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Mathematical Principles in Photonic Crystals (**)

Dedicated to the memory of Giulio Di Cola.

1 - Introduction

Photonic crystals are nano-structures exhibiting the interesting behavior that light at certain frequencies cannot travel in the crystal, whereas at other frequencies it does travel and is scattered. This phenomenon is due to the periodic variation in the index of refraction of the crystal [**17**], [8].

Such crystals also have the property that light at an allowed frequency may travel along a particular path, as a consequence of a small non-periodic variation (impurity) in the refractive index. The role of mathematics is crucial to the solution of several problems involving nano-structures. In particular, the design of photonic crystals is based on the identification of the refractive index of crystals when the allowed and forbidden frequencies are specified.

The purpose of this paper is to derive physically relevant mathematical results on the design of photonic crystals.

The outline of the paper is the following: in Section 2 we illustrate some physical

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properties, mention relevant applications and introduce the mathematical model that describes the propagation of light in photonic crystals. In Section 3 we give the basic mathematical results. In Section 4 we introduce the scattering matrix and the period map which allows us to characterize the propagation of the light in the crystal in terms of its behavior when propagating for only one period. In Section 5 we propose some new results on the design of photonic crystals and in Section 6 we draw some conclusions and mention some open problems.

2 - Physical properties, applications and mathematical modeling

2.1 - *Physical properties and applications*

Photonic crystals are mono, bi or tri-dimensional crystal lattice structures characterized by a periodic refractive index[1] $n(x, y, z) = \sqrt{(\varepsilon\mu/\varepsilon_0\mu_0)}$.

These crystals have many properties analogous to those of semiconductor crystals, such as the appearance of pass bands and band gaps and a complex dispersion relation [**7**]. Repeating the dielectric constant in a pure unbounded photonic crystal periodically generates allowed and forbidden photonic energy bands in the same way as the periodic potential in a semiconductor crystal affects the electron motion by defining allowed and forbidden electronic energy bands. Forbidden bands in photonic crystals are called *photonic band gaps* or *PBGs*. In Figure 1 we show a typical band structure.

Replacing the material in a bounded region by a different material or changing the size of a period while keeping the same material, we can put the (discrete) energies of allowed states into a band gap (crossed red dots in Figure 1). Besides the band gap structure, another analogy is between polarization and spin. The two orthogonal polarizations for photons are analogous to the two electron spins [**7**]. On the other hand, electrons have mass and charge while photons have neither mass nor change. Moreover, electrons follow the Fermi-Dirac distribution, whereas photons obey Bose-Einstein statistics.

The band gap structure allows us to design resonant cavities [**7**], [**5**], [**6**], waveguides [**7**], [**5**], [**6**] and optical fibers [**2**]. Introducing impurities we can either confine

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[1] ε and μ are the electric permittivity and magnetic permeability of the medium, respectively, whereas ε_0 and μ_0 are the electric permittivity and magnetic permeability of the vacuum. Recall that the permittivity ε and the permeability μ of a medium together determine the phase velocity v of electromagnetic radiation through that medium:

$$\varepsilon\mu = \frac{1}{v^2}\,.$$

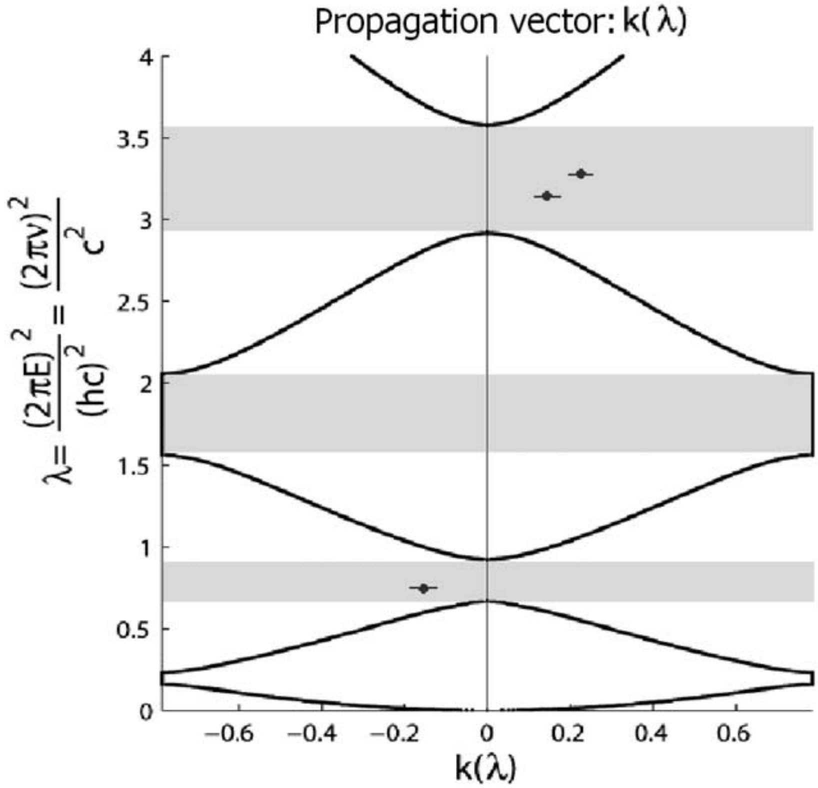

Fig. 1. The band gap structure of a photonic crystal. The band gap structure of a pure crystal is plotted in blue, crossed red dots are allowed energy levels introduced by an impurity. The axis units are arbitrary.

light (resonant cavity) or light can be guided in the crystal by using impurities to create preferred pathways.

Photonic crystals can also be used to design next generation optical fibers. Standard optical fibers rely on light being guided by the physical law known as *total internal reflection* (TIR) or *index guiding*. In order to achieve TIR in these fibers, which are formed from dielectrics or semiconductors, it is required that the refractive index of the core exceeds that of the surrounding media. In photonic crystal fibers light is confined to propagating along PBGs, while the core can be a different medium with a small index of refraction. These fibers have properties that differ from those of standard fibers: they allow bending by large angles and soliton propagation, both of which are very important to telecommunication.

Photonic crystals are also characterized by seemingly strange properties like negative refraction, negative diffraction and the superprism effect [**10**], [**12**] typical of a left-handed metamaterial. As to the first property, we can say that *"Snell's law is reversed."* As a matter of fact, in photonic crystals, for certain frequency intervals, the rays will be refracted on the same side of the normal upon entering the material. Negative diffraction is another unusual phenomenon: the luminous cone collimates inside photonic crystals unlike what occurs at ordinary diffraction. Finally, photonic crystals are characterized by a high dispersion capability. A prism made up of a photonic crystal would have a dispersion capability that is about 500 times stronger than that of a prism made of a conventional material [**9**]. Using these properties (negative refraction, negative diffraction and superprism) a research group at the Georgia Institute of Technology has designed an optical de-multiplexer [**13**].

Nonlinear optics also plays an important role in this kind of crystal. Some of the most interesting nonlinear phenomena are second and third harmonics generation (SHG and THG), optical parametric amplification (OPA), optical rectification and white-light supercontinuum generation (WLSCG).

In a linear medium the dielectric polarization vector $\boldsymbol{P}(\boldsymbol{r}, t)$ can be written as

$$\boldsymbol{P}(\boldsymbol{r}, t) = \varepsilon_0 \chi_e(\boldsymbol{r}, t) \boldsymbol{E}(\boldsymbol{r}, t),$$

where $\boldsymbol{r}$ is the position in space, t is the time, while ε_0 is the electric permittivity of free space and $\chi_e(\boldsymbol{r}, t)$ is the electric susceptibility of the medium.[2] If the medium is nonlinear then the previous formula is not correct and the susceptibility also depends on the electric field amplitude:

$$P_i(\boldsymbol{r}, t) = \sum_j \chi_{ij}^{(1)}(\boldsymbol{r}, t) E_j(\boldsymbol{r}, t) + \sum_{j,k} \chi_{i,j,k}^{(2)}(\boldsymbol{r}, t) E_j(\boldsymbol{r}, t) E_k(\boldsymbol{r}, t) + \dots$$

for $i, j, k = 1, 2, 3$, where the different χ's are electric susceptibilities.

Exciting a medium with two electromagnetic waves with different frequencies ω_1 and ω_2, the dielectric polarization vector becomes

$$\boldsymbol{P} = \boldsymbol{P}(\omega_1) + \boldsymbol{P}(\omega_2) + \boldsymbol{P}(\omega_1 + \omega_2) + \boldsymbol{P}(\omega_1 - \omega_2) + \dots$$

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[2] The electric susceptibility $\chi(\boldsymbol{r}, t)$ of a dielectric material is a measure of how easily the medium polarizes in response to an electric field. In an anisotropic medium $\chi_e(\boldsymbol{r}, t)$ is a tensor. We recall that $\chi_e = \varepsilon_r - 1$ and the electric displacement $\boldsymbol{D}$ is related to the polarization density $\boldsymbol{P}$ by

$$\boldsymbol{D} = \varepsilon_0 \boldsymbol{E} + \boldsymbol{P} = \varepsilon_0 (1 + \chi_e) \boldsymbol{E} = \varepsilon_0 \varepsilon_r \boldsymbol{E}.$$

In general, a material cannot polarize instantaneously in response to an applied field, and so the more general formulation as a function of time is

$$\boldsymbol{P}(\boldsymbol{r}, t) = \varepsilon_0 \int_{-\infty}^{t} \chi_e(t - t') \boldsymbol{E}(\boldsymbol{r}, t') \, dt'.$$

According to this we can generate light with a double or triple frequency (SHG or THG) and amplify a signal input in the presence of a higher-frequency wave (OPA). It is also possible to generate quasi-static electric fields or to produce an optical spectrum which covers all of the visible range (WLSCG). This last property is commonly used for spectroscopic purposes to produce a very broad spectrum of light starting from an initially spectrally much narrower light pulse (a few tenths of a nanometer or less).

Another important nonlinear phenomenon is the Kerr effect, according to which the refractive index depends on the electromagnetic amplitude, i.e.,

$$n = n(|\boldsymbol{E}|).$$

The Kerr effect is used to design optical transistors [**18**] that are the basic components of integrated optics. Research in photonic crystals is also enhanced by low energy loss ($50cm^{-1} = 2dB/100\mu m$, [**5**]).

2.2 - *Mathematical modeling*

Our mathematical model generalizes both the Schrödinger equation, which describes electron propagation in a semiconductor crystal, and the Maxwell and Helmholtz equations, which describe electromagnetic wave propagation. A mathematical model capable of merging both models is the following:

$$-\psi''(\lambda, x) + Q(x)\psi(\lambda, x) = \lambda n(x)^2 \psi(\lambda, x), \tag{2.1}$$

where $Q(x+p) = Q(x)$, $n(x+p) = n(x)$ and p is the period. Here $Q(x)$ is the potential energy and $n(x)$ is the refractive index. This approach allows us to extend the quantum mechanical postulates to describe light propagation rather than to adopt a classical model like the Helmholtz equation. In fact,

1. each eigenfunction furnishes an allowed state;
2. the state of a quantum mechanical system is completely specified by the wavefunction;
3. the squared absolute value of the wavefunction $|\psi(\lambda, x)|^2$ is proportional to the probability to find a particle within an infinitesimal interval centered at x.

We can use quantum mechanical operators to obtain a probabilistic interpretation of the wavefunction.

The Schrödinger equation[3] for electrons and the Helmholtz[4] equation for photons

[3] $-\dfrac{\hbar^2}{2m}\psi''(\lambda, x) + Q(x)\psi(\lambda, x) = E\psi(\lambda, x)$, with $Q(x+p) = Q(x)$ and p is the period.

[4] $-\psi''(\lambda, x) = \lambda n(x)^2 \psi(\lambda, x)$, with $n(x+p) = n(x)$ and p is the period.

in a crystal are both eigenvalue equations. Though very similar, the physical meaning of the eigenvalue λ is very different. We can appreciate the difference by considering two examples: electrons in free space ($Q(x) = 0$) and photons in an optically homogeneous medium ($n(x) = \text{const}$). In these cases we have

$$\begin{cases} -\dfrac{\hbar^2}{2m}\psi_e''(x) = E\psi_e(x) & \text{Schrödinger equation} \\ \\ \psi_{ph}''(x) + \omega^2\varepsilon_0\mu_0 n^2\psi_{ph}(x) = 0 & \text{Helmholtz equation.} \end{cases}$$

Recalling Plank's energy law for photons $E = \hbar\omega$ and $c^2 = \dfrac{1}{\mu_0\varepsilon_0}$ we can derive

$$\lambda = \begin{cases} \dfrac{2mE}{\hbar^2} & \text{electron in free space} \\ \omega^2\varepsilon_0\mu_0 = \dfrac{E^2}{\hbar^2 c^2} & \text{photon} \end{cases}$$

where λ is the eigenvalue parameter of the equations. We observe that in the first case the eigenvalue parameter λ is proportional to the electron energy, whereas in the second case the eigenvalue parameter is proportional to the square of the energy.

