{2\pi i l \cdot x} \rightarrow \sum_{l \in \mathbf{Z}^2} g_l e^{2\pi i l \cdot x}$$

(defined only on the range of the operator) is uniquely defined and continuous from  $L^2$  to  $H^1$  topology, provided again that  $k$  is not in  $2\pi\mathbf{Z}^2$ . Namely, the square of the  $H^1$ -norm of the right hand side can be estimated as follows:

$$\begin{aligned} \sum_{l \in \mathbf{Z}^2} |g_l|^2 (1 + |l|)^2 &= \sum_{l \in \mathbf{Z}^2} |g_l|^2 \frac{|2\pi l + k|^2 (1 + |l|)^2}{|2\pi l + k|^2} = \\ \sum_{l \in \mathbf{Z}^2} |g_l (2\pi l + k)|^2 \frac{(1 + |l|)^2}{|2\pi l + k|^2} &\leq C \sum_{l \in \mathbf{Z}^2} |g_l (2\pi l + k)|^2, \end{aligned}$$

which is the  $L^2$ -norm of  $i \sum_{l \in \mathbf{Z}^2} (2\pi l + k) g_l e^{2\pi i l \cdot x}$ . In the last inequality we employed the fact that for any  $k \notin 2\pi\mathbf{Z}^2$  we have  $|2\pi l + k| \geq C_k(1 + |l|)$  for all  $l \in \mathbf{Z}^2$ . Now the statement about the range follows from the estimates above.  $\square$

This lemma implies the following:

**Corollary 52** *The image of the morphism  $\nabla(k)$  is an analytic subbundle  $\text{Im}\nabla$  in the trivial bundle over  $\mathbf{C}^2 \setminus 2\pi\mathbf{Z}^2$  with the fiber  $[L^2(X')]^2$ .*

**Proof.** The statement is local in  $k$ . Locally we can assume that the base  $\mathcal{U}$  of our bundles is a polydisk (and hence is a Stein manifold). According to the lemma above, for  $k \in \mathcal{U}$  the operator  $\nabla(k)$  is left invertible. Hence, due to the results of [A] (see also Theorem 4.4 in [ZK]) there exists an analytic left inverse operator  $T(k)$  for  $k \in \mathcal{U}$ . The composition  $\nabla(k)T(k)$  provides an analytic projection operator onto  $\text{Im}\nabla(k)$ , which proves the statement.  $\square$

We introduce now another analytic subbundle of  $\mathbf{C}^2 \setminus 2\pi\mathbf{Z}^2 \times [L^2(X')]^2$  that has the fiber over the point  $k \in \mathbf{C}^2 \setminus 2\pi\mathbf{Z}^2$  equal to  $(\text{Im}\nabla(k))^\perp \subset [L^2(X')]^2$ . This new bundle is denoted by  $\mathcal{E}^0$ , and its fibers by  $\mathcal{E}_k^0$ . (We understand here orthogonality in the meaning of the **bilinear** form  $\int \mathbf{F} \cdot \mathbf{F}$  instead of the standard scalar product).

We are now ready to describe the image of the space  $S_E$  under the transform (332). Namely, comparing (337) with the statement of the last Corollary 52, we get the following statement.

**Lemma 53** *The image of the space  $S_E$  under the transform (332) coincides with the next space of sections:*

$$L^2(K', L^2(X')) \times L^2(K', \mathcal{E}^0).$$

**Remark.** The reason to consider the set  $K'$  instead of the whole fundamental domain  $K$  is now obvious: the bundle  $\mathcal{E}^0$  has singularities at the points of the dual lattice. This is an effect that does not arise in the general theory of elliptic equations (see [K93]), but naturally arises for operators that can be included into elliptic complexes (see the Floquet theory for such complexes in [P]).

Our next step is to describe the image of the domain  $D(M|_{S_E})$  of the operator  $M|_{S_E}$  under the transform (332). According to the Lemma 48,  $D(M|_{S_E})$  can be described as the kernel in the space  $[H^1(\mathbf{R}^2)]^3$  of the continuous operator

$$A : [H^1(\mathbf{R}^2)]^3 \rightarrow L^2(\mathbf{R}^2), \text{ where } A(E, H_1, H_2) = \operatorname{div} \mathbf{H}.$$

Let us apply now the transform (332). According to the lemmas 49 and 50 the spaces  $L^2(\mathbf{R}^2)$  and  $[H^1(\mathbf{R}^2)]^3$  transform correspondingly into  $L_2(K', L^2(X'))$  and  $[L_2(K', \mathcal{E}^1)]^3$ . The operator  $A$  transforms into the multiplication by the analytic morphism that is equal to zero on the first component of the vector function  $(E, H_1, H_2)$ , and coincides on  $[\mathcal{E}^1]^2$  with the analytic morphism of  $[\mathcal{E}^1]^2$  into  $L_2(K', L^2(X'))$  that on the fiber over  $k$  is equal to  $A(k) = \operatorname{div}|_{[\mathcal{E}^1]^2}$ . Switching to the transform (333) instead of (332), we can prove analogously to the Corollary 52 the following statement:

