On the Calculation of the Spectral Bands of One-Dimensional Photonic Crystals

V Barbera-Figueroa

Instituto Politécnico Nacional, SEPI-UPIITA.
Av. IPN 2580, Col. Barrio la Laguna Ticomán CP. 07340, CDMX, México.
E-mail: vbarreraf@ipn.mx

Abstract. In this work we consider the propagation of transverse electromagnetic waves in one-dimensional photonic crystals consisting of periodic arrays of slabs. On the basis of the Floquet theory we obtain the characteristic function of the periodic medium, which defines the photonic bands of the crystal. The characteristic function is constructed from the monodromy matrices of the slabs. Entries of monodromy matrices are explicitly given as power series of the spectral parameter. The present analysis can be applied not only to homogeneous slabs, but also to slabs with varying refractive indexes. The power series representation of the entries of monodromy matrices leads to an effective numerical method for the calculation of the spectral bands of one-dimensional photonic crystals.

1. Introduction

Let us consider the differential equation

\[(pu')' + r(\lambda - q)u = 0,\]  \hspace{1cm} (1)

where \(p, p', q, r\) are complex-valued, piecewise continuous, periodic functions of the real variable \(x \in \mathbb{R}\), all with the same period \(\ell\). It is assumed that \(p\) is nowhere zero, so that no singular points are involved. The spectral parameter is denoted by \(\lambda\). This \(\ell\)-periodic Sturm-Liouville equation is often called the Hill’s equation [1]. The spectral analysis of the Hill’s equation relies on the so-called Hill’s discriminant \(D(\lambda) := f_1(\ell, \lambda) + f_2(\ell, \lambda)\), where \(f_1\) and \(f_2\) are two linearly independent solutions of (1) in \((0, \ell)\) satisfying the Cauchy conditions \(f_1(0, \lambda) = 1, f_1'(0, \lambda) = 0, f_2(0, \lambda) = 0,\) and \(f_2'(0, \lambda) = 1\). The values of \(\lambda\) for which \(|D(\lambda)| < 2\) define stability intervals also called allowed spectral bands. Solutions of (1) corresponding to these values of \(\lambda\) are bounded in the real axis \(\mathbb{R}\). If \(|D(\lambda)| > 2\) then \(\lambda\) lies in an interval of instability or forbidden band. The band edges are those values of \(\lambda\) such that \(|D(\lambda)| = 2\). Though the theory of the Hill’s discriminant is well known, its numerical treatment is rather limited.

Problems of wave propagation in periodic media frequently lead to periodic Sturm-Liouville equations. This is the result of performing a separation of variables, of considering the underlying symmetries of the problem, or of using some transformation such as the Fourier or Floquet transform. The physical sense of the spectral bands indeed depends on the nature of the waves. Mathematical methods are always necessary to accurately determine the spectral bands for a given periodic problem. In this sense the paper [2] provides an explicit representation of the
Hill’s discriminant $\mathcal{D}$ by using the spectral parameter power series method [3] (SPPS method for short). In that paper it is assumed that $p, q$ are real-valued continuous function, with $r(x) \equiv 1$. In the paper [4] the SPPS method as well as the limit operators method [5] were used for the spectral analysis of periodic Schrödinger operators with potentials including both a regular and a singular part. In that work the regular part of the potential is perturbed by a slowly oscillating at infinity function. In addition, the works [6, 7] approached periodic quantum graphs involving one-dimensional Schrödinger operators with the previously mentioned methods for the study of the essential spectra of perturbed operators.

In the present paper we consider Sturm-Liouville operators of the form

$$L_\nu u := \nu(z) \frac{d}{dz} \left( \nu^{-1}(z) \frac{du(z)}{dz} \right) + k_0^2 n^2(z) u(z),$$

where $n > 0$ and $\nu > 0$ are real-valued, piecewise continuous, periodic functions. The function $n$ represents the refractive index of the electromagnetic medium, and $\nu$ represents either its permittivity $\varepsilon$ or permeability $\mu$. Operator $L_\nu$ can be used to analyze the propagation of transverse electromagnetic waves in one-dimensional photonic crystals. The main interest of the paper is to provide a method to accurately determine the photonic bands of a crystal. This method is based on the calculation of certain monodromy matrices that carry the information of the (finite) jumps of the functions $n$ and $\nu$ at the slabs forming the cells of the crystal. The entries of these matrices are represented in the form of convergent power series of the wave-number. In the numerical implementation of the method, the band edges are approximately calculated from the polynomial roots of certain polynomial equation. Hence the numerical determination of the photonic bands of one-dimensional photonic crystals reduces to calculating polynomial roots.

The outline of this work is as follows. In Section 2 we obtain the wave equations for the electromagnetic transverse waves in planar layered media. In Section 3 we focus on the Sturm-Liouville equation governing the propagation in periodic media. In Section 4 we obtain the dispersion equation for one-dimensional photonic crystals in terms of monodromy matrices and define the photonic spectra of these structures. In Section 5 we employ the SPPS method for deriving a numerical method for calculating the photonic bands.

2. Wave equations for the electromagnetic field in planar layered media

The time-harmonic Maxwell’s equations for a free of sources isotropic medium are

$$\nabla \times H = -i \omega \varepsilon E, \quad \nabla \times E = i \omega \mu H, \quad (2)$$

$$\nabla \cdot (\mu H) = 0, \quad \nabla \cdot (\varepsilon E) = 0, \quad (3)$$

where $E$ and $H$ denote the complex amplitudes of the electric and magnetic fields, respectively. The constitutive parameters of the medium are represented by $\varepsilon := \varepsilon_0 \varepsilon_r$ (permittivity) and $\mu := \mu_0 \mu_r$ (permeability). The relative constitutive parameters $\varepsilon_r$ and $\mu_r$ are assumed to be positive functions of the position $r \in \mathbb{R}^3$. The phase velocity of the electromagnetic field in the free space is defined by $c_0 := 1/\sqrt{\varepsilon_0 \mu_0}$. The time variation is referred to the $e^{-i\omega t}$ time convention, being $\omega \neq 0$ the angular frequency of the field. The application of the curl operator on both sides of equations (2) leads to decoupled vector wave equations [8, Chap. 2]

$$\nabla \times \mu^{-1} \nabla \times E - \omega^2 \varepsilon E = 0, \quad (4a)$$

$$\nabla \times \varepsilon^{-1} \nabla \times H - \omega^2 \mu H = 0. \quad (4b)$$