In this work we introduce the period map as a matrix operator that allows us to obtain the solution at any location in the crystal by analysing only one period. Our primary purpose is to calculate the refractive index from the left and right reflection and transmission coefficients, which is a typical inverse problem. To do so, we introduce the scattering matrix, that is the matrix uniquely characterized by the reflection and transmission coefficients, and then divide this inverse problem into the following two subproblems:

1. determining the period map from the scattering matrix;
2. determining the refractive index from the period map.

In particular, we analyse the piecewise-constant case for the refractive index $n(x)$ in a mono-dimensional crystal and consider the impurities confined to an interval of length less than a crystal period.

3 - Basic properties

In the following subsections we consider equation (2.1) determine its solution and analyse the case of a crystal without impurities.

3.1 - *Floquet's solutions and Hill's discriminant*

Let us first derive Floquet's theorem (**[15, Ch. XXI]** and [**11**], [**3**]) and Hill's discriminant. There exist unique linearly independent solutions $\theta(\lambda, x)$ and $\phi(\lambda, x)$ of equation (2.1) satisfying the initial conditions

$$\theta(\lambda, 0) = 1, \qquad \theta'(\lambda, 0) = 0, \tag{3.1a}$$

$$\phi(\lambda, 0) = 0, \qquad \phi'(\lambda, 0) = 1. \tag{3.1b}$$

Let $\psi(x) \not\equiv 0$ be a solution of equation (2.1) satisfying the τ-periodicity or Born-Von Kármán's condition

$$\psi(\lambda, x + p) = \tau\psi(\lambda, x), \tag{3.2}$$

where τ is a constant. Since $\psi \in C^1$, by substituting $x = 0$ in (3.2) and its x-derivative we have

$$\psi(\lambda, p) = \tau\psi(\lambda, 0), \tag{3.3a}$$

$$\psi'(\lambda, p) = \tau\psi'(\lambda, 0), \tag{3.3b}$$

for some constants $0 \neq \tau \in \mathbb{C}$. Obviously $\psi(\lambda, x)$ is a linear combination of $\theta(\lambda, x)$ and $\phi(\lambda, x)$:

$$\psi(\lambda, x) = c_1\theta(\lambda, x) + c_2\phi(\lambda, x).$$

This linear combination satisfies the boundary conditions (3.3) if and only if the linear system

$$\begin{pmatrix} \tau - \theta(\lambda, p) & -\phi(\lambda, p) \\ -\theta'(\lambda, p) & \tau - \phi'(\lambda, p) \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

has a nontrivial solution. This is the case if and only if the system determinant

$$\tau^2 - [\theta(\lambda, p) + \phi'(\lambda, p)]\tau + 1 \tag{3.4}$$

vanishes. Here we have used the constancy of the Wronskian[5] $w = \theta\phi' - \theta'\phi$ and condition (3.1). Introducing *Hill's discriminant*

$$\Delta(\lambda) = \theta(\lambda, p) + \phi'(\lambda, p), \tag{3.5}$$

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[5] Using equation (2.1) we easily show that

$$w' = \left(\theta\phi' - \theta'\phi\right)' = \theta\phi'' - \theta''\phi = \theta(Q - \lambda n^2)\phi - (Q - \lambda n^2)\theta\phi = 0.$$

To be more precise, $w(x) = \text{const.} = w(0)$. From conditions (3.1) it follows that $w(x) = 1$.

we have

$$\tau^2 - \Delta(\lambda)\tau + 1 = 0 \tag{3.6}$$

as well as

$$\begin{cases} \tau_1 + \tau_2 = \Delta(\lambda), \\ \tau_1 \tau_2 = 1, \end{cases}$$

where τ_1 and τ_2 are the roots of equation (3.6). Generalizing Born-Von Kármán's condition to m periods we get:

$$\psi(\lambda, x + mp) = \tau^m \psi(\lambda, x).$$

When nontrivial, such solutions are unbounded as $x \to +\infty$ if $|\tau| > 1$ and as $x \to -\infty$ if $|\tau| < 1$. Thus boundedness of such nontrivial solutions requires $|\tau| = 1$, so $\tau_1 = e^{ikp}$ and $\tau_2 = e^{-ikp}$ with $k \in \mathbb{R}$. Hill's discriminant becomes

$$\Delta(\lambda) = \tau_1 + \tau_1^{-1} = e^{ikp} + e^{-ikp} = 2\cos(kp). \tag{3.7}$$

Hence we have bounded solutions if and only if $\Delta(\lambda)$ is in $[-2, 2]$. For such values of λ a *bounded solution* exists and hence an electromagnetic wave can propagate inside the crystal. Outside this range there is no physical solution, because these waves, which are called *unbounded solutions*, would have infinite energy. By the Schrödinger-Helmholtz Spectrum, denoted by $\{\sigma\}$, we mean the set of λ values such that $\psi(\lambda, x)$ is bounded in $x \in \mathbb{R}$.

The natural extension of a solution of equation (2.1) has the *Bloch representation*

$$\psi(\lambda, x) = e^{ikx}\chi(\lambda, x), \tag{3.8}$$

where $\chi(\lambda, x)$ is periodic with period p. This is easily verified by checking the periodicity of $e^{-ikx}\psi(\lambda, x)$. We observe that k can be interpreted as a propagation vector of Bloch's wave. Generalizing Firsova's formula [**4**], defined for $n(x) = 1$, we can write k as follows[6]

$$k(\lambda) = \frac{1}{p}\arcsin\left(\frac{i}{2}\sqrt{\Delta(\lambda)^2 - 4}\right), \tag{3.9}$$

and state Floquet's Theorem [**11**] in terms of $k = k(\lambda)$ and λ.

Theorem 3.1 [Floquet]. *If the roots τ_1 and τ_2 of the quadratic polynomial* (3.4) *are distinct, then equation* (2.1) *has two linearly independent solutions of the type*

$$e^{ikx}\chi_1(\lambda, x) \quad \textit{and} \quad e^{-ikx}\chi_2(\lambda, x),$$

[6] Formula (3.9) can be derived from equation (3.7).

where $\chi_1(\lambda, x)$ and $\chi_2(\lambda, x)$ are both periodic with period p. If $\tau_1 = \tau_2$, then equation (2.1) *has a nontrivial periodic solution* ($\tau_1 = \tau_2 = 1$) *or an antiperiodic solution* ($\tau_1 = \tau_2 = -1$). *Let $\chi(x)$ denote such a solution and let $\phi(x)$ be another solution that is linearly independent of $\chi(x)$. Then there exists a constant ϑ such that $\phi(x+p) = \tau_1\phi(x) + \vartheta\chi(x)$, while $\vartheta = 0$ is equivalent to*

$$\theta(\lambda, p) = \phi'(\lambda, p) = \pm 1 \quad \textit{and} \quad \phi(\lambda, p) = \theta'(\lambda, p) = 0.$$

Further, the solutions of equation (2.1) *are all bounded if and only if*

(*a*) *either $\theta(\lambda, p) + \phi'(\lambda, p)$ belongs to $(-2, 2)$,*
(*b*) *or $\theta(\lambda, p) = \phi'(\lambda, p) = \pm 1$ and $\phi(\lambda, p) = \theta'(\lambda, p) = 0$.*

We can calculate τ as a function of λ from equation (3.6),

$$\tau(\lambda) = \frac{1}{2}\left[\Delta(\lambda) \mp \sqrt{\Delta(\lambda)^2 - 4}\right].$$

Assuming $\lambda \notin \{\sigma\}$, let us set $\tau_1(\lambda)$ and $\tau_2(\lambda)$ such as

$$|\tau_1(\lambda)| < 1 \quad \text{and} \quad |\tau_2(\lambda)| > 1,$$

then for any λ with $\Delta(\lambda) \notin [-2, 2]$

$$\tau_1(\lambda) = \begin{cases} \frac{1}{2}\left[\Delta(\lambda) - \sqrt{\Delta(\lambda)^2 - 4}\right], & \Delta(\lambda) > 2, \\ \frac{1}{2}\left[\Delta(\lambda) + \sqrt{\Delta(\lambda)^2 - 4}\right], & \Delta(\lambda) < -2, \end{cases} \tag{3.10a}$$

$$\tau_2(\lambda) = \begin{cases} \frac{1}{2}\left[\Delta(\lambda) + \sqrt{\Delta(\lambda)^2 - 4}\right], & \Delta(\lambda) > 2, \\ \frac{1}{2}\left[\Delta(\lambda) - \sqrt{\Delta(\lambda)^2 - 4}\right], & \Delta(\lambda) < -2, \end{cases} \tag{3.10b}$$

where the square root is positive. If $\lambda \in \{\sigma\}$ we can write

$$\tau_1(\lambda) = \frac{1}{2}\left[\Delta(\lambda) + \sqrt{\Delta(\lambda)^2 - 4}\right] = \tau_2^*(\lambda), \qquad -2 < \Delta(\lambda) < 2, \tag{3.11}$$

where the asterisk denotes the complex conjugate. Recalling that

$$\tau_1(\lambda) = e^{ikp} \quad \text{and} \quad \tau_2(\lambda) = e^{-ikp}, \tag{3.12}$$

we have

$$\begin{cases} k \in \mathbb{R}, & \Delta(\lambda) \in [-2, 2] \text{ or equivalently } \lambda \in \{\sigma\}, \\ k \in \mathbb{C} \setminus \mathbb{R}, & \Delta(\lambda) \notin [-2, 2] \text{ or equivalently } \lambda \notin \{\sigma\}. \end{cases} \tag{3.13}$$

Hereafter in the paper we shall assume $\mathbb{I}m\{k\} \geq 0$ if $\Delta(\lambda) \notin [-2, 2]$.

3.2 - *Eigenvalues: properties*

Proposition 3.2. *Given the following eigenvalue problem:*

$$\begin{cases} -\psi''(\lambda,x)+Q(x)\psi(\lambda,x)=\lambda n(x)^2\psi(\lambda,x), \\ \psi(\lambda,p)=\tau\psi(\lambda,0), \\ \psi'(\lambda,p)=\tau\psi'(\lambda,0), \end{cases}$$

if $Q(x)$ and $n(x)$ are real functions, then λ is real for every τ such that $|\tau|=1$.

Proof. Multiplying equation (2.1) by $\psi^*(\lambda,x)$ and integrating the resulting equation from 0 to p we obtain:

$$\int_0^p \left(-\psi''\psi^* + Q|\psi|^2\right) dx = \lambda \int_0^p n^2|\psi|^2\, dx,$$

from which we can derive

$$-\psi'\psi^*|_0^p + \int_0^p \left(|\psi'|^2 + Q|\psi|^2\right) dx = \lambda \int_0^p n^2|\psi|^2\, dx,$$

$$-\psi'(\lambda,p)\psi^*(\lambda,p) + \psi'(\lambda,0)\psi^*(\lambda,0) + \int_0^p \left(|\psi'|^2+Q|\psi|^2\right) dx = \lambda \int_0^p n^2|\psi|^2\, dx,$$

that is

$$-\tau\psi'(\lambda,0)\tau^*\psi^*(\lambda,0)+\psi'(\lambda,0)\psi^*(\lambda,0)+\int_0^p \left(|\psi'|^2+Q|\psi|^2\right) dx=\lambda \int_0^p n^2|\psi|^2\, dx.$$

Recalling that $|\tau|=1$,

$$\int_0^p \left(|\psi'(\lambda,x)|^2 + Q(x)|\psi(\lambda,x)|^2\right) dx = \lambda \int_0^p n(x)^2|\psi(\lambda,x)|^2\, dx \tag{3.14}$$

from which we can conclude that λ is real. □

Theorem 3.3. *The eigenvalues of equation* (2.1) *under the boundary conditions* (3.3) *form a nondecreasing sequence of numbers $\lambda \geq \lambda^*$ where*

$$\lambda^* = \min_{0\leq x\leq p} \frac{Q(x)}{n(x)^2}, \tag{3.15}$$

which tends to $+\infty$. *For* $|\tau| = 1$ *and* $\tau \neq \pm 1$ *these eigenvalues are simple, while for* $\tau = \pm 1$ *they have multiplicity one or two. The eigenvalue* λ^* *can only occur if the corresponding eigenfunction is constant,* $Q(x) \equiv \lambda^* n(x)^2$, *and the boundary conditions are periodic.*