**Lemma 54** *The kernel of the morphism  $A(k)$  is an analytic subbundle  $\tilde{\mathcal{E}}^1$  in the bundle  $[\mathcal{E}^1]^2|_{\mathbf{C}^2 \setminus 2\pi\mathbf{Z}^2}$  over  $\mathbf{C}^2 \setminus 2\pi\mathbf{Z}^2$ .*

**Proof.** First of all, the statement is local in  $k$ , so we will consider a small bidisk neighborhood of a point  $k \in K'$ . Let us switch to the transform (333) and expand into Fourier series on  $\mathbf{T}^2$ . After that we get the operator function

$$g \in [H^1(\mathbf{T}^2)]^2 \rightarrow (\nabla + ik) \cdot g \in L^2(\mathbf{T}^2).$$

Expanding the function  $g$  into Fourier series

$$\sum_{l \in \mathbf{Z}^2} g_l e^{2\pi i l \cdot x}, \quad g_l \in \mathbf{C}^2,$$

we can represent the operator as

$$(\nabla + ik) \cdot g = \sum i(2\pi l + k) \cdot g_l e^{2\pi i l \cdot x}.$$

Assuming that  $k \notin 2\pi\mathbf{Z}^2$ , one can easily show surjectivity of this operator. Namely, let

$$f = \sum_{l \in \mathbf{Z}^2} f_l e^{2\pi i l \cdot x} \in L^2(\mathbf{T}^2).$$

Since  $(2\pi l + k) \neq 0$ , we can find a vector  $g_l$  such that  $i(2\pi l + k) \cdot g_l = f_l$ , and  $|g_l| = \frac{|f_l|}{|(2\pi l + k)|}$ . Then obviously  $g = \sum_{l \in \mathbf{Z}^2} g_l e^{2\pi i l \cdot x}$  belongs to  $[H^1(\mathbf{T}^2)]^2$  and solves the equation  $(\nabla + ik) \cdot g = f$ , which shows the surjectivity. Now, like in the Corollary 52, we use the G. Allan's theorem (this time for the right inverse operators), and get the statement of the lemma.  $\square$

**Remark.** We notice that for  $g \in \operatorname{Ker} A(k)$  we have  $g_l \perp (2\pi l + k)$ . We are ready to describe the image of the domain  $D(M|_{S_E})$  of the operator  $M|_{S_E}$  under the Floquet transform (332).

**Lemma 55** *The image of  $D(M|_{S_E})$  under the transform (332) coincides with*

$$L^2(K', \mathcal{E}^1) \oplus L_2(K, \tilde{\mathcal{E}}^1) = L^2(K', \mathcal{E}^1 \oplus \tilde{\mathcal{E}}^1).$$

Now we have to consider the action of our operator  $M|_{S_E} : D(M|_{S_E}) \rightarrow S_E$ , where  $D(M|_{S_E})$  denotes the domain of the operator  $M|_{S_E}$  described in the Lemma 48. First of all, the differential expression (323) defines a continuous operator from the space  $[H^1(\mathbf{R}^2)]^3$  into the space  $[L^2(\mathbf{R}^2)]^3$ , and from the space  $[H^1(X')]^3$  into  $[L^2(X')]^3$ . In the first of these two cases, restricting the operator to the space  $S_E$ , we get the operator  $M|_{S_E}$ . In the second one, for  $k \in K'$  we restrict the operator to the fiber over  $k$  of

the bundle  $\mathcal{E}^1 \times \tilde{\mathcal{E}}^1$ , and get some analytic morphism  $M(k)$  over  $K'$  between the bundles  $\mathcal{E}^1 \oplus \tilde{\mathcal{E}}^1$  and  $(K' \times L^2(X')) \oplus \mathcal{E}^0$ . This is an analytic morphism, since it is the restriction to an analytic subbundle of a constant morphism of trivial bundles. A simple exercise is to check that multiplication by  $M(k)$  is the image of the operator  $M|_{S_E}$  under the Floquet transform (332):

$$\widehat{(M\mathbf{F})}(k, \cdot) = M(k)\widehat{(\mathbf{F})}(k, \cdot). \quad (338)$$

This formula is another way of saying that the decomposition (331) holds.

We need to establish some properties of the operator  $M(k)$  now.