In a Cartesian system of coordinates $(x, y, z) \in \mathbb{R}^3$ we choose the axis $z$ as the propagation axis of the electromagnetic waves. The electric field of transverse electric (TE) waves lies on
If the electric field is linearly polarized, say \( \mathbf{E} = E_y \mathbf{a}_y \), then it is described by the scalar wave equation
\[
\frac{\partial}{\partial z} \mu^{-1} \frac{\partial E_y}{\partial z} + \frac{\partial}{\partial x} \mu^{-1} \frac{\partial E_y}{\partial x} + \omega^2 \varepsilon E_y = 0,
\]
which is obtained from the \( y \) component of vector equation (4a). Similarly, the wave equation
\[
\frac{\partial}{\partial z} \varepsilon^{-1} \frac{\partial H_y}{\partial z} + \frac{\partial}{\partial x} \varepsilon^{-1} \frac{\partial H_y}{\partial x} + \omega^2 \mu H_y = 0
\]
(6)
describes the transverse magnetic (TM) waves \((H_z \equiv 0)\) in which the magnetic field is linearly polarized, \( \mathbf{H} = H_y \mathbf{a}_y \). Let us assume that the constitutive parameters depend on only the coordinate \( z \), that is, \( \varepsilon = \varepsilon (z) \) and \( \mu = \mu (z) \). Hence equations (5) and (6) can collectively be written as
\[
\frac{\partial^2 U}{\partial x^2} + \nu \frac{\partial}{\partial z} \nu^{-1} \frac{\partial U}{\partial z} + k_0^2 n^2 (z) U = 0,
\]
where \( U \) and \( \nu \) stand for \( U (x, z) = \begin{cases} E_y (x, z), & \text{TE waves} \\ H_y (x, z), & \text{TM waves} \end{cases} \) \( \nu (z) = \begin{cases} \mu (z), & \text{TE waves} \\ \varepsilon (z), & \text{TM waves} \end{cases} \).

The function \( \nu \) is assumed to be positive for each \( z \in \mathbb{R} \). We have introduced the quantity \( k_0^2 n^2 (z) \equiv \omega^2 \mu (z) \varepsilon (z) \), where \( n (z) := \sqrt{\mu_r (z) \varepsilon_r (z)} \) is the refractive index of the medium, and \( k_0 = \omega / c_0 \) is the free-space wave-number. For non-magnetic media such as dielectrics \((\mu_r = 1)\), the refractive index is calculated by \( n (z) = \sqrt{\varepsilon_r (z)} \).

**Figure 1.** Linearly polarized: (a) TE waves (b) TM waves (c) planar layered medium (d) jump discontinuities of the constitutive parameters.

Constitutive parameters can be discontinuous at \( z = z_0 \). In this case the function \( U \) should satisfy the continuity conditions
\[
[U (x, z)]_{z=z_0} = 0, \quad \left[ \nu^{-1} (z) \frac{\partial U (x, z)}{\partial z} \right]_{z=z_0} = 0,
\]
where the notation \([f]_{z_0} := f (z_0^+) - f (z_0^-)\) represents the (finite) jump of \( f \) at \( z_0 \), being \( f (z_0^+) \) the one-sided limits of \( f \) to the point \( z_0 \) if exist. Continuity conditions (8) follow from the boundary conditions of the electromagnetic field between two distinct media. Indeed for TE waves, the tangential components \( E_y, H_x \) and the normal component \( B_z = \mu H_z \) must remain continuous on the plane \( z = z_0 \), see Figure 1-(a), where
\[
H_x = i \omega^{-1} \mu^{-1} \frac{\partial E_y}{\partial z}, \quad H_z = -i \omega^{-1} \mu^{-1} \frac{\partial E_y}{\partial x}.
\]
Similarly for TM waves, the tangential components \( H_y, E_z \) and the normal component \( D_z = \varepsilon E_z \) must remain continuous at \( z = z_0 \), see Figure 1-(b), where

\[
E_x = -i\omega^{-1}\varepsilon^{-1}\frac{\partial H_y}{\partial x}, \quad E_z = i\omega^{-1}\varepsilon^{-1}\frac{\partial H_y}{\partial x}.
\]

Since the medium is invariant with respect to the displacements in the \( x \) direction, equation (7) admits harmonic solutions of the form

\[
U(x, z) = u(z) e^{\pm ikx},
\]

where \( \kappa > 0 \ [\text{rad/m}] \) is the propagation constant in the \( x \) direction, and \( u(z) \) is an amplitude satisfying the Sturm-Liouville equation

\[
\nu(z) \frac{d}{dz} \left( \nu^{-1}(z) \frac{du(z)}{dz} \right) + k_0^2 n^2(z) u(z) = \beta u(z),
\]

where \( \beta := \kappa^2 \in \mathbb{R} \) is the spectral parameter, and the amplitude \( u \) stands for

\[
u u(z) = \begin{cases} e_y(z), & \text{TE waves} \\ h_y(z), & \text{TM waves} \end{cases}
\]

being \( e_y (h_y) \) the electric (magnetic) field intensity that points in the \( y \) direction.

**Remark.** For non-magnetic media, equation (7) describing TE waves takes the form of a Helmholtz equation

\[
\Delta_{(x,z)} E_y + k_0^2 n^2(z) E_y = 0,
\]

where \( \Delta_{(x,z)} \) is the Laplacian with respect to \( (x, z) \in \mathbb{R}^2 \). Let the refractive index \( n \) be represented in the form \( n(z) = n_0 + \mathcal{O}(z) \), where \( n_0 > 0 \). If the refractive index shows small variations with respect to the constant level \( n_0 \) the terms of the order \( \mathcal{O}(z) \) can be neglected, so that a rough approximation is given by \( n(z) \approx n_0 \). Helmholtz equation (10) admits harmonic solutions \( E_y(x, z) = e_y(z) e^{\pm ikx} \), where the amplitude \( e_y(z) \) satisfies the Schrödinger equation

\[
-\frac{1}{2k_0^2 n_0} \frac{d^2 e_y(z)}{dz^2} - n(z) e_y(z) = \xi e_y(z),
\]

being \( \xi = -\frac{\kappa^2 e_y^2}{2n_0 k_0^2} \) a negative eigen-energy of a particle of mass \( n_0 \) subjected to an attractive potential \(-n(z)\), cf. [9]. The role of the Planck’s constant \( \hbar \) is assumed by \( k_0^{-1} \).