Proof. For a noneigenvalue $\lambda_0 \in \mathbb{R}$, let $f(x)$ be an electromagnetic pulse, so that the right hand side of equation (2.1) is $\lambda n(x)^2[\psi(\lambda, x) + f(x)]$. In this case equation (2.1) with boundary conditions (3.3) (see Appendix A) can be written as the equivalent integral equation

$$\psi(\lambda, x) - (\lambda - \lambda_0) \int_0^p \mathcal{G}(x, y; \lambda_0) n(y)^2 \psi(\lambda, y)\, dy = \int_0^p \mathcal{G}(x, y; \lambda_0) n(y)^2 f(y)\, dy, \tag{3.16}$$

where $\mathcal{G}(x, y; \lambda)$ is the associated Green's function. In this integral equation the Green's function kernel $\mathcal{G}(x, y; \lambda)$ has the form

$$\mathcal{G}(x, y; \lambda) = \sum_j \frac{\phi_j(x)\overline{\phi_j(y)}}{\lambda^{(j)} - \lambda},$$

where $\{\phi_j\}$ is an orthonormal basis of $L^2((0, p); n(x)^2 dx)$ consisting of eigenfunctions corresponding to (real) eigenvalues $\{\lambda^{(j)}\}$. The summation is finite for degenerate kernels and infinite for nondegenerate kernels. Since $\mathcal{G}(x, y; \lambda)$ cannot be C^1 in (x, y) [because this would contradict relation (A.9)], the summation and hence the number of eigenvalues must be infinite. Furthermore, from (3.14) it follows that the eigenvalues λ are real, satisfy $\lambda \geq \lambda^*$ with λ^* as in (3.15), and can only coincide with λ^* if the eigenfunction is constant, $Q(x) \equiv \lambda^* n(x)^2$, and the boundary conditions are periodic. Thus there exist two infinite sequences, one of eigenvalues

$$\lambda^* \leq \lambda_0 \leq \lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \cdots, \qquad \lambda_n \to +\infty,$$

under periodic boundary conditions and the other one of eigenvalues

$$\lambda^* < \mu_1 \leq \mu_2 \leq \mu_3 \leq \ldots, \qquad \mu_n \to +\infty,$$

under anti-periodic boundary conditions. For $\tau \neq 1$ there also exists an infinite sequence of eigenvalues

$$\lambda_1^{(\tau)} \leq \lambda_2^{(\tau)} \leq \lambda_3^{(\tau)} \leq \ldots, \qquad \lambda_n^{(\tau)} \to +\infty,$$

under the boundary conditions (3.3). The multiplicity of an eigenvalue is at most 2, because the differential equation (2.1) has order 2. For $\tau \neq \pm 1$ the multiplicity is always one, because the eigenvalues λ follow from (3.6), so that one differential equation has both a τ-periodic and a τ^{-1}-periodic solution. $\square$

Now we state the following important theorem concerning a very important relation between the eigenvalues $\{\lambda_i\}$ and $\{\mu_i\}$ [**11**]:

Theorem 3.4 [Oscillation theorem]. *To each differential equation* (2.1) *we associate two monotonically increasing infinite sequences of real numbers* $\{\lambda_n\}_{n=0}^{\infty}$ *and* $\{\mu_n\}_{n=1}^{\infty}$ *such that equation* (2.1) *has a solution of period* p *if and only if* $\lambda = \lambda_n$ $(n = 0, 1, 2, \ldots)$ *and a solution of primitive period* $2p$ *if, and only if,* $\lambda = \mu_n$ $(n = 1, 2, 3, \ldots)$. *These sequences satisfy the inequalities*

$$\lambda_0 < \mu_1 \leq \mu_2 < \lambda_1 \leq \lambda_2 < \mu_3 \leq \mu_4 < \lambda_3 \leq \lambda_4 < \ldots \tag{3.17}$$

and the relations

$$\lim_{n\to\infty} \lambda_n = +\infty, \qquad \lim_{n\to\infty} \mu_n = +\infty. \tag{3.18}$$

The solutions are all bounded for λ *in the intervals*

$$(\lambda_0, \mu_1), \quad (\mu_2, \lambda_1), \quad (\lambda_2, \mu_3), \quad (\mu_4, \lambda_3), \ldots. \tag{3.19}$$

For λ *at the endpoints of these intervals* (*and always for* $\lambda = \lambda_0$) *there exist unbounded solutions. The solutions are all bounded for* $\lambda = \lambda_{2n+1}$ *or* $\lambda = \lambda_{2n+2}$ *if and only if* $\lambda_{2n+1} = \lambda_{2n+2}$ *and they are all bounded for* $\lambda = \mu_{2n+1}$ *or* $\lambda = \mu_{2n+2}$ *if and only if* $\mu_{2n+1} = \mu_{2n+2}$. *The numbers* λ_n *are the zeros of* $\Delta(\lambda) = 2$ *and the numbers* μ_n *are the zeros of* $\Delta(\lambda) = -2$.

We call λ_n the *characteristic values of the first kind* and μ_n the *characteristic values of the second kind*. The intervals in (3.19) are called *bands*. We consider an endpoint as belonging to a band if for that value of λ all solutions of equation (2.1) are bounded. The gaps between the stability intervals are called *band gaps*, one of which is the zero-th band gap $(-\infty, \lambda_0]$. The bands are numbered consecutively $1, 2, 3, \ldots$ and may line up. The band gaps are numbered consecutively $0, 1, 2, \ldots$ and may be empty.

3.3 - *Analysis of Hill's discriminant*

In the previous section, we showed that analysis of Hill's discriminant permits us to calculate the bands. We report the same important results about Hill's discriminant without proof [**11**]. First of all we extend $\Delta(\lambda)$ to the complex λ-plane which we indicate by Λ. More precisely we mention the following properties:

(a) $\Delta(\lambda) \to +\infty$ if $\lambda \in \mathbb{R}$ and $\lambda \to -\infty$;

(b) in each band-gap, excluding band-gap 0, there is a unique relative maximum or a unique relative minimum $\{\xi_i\}$: ($\xi_i \in$ band-gap i, $i \geq 1$). If a band-gap is empty and

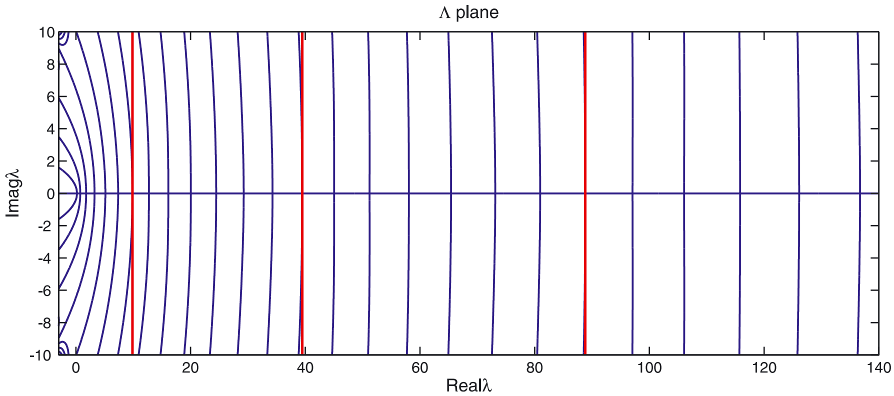

Fig. 2. Λ plane. The real axis and the Γ-curve are plotted in blue. The vertical asymptotes, $Real\{\lambda\} = (i\pi)^2$, where $i = 1, 2, ...$, are plotted in red.

$\Delta(\xi_i)$ is a relative maximum then $\xi_i \equiv \lambda_{i-1} \equiv \lambda_i$; conversely if a band-gap is empty and $\Delta(\xi_i)$ is a relative minimum then $\Delta(\xi_i) = -2$ and $\xi_i \equiv \mu_i \equiv \mu_{i+1}$;

(c) the function $\Delta(\lambda)$ is strictly decreasing in band-gap 0 and strictly increasing between a relative minimum and a relative maximum, while it is strictly increasing between a relative minimum and a relative maximum.

If $\lambda \in \Lambda \setminus \{\sigma\}$, the solution $\psi(\lambda, x)$ is unbounded as $x \to +\infty$ or as $x \to -\infty$, while it is bounded for any x if, and only if, $\lambda \in \{\sigma\}$.

Let us consider the Λ plane, we call *Γ_i-curve* [4] the i-th curve in the complex plane $\Lambda \setminus \mathbb{R}$ where Hill's discriminant is real. The Γ_i-curve crosses the real axis in ξ_i and approaches the vertical asymptote $Real\{\lambda\} = (i\pi)^2$, where $i = 1, 2, \ldots$. Then Hill's discriminant is real if $\lambda \in \mathbb{R}$ or if λ belong to Γ-curve, where Γ-curve denotes the set of all Γ_i-curves.

4 - Direct scattering theory

4.1 - *Jost's functions*

Let us now consider a photonic crystal with impurities, where both $Q(x)$ and $n(x)$ have a periodic component and a component describing the effect of impurities. In this case we have the equation

$$-\psi''(\lambda, x) + [Q_0(x) + Q_i(x)]\psi(\lambda, x) = \lambda n_0(x)^2[1 + \varepsilon(x)]\psi(\lambda, x), \tag{4.1}$$

where $Q_0(x)$ and $n_0(x)$ are assumed to be real piecewise continuous periodic functions of period p, $\varepsilon(x)$ is piecewise continuous and vanishes as $x \to \pm\infty$, the lower bound $\inf\{\varepsilon(x) : x \in \mathbb{R}\} > -1$ and $Q_i(x)$ is a Faddeev class potential (i.e., $Q_i(x)$ is real and satisfies $\int_{-\infty}^{\infty} (1+|x|)|Q_i(x)|\,dx < \infty$). We also assume that $\int_{-\infty}^{\infty} (1+|x|)|\varepsilon(x)| < \infty$.

In this context the Jost functions $f_{1,2}$ play a very important role. Indeed, the Jost functions are needed to describe the asymptotic scattering effect and must coincide with appropriate $\tau_{1,2}$-periodic solutions $\psi_{1,2}$ for large $|x|$ if the impurity is confined to a bounded region. To analyse these solutions let us first consider the two $\tau_{1,2}-$periodic solutions $\psi_{1,2}$ of (2.1) satisfying $\psi_1(\lambda,0) = \psi_2(\lambda,0) = 1$. Then

$$\psi_1(\lambda,x) = \theta(\lambda,x) + m_1(\lambda)\phi(\lambda,x), \tag{4.2a}$$

$$\psi_2(\lambda,x) = \theta(\lambda,x) + m_2(\lambda)\phi(\lambda,x), \tag{4.2b}$$

where $m_{1,2}(\lambda)$ are called *Weyl coefficients* and $\theta(\lambda,x)$ and $\phi(\lambda,x)$ are the Floquet solutions.

Unlike $\theta(\lambda,x)$ and $\phi(\lambda,x)$, the functions $\psi_{1,2}(\lambda,x)$ are independent of the initial conditions 3.2. The Weyl coefficients can be calculated by considering the Born-Von Kármán condition in the form

$$\begin{pmatrix} \tau_{1,2} - \theta(\lambda,p) & -\phi(\lambda,p) \\ -\theta'(\lambda,p) & \tau_{1,2} - \phi'(\lambda,p) \end{pmatrix} \begin{pmatrix} 1 \\ m_{1,2}(\lambda) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \tag{4.3}$$

from which

$$m_{1,2}(\lambda) = \frac{\tau_{1,2} - \theta(\lambda,p)}{\phi(\lambda,p)}, \tag{4.4}$$

where $\tau_{1,2}$ are defined by equations (3.10) and (3.12). The solutions $\psi_{1,2}$ can be written according to Bloch's description:

$$\psi_{1,2}(k,x) = e^{\pm ikx}\chi_{1,2}(\lambda,x). \tag{4.5}$$

Recalling that for $\lambda \in \mathbb{C}\setminus\{\sigma\}$ we have $\mathbb{I}m\{k\} \geq 0$ and that $\chi_{1,2}$ are periodic functions, we can easily prove that $\psi_1(\lambda,x)$ diverges as $x \longrightarrow -\infty$ and $\psi_2(\lambda,x)$ diverges as $x \longrightarrow +\infty$. Thus if $\lambda \in \mathbb{C}\setminus\{\sigma\}$ we have $\psi_1 \in L^2(\mathbb{R}^+)$ and $\psi_2 \in L^2(\mathbb{R}^-)$, that is:

$$\int_0^{+\infty} |\psi_1(\lambda,x)|^2\,dx < \infty \quad \text{and} \quad \int_{-\infty}^{0} |\psi_2(\lambda,x)|^2\,dx < \infty. \tag{4.6}$$

In the next part we shall consider all functions to depend on k instead of λ, according to formula (3.9). If we consider functions depending on k we can interpret solutions of equations (2.1) and (4.1) as waves.