**Lemma 56** *Operator  $M(k)$  defined in  $L^2(X'; \varepsilon dx) \oplus \mathcal{E}_k^0$  by the formula (323) with the domain  $\mathcal{E}_k^1 \times \tilde{\mathcal{E}}_k^1$  is self-adjoint, and has discrete spectrum.*

**Proof.** First of all, direct calculation shows that  $M(k)$  is symmetric on its domain. Its self-adjointness, after switching to the transform (333) amounts to the fact that any weak solution  $\mathbf{F} = (E, H_1, H_2)$  in  $[L^2(\mathbf{T}^2)]^3$  of the system of equations

$$\begin{aligned} -ic\varepsilon^{-1}(\partial/\partial x_2 + ik_2)H_1 + ic\varepsilon^{-1}(\partial/\partial x_1 + ik_1)H_2 &= 0 \\ (\partial/\partial x_1 + ik_1)H_1 + (\partial/\partial x_2 + ik_2)H_2 &= 0 \\ -ic(\partial/\partial x_2 + ik_2)E &= \psi_1 \\ ic(\partial/\partial x_2 + ik_2)E &= \psi_2 \\ \varphi, \psi_1, \psi_2 &\in L^2(\mathbf{T}^2) \end{aligned}$$

belongs to  $[H^1(\mathbf{T}^2)]^3$ . Expanding into Fourier series, and using estimates like in the proof of the Lemma 48, one can easily show that  $\mathbf{F} \in [H^1(\mathbf{T}^2)]^3$ , as soon as  $k$  is not on the dual lattice.

Discreteness of the spectrum follows from the fact that the domain of  $M(k)$  equipped with the graph norm (see Lemma 48) is compactly embedded into the space where the operator acts.  $\square$

**Corollary 57** *The following equality holds:*

$$\sigma_E(M) = \sigma(M|_{S_E}) = \overline{\cup_{k \in K'} \sigma(M(k))}, \quad (339)$$

where the bar denotes closure.

**Proof.** Let first  $\lambda \in \mathbf{R}$  is not in  $\overline{\cup_{k \in K'} \sigma(M(k))}$  (non-real values of  $\lambda$  are not interesting due to self-adjointness). We will show that then  $\lambda$  does not belong to  $\sigma(M|_{S_E})$ . Let  $\rho = \text{dist}(\lambda, \overline{\cup_{k \in K'} \sigma(M(k))})$ . Consider the morphism that on the fiber over the point  $k \in K'$  is equal to  $M(k) - \lambda$ . Due to the assumption, it is invertible in each fiber. Hence, there is the inverse analytic morphism  $(M(k) - \lambda)^{-1}$ . Due to self-adjointness, we get that the norm of  $(M(k) - \lambda)^{-1}$ , as an operator in  $L^2(X') \oplus \mathcal{E}_k^0$ , is at most  $\rho^{-1}$  (uniformly with respect to  $k$ ). Then we conclude that the operator of multiplication by  $(M(k) - \lambda)$  is invertible in  $L^2(K', L^2(X') \oplus \mathcal{E}^0)$ , and its inverse is the operator of multiplication by  $(M(k) - \lambda)^{-1}$ . Since the multiplication by  $(M(k) - \lambda)$  is the Floquet image of the operator  $M|_{S_E} - \lambda$ , the latter one is also invertible, so  $\lambda \notin \sigma(M|_{S_E})$ .

The converse statement is: if  $\lambda \in \overline{\cup_{k \in K'} \sigma(M(k))}$ , then  $\lambda \in \sigma(M|_{S_E})$ . This part is in general more delicate than the first one, but it follows as in the Theorem 4.5.1 in [K93].  $\square$

We are prepared now to prove the Theorem 47.

**Proof of the Theorem 47.** Let  $\lambda \in \sigma(M|_{S_E})$ , and due to the lemma above  $\lambda \in \overline{\cup_{k \in K'} \sigma(M(k))}$ . We will have to show that  $\lambda \in \sigma(M_E)$ . Due to the closedness of the spectra, it is sufficient to assume that  $\lambda \in \cup_{k \in K'} \sigma(M(k))$ . According to the Lemma 56, there is  $k \in K'$  such that  $\lambda$  is an eigenvalue of the

operator  $M(k)$ . Hence, there exists a vector function  $\mathbf{F} = (E, H_1, H_2) \in \mathcal{E}_k^1 \times \widetilde{\mathcal{E}}_k^1$  such that  $M(k)\mathbf{F} = \lambda\mathbf{F}$ . In other words, all three components  $E, H_1$ , and  $H_2$  belong to the space  $H^1(X')$ , they all satisfy the cyclic conditions (334), the last two components satisfy the condition