### 3. Sturm-Liouville operator with discontinuous coefficients

Let us consider the Sturm-Liouville operator \( \mathcal{L}_\nu \) defined by the differential expression

\[
\mathcal{L}_\nu u := \nu(z) \frac{d}{dz} \left( \nu^{-1}(z) \frac{du(z)}{dz} \right) + k_0^2 n^2(z) u(z),
\]

where \( u \) is the amplitude of the transverse wave \( U(x, z) = u(z) e^{\pm ikx} \) propagating in a planar layered medium. Assume that the medium consists of stacked slabs with variable refractive indexes depending on \( z \), see Figures 1-(c) and -(d). The stack will be dotted by a periodic structure. By means of the Floquet theory we will determine the band spectrum of operator \( \mathcal{L}_\nu \). Such periodic media will serve to model one-dimensional photonic crystals.
3.1. Structure of the planar layered medium

Let \( z = z_j \) be a plane between adjacent slabs. We assume that the finite jump \([\nu]_{z_j} \) is well defined. The amplitude \( u \) at \( z_j \) is governed by conditions

\[
[u(z)]_{z_j} = 0, \quad \left[ \nu^{-1}(z) \frac{du(z)}{dz} \right]_{z_j} = 0,
\]

which can be written in a matrix form

\[
\begin{pmatrix}
  u(z_j^+) \\
  u'(z_j^+)
\end{pmatrix} = A(z_j) \begin{pmatrix}
  u(z_j^-) \\
  u'(z_j^-)
\end{pmatrix}, \quad \text{where} \quad A(z) := \begin{pmatrix}
  1 & 0 \\
  0 & \gamma(z)
\end{pmatrix}, \tag{12}
\]

and \( \gamma(z) := \nu(z^+)/\nu(z^-) \). For TE waves boundary conditions (12) specify the continuity of both \( u \) and \( u' \) at \( z_j \) since \( \gamma(z_j) \equiv 1 \).

Let \( \zeta := \{z_j\}_{j \in \mathbb{Z}} \) be the set of planes of discontinuity, such that \( z_j < z_{j+1}, \ j \in \mathbb{Z} \). The thickness \( |d_j| := z_{j+1} - z_j \) of a slab located in between the interval \( d_j := (z_j, z_{j+1}) \) satisfies \( 0 < |d_j| < \infty \) for each \( j \in \mathbb{Z} \). Let \( \Gamma \) be the union of all intervals \( d_j \), that is

\[
\Gamma := \mathbb{R} \setminus \zeta = \bigcup_{j \in \mathbb{Z}} d_j.
\]

On \( \Gamma \) we introduce the Hilbert space

\[
H^2(\Gamma) := \bigoplus_{j \in \mathbb{Z}} H^2(d_j),
\]

where \( H^2(d_j) \) is the Sobolev space of order 2 on the interval \( d_j \). As an unbounded operator in \( L^2(\mathbb{R}) \), a domain of Sturm-Liouville operator \( \mathcal{L}_\nu \) is given by

\[
\text{Dom}(\mathcal{L}_\nu) = \left\{ u \in H^2(\Gamma) : \begin{pmatrix}
  u(z_j^+) \\
  u'(z_j^+)
\end{pmatrix} = A(z_j) \begin{pmatrix}
  u(z_j^-) \\
  u'(z_j^-)
\end{pmatrix}, \ \forall z_j \in \zeta \right\}.
\]

3.2. Floquet theory for periodic Sturm-Liouville operators

From now on we will assume that:

(a) the sequence of planes \( \zeta := \{z_j\}_{j \in \mathbb{Z}} \) is periodic with respect to the group \( \mathbb{G} := \ell \mathbb{Z}, \ \ell > 0 \);

(b) matrices \( z_j \mapsto A_j := A(z_j) \) are periodic with respect to \( \mathbb{G} \), where

\[
A_j = \begin{pmatrix}
  1 & 0 \\
  0 & \gamma_j
\end{pmatrix}, \quad j = 1, \ldots, n
\]

and \( \gamma_j := \nu(z_j^+)/\nu(z_j^-) \) is well-defined;

(c) functions \( \nu(z) > 0 \) and \( n(z) > 0 \) are piecewise continuous, and periodic with respect to \( \mathbb{G} \).
Let \( V_g u (z) := u(\theta + g) \), \( z \in \mathbb{R} \), \( g \in \mathbb{G} \), be the shift operator. Sturm-Liouville operator \( \mathcal{L}_\nu \) is invariant with respect to the shifts on the elements of group \( \mathbb{G} \),

\[
V_g \mathcal{L}_\nu u (z) = \nu (z + g) \frac{d}{dz} \left( \nu^{-1} (z + g) \frac{du(z + g)}{dz} \right) + k_0^2 n^2 (z + g) u(z + g)
\]

\[
= \nu (z) \frac{d}{dz} \left( \nu^{-1} (z) \frac{du(z + g)}{dz} \right) + k_0^2 n^2 (z) u(z + g) = \mathcal{L}_\nu V_g u (z).
\]

Given that \( V_g \mathcal{L}_\nu = \mathcal{L}_\nu V_g \) for every \( g \in \mathbb{G} \) it follows that \( \text{sp}_{\text{ess}} \mathcal{L}_\nu = \text{sp} \mathcal{L}_\nu \) and \( \text{sp}_{\text{dis}} \mathcal{L}_\nu = \emptyset \). The Sturm-Liouville operator \( \mathcal{L}_\nu \) thus defined is self-adjoint in \( L^2 (\mathbb{R}) \) by the conditions imposed on the coefficients \( n, \nu, \nu^{-1} \), as well as on the matrices \( A_j \), see [1].