Since the Jost functions are solutions that must converge to 0 as $x \to \pm\infty$, we can set

$$f_1(k,x) = \psi_1(k,x)[1+o(1)], \qquad x \to +\infty, \tag{4.7a}$$

$$f_2(k,x) = \psi_2(k,x)[1+o(1)], \qquad x \to -\infty. \tag{4.7b}$$

To calculate the Jost functions we use the method of variation of parameters. To do so, let us write the Schrödinger-Helmholtz equation with impurities in the following way:

$$-\psi''(k,x) + Q_0(x)\psi(k,x) = \lambda n_0(x)^2\psi(k,x) + g(x), \tag{4.8}$$

where

$$g(x) = [\lambda n_i(x)^2\varepsilon(x) - Q_i(x)]\psi(x,k) \tag{4.9}$$

Writing the general solution in the form

$$\psi(k,x) = c_1(x)\psi_1(k,x) + c_2(x)\psi_2(k,x), \tag{4.10}$$

by the method of variation of parameters method, we obtain

$$\begin{pmatrix} \psi_1(k,x) & \psi_2(k,x) \\ \psi_1'(k,x) & \psi_2'(k,x) \end{pmatrix} \begin{pmatrix} c_1'(x) \\ c_2'(x) \end{pmatrix} = \begin{pmatrix} 0 \\ -g(x) \end{pmatrix}.$$

Then

$$c_1(x) = c_1 + \frac{1}{w(k)} \int_{-\infty}^{x} \psi_2(k,t)g(t)\,dt,$$

$$c_2(x) = c_2 + \frac{1}{w(k)} \int_{x}^{\infty} \psi_1(k,t)g(t)\,dt.$$

Substituting them into equation (4.10),

$$\begin{aligned} \psi(k,x) = {} & \left[c_1 + \frac{1}{w(k)} \int_{-\infty}^{x} \psi_2(k,t)g(t)\,dt\right]\psi_1(k,x) \\ & + \left[c_2 + \frac{1}{w(k)} \int_{x}^{\infty} \psi_1(k,t)g(t)\,dt\right]\psi_2(k,x), \end{aligned} \tag{4.11}$$

where the constants c_1 and c_2 can be calculated by recalling that the solution must converge to $\psi_{1,2}(k,x)$ as $x \to \pm\infty$ if the impurity is confined to a bounded region. Considering

$$\lim_{x\to+\infty} \psi(k,x) = \psi_1(k,x), \tag{4.12}$$

we have $c_2 = 0$, so that

$$\lim_{x\to+\infty} \psi(k,x) = \left[\underbrace{c_1 + \frac{1}{w(k)} \int_{-\infty}^{\infty} \psi_2(k,t) g(t)\, dt}_{=1}\right] \psi_1(k,x).$$

Adding and subtracting $\dfrac{\psi_1(k,x)}{w(k)} \displaystyle\int_x^\infty \psi_2(k,t)g(t)\,dt$ to equation (4.11) we get

$$\psi(k,x) = \left[\underbrace{c_1 + \frac{1}{w(k)} \int_{-\infty}^{\infty} \psi_2(k,t) g(t)\, dt}_{=1}\right] \psi_1(k,x)$$
$$- \frac{\psi_1(k,x)}{w(k)} \int_x^\infty \psi_2(k,t) g(t)\, dt + \frac{\psi_2(k,x)}{w(k)} \int_x^\infty \psi_1(k,t) g(t)\, dt,$$

from which

$$\psi(k,x) = \psi_1(k,x) + \int_x^{+\infty} \frac{\psi_1(k,t)\psi_2(k,x) - \psi_2(k,t)\psi_1(k,x)}{w(k)} g(t)\, dt. \tag{4.13}$$

In the same way, using the condition

$$\lim_{x\to-\infty} \psi(k,x) = \psi_2(k,x), \tag{4.14}$$

we obtain

$$\psi(k,x) = \psi_2(k,x) - \int_{-\infty}^{x} \frac{\psi_1(k,t)\psi_2(k,x) - \psi_2(k,t)\psi_1(k,x)}{w(k)} g(t)\, dt. \tag{4.15}$$

Defining by $A(x,t;k)$ the integral kernel of the above equations, that is putting

$$A(x,t;k) = \frac{\psi_1(k,t)\psi_2(k,x) - \psi_2(k,t)\psi_1(k,x)}{w(k)}, \tag{4.16}$$

we can write the solutions in the following way:

$$\psi(k,x) = \begin{cases} \psi_1(k,x) + \displaystyle\int_x^{+\infty} A(x,t;k) g(t)\, dt & \text{if } \displaystyle\lim_{x\to+\infty} \psi(k,x) = \psi_1(k,x), \\ \psi_2(k,x) - \displaystyle\int_{-\infty}^{x} A(x,t;k) g(t)\, dt & \text{if } \displaystyle\lim_{x\to-\infty} \psi(k,x) = \psi_2(k,x). \end{cases}$$

The Jost functions $f_{1,2}(k,x)$ satisfy conditions (4.12) and (4.14), so we can write

$$f_1(k,x) = \psi_1(k,x) + \int_x^{\infty} A(k;x,t)\Big[\lambda n_0(t)^2\varepsilon(t) - Q_i(t)\Big] f_1(k,t)\,dt, \tag{4.17a}$$

$$f_2(k,x) = \psi_2(k,x) - \int_{-\infty}^{x} A(k;x,t)\Big[\lambda n_0(t)^2\varepsilon(t) - Q_i(t)\Big] f_2(k,t)\,dt, \tag{4.17b}$$

or

$$\begin{aligned} f_1(k,x) = &\left[1 - w(k)^{-1}\int_x^{\infty} \psi_2(k,t)\Big[\lambda n_0(t)^2\varepsilon(t) - Q_i(t)\Big] f_1(k,t)\,dt\right]\psi_1(k,x) \\ &+ \left[w(k)^{-1}\int_x^{\infty} \psi_1(k,t)\Big[\lambda n_0(t)^2\varepsilon(t) - Q_i(t)\Big] f_1(k,t)\,dt\right]\psi_2(k,x), \end{aligned} \tag{4.18a}$$

$$\begin{aligned} f_2(k,x) = &\left[w(k)^{-1}\int_{-\infty}^{x} \psi_1(k,t)\Big[\lambda n_0(t)^2\varepsilon(t) - Q_i(t)\Big] f_2(k,t)\,dt\right]\psi_1(k,x) \\ &+ \left[1 - w(k)^{-1}\int_x^{\infty} \psi_2(k,t)\Big[\lambda n_0(t)^2\varepsilon(t) - Q_i(t)\Big] f_2(k,t)\,dt\right]\psi_2(k,x). \end{aligned} \tag{4.18b}$$

Letting $x \longrightarrow \pm\infty$ we obtain:

$$f_1(k,x) = a_1(k)\psi_1(k,x) + b_1(k)\psi_2(k,x) + o(1), \qquad x \to -\infty, \tag{4.19a}$$

$$f_2(k,x) = b_2(k)\psi_1(k,x) + a_2(k)\psi_2(k,x) + o(1), \qquad x \to +\infty, \tag{4.19b}$$

where

$$a_1(k) = 1 - w(k)^{-1}\int_{-\infty}^{\infty} \psi_2(k,t)\Big[\lambda n_0(t)^2\varepsilon(t) - Q_i(t)\Big] f_1(k,t)\,dt, \tag{4.20a}$$

$$b_1(k) = w(k)^{-1}\int_{-\infty}^{\infty} \psi_1(k,t)\Big[\lambda n_0(t)^2\varepsilon(t) - Q_i(t)\Big] f_1(k,t)\,dt, \tag{4.20b}$$

$$a_2(k) = 1 - w(k)^{-1}\int_{-\infty}^{\infty} \psi_2(k,t)\Big[\lambda n_0(t)^2\varepsilon(t) - Q_i(t)\Big] f_2(k,t)\,dt, \tag{4.20c}$$

$$b_2(k) = w(k)^{-1}\int_{-\infty}^{\infty} \psi_1(k,t)\Big[\lambda n_0(t)^2\varepsilon(t) - Q_i(t)\Big] f_2(k,t)\,dt. \tag{4.20d}$$

Finally, we can write all asymptotic expressions for the Jost functions

(4.21a) $f_1(k,x) \simeq \psi_1(k,x), \qquad x \to +\infty,$

(4.21b) $f_1(k,x) \simeq a_1(k)\psi_1(k,x) + b_1(k)\psi_2(k,x), \qquad x \to -\infty,$

(4.21c) $f_2(k,x) \simeq b_2(k)\psi_1(k,x) + a_2(k)\psi_2(k,x), \qquad x \to +\infty,$

(4.21d) $f_2(k,x) \simeq \psi_2(k,x), \qquad x \to -\infty.$

Considering equations (4.6) and equations (4.21) we can observe that $f_1(k,x)$ is bounded as $x \to -\infty$ if and only if $a_1(k) = 0$. In the same way we see that $f_2(k,x)$ is bounded as $x \to +\infty$ if and only if $a_2(k) = 0$. Finally, we have bounded solutions only for the k-values that are zeros of the functions $a_1(k)$ and $a_2(k)$. These k-values are the discrete eigenvalues inserted into the band gaps by impurities.

4.2 - *Symmetry*

Let us consider $\lambda \in \mathbb{C}$. We analyse symmetry for the principal functions depending on λ. From equation (2.1), replacing λ by its complex conjugate $\overline{\lambda}$ we have

$$-\psi''(\overline{\lambda},x) + Q(x)\psi(\overline{\lambda},x) = \overline{\lambda}n(x)^2\psi(\overline{\lambda},x).$$

If we conjugate the previous equation and recall that $Q(x)$ and $n(x)$ are real we have

$$-\overline{\psi''(\overline{\lambda},x)} + Q(x)\overline{\psi(\overline{\lambda},x)} = \lambda n(x)^2\overline{\psi(\overline{\lambda},x)}.$$

Then $\overline{\psi(\overline{\lambda},x)} = \psi(\lambda,x)$ is a solution of the Schrödinger-Helmholtz equation. Clearly we have

(4.22a) $$\overline{\theta(\overline{\lambda},x)} = \theta(\lambda,x), \qquad \overline{\theta'(\overline{\lambda},x)} = \theta'(\lambda,x),$$

(4.22b) $$\overline{\phi(\overline{\lambda},x)} = \phi(\lambda,x), \qquad \overline{\phi'(\overline{\lambda},x)} = \phi'(\lambda,x).$$

According to equations (4.22) it is possible to derive symmetry relations for Hill's discriminant:

(4.23) $$\overline{\Delta(\overline{\lambda})} = \Delta(\lambda)$$

According to equations (3.10), if $\lambda \notin \{\sigma\}$ we have

(4.24) $$\overline{\tau_1(\overline{\lambda})} = \tau_1(\lambda), \qquad \overline{\tau_2(\overline{\lambda})} = \tau_2(\lambda),$$

while if $\lambda \in \{\sigma\}$ we have

(4.25) $$\overline{\tau_1(\lambda)} = \tau_2(\lambda).$$

From Firsova's formula (3.9) it is easy to prove that

$$k(\overline{\lambda}) = -\overline{k(\lambda)}. \tag{4.26}$$

Let us now study symmetry properties of $\psi_{1,2}(k,x)$. According to equations (4.22) and 4.26 we have

$$\psi_{1,2}(k,x) = \psi_1(k(\lambda),x) = \overline{\psi_{1,2}(k(\overline{\lambda}),x)} = \overline{\psi_{1,2}(-\overline{k(\lambda)},x)} = \overline{\psi_{1,2}(-\overline{k},x)}.$$

Considering now $k \in \mathbb{R}$, from equation (4.2), we can write

$$\begin{aligned}\psi_1(\lambda,x) &= \theta(\lambda,x) + m_1(\lambda)\phi(\lambda,x)\\ &= \theta(\lambda,x) + \left(\frac{\tau_1 - \theta(\lambda,p)}{\phi(\lambda,p)}\right)\phi(\lambda,x)\\ &= \theta(\lambda,x) + \left(\frac{e^{-ikp} - \theta(\lambda,p)}{\phi(\lambda,p)}\right)\phi(\lambda,x).\end{aligned}$$