$$\frac{\partial H_1}{\partial x_1} + \frac{\partial H_2}{\partial x_2} = 0,$$

and besides they satisfy the system of equations

$$ic\varepsilon^{-1}\left(\frac{\partial H_2}{\partial x_1} - \frac{\partial H_1}{\partial x_2}\right) = \lambda E, \quad (340)$$

$$-ic\frac{\partial E}{\partial x_2} = \lambda H_1, \quad (341)$$

$$ic\frac{\partial E}{\partial x_1} = \lambda H_2. \quad (342)$$

If  $\lambda \neq 0$ , then we can express  $H_1$  and  $H_2$  from the equations (341), (342) and plug them into (340). This will lead to the equality  $-c^2\varepsilon^{-1}\Delta E = \lambda^2 E$ . At the same time, from the equalities (341) and (342) we conclude, first, that  $E \in H^2(X')$ , and second, that not only the function  $E$  itself, but also its partial derivatives satisfy the Floquet cyclic conditions (334). Since  $E \neq 0$  (otherwise  $\mathbf{F}$  would be also equal to zero), we conclude that the equation  $(-c^2\Delta - \lambda^2\varepsilon)E = 0$  has a non-zero solution in  $H^2(X')$  with the conditions (334) on the function and its partial derivatives. Then Theorem 4.5.1 in [K93] says that zero is in the spectrum in  $L^2(\mathbf{R}^2)$  of the operator  $(-c^2\Delta - \lambda^2\varepsilon)$ , and hence of the operator  $(-c^2\varepsilon^{-1}\Delta - \lambda^2)$ . The last remark is that the spaces  $L^2(\mathbf{R}^2)$  and  $L^2(\mathbf{R}^2, \varepsilon dx)$  have the same elements and equivalent norms. We conclude, therefore, that  $\lambda^2 \in \sigma(M_E)$ .

Now, let us assume that  $\lambda^2 (\neq 0) \in \sigma(M_E)$ . According to the same Theorem 4.5.1 in [K93], applied to the operator  $(-c^2\Delta - \lambda^2\varepsilon)$ , this means that there exists a point  $k \in K$  such that the equation  $(-c^2\Delta - \lambda^2\varepsilon)E = 0$  and, hence, the equation  $(-c^2\varepsilon^{-1}\Delta - \lambda^2)E = 0$  have a nontrivial solution in  $H^2(X')$  that satisfies together with its partial derivatives the conditions (334). Since the spectra of these boundary value problems  $M_E(k)$  depend continuously on  $k \in K$ , we conclude that  $\lambda^2 \in \overline{\cup_{k \in K'} \sigma(M_E(k))}$ . Hence, it is sufficient to show that if  $\lambda \in \overline{\cup_{k \in K'} \sigma(M_E(k))}$ , then  $\lambda \in \overline{\cup_{k \in K'} \sigma(M(k))}$ . So, let  $k \in K'$ , and  $\lambda^2$  and  $E$  are an eigenvalue and the corresponding eigenfunction of the cyclic boundary value problem

$$\begin{aligned} (-c^2\varepsilon^{-1}\Delta - \lambda^2)E &= 0 \text{ in } X', \\ E(1 + \delta/2, x_2) &= e^{ik_1}E(\delta/2, x_2), \quad E(x_1, 1 + \delta/2) = e^{ik_2}E(x_1, \delta/2), \\ \nabla E(1 + \delta/2, x_2) &= e^{ik_1}\nabla E(\delta/2, x_2), \quad \nabla E(x_1, 1 + \delta/2) = e^{ik_2}\nabla E(x_1, \delta/2). \end{aligned}$$

Determining  $H_1$  and  $H_2$  according to (341) and (342), we conclude that the equation (340), and the condition (325) are also satisfied, so  $\lambda \in \sigma(M(k)) \subset \overline{\cup_{k \in K'} \sigma(M(k))}$ .

We have to consider the case of  $\lambda = 0$  separately. The thing is that zero belongs to both spectra: to  $\sigma(M_E)$  as well as to  $\sigma_E(M)$ . For the operator  $M_E$  this is obvious, since zero belongs to the spectrum of the Laplacian in  $L^2(\mathbf{R}^2)$ . Consider now the operator  $M|_{S_E}$ . We choose a vector  $k \in K'$  with arbitrarily small norm, and a unit vector  $\mathbf{a}$  that is orthogonal to  $k$ . Consider now the vector function  $\mathbf{F} = e^{ik \cdot x} \mathbf{a}$ . Then  $\mathbf{F}$  belongs to the domain of  $M(k)$ , and the  $L^2$ -norm  $\|M(k)\mathbf{F}\|$  is small (though the  $L^2$ -norm of  $\mathbf{F}$  is fixed). Hence,  $0 \in \overline{\cup_{k \in K'} \sigma(M(k))}$ .  $\square$

Analogously to the Theorem 47, one the following can be proven.