Let \( \Lambda := [0, \ell) \) be a fundamental domain with respect to the action of the group \( \mathbb{G} \). The set of planes of discontinuity inside \( \Lambda \) is denoted by \( \zeta_0 := \zeta \cap \Lambda = \{z_1, \ldots, z_n\} \), where \( 0 < z_1 < \cdots < z_n < \ell \). By abusing the notation, we set \( z_0 \equiv 0 \), and \( z_{n+1} \equiv \ell \), so that

\[
\Gamma_0 := \Lambda \setminus \zeta_0 = \bigcup_{j=0}^{n} d_j
\]

represents the union of the intervals inside \( \Lambda \).

Consider the equation

\[
\mathcal{L}_\nu u (z) = \beta u (z), \quad z \in \Gamma,
\]

(13)

where \( \mathcal{L}_\nu \) is a \( \mathbb{G} \)-periodic Sturm-Liouville operator and \( \beta \) is the spectral parameter. Recall that a Bloch function is an eigenfunction of operator \( V_\ell \), that is, a non-vanishing solution of the equation \( V_\ell u(z) = \chi u(z) \) associated to the eigenvalue \( \chi \in \mathbb{C} \setminus \{0\} \) (see, e.g., [10, §2.8]). On choosing \( \chi \) in the form \( \chi = e^{i\theta t} \), \( p \in \mathbb{C} \), Bloch functions satisfy the quasi-periodic properties

\[
u(z + \ell) = e^{i\ell p} u(z) \quad \text{and} \quad u'(z + \ell) = e^{i\ell p} u'(z).
\]

The parameter \( p \) can be chosen as real, say \( p = \theta \in \mathbb{R} \), where \( \theta \) is called quasi-momentum. Hence \( \chi = e^{i\theta t} \) is uniquely determined if \( \theta \in [-\pi/\ell, \pi/\ell] \). This implies that \( \phi(z) = e^{-it\theta} u(z) \) is \( \ell \)-periodic. By \( \mathbb{B} := [-\pi/\ell, \pi/\ell] \) we denote the reciprocal unit cell (also known as Brillouin zone) of \( \Lambda \).

Let \( \mathcal{L}^\theta_\nu \) be a family of unbounded operators in \( L^2 (\Lambda) \) defined by differential expression (11) in \( \Gamma_0 \), with domain

\[
\text{Dom} \left( \mathcal{L}^\theta_\nu \right) = \left\{ u \in H^2 (\Gamma_0): \begin{pmatrix} u(z_j^+; \theta) \\ u'(z_j^-; \theta) \end{pmatrix} = A_j \begin{pmatrix} u(z_j^-; \theta) \\ u'(z_j^-; \theta) \end{pmatrix}, \quad z_j \in \zeta_0, j = 1, \ldots, n, \\
\right.
\]

\[
u(\ell; \theta) = e^{i\ell \theta} u(0; \theta), \quad u'(\ell; \theta) = e^{i\ell \theta} u'(0; \theta), \quad \theta \in \mathbb{B}
\]

where

\[
H^2 (\Gamma_0) := \bigoplus_{j=0}^{n} H^2 (d_j)
\]

For each \( \theta \in \mathbb{B} \), operator \( \mathcal{L}^\theta_\nu \) has a discrete spectrum

\[
\text{sp} \mathcal{L}^\theta_\nu = \{ \beta_1 (\theta) < \beta_2 (\theta) < \cdots < \beta_j (\theta) < \cdots \}
\]

where \( \beta_j (\theta) \) is the eigenvalue associated to the eigenfunction \( u_j (z; \theta) \), which satisfy the equation

\[
\mathcal{L}^\theta_\nu u_j (z; \theta) = \beta (\theta) u_j (z; \theta), \quad u \in \text{Dom} \left( \mathcal{L}^\theta_\nu \right).
\]

(14)
The functions $\mathbb{B} \ni \theta \mapsto \beta_j (\theta)$, called dispersion curves, are continuous functions on $\mathbb{B}$. As the quasi-momentum $\theta$ covers the whole Brillouin zone $\mathbb{B}$ the dispersion curves render spectral bands. In this way, the spectrum of the $G$-periodic Sturm-Liouville operator $L_\nu$ is

$$\text{sp} L_\nu = \bigcup_{\theta \in \mathbb{B}} \text{sp} L^\theta_\nu. \quad (15)$$

On the other hand, if $[a_j, b_j] \ (a_j \leq b_j, \ j \in \mathbb{N})$ is the image of the Brillouin zone $\mathbb{B}$ under the function $\beta_j$, then formula (15) gives

$$\text{sp} L_\nu = \bigcup_{j=1}^\infty [a_j, b_j],$$

that is, $L_\nu$ has a band spectrum.

4. Dispersion equation for $G$-periodic Sturm-Liouville operators

Let $\varphi_1, \varphi_2$ be two linearly independent solutions of equation $L^\theta_\nu u (z; \theta) = \beta (\theta) u (z; \theta)$, $z \in \Gamma_0$, that satisfy the Cauchy conditions

$$\varphi_1 (0, \kappa) = 1, \quad (\varphi_1)'_z (0, \kappa) = 0, \quad (16a)$$

$$\varphi_2 (0, \kappa) = 0, \quad (\varphi_2)'_z (0, \kappa) = 1, \quad (16b)$$

as well as the point conditions

$$\begin{pmatrix} u (z_j^+) \\ u' (z_j^+) \end{pmatrix} = A_j \begin{pmatrix} u (z_j^-) \\ u' (z_j^-) \end{pmatrix}, \quad j = 1, \ldots, n. \quad (17)$$