Conjugating the equation and replacing λ with $\overline{\lambda}$, we have

$$\overline{\psi_1(\overline{\lambda},x)} = \overline{\theta(\overline{\lambda},x)} + \left(\frac{e^{ik(\overline{\lambda})p} - \overline{\theta(\overline{\lambda},p)}}{\overline{\phi(\overline{\lambda},p)}}\right)\overline{\phi(\overline{\lambda},x)}.$$

If we consider $k \in \mathbb{R}$ or, equally, $\lambda \in \{\sigma\}$

$$\begin{aligned}\overline{\psi_1(\overline{\lambda},x)} &= \theta(\lambda,x) + \left(\frac{e^{ik(\lambda)p} - \theta(\lambda,p)}{\phi(\lambda,p)}\right)\phi(\lambda,x)\\ &= \theta(\lambda,x) + \left(\frac{\tau_2 - \theta(\lambda,p)}{\phi(\lambda,p)}\right)\phi(\lambda,x)\\ &= \psi_2(\lambda,x)\end{aligned}$$

we get

$$\psi_{1,2}(k,x) = \begin{cases}\overline{\psi_{1,2}(-\overline{k},x)}\\ \psi_{2,1}(-k,x), \quad k \in \mathbb{R}.\end{cases} \tag{4.27}$$

Considering the previous relations and equations (4.18) we can write

$$f_{1,2}(k,x) = \begin{cases}\overline{f_{1,2}(-\overline{k},x)}\\ f_{2,1}(-k,x), \quad k \in \mathbb{R}.\end{cases} \tag{4.28}$$

To study symmetry properties of $a_1(k)$, $a_2(k)$, $b_1(k)$ and $b_2(k)$ we introduce the operator W which evaluates the Wronskian of a pair of functions:

$$W[f(k,\cdot),g(k,\cdot)] = \begin{vmatrix} f(k,\cdot) & g(k,\cdot) \\ f'(k,\cdot) & g'(k,\cdot) \end{vmatrix}$$

We also get for the Wronskian

$$\begin{aligned} w(k) &\stackrel{\text{def}}{=} W[\psi_1(k,\cdot),\psi_2(k,\cdot)] = W[\theta(\lambda,\cdot)+m_1(\lambda)\phi(\lambda,\cdot),\theta(k,\cdot)+m_2(\lambda)\phi(k,\cdot)] \\ &= \{m_2(\lambda)-m_1(\lambda)\}W[\theta(\lambda,\cdot),\phi(\lambda,\cdot)] \\ &= m_2(\lambda)-m_1(\lambda). \end{aligned} \tag{4.29}$$

By the inversion and conjugation symmetries (4.27) we get

$$w(k) = W[\psi_1(k,\cdot),\psi_2(k,\cdot)] = \begin{cases} W[\psi_2(-k,\cdot),\psi_1(-k,\cdot)] = -w(-k), & k\in\mathbb{R}, \\ W[\overline{\psi_1(-\overline{k},\cdot)},\overline{\psi_2(-\overline{k},\cdot)}] = \overline{w(-\overline{k})}. \end{cases} \tag{4.30}$$

With the help of equations (4.21) we find

$$\begin{aligned} W[f_1(k,\cdot),f_2(k,\cdot)] &= W[\psi_1, b_2\psi_1+a_2\psi_2] = a_2(k)w(k), \\ &= W[a_1\psi_1+b_1\psi_2,\psi_2] = a_1(k)w(k), \end{aligned}$$

so that

$$a(k) \stackrel{\text{def}}{=} a_1(k) = a_2(k), \qquad k\in\mathbb{C}. \tag{4.31}$$

Using the symmetry relation (4.28) we obtain

$$\overline{w(-\overline{k})a(-\overline{k})} = W[\overline{f_1(-\overline{k},\cdot)},\overline{f_2(-\overline{k},\cdot)}] = W[f_1(k,\cdot),f_2(k,\cdot)] = w(k)a(k),$$

so that

$$\overline{a(-\overline{k})} = a(k), \qquad k\in\mathbb{C}. \tag{4.32}$$

Let us now look for relations involving $b_1(k)$ and $b_2(k)$. For $k\in\mathbb{R}$ we have

$$W[f_1(k,\cdot),\ f_1(-k,\cdot)]$$
$$= \begin{cases} W[\psi_1(k,\cdot),\psi_1(-k,\cdot)] = W[\psi_1(k,\cdot),\psi_2(k,\cdot)] = w(k), \\ W[a_1(k)\psi_1(k,\cdot)+b_1(k)\psi_2(k,\cdot),a_1(-k)\psi_1(-k,\cdot)+b_1(-k)\psi_2(-k,\cdot)] \\ = W[a_1(k)\psi_1(k,\cdot)+b_1(k)\psi_2(k,\cdot),a_1(-k)\psi_2(k,\cdot)+b_1(-k)\psi_1(k,\cdot)] \\ = \{a_1(k)a_1(-k)-b_1(k)b_1(-k)\}w(k), \end{cases}$$

and hence

$$a_1(k)a_1(-k)-b_1(k)b_1(-k) = 1, \qquad k\in\mathbb{R}. \tag{4.33}$$

Similarly, for $k \in \mathbb{R}$ we have

$$W[f_2(k,\cdot), f_2(-k,\cdot)]$$

$$= \begin{cases} W[\psi_2(k,\cdot), \psi_2(-k,\cdot)] = W[\psi_2(k,\cdot), \psi_1(k,\cdot)] = -w(k), \\ W[a_2(k)\psi_2(k,\cdot) + b_2(k)\psi_1(k,\cdot), a_2(-k)\psi_2(-k,\cdot) + b_2(-k)\psi_1(-k,\cdot)] \\ = W[a_2(k)\psi_2(k,\cdot) + b_2(k)\psi_1(k,\cdot), a_2(-k)\psi_1(k,\cdot) + b_2(-k)\psi_2(k,\cdot)] \\ = -\{a_2(k)a_2(-k) - b_2(k)b_2(-k)\}w(k), \end{cases}$$

and hence

$$a_2(k)a_2(-k) - b_2(k)b_2(-k) = 1, \qquad k \in \mathbb{R}. \tag{4.34}$$

Analogously, for $k \in \mathbb{R}$ we have

$$W[f_1(k,\cdot), f_2(-k,\cdot)]$$

$$= \begin{cases} W[\psi_1(k,\cdot), a_2(-k)\psi_2(-k,\cdot) + b_2(-k)\psi_1(-k,\cdot)] \\ W[\psi_1(k,\cdot), a_2(-k)\psi_1(k,\cdot) + b_2(-k)\psi_2(k,\cdot)] = b_2(-k)w(k), \\ W[a_1(k)\psi_1(k,\cdot) + b_1(k)\psi_2(k,\cdot), \psi_2(-k,\cdot)] \\ = W[a_1(k)\psi_1(k,\cdot) + b_1(k)\psi_2(k,\cdot), \psi_1(k,\cdot)] = -b_1(k)w(k), \end{cases}$$

which implies

$$b_2(-k) = -b_1(k), \qquad k \in \mathbb{R}. \tag{4.35}$$

For $k \in \mathbb{R}$ we can now write $b(k) \overset{\text{def}}{=} b_1(k) = -b_2(-k)$. We do not define $b(k)$ off the real line. Using (4.28) and (4.29) for $k \in \mathbb{R}$ we get for $k \in \mathbb{R}$

$$\overline{b(-k)w(-k)} = -W[\overline{f_1(-k,x)}, \overline{f_2(-k,x)}] = b(-k)w(-k),$$

which yields

$$b(-k) = \overline{b(k)}, \qquad k \in \mathbb{R}. \tag{4.36}$$

Finally, considering equations (4.32), (4.33) and (4.36) we get for $k \in \mathbb{R}$ the crucial relation

$$|a(k)|^2 - |b(k)|^2 = 1, \qquad k \in \mathbb{R}. \tag{4.37}$$

4.3 - *Scattering matrix S*

Let us consider coefficients $d_{ij}(k)$ $(i,j = 1,2)$ such that

$$f_1(-k,x) = d_{11}(k)f_1(k,x) + d_{12}(k)f_2(k,x), \tag{4.38a}$$

$$f_2(-k,x) = d_{21}(k)f_1(k,x) + d_{22}(k)f_2(k,x). \tag{4.38b}$$

Writing the asymptotic expressions ($x \to \pm\infty$) for $\psi_{1,2}$ we get

$$\begin{aligned}
\psi_1(-k,x) &= d_{11}(k)\psi_1(k,x) + d_{12}(k)[-b(-k)\psi_1(k,x) + a(k)\psi_2(k,x)],\\
a(-k)\psi_1(-k,x) + b(-k)\psi_2(-k,x) &= d_{11}(k)[a(k)\psi_1(k,x) + b(k)\psi_2(k,x)]\\
&\quad + d_{12}(k)\psi_2(k,x),\\
-b(k)\psi_1(-k,x) + a(-k)\psi_2(-k,x) &= d_{21}(k)\psi_1(k,x)\\
&\quad + d_{22}(k)[-b(-k)\psi_1(k,x) + a(k)\psi_2(k,x)],\\
\psi_2(-k,x) &= d_{21}(k)[a(k)\psi_1(k,x) + b(k)\psi_2(k,x)] + d_{22}(k)\psi_2(k,x).
\end{aligned}$$

Using that $\psi_{1,2}(-k,x) = \psi_{2,1}(k,x)$ and using the linear independence of the Floquet solutions to equate coefficients of $\psi_1(k,x)$ and $\psi_2(k,x)$ we get

$$\begin{aligned}
0 &= d_{11}(k) - d_{12}(k)b(-k), & 1 &= d_{12}(k)a(k),\\
b(-k) &= d_{11}(k)a(k), & a(-k) &= d_{11}(k)b(k) + d_{12}(k),\\
a(-k) &= d_{21}(k) - d_{22}(k)b(-k), & -b(k) &= d_{22}(k)a(k),\\
1 &= d_{21}(k)a(k), & 0 &= d_{21}(k)b(k) + d_{22}(k).
\end{aligned}$$

Therefore,

$$\begin{pmatrix} d_{11}(k) & d_{12}(k) \\ d_{21}(k) & d_{22}(k) \end{pmatrix} = \frac{1}{a(k)} \begin{pmatrix} b(-k) & 1 \\ 1 & -b(k) \end{pmatrix}, \qquad k \in \mathbb{R}.$$

We now define the *transmission coefficient* $T(k)$, the *reflection coefficient from the right* $R(k)$, and the *reflection coefficient from the left* $L(k)$ as follows

$$\begin{cases} T(k) = d_{12}(k) = d_{21}(k) = \dfrac{1}{a(k)}, \\[2ex] R(k) = -d_{11}(k) = -\dfrac{b(-k)}{a(k)}, \qquad L(k) = -d_{22}(k) = \dfrac{b(k)}{a(k)}, \end{cases} \tag{4.39}$$

where $k \in \mathbb{R}$. Then (4.37) implies that the *scattering matrix* is

$$S(k) = \begin{pmatrix} T(k) & R(k) \\ L(k) & T(k) \end{pmatrix}, \qquad k \in \mathbb{R}, \tag{4.40}$$

that is the matrix characterizing the primary scattering parameters. According to relations (4.37), (4.39) and (4.40) we can show that S is unitary. All of these facts lead to the Riemann-Hilbert problem

$$\begin{pmatrix} f_1(-k,x) \\ f_2(-k,x) \end{pmatrix} = JS(k)J\begin{pmatrix} f_2(k,x) \\ f_1(k,x) \end{pmatrix}, \qquad k \in \mathbb{R}, \tag{4.41}$$

where $J = \mathrm{diag}(1, -1)$. From (4.32), (4.36), and (4.39) we get for $k \in \mathbb{R}$

$$T(-k) = \overline{T(k)}, \qquad R(-k) = \overline{R(k)}, \qquad L(-k) = \overline{L(k)}. \tag{4.42}$$