**Theorem 58** *A real number  $\lambda$  belongs to the spectrum  $\sigma_H(M)$  of the self-adjoint operator  $M|_{S_H}$  if and only if  $\lambda^2$  belongs to the spectrum  $\sigma(M_H)$  of the operator*

$$M_H u = -\nabla \cdot (\varepsilon^{-1} \nabla u),$$

where the operator  $M_H$  is defined in  $L^2(\mathbf{R}^2)$  in an appropriate weak sense (see details in [FK]).

The spectrum  $\sigma(M_H)$  (and hence  $\sigma_H(M)$ ) was described in [FK], so according to (320), and to the Theorems 47 and 58 our task is reduced to investigation of  $\sigma(M_E)$  only.

## 7.2 Proof of the main results

All the statements of Theorems 2 and 3 (except for (28)) on the spectrum of Maxwell operator  $\sigma(M)$  follow immediately from (13), Theorems 30, 31 for the operator  $\Theta_\varepsilon$  (i.e. for  $E$ -polarized fields), and Theorem 1 from our paper [FK] for the operator  $\Gamma_\varepsilon$ , associated with  $H$ -polarized fields. As far as the estimate (28) for the very first band of the operator  $\Gamma_\varepsilon$  is concerned, we can mention that in [FK] we estimated the width of this band by  $Cw$  for some constant  $C$ . Now based on our results for one-dimensional problems, we can make this estimate more precise and come to (28).

We showed in [FK] that the upper limit of the first band of the operator  $\Gamma_\varepsilon$  is smaller than the upper limit of the first band of the following operator with separate variables:

$$\begin{aligned} \overset{\circ}{\Gamma}_\varepsilon &= -\partial_1 \varepsilon_1^{-1}(x_1) \partial_1 - \partial_2 \varepsilon_1^{-1}(x_2) \partial_2, \text{ where} \\ \varepsilon_1(y) &= \begin{cases} \zeta & \text{if } 0 \leq y < \delta \\ 1 & \text{if } \delta \leq y < 1 \end{cases}, \quad \varepsilon_1(y) = \varepsilon_1(y+n), n \in \mathbf{Z}, y \in \mathbf{R}. \end{aligned}$$

Analysis of the spectral structure of the operator  $\overset{\circ}{\Gamma}_\varepsilon$  boils down to analysis of the one-dimensional operator  $-\partial_y \varepsilon_1^{-1} \partial_y$  acting in  $L_2(\mathbf{R})$ . We notice that the spectrum of that one-dimensional operator is the same as the spectrum of the operator  $\Theta_{1,\varepsilon_1} = -\varepsilon_1^{-1} \partial_y^2$  acting in  $L_2(\mathbf{R}, \varepsilon_1(y) dy)$ . Spectral analysis of the operator  $\Theta_{1,\varepsilon_1}$ , in turn, can be reduced to the analysis of a Schrödinger operator in the same fashion as we did for the two-dimensional operator  $\Theta_\varepsilon$ . In fact, it is easier. Thus, in order to find the spectrum of the operator  $\Theta_\varepsilon$ , we introduce the Schrödinger operator  $Q_g^1 = -\frac{\partial^2}{\partial y^2} - g(\varepsilon_1(y) - 1)$ . This operator is almost the same as the operator  $Q_{\kappa,g}$  defined by (239), and we can represent it in terms of the operator  $Q(\kappa, D, \delta)$  as  $Q_g^1 = Q(\kappa, g(w^{-1} - \delta), \delta)$ ,  $g \geq 0$ . Therefore, the upper limit  $u$  of first band of the operator  $Q_g^1$  solves the next equation for  $g$ :

$$u : \xi_0(\pi, g\hat{w}^{-1}, \delta) = g, \quad \hat{w} = w(1 - w\delta)^{-1}.$$

If we denote  $u = D\hat{w}^{-1}$ , we obtain the equation for  $D : \xi_0(\pi, D, \delta) = D\hat{w}$ . Using Lemma 6 (ii) and Lemma 24 (iii), we conclude that  $D = 4 + O(w)$ . Hence, the upper limit for the first band of the operator  $\Theta_\varepsilon$  equals  $4 + O(w)$  and, therefore, the upper limit of the operator  $\overset{\circ}{\Gamma}_\varepsilon$  is  $8 + O(w)$ . This leads straightforwardly to the desired estimate (28) which completes the proof of Theorem 2.