The function $u (z; \theta; \kappa) = C_1 (\theta, \kappa) \varphi_1 (z, \kappa) + C_2 (\theta, \kappa) \varphi_2 (z, \kappa)$ is a general solution of equation (14), being $C_1, C_2$ arbitrary coefficients. Quasi-periodic conditions $u (\ell, \theta) = e^{i \ell \theta} u (0, \theta)$ and $u_z (\ell, \theta) = e^{i \ell \theta} u_z (0, \theta)$ lead to the system of linear equations

$$C_1 (\theta, \kappa) \varphi_1 (\ell, \kappa) + C_2 (\theta, \kappa) \varphi_2 (\ell, \kappa) = e^{i \ell \theta} C_1 (\theta, \kappa), \quad (18a)$$

$$C_1 (\theta, \kappa) (\varphi_1)'_z (\ell, \kappa) + C_2 (\theta, \kappa) (\varphi_2)'_z (\ell, \kappa) = e^{i \ell \theta} C_2 (\theta, \kappa), \quad (18b)$$

so that $(C_1 (\theta, \kappa) \quad C_2 (\theta, \kappa))^T$ is an eigenvector of the monodromy matrix

$$M_\nu (\kappa) = \begin{pmatrix} \varphi_1 (\ell, \kappa) & \varphi_2 (\ell, \kappa) \\ (\varphi_1)'_z (\ell, \kappa) & (\varphi_2)'_z (\ell, \kappa) \end{pmatrix},$$

associated to the eigenvalue $\chi = e^{i \ell \theta}$. System (18) shall possess non-trivial solutions if

$$\det \begin{pmatrix} \varphi_1 (\ell, \kappa) - \chi & \varphi_2 (\ell, \kappa) \\ (\varphi_1)'_z (\ell, \kappa) & (\varphi_2)'_z (\ell, \kappa) - \chi \end{pmatrix} = 0.$$

This gives the dispersion equation

$$\chi^2 - 2 \chi D_\nu (\kappa) + 1 = 0, \quad (19)$$

where $D_\nu (\kappa) := \frac{1}{2} (\varphi_1 (\ell, \kappa) + (\varphi_2)'_z (\ell, \kappa))$ is the characteristic function of $G$-periodic Sturm-Liouville operator $L_\nu$. Equation (19) has solutions of the form $\chi = e^{i \ell \theta}, \ \theta \in \mathbb{B}$, if and only if $|D_\nu (\kappa)| \leq 1$. Hence, the spectrum of $L_\nu$ is given by the set

$$\text{sp} L_\nu = \{ \beta = \kappa^2 \geq 0 : |D_\nu (\kappa)| \leq 1 \}.$$
4.1. Construction of the characteristic function $D_\nu(\kappa)$

Solutions of equation (14) can be constructed as piecewise continuous functions. Let $\nu_j := \nu|_{d_j}$ and $n_j := n|_{d_j}$ be the restrictions of $\nu$ and $n$ on the interval $d_j$, respectively. By $\phi_{1,j}$, $\phi_{2,j}$ ($j = 0, \cdots, n$) we denote two linearly independent solutions of the equation

$$\nu_j (z) \frac{d}{dz} \left( \nu_j^{-1} (z) \frac{du_j (z)}{dz} \right) + k_0^2 u_j^2 (z) u_j (z) = \kappa^2 u_j (z), \quad z \in d_j,$$

which satisfy the Cauchy conditions

$$\begin{align*}
\phi_{1,j} (z_j) &= 1, & \phi_{2,j} (z_j) &= 0, \\
\phi'_{1,j} (z_j) &= 0, & \phi'_{2,j} (z_j) &= 1.
\end{align*}$$

A general solution of (20) in the interval $d_j$ is given by $u_j (z) = u_j (z_j) \phi_{1,j} (z) + u'_j (z_j) \phi_{2,j} (z)$. Hence, the piecewise continuous function

$$u (z) = \begin{cases} 
  u_0 (z_0) \phi_{1,0} (z) + u_0' (z_0) \phi_{2,0} (z), & z \in d_0 \\
  u_1 (z_1) \phi_{1,1} (z) + u_1' (z_1) \phi_{2,1} (z), & z \in d_1 \\
  \vdots \\
  u_n (z_n) \phi_{1,n} (z) + u_n' (z_n) \phi_{2,n} (z), & z \in d_n
\end{cases}$$

is a general solution of (14) in $\Gamma_0 = \bigcup_{j=0}^{n} d_j$. At $z_j \in \zeta_0$ point conditions (17) take the form

$$\begin{pmatrix} u_j (z_j) \\ u'_j (z_j) \end{pmatrix} = A_j \begin{pmatrix} u_{j-1} (z_{j-1}) \phi_{1,j-1} (z_j) + u'_{j-1} (z_{j-1}) \phi'_{2,j-1} (z_j) \\ u_{j-1} (z_{j-1}) \phi'_{1,j-1} (z_j) + u'_{j-1} (z_{j-1}) \phi'_{2,j-1} (z_j) \end{pmatrix} = A_j M_{j-1,j} \begin{pmatrix} u_{j-1} (z_{j-1}) \\ u'_{j-1} (z_{j-1}) \end{pmatrix},$$

where

$$M_{j,j+1} := \begin{pmatrix} \phi_{1,j} (z_{j+1}) & \phi_{2,j} (z_{j+1}) \\ \phi'_{1,j} (z_{j+1}) & \phi'_{2,j} (z_{j+1}) \end{pmatrix}, \quad j = 0, \cdots, n$$

is the monodromy matrix associated to the interval $d_j = (z_j, z_{j+1})$. The recursive use of previous expression leads to the matrix equation

$$\begin{pmatrix} u (\ell; \kappa) \\ u' (\ell; \kappa) \end{pmatrix} = T_\nu (\kappa) \begin{pmatrix} u (0; \kappa) \\ u' (0; \kappa) \end{pmatrix} = \begin{pmatrix} T_{11} (\kappa) & T_{12} (\kappa) \\ T_{21} (\kappa) & T_{22} (\kappa) \end{pmatrix} \begin{pmatrix} u (0; \kappa) \\ u' (0; \kappa) \end{pmatrix},$$

where $T_\nu := M_{n,n+1} A_n M_{n-1,n} \cdots A_2 M_{1,2} A_1 M_{0,1}$ is the transfer matrix of the unit cell of the periodic medium.