4.4 - *Period map*

Let us now introduce the period map, i.e. the matrix operator that allows us to obtain the solution at any location in the crystal by analysing only one period. Let us consider an unbounded mono-dimensional photonic crystal under the hypothesis of a linear, stationary, isotropic and lossless medium ($n(x) \in \mathbb{R}$ and $Q(x) = 0$). Let $n(x)$ be a piecewise constant function, so that we can write $n(x) = n_j$ $(b_{j-1} < x < b_j,\ \ j = 1, \ldots, m)$. Here $0 = b_0 < b_1 < \ldots < b_m = p$ and $a_j = b_j - b_{j-1}$ $(j = 1, \ldots, m)$. Then any solution $\psi_j(\lambda, x)$ of (3.1) on (b_{j-1}, b_j) satisfies

$$\psi_j(\lambda, x) = c_{1j} \cos\left(n_j\sqrt{\lambda}\,(x - b_{j-1})\right) + c_{2j}\,\frac{\sin\left(n_j\sqrt{\lambda}\,(x - b_{j-1})\right)}{n_j\sqrt{\lambda}}, \tag{4.43a}$$

$$\psi_j'(\lambda, x) = -n_j\sqrt{\lambda}\,c_{1j} \sin\left(n_j\sqrt{\lambda}\,(x - b_{j-1})\right) + c_{2j} \cos\left(n_j\sqrt{\lambda}\,(x - b_{j-1})\right), \tag{4.43b}$$

where $j = 1, \ldots, m$. The requirement that $\psi(\lambda, x)$ is C^1 at the points $b_1, \ldots, b_{m-1}$ leads to the identities

$$\begin{pmatrix} \psi(\lambda, b_{j-1}^+) \\ \psi'(\lambda, b_{j-1}^+) \end{pmatrix} = \begin{pmatrix} \psi(\lambda, b_{j-1}^-) \\ \psi'(\lambda, b_{j-1}^-) \end{pmatrix},$$

or also

$$\begin{pmatrix} c_{1j} \\ c_{2j} \end{pmatrix} = \begin{pmatrix} \cos(n_{j-1}a_{j-1}\sqrt{\lambda}) & \dfrac{\sin(n_{j-1}a_{j-1}\sqrt{\lambda})}{n_{j-1}\sqrt{\lambda}} \\ -n_{j-1}\sqrt{\lambda}\,\sin(n_{j-1}a_{j-1}\sqrt{\lambda}) & \cos(n_{j-1}a_{j-1}\sqrt{\lambda}) \end{pmatrix}\begin{pmatrix} c_{1,j-1} \\ c_{2,j-1} \end{pmatrix}.$$

Let $A_{j-1}(\lambda)$ be the matrix that links coefficients belonging to $(j-1)$-th and j-th interval respectively. Then we can write

$$
\begin{aligned}
\begin{pmatrix} c_{1m} \\ c_{2m} \end{pmatrix} &= A_{m-1}(\lambda)\begin{pmatrix} c_{1m-1} \\ c_{2m-1} \end{pmatrix} \\
&= A_{m-1}(\lambda)A_{m-2}(\lambda)\begin{pmatrix} c_{1m-2} \\ c_{2m-2} \end{pmatrix} \\
&\ \ \vdots \\
&= A_{m-1}(\lambda)\dots A_2(\lambda)A_1(\lambda)\begin{pmatrix} c_{11} \\ c_{21} \end{pmatrix}.
\end{aligned} \tag{4.44}
$$

On the other hand, $\psi(\lambda, x)$ is C^1 also in p, so that setting

$$
\begin{pmatrix} \psi(\lambda, p) \\ \psi'(\lambda, p) \end{pmatrix} = A_m(\lambda)\begin{pmatrix} c_{1m} \\ c_{2m} \end{pmatrix},
$$

we have

$$
\begin{pmatrix} \psi(\lambda, p) \\ \psi'(\lambda, p) \end{pmatrix} = \underbrace{A_m(\lambda)A_{m-1}(\lambda)\dots A_2(\lambda)A_1(\lambda)}_{\stackrel{\text{def}}{=} M(\lambda)}\begin{pmatrix} \psi(\lambda, 0) \\ \psi'(\lambda, 0) \end{pmatrix}. \tag{4.45}
$$

We define $M(\lambda)$ as the *period map*. Since equation (2.1) is a second order linear ordinary differential equation we can write

$$
\psi(\lambda, x) = c_{1,tot}\, \theta(\lambda, x) + c_{2,tot}\, \phi(\lambda, x),
$$

or

$$
\begin{pmatrix} \psi(\lambda, x) \\ \psi'(\lambda, x) \end{pmatrix} = \begin{pmatrix} \theta(\lambda, x) & \phi(\lambda, x) \\ \theta'(\lambda, x) & \phi'(\lambda, x) \end{pmatrix}\begin{pmatrix} c_{1,tot} \\ c_{2,tot} \end{pmatrix}.
$$

By substituting into equation (4.45) we get

$$
\begin{pmatrix} \theta(\lambda, p) & \phi(\lambda, p) \\ \theta'(\lambda, p) & \phi'(\lambda, p) \end{pmatrix} = M(\lambda)\begin{pmatrix} \theta(\lambda, 0) & \phi(\lambda, 0) \\ \theta'(\lambda, 0) & \phi'(\lambda, 0) \end{pmatrix} = M(\lambda). \tag{4.46}
$$

From the preceding equation we can obtain the following relationship

$$
\Delta(\lambda) = \theta(\lambda, p) + \phi'(\lambda, p) = \operatorname{Tr} M(\lambda), \tag{4.47}
$$

where *Tr* stands for the matrix trace. The behavior of Hill's discriminant $\Delta(\lambda)$, in the particular case of a piecewise constant case with $m = 2$, is depicted in Figure 3. Using the function $\Delta(\lambda)$ we can evaluate the allowed and forbidden bands.

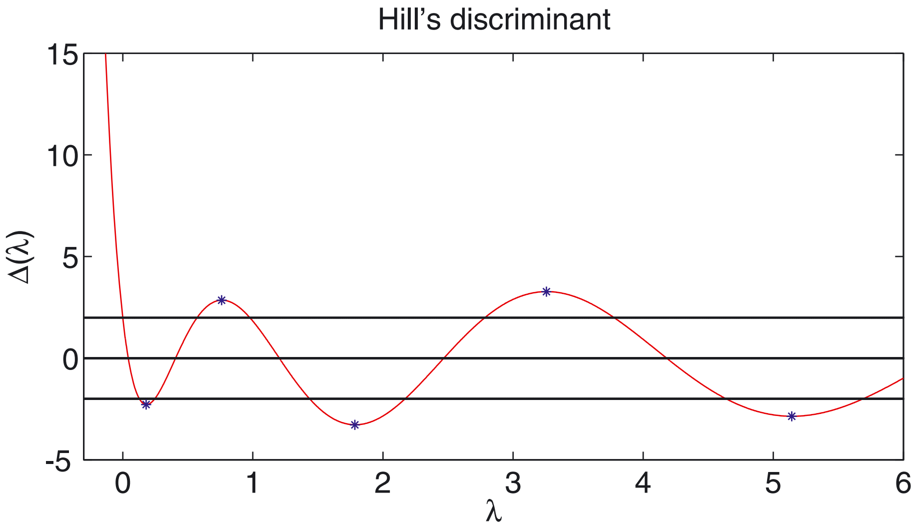

Fig. 3. Hill's discriminant if $n(x)$ is piecewise constant. $n_1 = 3$, $n_2 = 1$, $a_1 = 2$ and $a_2 = 1$. $\Delta(\lambda)$ is unbounded as $x \to -\infty$. Relative maxima and minima are labeled as ' * '.

In the piecewise continuous case it is clear that the period map $M(\lambda)$ has the following property

$$\begin{pmatrix} \sqrt{\lambda} & 0 \\ 0 & 1 \end{pmatrix} M(\lambda) \begin{pmatrix} \frac{1}{\sqrt{\lambda}} & 0 \\ 0 & 1 \end{pmatrix} = \prod_{j=m,m-1,\dots,1} \begin{pmatrix} \cos(n_j a_j \sqrt{\lambda}) & \dfrac{\sin(n_j a_j \sqrt{\lambda})}{n_j} \\ -n_j \sin(n_j a_j \sqrt{\lambda}) & \cos(n_j a_j \sqrt{\lambda}) \end{pmatrix}.$$

We can observe that this matrix has determinant 1 and its entries are almost periodic polynomials in $\sqrt{\lambda}$. The diagonal entries are even real functions of $\sqrt{\lambda}$ and the off-diagonal entries are odd real functions of $\sqrt{\lambda}$ vanishing at $\sqrt{\lambda} = 0$. Let us write

$$\mu_j = n_j a_j > 0 \qquad \text{and } z = \sqrt{\lambda}.$$

Then we can introduce the *modified period map* $\boldsymbol{M}(z)$ as

$$\boldsymbol{M}(z) = \begin{pmatrix} z & 0 \\ 0 & 1 \end{pmatrix} M(\lambda) \begin{pmatrix} z^{-1} & 0 \\ 0 & 1 \end{pmatrix}. \tag{4.48}$$

More precisely, we can write

$$\boldsymbol{M}(z) = \prod_{j=m,m-1,\dots,1} \begin{pmatrix} \cos(\mu_j z) & \dfrac{\sin(\mu_j z)}{n_j} \\ -n_j \sin(\mu_j z) & \cos(\mu_j z) \end{pmatrix}.$$

If we take a homogeneous medium with refractive index n_1 and consider the period[7] p

$$\boldsymbol{M}(z) = \begin{pmatrix} \cos(\mu_j z) & \dfrac{\sin(\mu_j z)}{n_j} \\ -n_j \sin(\mu_j z) & \cos(\mu_j z) \end{pmatrix}.$$

Considering a crystal with 2 different media with refractive indices n_1 and n_2. Respectively, we have the following modified period map matrix

$$\boldsymbol{M}(z) = \frac{1}{2}\begin{pmatrix} \left(1+\dfrac{n_1}{n_2}\right)\cos((\mu_1+\mu_2)z) & \left(\dfrac{1}{n_1}+\dfrac{1}{n_2}\right)\sin((\mu_1+\mu_2)z) \\ +\left(1-\dfrac{n_1}{n_2}\right)\cos((\mu_1-\mu_2)z) & +\left(\dfrac{1}{n_1}-\dfrac{1}{n_2}\right)\sin((\mu_1-\mu_2)z) \\ -(n_1+n_2)\sin((\mu_1+\mu_2)z) & \left(1+\dfrac{n_2}{n_1}\right)\cos((\mu_1+\mu_2)z) \\ -(n_1-n_2)\sin((\mu_1-\mu_2)z) & +\left(1-\dfrac{n_2}{n_1}\right)\cos((\mu_1-\mu_2)z) \end{pmatrix}.$$

We can now generalize the modified period map for a crystal with m different media with refractive indices n_1, n_2, …, n_m, respectively, by writing

$$\boldsymbol{M}_{11}(z) = +\sum_{\sigma_1=1} c^{11}_{\sigma_1,\sigma_2,\ldots,\sigma_m} \cos((\sigma_1\mu_1+\sigma_2\mu_2+\ldots+\sigma_m\mu_m)z),$$

$$\boldsymbol{M}_{12}(z) = +\sum_{\sigma_1=1} c^{12}_{\sigma_1,\sigma_2,\ldots,\sigma_m} \sin((\sigma_1\mu_1+\sigma_2\mu_2+\ldots+\sigma_m\mu_m)z),$$

$$\boldsymbol{M}_{21}(z) = -\sum_{\sigma_1=1} c^{21}_{\sigma_1,\sigma_2,\ldots,\sigma_m} \sin((\sigma_1\mu_1+\sigma_2\mu_2+\ldots+\sigma_m\mu_m)z),$$

$$\boldsymbol{M}_{22}(z) = +\sum_{\sigma_1=1} c^{22}_{\sigma_1,\sigma_2,\ldots,\sigma_m} \cos((\sigma_1\mu_1+\sigma_2\mu_2+\ldots+\sigma_m\mu_m)z),$$

where we sum over all $(\sigma_2,\ldots,\sigma_m) \in \{-1,+1\}^{m-1}$. The entries of the previous matrix are almost periodic functions [**1**]. For an almost periodic function

$$\phi(t) = \sum_j c_j e^{i\mu_j t},$$

where μ_j are distinct real numbers and the set of Fourier coefficients $\{c_j\}$ is bounded, we define the Fourier spectrum as the set of those real numbers μ for which the

[7] For a homogeneous medium the choice of the period p is arbitrary.