## 7.3 Space distribution of the electric field energy

In this section we consider how the electric field energy is distributed in the space for the  $E$ -polarized eigenmodes of the Maxwell operator. We are interested in the portion of the energy residing in the areas with high dielectric constant (i.e., in thin “walls” in our medium) in comparison with the energy residing in the areas with low dielectric constant (air columns). We consider the sell of periods  $X$  (see (5)) and the eigenfunctions of the operator  $\overset{\circ}{\Theta}_{\zeta,\delta}$ . We pick the operator  $\overset{\circ}{\Theta}_{\zeta,\delta}$  with separate variables instead of  $\Theta_\varepsilon$ , since it is simpler. We have already shown that these operators have practically the same spectra and so we expect that the properties of the eigenfunctions are similar too. Let us denote the portion of the electric field energy associated with an eigenmode  $\Psi$  and high dielectric constant area in  $X$  by  $\mathcal{E}_d(\Psi, X)$  and the corresponding energy in low dielectric constant area filled by air by  $\mathcal{E}_a(\Psi, X)$ . Let us pick now



an eigenfunction  $\mathring{\Psi}_{\mathbf{n}}(\mathbf{k}, \zeta, \delta, \mathbf{x})$  of the operator  $\mathring{\Theta}_{\mathbf{k}, \zeta, \delta}$ . Since the density of the electric field energy is  $\varepsilon(\mathbf{x})E_3^2(\mathbf{x})$ ,  $\mathbf{x} = (x_1, x_2)$ , we have

$$\mathcal{E}_d(\mathring{\Psi}_{\mathbf{n}}, X) = \zeta \int_{X-O_\delta} \left| \mathring{\Psi}_{\mathbf{n}}(\mathbf{k}, \zeta, \delta, \mathbf{x}) \right|^2 d\mathbf{x}, \quad (343)$$

$$\mathcal{E}_a(\mathring{\Psi}_{\mathbf{n}}, X) = \zeta \int_{O_\delta} \left| \mathring{\Psi}_{\mathbf{n}}(\mathbf{k}, \zeta, \delta, \mathbf{x}) \right|^2 d\mathbf{x}. \quad (344)$$

The ratio  $\mathcal{E}_d(\mathring{\Psi}_{\mathbf{n}}, X)/\mathcal{E}_a(\mathring{\Psi}_{\mathbf{n}}, X)$  significantly depends on whether  $\mathring{\Psi}_{\mathbf{n}}$  is associated with  $E$ -subpectrum or  $H$ -subpectrum. Our main tools here will be Lemmas 28 and 29. Let us consider first an eigenfunction  $\mathring{\Psi}_{(0,n)}$  as in the formula (299). Then

$$\int_{X-O_\delta} \left| \mathring{\Psi}_{(0,n)}(\mathbf{k}, \zeta, \delta, \mathbf{x}) \right|^2 d\mathbf{x} \geq \quad (345)$$

$$\left. \int_0^\delta |f_0(k_1, D, \delta; x)|^2 dx \int_0^1 |f_n(k_1, D, \delta, x)|^2 dx \right|_{D=D(n, \mathbf{k}, \zeta, \delta)} \cdot$$

$$\int_{O_\delta} \left| \mathring{\Psi}_{(0,n)}(\mathbf{k}, \zeta, \delta, \mathbf{x}) \right|^2 d\mathbf{x} \leq \quad (346)$$

$$\left. \int_1^\delta |f_0(k_1, D, \delta; x)|^2 dx \int_0^1 |f_n(k_1, D, \delta, x)|^2 dx \right|_{D=D(n, \mathbf{k}, \zeta, \delta)} \cdot$$

Combining formulas (343)-(346) with Lemma 29 and with the bound (273) for  $D(n, \mathbf{k}, \zeta, \delta)$ , we get

$$\frac{\mathcal{E}_d(\mathring{\Psi}_{(0,n)}, X)}{\mathcal{E}_a(\mathring{\Psi}_{(0,n)}, X)} \geq w^{-1} \left[ \frac{\nu^{-2} \sinh \nu}{I(k_1, \nu)} + o(1) \right], \quad \nu = \sqrt{-\xi_0(k_1, D(n, \mathbf{k}, \zeta, \delta))}. \quad (347)$$

Since  $w \rightarrow 0$ , the last relationships say that *for the eigenmodes from  $E$ -subpectrum the overwhelming portion of their electric field energy resides in thin walls with large dielectric constant.*

Let us consider now an eigenfunction  $\mathring{\Psi}_{\mathbf{n}}, \mathbf{n} = (n_1, n_2) > 0$  associated with the  $H$ -subpectrum. It has the following form (see (255) and (256)):

$$\Psi(\mathbf{x}) = \mathring{\Psi}_{\mathbf{n}}(\mathbf{x}) = f_{n_1}(k_1, D, \delta; x_1) f_{n_2}(k_2, D, \zeta, \delta; x_2) \Big|_{D=g(\mathbf{n}, \mathbf{k}, \zeta, \delta) \tilde{w}^{-1}}.$$