Thus, solutions $\varphi_1$ and $\varphi_2$ that fulfill conditions (16) are defined by

$$\begin{pmatrix} \varphi_1 (\ell, \kappa) \\ (\varphi_1)' (\ell, \kappa) \end{pmatrix} = T_\nu (\kappa) \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} T_{11} (\kappa) \\ T_{21} (\kappa) \end{pmatrix}, \quad \begin{pmatrix} \varphi_2 (\ell, \kappa) \\ (\varphi_2)' (\ell, \kappa) \end{pmatrix} = T_\nu (\kappa) \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} T_{12} (\kappa) \\ T_{22} (\kappa) \end{pmatrix},$$

thereby function $D_\nu (\kappa)$ is given by the expression

$$D_\nu (\kappa) = \frac{1}{2} \left( T_{11} (\kappa) + T_{22} (\kappa) \right).$$
4.2. Monodromy matrices for homogeneous slabs

Let \( n_j := \sqrt{\varepsilon_{r,j}\mu_{r,j}} \) \((\varepsilon_{r,j} > 0, \mu_{r,j} > 0)\) be a constant refractive index corresponding to a homogeneous slab at the interval \( d_j \). The corresponding monodromy matrix can be obtained in a closed-form. Equation (20) reads

\[
\frac{d^2 u_j(z)}{dz^2} = - \left( k_0^2 n_j^2 - \kappa^2 \right) u_j(z), \quad z \in d_j,
\]

thereby

\[
\phi_{1,j}(z) = \cos \left( (z - z_j) \sqrt{k_0^2 n_j^2 - \kappa^2} \right), \quad \phi_{2,j}(z) = \frac{1}{\sqrt{k_0^2 n_j^2 - \kappa^2}} \sin \left( (z - z_j) \sqrt{k_0^2 n_j^2 - \kappa^2} \right) \tag{26}
\]

are linearly independent solutions satisfying conditions (21). These solutions are oscillatory if \( k_0^2 n_j^2 - \kappa^2 > 0 \), that is, if \( \omega > \omega_{j}^{(c)} = \kappa c_0 / n_j \). Therefore the condition \( \omega_{j}^{(c)} \) defines a cutoff frequency, where \( v_j := c_0 / n_j \) is the phase velocity in a medium with constant refractive index \( n_j \). If \( \omega > \omega_{j}^{(c)} \) solutions (26) will be oscillatory. In the optical regime, frequencies and wavelengths are of the order of \( \times 10^{15} \) Hz and \( \times 10^{-7} \) m, respectively. Such magnitudes hold extreme positions. Hence, it would be convenient to express the matrix \( M_{j,j+1} \) in terms of numbers from a more suitable scale. Let us introduce the dimensionless parameters \( \kappa := \kappa / k_0 \) and \( \tilde{d}_j := |d_j| / \lambda \), where \( \lambda \) is the (optical) working wavelength. The wavelength \( \lambda \) is linked with the free-space wave-number \( k_0 \) by the relation \( k_0 = 2\pi / \lambda \). In terms of the new parameters the monodromy matrix reads

\[
\tilde{M}_{j,j+1}(\kappa) = \begin{pmatrix}
\cos \left( 2\pi \tilde{d}_j \sqrt{n_j^2 - \kappa^2} \right) & \frac{1}{k_0 \sqrt{n_j^2 - \kappa^2}} \sin \left( 2\pi \tilde{d}_j \sqrt{n_j^2 - \kappa^2} \right) \\
-k_0 \sqrt{n_j^2 - \kappa^2} \sin \left( 2\pi \tilde{d}_j \sqrt{n_j^2 - \kappa^2} \right) & \cos \left( 2\pi \tilde{d}_j \sqrt{n_j^2 - \kappa^2} \right)
\end{pmatrix},
\]

where \( \tilde{M}_{j,j+1}(\kappa) := M_{j,j+1} \left( k_0 \kappa \right) = M_{j,j+1}(\kappa) \). The condition \( 0 \leq \kappa < n_j \) implies oscillatory solutions.

4.3. Example

Let us consider a periodic medium consisting of two distinct media with constant refractive indexes \( n_0 \) and \( n_1 \). The slabs alternate each other as is shown in Figure 2-(a).

![Figure 2](image-url)

Figure 2. (a) Refractive index profile of the photonic crystal. (b) Determination of the photonic bands for TE waves at \( \omega = 2.250 \times 10^{15} \) rad/s.

In this case \( \zeta = \{ z_1 \} \) and \( \Gamma_0 = d_0 \cup d_1 \). The transfer matrix for this structure is

\[
\tilde{T}_\nu(\kappa) = \tilde{M}_{1,2}(\kappa) A_1 \tilde{M}_{0,1}(\kappa),
\]
where $\tilde{T}_\nu(\kappa) := T_\nu(k_0\kappa) = T_\nu(\kappa)$. The characteristic function is given in a closed form by

$$\tilde{D}_\nu(\kappa) = \left(1 + \gamma_1\right) \cos\left(2\pi \sqrt{n_0^2 - \frac{n_0^2}{n_0^2} - \kappa^2}\right) \cos\left(2\pi \sqrt{n_1^2 - \sqrt{n_1^2 - \kappa^2}}\right)$$

$$- \sin\left(2\pi \sqrt{n_0^2 - \kappa^2}\right) \sin\left(2\pi \sqrt{n_1^2 - \sqrt{n_1^2 - \kappa^2}}\right) \left(\frac{n_0^2 - \kappa^2 + \gamma_1 (n_0^2 - \kappa^2)}{2(n_0^2 - \kappa^2)(n_1^2 - \kappa^2)}\right),$$

where $0 \leq \kappa < \min\{n_0, n_1\}$, $\gamma_1 = 1$ for TE waves, and $\gamma_1 = \frac{\varepsilon(z_1^+)}{\varepsilon(z_1^-)} = \frac{\varepsilon_{r,1}}{\varepsilon_{r,0}} = \frac{n_1^2}{n_0^2}$ for TM waves.

In the new variables the function $\tilde{D}_\nu$ is defined by $\tilde{D}_\nu(\kappa) := D_\nu(k_0\kappa) = D_\nu(\kappa)$.