related coefficients

$$c(\mu) \stackrel{\text{def}}{=} \lim_{T\to+\infty} \frac{1}{2T} \int_{-T}^{T} f(t)e^{-i\mu t}\,dt$$

are $\neq 0$. The Fourier spectrum of an almost periodic function is an, at most countably, infinite subset of $\mathbb{R}$. The Fourier spectrum of the entries of the product matrix is contained in the set

$$\left\{\sum_{j=1}^{m} \sigma_j n_j a_j : \sigma_j = \pm 1\right\},$$

where zero may (resp. cannot) belong to the Fourier spectrum of the diagonal (resp. off-diagonal) entries. Thus the Fourier spectrum has at most 2^m points and its maximum is $\mu_1 + \ldots + \mu_m$. Among the above Fourier coefficients we have the recurrence relations[8]

$$\begin{aligned} c^{11}_{\sigma_1,\ldots,\sigma_{m-1},\pm 1} &= \frac{1}{2} c^{11}_{\sigma_1,\ldots,\sigma_{m-1}} \pm \frac{1}{2n_m} c^{21}_{\sigma_1,\ldots,\sigma_{m-1}}, \\ c^{22}_{\sigma_1,\ldots,\sigma_{m-1},\pm 1} &= \frac{1}{2} c^{22}_{\sigma_1,\ldots,\sigma_{m-1}} \pm \frac{1}{2} n_m c^{12}_{\sigma_1,\ldots,\sigma_{m-1}}. \end{aligned}$$

In the same way we derive the recurrence relations

$$\begin{aligned} c^{12}_{\sigma_1,\ldots,\sigma_{m-1},\pm 1} &= \frac{1}{2} c^{12}_{\sigma_1,\ldots,\sigma_{m-1}} \pm \frac{1}{2n_m} c^{22}_{\sigma_1,\ldots,\sigma_{m-1}}, \\ c^{21}_{\sigma_1,\ldots,\sigma_{m-1},\pm 1} &= \frac{1}{2} c^{21}_{\sigma_1,\ldots,\sigma_{m-1}} \pm \frac{1}{2} n_m c^{11}_{\sigma_1,\ldots,\sigma_{m-1}}. \end{aligned}$$

In general,

$$\begin{aligned} \boldsymbol{c}_{\sigma_1,\ldots,\sigma_m} &\stackrel{\text{def}}{=} \begin{pmatrix} c^{11}_{\sigma_1,\ldots,\sigma_m} & c^{12}_{\sigma_1,\ldots,\sigma_m} \\ c^{21}_{\sigma_1,\ldots,\sigma_m} & c^{22}_{\sigma_1,\ldots,\sigma_m} \end{pmatrix} \\ &= \frac{1}{2^{m-1}} \begin{pmatrix} 1 & \dfrac{\sigma_m}{n_m} \\ \sigma_m n_m & 1 \end{pmatrix} \cdots \begin{pmatrix} 1 & \dfrac{\sigma_2}{n_2} \\ \sigma_2 n_2 & 1 \end{pmatrix} \begin{pmatrix} 1 & \dfrac{\sigma_1}{n_1} \\ \sigma_1 n_1 & 1 \end{pmatrix}. \end{aligned} \tag{4.49}$$

[8] Here we used $2\cos a \cos\beta = \cos(\beta + a) + \cos(\beta - a)$, $2\sin a \sin\beta = -\cos(\beta + a) + \cos(\beta - a)$, $2\sin a \cos\beta = \sin(\beta + a) - \sin(\beta - a)$, and $2\cos a \sin\beta = \sin(\beta + a) + \sin(\beta - a)$, where $a = \mu_m z$ and $\beta = (\mu_1 + \ldots + \mu_{m-1})z$.

By induction on the number of factors we can easily prove that

$$\frac{c^{11}_{\sigma_1,\dots,\sigma_m}}{c^{21}_{\sigma_1,\dots,\sigma_m}}=\frac{c^{21}_{\sigma_1,\dots,\sigma_m}}{c^{22}_{\sigma_1,\dots,\sigma_m}}=\sigma_1 n_1,\qquad \frac{c^{21}_{\sigma_1,\dots,\sigma_m}}{c^{11}_{\sigma_1,\dots,\sigma_m}}=\frac{c^{22}_{\sigma_1,\dots,\sigma_m}}{c^{21}_{\sigma_1,\dots,\sigma_m}}=\sigma_m n_m. \tag{4.50}$$

Lemma 4.1.

$$\boldsymbol{c}_{\sigma_1,\dots,\sigma_i,\dots,\sigma_m}+\boldsymbol{c}_{\sigma_1,\dots,-\sigma_i,\dots,\sigma_m}=\boldsymbol{c}_{\sigma_1,\dots,\sigma_{i-1},\sigma_{i+1},\dots,\sigma_m}$$

Proof. It is easy to prove the preceding relation using the formula (4.49). □

4.5 - *Recovering the period map from the scattering matrix*

In this section we indicate how the period map of the periodic-plus-impurity problem can be recovered from the scattering coefficients $a(k)$ and $b(k)$. We shall restrict ourselves to the piecewise constant case, although the reduction of the scattering coefficients to the period map goes through in general.

As the periodic part we consider $Q_0(x)\equiv 0$ and $n_0(x)=n_j$ $(b_{j-1}<x<b_j$, $j=1,\dots,m)$. Here $0=b_0<b_1<\dots<b_m=p$ and $a_j=b_j-b_{j-1}$ $(j=1,\dots,m)$. The impurity consists of defining $Q_i(x)\equiv 0$ and

$$1+\varepsilon(x)=\begin{cases}(N_j/n_j), & b_{j-1}<x<b_j,\ j=1,\dots,m,\\ 0, & x\notin[0,p].\end{cases}$$

Now let us define $M_i(\lambda)$ as the matrix $M(\lambda)$ in the period with impurities with n_j replaced by N_j $(j=1,\dots,m)$.[9] Then outside the interval $[0,p]$ the Jost solutions can be expressed in the Floquet solutions as follows:

$$f_1(k,x)=\begin{cases}\psi_1(k,x), & x\ge p,\\ \quad a(k)\psi_1(k,x)+b(k)\psi_2(k,x), & x\le 0,\end{cases}$$

$$f_2(k,x)=\begin{cases}-\overline{b(\overline{k})}\psi_1(k,x)+a(k)\psi_2(k,x), & x\ge p,\\ \psi_2(k,x), & x\le 0.\end{cases}$$

Putting

$$W(k,x)\overset{\text{def}}{=}\begin{pmatrix}\psi_1(k,x) & \psi_2(k,x)\\ \psi_1'(k,x) & \psi_2'(k,x)\end{pmatrix}, \tag{4.51}$$

---

[9] We could just consider any periodic and periodic-plus-impurity problem, because we only need to work with the period maps $M(\lambda)$ and $M_i(\lambda)$.

we obtain

$$W(k,0)\begin{pmatrix} a(k) \\ b(k) \end{pmatrix} = \begin{pmatrix} f_1(k,0) \\ f_1'(k,0) \end{pmatrix} = M_i(\lambda)^{-1}\begin{pmatrix} f_1(k,p) \\ f_1'(k,p) \end{pmatrix}$$
$$= M_i(\lambda)^{-1}\begin{pmatrix} \psi_1(k,p) \\ \psi_1'(k,p) \end{pmatrix} = M_i(\lambda)^{-1}M(\lambda)\begin{pmatrix} \psi_1(k,0) \\ \psi_1'(k,0) \end{pmatrix}$$

and

$$W(k,0)\begin{pmatrix} -\overline{b(\overline{k})} \\ a(k) \end{pmatrix} = M(\lambda)^{-1}W(k,p)\begin{pmatrix} -\overline{b(\overline{k})} \\ a(k) \end{pmatrix} = M(\lambda)^{-1}\begin{pmatrix} f_2(k,p) \\ f_2'(k,p) \end{pmatrix}$$
$$= M(\lambda)^{-1}M_i(\lambda)\begin{pmatrix} f_2(k,0) \\ f_2'(k,0) \end{pmatrix} = M(\lambda)^{-1}M_i(\lambda)\begin{pmatrix} \psi_2(k,0) \\ \psi_2'(k,0) \end{pmatrix}.$$

As a result of $w(k) = m_2(\lambda) - m_1(\lambda)$, $\psi_1(k,0) = \psi_2(k,0) = 1$, $\psi_1'(k,0) = m_1(\lambda)$, and $\psi_2'(k,0) = m_2(\lambda)$ we get

$$\begin{pmatrix} a(k) \\ b(k) \end{pmatrix} = \frac{1}{w(k)}\begin{pmatrix} m_2(\lambda) & -1 \\ -m_1(\lambda) & 1 \end{pmatrix} M_i(\lambda)^{-1}M(\lambda)\begin{pmatrix} 1 \\ m_1(\lambda) \end{pmatrix}, \tag{4.52a}$$

$$\begin{pmatrix} -\overline{b(\overline{k})} \\ a(k) \end{pmatrix} = \frac{1}{w(k)}\begin{pmatrix} m_2(\lambda) & -1 \\ -m_1(\lambda) & 1 \end{pmatrix} M_i(\lambda)M(\lambda)^{-1}\begin{pmatrix} 1 \\ m_2(\lambda) \end{pmatrix}. \tag{4.52b}$$

Equations (4.52) allow us to compute the period map $M_i(\lambda)$ of the periodic-plus-impurity problem if the impurity is concentrated in one period, the periodic data are known, and $a(k)$ and $b(k)$ are known. The latter scattering data can easily be computed from one reflection coefficient and the transmission coefficient by using (4.37) and (4.39).

More generally, let the impurity be concentrated in $[-Mp, Np]$, where M is a nonnegative integer and N a positive integer. Then $f_1(k,x) = \psi_1(k,x)$ for $x \geq Np$ and $f_2(k,x) = \psi_2(k,x)$ for $x \leq -Mp$. Now let $M_{i+}(\lambda)$ be the period map of the periodic-plus-impurity problem for computing solutions at $x = Np$ from those at $x = 0$, and let $M_{i-}(\lambda)$ be the period map of the periodic-plus-impurity problem to compute solutions at $x = 0$ from those at $x = -Mp$. Then

$$W(k,0)\begin{pmatrix} a(k) \\ b(k) \end{pmatrix} = \begin{pmatrix} f_1(k,0) \\ f_1'(k,0) \end{pmatrix} = M_{i+}(\lambda)^{-1}\begin{pmatrix} f_1(k,Np) \\ f_1'(k,Np) \end{pmatrix}$$
$$= M_{i+}(\lambda)^{-1}\begin{pmatrix} \psi_1(k,Np) \\ \psi_1'(k,Np) \end{pmatrix} = M_{i+}(\lambda)^{-1}M(\lambda)^N\begin{pmatrix} \psi_1(k,0) \\ \psi_1'(k,0) \end{pmatrix}$$

and

$$\begin{aligned}
W(k,0)\begin{pmatrix} -\overline{b(\overline{k})} \\ a(k) \end{pmatrix} &= M(\lambda)^{-N} W(k,Np)\begin{pmatrix} -\overline{b(k)} \\ a(k) \end{pmatrix} = M(\lambda)^{-N}\begin{pmatrix} f_2(k,Np) \\ f_2'(k,Np) \end{pmatrix} \\
&= M(\lambda)^{-N} M_{i+}(\lambda) M_{i-}(\lambda)\begin{pmatrix} f_2(k,-Mp) \\ f_2'(k,-Mp) \end{pmatrix} \\
&= M(\lambda)^{-N} M_{i+}(\lambda) M_{i-}(\lambda)\begin{pmatrix} \psi_2(k,-Mp) \\ \psi_2'(k,-Mp) \end{pmatrix} \\
&= M(\lambda)^{-N} M_{i+}(\lambda) M_{i-}(\lambda) M(\lambda)^{-M}\begin{pmatrix} \psi_2(k,0) \\ \psi_2'(k,0) \end{pmatrix}.
\end{aligned}$$

Instead of (4.52) we now get

$$\begin{pmatrix} a(k) \\ b(k) \end{pmatrix} = \frac{1}{w(k)}\begin{pmatrix} m_2(\lambda) & -1 \\ -m_1(\lambda) & 1 \end{pmatrix} M_{i+}(\lambda)^{-1} M(\lambda)^N \begin{pmatrix} 1 \\ m_1(\lambda) \end{pmatrix}, \tag{4.53a}$$

$$\begin{pmatrix} -\overline{b(\overline{k})} \\ a(k) \end{pmatrix} = \frac{1}{w(k)}\begin{pmatrix} m_2(\lambda) & -1 \\ -m_1(\lambda) & 1 \end{pmatrix} M(\lambda)^{-N} M_{i+}(\lambda) M_{i-}(\lambda) M(\lambda)^{-M}\begin{pmatrix} 1 \\ m_2(\lambda) \end{pmatrix}. \tag{4.53b}$$