This representation implies

$$\int_{X-O_\delta} \left| \mathring{\Psi}_{\mathbf{n}}(\mathbf{k}, \zeta, \delta, \mathbf{x}) \right|^2 d\mathbf{x} \leq$$

$$\sum_{j=1,2} \int_0^\delta |f_{n_j}(k_j, D, \delta; x)|^2 dx \int_0^1 |f_{n_{3-j}}(k_{3-j}, D, \delta, x)|^2 dx \Big|_{D=g(\mathbf{n}, \mathbf{k}, \zeta, \delta) \tilde{w}^{-1}}, \quad (348)$$

$$\int_{O_\delta} \left| \mathring{\Psi}_{(0,n)}(\mathbf{k}, \zeta, \delta, \mathbf{x}) \right|^2 d\mathbf{x} =$$

$$\int_1^\delta |f_{n_1}(k_1, D, \delta; x)|^2 dx \int_1^\delta |f_{n_2}(k_1, D, \delta, x)|^2 dx \Big|_{D=g(\mathbf{n}, \mathbf{k}, \zeta, \delta) \tilde{w}^{-1}}. \quad (349)$$

Combining the inequalities (348) and (349) with Lemma 28 and with the inequality (280), we come to the estimate

$$\frac{\mathcal{E}_d(\overset{\circ}{\Psi}_{\mathbf{n}}, X)}{\mathcal{E}_a(\overset{\circ}{\Psi}_{\mathbf{n}}, X)} \leq \sum_{j=1,2} (1 - \cos k_j)^{-1} O(w + \beta_1^{-2}). \quad (350)$$

Here we took into account that  $\beta w = \beta_1^2$  (see (19)). The last inequality implies that if  $0 < k_j < \pi$ ,  $j = 1, 2$  and if  $w, \beta_1^{-1} \rightarrow 0$ , then for the eigenmodes from  $H$ -subpectrum the overwhelming portion of their energy resides in the air columns with dielectric constant 1.

## References

- [A] G. R. Allan, *Holomorphic vector-valued functions on a domain of holomorphy*, J. London Math. Soc. **42**: 509-513, 1967.
- [AM] N.W. Ashcroft and N.D. Mermin, *Solid State Physics*, Holt, Rinehart and Winston, New York-London, 1976.
- [BS] M. Birman and M. Solomyak,  *$L_2$ -Theory of the Maxwell operator in arbitrary domains*, Russian Math. Surveys **42**, no 6: 75-96, 1987.
- [1B] L. C. Botten, M. S. Craig, R. C. McPhedran, J. L. Adams and J. R. Andrewartha, *The dielectric lamellar diffraction grating*, Optica Acta, **28**(8), 413-428, 1981.
- [2B] L. C. Botten, M. S. Craig, R. C. McPhedran, J. L. Adams and J. R. Andrewartha, *The finetly conducting lamellar diffraction grating*, Optica Acta, **28**(8), 1087-1102, 1981.
- [DE] *Development and Applications of Materials Exhibiting Photonic Band Gaps*, Journal of the Optical Society of America **B**, **10**: 280-413, 1993.
- [DG] J. Drake and A. Genack, *Observation of Nonclassical Optical Diffusion*, Phys. Rev. Lett. **63**: 259, 1989.
- [E] M. S. P. Eastham, *The Spectral Theory of Periodic Differential Equations*, Scottish Acad. Press, Edinburgh-London, 1973.
- [EZ] E. N. Economou and A. Zdetsis, *Classical wave propagation in periodic structures*, Phys. Rev. **B**, **40**: 1334, 1989.
- [F94] A. Figotin, *Photonic Pseudogaps in Periodic Dielectric Structures*, J. Stat. Phys., **74**(1/2): 443-446, 1994.
- [FK94] A. Figotin and P. Kuchment, *Band-Gap Structure of the Spectrum of Periodic Maxwell Operators*, J. Stat. Physics, **74**(1/2): 447-458, 1994.
- [FK] A. Figotin and P. Kuchment, *Band-Gap Structure of the Spectrum of Periodic and Acoustic Media. I. Scalar Model*, (to appear in SIAM Journal on Applied Mathematics).
- [FK95] A. Figotin and P. Kuchment, *Band-Gap Structure of the Spectrum of Periodic and Acoustic Media. II. 2D Photonic Crystals*, Preprint, UNCC, 1995.
- [HCS] K. M. Ho, C. T. Chan and C. M. Soukoulis, *Existence of a Photonic Gap in Periodic Dielectric Structures*, Phys. Rev. Lett. **65**: 3152, 1990.