Photonic bands are determined from the normalised propagation constant $\kappa$ satisfying $\left|\tilde{D}_\nu(\kappa; \omega)\right| \leq 1$, see Figure 2-(b). The band edges $\kappa_{\text{edge}}$ are calculated from the equation $\left|\tilde{D}_\nu(\kappa_{\text{edge}}; \omega)\right| = 1$. Note that the frequency $\omega$ has been indicated explicitly. This means that for each $\omega \in [\omega_i, \omega_f]$ the photonic bands should be calculated, which results in a $\omega - \kappa$ diagram. For instance, in Figure 3-(a), -(b) we have the $\omega - \kappa$ diagrams for both TE and TM waves for a photonic crystal with the following settings [11]: $d_0 = 815$ nm, $d_1 = 680$ nm, $n_0 = 1.4585$ (SiO$_2$), $n_1 = 3.9766$ (Si), [12, 13]. The considered interval of frequencies ranges from $\omega_i = 0.025 \times 10^{15}$ rad/s to $\omega_f = 2.400 \times 10^{15}$ rad/s, which lie in the infrared spectrum. The $\omega - \kappa$ diagrams were obtained by taking equidistant increments of frequency $\Delta \omega = 0.025 \times 10^{15}$ rad/s on calculating the photonic bands. In these diagrams the dashed line $\kappa = n_0$ separates the oscillatory region from the non-oscillatory region (indicated by the grey background).

5. Monodromy matrices for arbitrary refractive indexes

In Subsection 4.2 it was possible to obtain a closed-form expression for the monodromy matrices since differential equation (25) has constant coefficients. For second order differential equations with variable coefficients it is possible to obtain closed-form solutions in terms of special functions in some cases. Regarding Sturm-Liouville equations, numerical techniques for determining
approximate solutions are at hand (see, e.g., [14]). Nonetheless in this work we employ the SPPS method [3] for obtaining solutions of equation (20) in the form of power series of the spectral parameter \( \beta = \kappa^2 \). This method gives exact solutions but a numerical method can be derived by truncating the convergent power series, as is shown next.

Let us assume that the homogeneous equation

\[
\frac{d}{dz} \left( \nu_j^{-1}(z) \frac{d \nu_j}{dz}(z) \right) + k_0^2 n_0^{2j}(z) \nu_j(z) = 0, \quad z \in d_j,
\]

possesses a particular solution \( \nu_{0,j} \) satisfying the smoothness conditions \( \nu_j^{-1} \nu_{0,j}^{-2}, \nu_j \nu_{0,j}^{-2} \in C(d_j) \).

The power series

\[
v_{1,j}(z) = \nu_{0,j}(z) \sum_{m=0}^{\infty} \kappa^{2m} \tilde{Z}_j^{(2m)}(z), \quad v_{2,j}(z) = \nu_{0,j}(z) \sum_{m=0}^{\infty} \kappa^{2m} Z_j^{(2m+1)}(z),
\]

with the functions \( \tilde{Z}_j^{(n)} \), \( Z_j^{(n)} \) defined by the recursive integration procedure [3]:

\[
\tilde{Z}_j^{(0)} = 1, \quad \tilde{Z}_j^{(n)}(z) = \begin{cases} 
\int_{z_j}^z \tilde{Z}_j^{(n-1)}(s) \nu_{0,j}^{-2}(s) \nu_j^{-1}(s) ds, & n \text{ odd} \\
\int_{z_j}^z \tilde{Z}_j^{(n-1)}(s) \nu_{0,j}^{-2}(s) \nu_j(s) ds, & n \text{ even}
\end{cases},
\]

\[
Z_j^{(0)} = 1, \quad Z_j^{(n)}(z) = \begin{cases} 
\int_{z_j}^z Z_j^{(n-1)}(s) \nu_{0,j}^{-2}(s) \nu_j(s) ds, & n \text{ odd} \\
\int_{z_j}^z Z_j^{(n-1)}(s) \nu_{0,j}^{-2}(s) \nu_j^{-1}(s) ds, & n \text{ even}
\end{cases},
\]

satisfy the Sturm-Liouville equation (20) in \( d_j = (z_j, z_{j+1}) \). In addition, these series converge uniformly in \( d_j \). Since series \( v_{1,j}, v_{2,j} \) satisfy the Cauchy conditions

\[
v_{1,j}(z_j) = \nu_{0,j}(z_j), \quad v_{2,j}(z_j) = \nu_{0,j}(z_j),
\]

\[
v_{1,j}(z_j) = 0, \quad v_{2,j}(z_j) = \frac{\nu_j(z_j)}{\nu_{0,j}(z_j)}
\]

it follows that the solutions

\[
\phi_{1,j}(z) = \frac{1}{\nu_{0,j}(z_j)} v_{1,j}(z) - \frac{\nu_{0,j}(z_j)}{\nu_j(z_j)} v_{2,j}(z), \quad \phi_{2,j}(z) = \frac{\nu_{0,j}(z_j)}{\nu_j(z_j)} v_{2,j}(z)
\]

(27a)

fulfill conditions (21). Derivatives of these solutions read

\[
\phi'_{1,j}(z) = \frac{\nu_{0,j}(z)}{\nu_{0,j}(z_j)} \phi_{1,j}(z) + \frac{1}{\nu_{0,j}(z_j)} v_{3,j}(z) - \frac{\nu_{0,j}(z_j)}{\nu_j(z_j)} v_{4,j}(z),
\]

\[
\phi'_{2,j}(z) = \frac{\nu_{0,j}(z)}{\nu_{0,j}(z_j)} \phi_{2,j}(z) + \frac{\nu_{0,j}(z_j)}{\nu_j(z_j)} v_{3,j}(z),
\]

(27b)

(27c)

where \( v_{3,j} \) and \( v_{4,j} \) are series defined by

\[
v_{3,j}(z) := \frac{\nu_j(z)}{\nu_{0,j}(z_j)} \sum_{m=1}^{\infty} \kappa^{2m} \tilde{Z}_j^{(2m-1)}(z), \quad v_{4,j}(z) := \frac{\nu_j(z)}{\nu_{0,j}(z_j)} \sum_{m=0}^{\infty} \kappa^{2m} Z_j^{(2m)}(z).
\]