- [J87] S. John, *Strong Localization of Photons in Certain Disordered Dielectric Superlattices*, Phys. Rev. Lett. **58**: 2486, 1987.
- [J91] S. John, *Localization of Light*, Phys. Today, (May 1991).
- [JMW] J. Joannopoulos, R. Meade, and J. Winn, *Photonic Crystals. Molding the Flow of Light*, Princeton University Press, 1995.
- [K82] P. Kuchment, *Floquet Theory for Partial Differential Equations*, Russian Math. Surveys, **37**, no.4, 1-60, 1982.
- [K93] P. Kuchment, *Floquet Theory for Partial Differential Equations*, Birkhäuser Verlag, Basel, 1993.
- [LL] K. M. Leung and Y. F. Liu, *Full Vector Wave Calculation of Photonic Band Structures in Face-Centered-Cubic Dielectric Media*, Phys. Rev. Lett. **65**: 2646, 1990.
- [M] R. C. McPhedran, L. C. Botten, M. S. Craig, M. Nevière and D. Maystre, *Lossy lamellar gratings in the quasistatic limit*, Optica Acta, **29**(3), 289-312, 1982.
- [MM] A. A. Maradudin, A. R. McGurn, *Photonic band gaps of a truncated, two-dimensional periodic dielectric media*, Journal of the Optical Society of America **B**, **10**: 307-313, 1993.
- [MPD] S. L. McCall, P. M. Platzman, R. Dalichaouch, D. Smith and S. Schultz, *Microwave Propagation in Two-Dimensional Dielectric Lattices*, Phys. Rev. Lett., **67**(17): 2017-2020, 1991.
- [MBRJ] R. D. Meade, K. D. Brommer, A. M. Rapper and J. D. Joannopoulos, *Existence of Photonic Band Gap in Two Dimensions*, Appl. Phys. Lett., **61**, 495-497, 1992.
- [P] V. Palamodov, *Harmonic synthesis of solutions of elliptic equations with periodic coefficients*, Ann. Inst. Fourier, 1994.
- [PSS] Ping Sheng, R. S. Stepleman and P. N. Sanda, *Exact Solutions for square-wave gratings: Applications to diffraction and surface-plasmon calculation*, Phys. Rev. **B** **28**(6), 2907-2916, 1982.
- [PM] M. Plihal and A. A. Maradudin, *Photonic band structure of two-dimensional systems: The triangular lattice*, Phys. Rev. **B**, **44**: 8565-8571, 1991.
- [RS] M. Reed, B. Simon, *Methods of Modern Mathematical Physics, Vol.IV: Analysis of Operators*, Academic Press, 1978.
- [RMP] A. Roberts and R. C. McPhedran, *Power losses in highly conducting lamellar gratings*, Journal of Modern Optics, **34**(4), 511-538, 1987.
- [SSE] M. Sigalas, C. M. Soukoulis, E. N. Economou, C. T. Chan, and K. M. Ho, *Photonic Band Gaps and Defects in Two Dimensions: Studies of the Transmission coefficient*, Phys. Rev. **B** **48**(19), 14121-14126, 1993.
- [vAL] M. P. Van Albada and A. Lagendijk, *Observation of Weak Localization of Light in Random Medium*, Phys. Rev. Lett. **55**:2692, 1985.
- [VP] P. R. Villeneuve and M. Piché, *Photonic band gaps of transverse-electric models in two-dimensionally periodic Media*, Journal of the Optical Society of America **A**, **8**: 1296-1305, 1991.
- [WVG] J. R. Wendt, G. A. Vawter, P. L. Gourley, T. M. Brennan and B. E. Hammons, *Nanofabrication of photonic lattice structures in GaAs/AlGaAs*, J. Vac. Sci. Technol, **B** **11**(6), 2637-2640, 1993.

- [Y] E. Yablonovitch, *Inhibited Spontaneous Emission in Solid-State Physics and Electronics*, Phys. Rev. Lett. **58**: 2059, 1987.
- [YG] E. Yablonovitch and T. J. Gmitter, *Photonic Band Structure: The Face-Centered-Cubic Case*, Phys. Rev. Lett. **63**:1950, 1989.
- [ZK] M. Zaidenberg, S. Krein, P. Kuchment, and A. Pankov, *Banach bundles and linear operators*, Russian Math. Surveys **30**, no.5, 115-175, 1975.
- [ZS] Ze Zhang and S. Sathpathy, *Electromagnetic Wave Propagation in Periodic Structures: Bloch Wave Solution of Maxwell's Equations*, Phys. Rev. Lett. **65**: 2650, 1990.