Monodromy matrices \( M_{j,j+1} \) \( (j = 0, \ldots, n) \) are constructed from functions (27) evaluated at \( z = z_{j+1} \) according to (23).
5.1. Numerical implementation

The numerical implementation of monodromy matrices $M_{j,j+1}$ needs the uniformly convergent series $v_{1,j}(z)$, $v_{2,j}(z)$, $v_{3,j}(z)$ and $v_{4,j}(z)$ to be truncated up to $N$ terms. Let $v_{1,j}^{(N)}$ denote the truncated version of series $v_{1,j}$, then an estimate of the truncation error is

$$\left|v_{1,j}(z) - v_{1,j}^{(N)}(z)\right| \leq \max_{0 \leq m \leq N} \left|v_{0,j}\right| \cosh \sqrt{\eta_j} - \sum_{m=0}^{N} \frac{\eta_j^m}{(2m)!},$$

where $\eta_j := |\kappa|^2 \left( \max \left| v_{0,j}^2 \nu_j^{-1} \right| \right) \left( \max \left| v_{0,j}^{-2} \nu_j \right| \right) |d_j|^2$.

Similarly, truncation error for $v_{2,j}$ is estimated by the tail of the Taylor series of $\sinh \sqrt{\eta_j}$, see [3]. Since $|d_j|$ and $\nu_j$ are specified for a given problem, the truncation error can be mainly reduced by increasing the number $N$ of terms of truncated series. In addition, the accuracy of particular solution $v_{0,j}$ influences the error, but this solution can also be constructed accurately by means of the SPPS method itself. Let $M_{j,j+1}^{(N)}$ ($j = 0, 1, \cdots, n$) denote the monodromy matrices constructed from truncated series $v_{i,j}^{(N)}(z)$ ($i = 1, \cdots, 4$), then the matrix $T^{(N)}_{\nu} := M_{n,n+1}^{(N)}A_nM_{n-1,n}^{(N)} \cdots A_2M_{1,2}A_1M_{0,1}^{(N)}$ is an approximation of the transfer matrix $T_{\nu}$, and

$$D_{\nu}^{(N)}(\kappa) = \frac{1}{2} \left( T_{11}^{(N)}(\kappa) + T_{22}^{(N)}(\kappa) \right)$$

is an approximation for the characteristic function $D_{\nu}(\kappa)$. Note that $D_{\nu}^{(N)}(\kappa)$ is a polynomial of the (complex) variable $\kappa$ thereby the band edges $\kappa_{\text{edge}}$ are calculated from the polynomial roots of the equations $D_{\nu}^{(N)}(\kappa) = 0$. One would expect the band edges to be real roots, but in general such roots will be complex numbers of the form $\kappa = \kappa' + \kappa'',$ where $\kappa', \kappa'' \in \mathbb{R}$. For the correct discrimination of accurate approximations of the band edges we fix an arbitrarily small tolerance $\epsilon_\nu > 0$ so that if $|\kappa''| < \epsilon_\nu$ then $\kappa_{\text{edge}} \approx \kappa'$ is an approximate band edge.

6. Conclusions

In this work we have derived the characteristic function $D_{\nu}$ of one-dimensional photonic crystals in terms of the monodromy matrices $M_{j,j+1}$ corresponding to the segments $d_j \in \Gamma_0$ of the fundamental cell $\Gamma_0$. An explicit representation for the entries of matrices $M_{j,j+1}$ was provided in the form of uniformly convergent power series of the spectral parameter $\kappa^2$. For their numerical treatment, the previously mentioned series should be truncated up to some $N$ terms. This leads to a characteristic polynomial $D_{\nu}^{(N)}(\kappa)$, whereby the numerical calculation of the edges of the photonic bands reduces to calculating polynomial roots of the equations $D_{\nu}^{(N)}(\kappa) = 0$. In spite the simplicity of this result, the theory here presented is robust enough to be applied on crystals involving slabs with (almost) arbitrary varying refractive indexes. A natural path to follow in this research is to consider two- and three-dimensional photonic crystals. We would expect to derive a similar result, that is to be able to calculate the spectra of the crystals from the zeros of an analytic function of the complex variable $\kappa$, or numerically from the roots of certain polynomial.

Acknowledgments

VBF acknowledges CONACyT for support via grant 283133.

References

[1] Eastham M S P 1973 The Spectral Theory of Periodic Differential Equations (Edinburgh: Scottish Academic Press).
[2] Khmelnitskaya K V and Rosu H C 2010 Ann. Phys. 325 2512.
[3] Kravchenko V V and Porter R M 2010 Math. Method. Appl. Sci. 33 459.
[4] Rabinovich V S, Barrera-Figueroa V and Olivera Ramírez L 2019 Front. Phys. 7 57.
[5] Rabinovich V S, Roch S and Silbermann B 2004 Limit Operators and Their Applications in Operator Theory (Basel: Birkhäuser).
[6] Barrera-Figueroa V and Rabinovich V S 2017 J. Phys. A: Math. Theor. 50 215207.
[7] Barrera-Figueroa V, Rabinovich V S and Maldonado Rosas M 2019 Appl. Anal. 98 458.
[8] Chew W C 1995 Waves and Fields in Inhomogeneous Media (New York: IEEE Press).
[9] Cruz y Cruz S and Razo R 2015 J. Phys. Conf. Ser. 624 012018.
[10] Berezin F A and Shubin M A 1991 The Schrödinger Equation (Dordrecht: Kluwer Academic Publ.)
[11] Gao W, Hu X, Li C, Yang J, Chai Z, Xie J and Gong Q 2018 Opt. Express 26 8634.
[12] Malitson I H 1965 J. Opt. Soc. Am. 55 1205.
[13] Tan C Z 1998 J. Non-Cryst. Solids 223 158.
[14] Pryce J D 1993 Numerical Solution of Sturm-Liouville Problems (Oxford: Clarendon Press).