Equations (4.53) allow us to compute the period maps $M_{i+}(\lambda)$ and $M_{i-}(\lambda)$ of the periodic-plus-impurity problem if the impurity is concentrated in finitely many (known) periods, the periodic data are known, and $a(k)$ and $b(k)$ are known. The latter scattering data can easily be computed from one reflection coefficient and the transmission coefficient by using (4.37) and (4.39). Let us write $N(\lambda) = M_i(\lambda)^{-1}M(\lambda)$ as in (4.52a). Then

$$\begin{aligned}
a(\lambda) = \frac{1}{w(\lambda)}\Big(&[m_2(\lambda) + m_1(\lambda)]\frac{1}{2}[N_{11}(\lambda) - N_{22}(\lambda)] - N_{21}(\lambda) \\
&+ m_2(\lambda) m_1(\lambda) N_{12}(\lambda) + [m_2(\lambda) - m_1(\lambda)]\frac{1}{2}[N_{11}(\lambda) + N_{22}(\lambda)]\Big).
\end{aligned} \tag{4.54}$$

Now for $\Delta(\lambda) \notin [-2,2]$ we have

$$w(\lambda) = m_2(\lambda) - m_1(\lambda) = \frac{\tau_2(\lambda) - \tau_1(\lambda)}{\phi(\lambda,p)},$$

$$m_2(\lambda) + m_1(\lambda) = \frac{\Delta(\lambda) - 2\theta(\lambda,p)}{\phi(\lambda,p)} = \frac{\phi'(\lambda,p) - \theta(\lambda,p)}{\phi(\lambda,p)},$$

$$\begin{aligned}
m_2(\lambda) m_1(\lambda) &= \frac{\tau_2(\lambda)\tau_1(\lambda) - [\tau_2(\lambda) + \tau_1(\lambda)]\theta(\lambda,p) + \theta(\lambda,p)^2}{\phi(\lambda,p)^2} \\
&= \frac{1 - [\theta(\lambda,p) + \phi'(\lambda,p)]\theta(\lambda,p) + \theta(\lambda,p)^2}{\phi(\lambda,p)^2} = -\frac{\theta'(\lambda,p)}{\phi(\lambda,p)}.
\end{aligned}$$

Consequently,

$$\begin{aligned} a(\lambda)w(\lambda)\phi(\lambda,p) &= \frac{1}{2}[N_{11}(\lambda)+N_{22}(\lambda)]w(\lambda)\phi(\lambda,p) - N_{21}(\lambda)\phi(\lambda,p) \\ &+ \frac{1}{2}[N_{11}(\lambda)-N_{22}(\lambda)][\phi'(\lambda,p)-\theta(\lambda,p)] - N_{12}(\lambda)\theta'(\lambda,p). \end{aligned} \tag{4.55}$$

5 - First results on the identification of the refractive index

In this section we propose a method to determine the refractive indices n_j and the layer amplitudes a_j knowing the period map, in the piecewise constant case when each crystal period is made of two or three different materials with constant index.

This kind of heterostructure is generally made of no more than three layers per period [**7**], [**14**]. An example of periodic structure with period p in the case of piecewise constant refractive index is depicted in Figure 4.

5.1 - *Piecewise constant with two different materials*

Let us consider a crystal where in each period there are two different media with refractive indices n_1 and n_2, respectively, where $n_1 \neq n_2$ (the $n_1 = n_2$ case is trivial).

We can evaluate n_1 and n_2 by equations (4.50):

$$\frac{c^{11}_{++}}{c^{12}_{++}} = \frac{c^{21}_{++}}{c^{22}_{++}} = \frac{c^{11}_{+-}}{c^{12}_{+-}} = \frac{c^{21}_{+-}}{c^{22}_{+-}} = n_1,$$

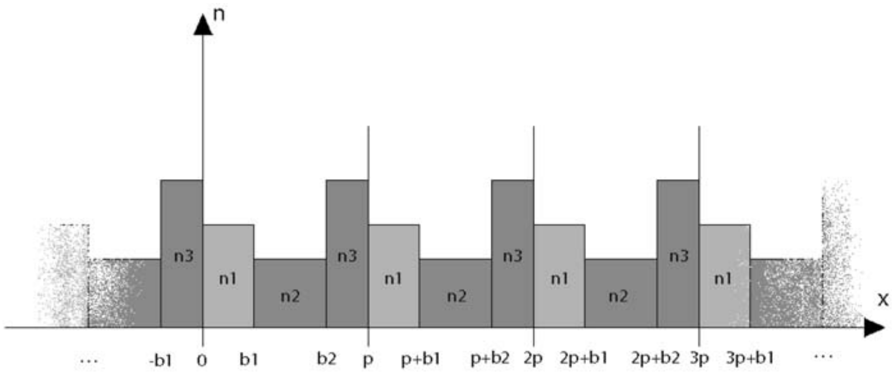

Fig. 4. Example of a periodic structure with period p in the case of a piecewise constant refractive index.

and

$$\frac{c^{21}_{++}}{c^{11}_{++}} = \frac{c^{22}_{++}}{c^{12}_{++}} = n_2, \qquad \frac{c^{21}_{+-}}{c^{11}_{+-}} = \frac{c^{22}_{+-}}{c^{12}_{+-}} = -n_2.$$

Setting $\mu_{max} = \mu_1 + \mu_2$ the maximum of the spectrum, we can calculate the layer amplitudes by solving the following system:

$$\begin{cases} n_1 a_1 + n_2 a_2 = \mu_{max} \\ a_1 + a_2 = p\,. \end{cases} \tag{5.1}$$

5.2 - *Piecewise constant with three different materials*

Let us now consider a crystal with period p where each period is made of three different materials with refractive indices n_1, n_2 and n_3. If $n_i = n_j$ for $i \neq j$ we have the preceding case, so we consider $n_i \neq n_j$ for $i \neq j$.

As in the previous example we can evaluate the refraction indices by using the following formulas

$$\frac{c^{11}_{+++}}{c^{12}_{+++}} = \frac{c^{21}_{+++}}{c^{22}_{+++}} = n_1, \qquad \frac{c^{21}_{+++}}{c^{11}_{+++}} = \frac{c^{22}_{+++}}{c^{12}_{+++}} = n_3.$$

Let us now consider the following inequality

$$0 < \mu_{\gamma_3} \leq \mu_{\gamma_2} \leq \mu_{\gamma_1},$$

where the set $\{\gamma_1, \gamma_2, \gamma_3\}$ is one of the possible permutations of indices $\{1, 2, 3\}$.

Let μ_{γ_3} be the minimal value of μ_j. Then the two largest numbers in the spectrum are

$$\mu_{max} = \mu_1 + \mu_2 + \mu_3 = \mu_{\gamma_1} + \mu_{\gamma_2} + \mu_{\gamma_3}$$

and

$$\widetilde{\mu} = \mu_{\gamma_1} + \mu_{\gamma_2} - \mu_{\gamma_3} = \mu_{max} - 2\mu_{\gamma_3}.$$

From lemma 4.1 we have

$$\boldsymbol{c}_{\sigma_{\gamma_1},\sigma_{\gamma_2},\sigma_{\gamma_3}} + \boldsymbol{c}_{\sigma_{\gamma_1},\sigma_{\gamma_2},-\sigma_{\gamma_3}} = \boldsymbol{c}_{\sigma_{\gamma_1},\sigma_{\gamma_2}},$$

where $\boldsymbol{c}_{1_{\gamma_1},1_{\gamma_2},1_{\gamma_3}}$ and $\boldsymbol{c}_{1_{\gamma_1},1_{\gamma_2},-1_{\gamma_3}}$ are the matrix Fourier coefficient matrices evaluated in μ_{max} and $\widetilde{\mu}$, respectively. $\boldsymbol{c}_{\sigma_{\gamma_1},\sigma_{\gamma_2}}$ is the matrix of Fourier coefficients of a "virtual" crystal made up of two layers with refractive indices n_{γ_1} and n_{γ_2}, respectively, and period $a_{\gamma_1} + a_{\gamma_2}$.

Let us calculate

$$\boldsymbol{c}_{\sigma_{\gamma_1},\sigma_{\gamma_2}} + \boldsymbol{c}_{\sigma_{\gamma_1},-\sigma_{\gamma_2}} = \boldsymbol{c}_{\sigma_{\gamma_1}}.$$

Then the matrix $\boldsymbol{c}_{\sigma_{\gamma_1}}$ is the matrix of Fourier coefficients of a "virtual" homogeneous crystal made of a medium with refractive index n_{γ_1} and period a_{γ_1}.

If $n_{\gamma_1} = n_1$ ($n_{\gamma_1} = n_3$) then $\gamma_1 = 1$ ($\gamma_1 = 3$); otherwise (i.e., if $n_{\gamma_1} \neq n_1$ and $n_{\gamma_1} \neq n_3$) the value of γ_1 is 2.

From $\boldsymbol{c}_{1_{\gamma_1}, 1_{\gamma_2}}$ we can evaluate n_{γ_1} and n_{γ_2} by using relations (4.50). Knowing γ_1 we can estimate γ_2 comparing n_{γ_2} with n_1, n_2 and n_3; the value of γ_3 is determined as a result.

To calculate a_1, a_2 and a_3 we can solve the following system

$$\begin{cases} n_1 a_1 + n_2 a_2 + n_3 a_3 = \mu_{max} \\ n_{\gamma_1} a_{\gamma_1} + n_{\gamma_2} a_{\gamma_2} - n_{\gamma_3} a_{\gamma_3} = \widetilde{\mu} \\ a_1 + a_2 + a_3 = p \end{cases} \tag{5.2}$$

and observe that in the second equation the indices $\{\gamma_1, \gamma_2, \gamma_3\}$ are known from the previous analysis.

6 - Conclusions

In this paper, a complete characterization of mono-dimensional photonic crystals has been given. We have calculated the solutions in a photonic crystal with and without impurities. In particular, we have analysed a structure consisting of a finite number of periodic layers with constant refractive index.

We have paid particular attention to the period map and determined the relation with the scattering matrix and the scattering coefficients $a(k)$ and $b(k)$. We have estimated the discrete eigenvalues introduced in band gaps by impurities.

Finally, we have developed an algorithm to recover the refractive index in the piecewise constant case when each period of the crystal is made of two or three different materials.

It is an open problem how to develop an algorithm for refractive index recovery when each period is composed of more than three layers. Moreover it could be very interesting to extend the formalism of Hill's discriminant to determine band gaps in a bi-dimensional or three-dimensional crystal.

Appendix

A - Green's function

The Green's function represents the impulse response, i.e., the system output when subjected to an impulsive signal. If the photonic crystal is excited by an electromagnetic wave $f(x)$ we can write:

$$-\psi''(\lambda, x) + Q(x)\psi(\lambda, x) = \lambda n(x)^2 \psi(\lambda, x) + n(x)^2 f(x), \tag{A.1}$$

where $n(x)$ is a positive piecewise continuous function and $Q(x)$ is a real piecewise continuous function, both periodic with period p. For $\tau \in \mathbb{C}$ with $|\tau| = 1$, we consider the self-adjoint boundary conditions (3.3), where the solution is given by

$$\psi(\lambda, x) = \int_0^p \mathcal{G}(x, y; \lambda) n(y)^2 f(y)\, dy \tag{A.2}$$

and $\mathcal{G}(x, y; \lambda)$ is the Green's function of the system, that is

$$\begin{aligned} \mathcal{G}(x, y; \lambda) &= \frac{\phi_1'(\lambda, p)\phi_1(\lambda, x)\phi_2(\lambda, y) - \phi_2'(\lambda, p)\phi_1(\lambda, x)\phi_1(\lambda, y)}{w[\tau\phi_1'(\lambda, 0) - \phi_1'(\lambda, p)]} \\ &+ \frac{\phi_1(\lambda, p)\phi_2(\lambda, x)\phi_2(\lambda, y) - \phi_2(\lambda, p)\phi_2(\lambda, x)\phi_1(\lambda, y)}{w[\tau\phi_2(\lambda, 0) - \phi_2(\lambda, p)]} \end{aligned} \tag{A.3a}$$

for $0 \le x < y \le p$, and

$$\begin{aligned} \mathcal{G}(x, y; \lambda) &= \frac{\tau\phi_1'(\lambda, 0)\phi_1(\lambda, x)\phi_2(\lambda, y) - \phi_2'(\lambda, p)\phi_1(\lambda, x)\phi_1(\lambda, y)}{w[\tau\phi_1'(\lambda, 0) - \phi_1'(\lambda, p)]} \\ &+ \frac{\phi_1(\lambda, p)\phi_2(\lambda, x)\phi_2(\lambda, y) - \tau\phi_2(\lambda, 0)\phi_2(\lambda, x)\phi_1(\lambda, y)}{w[\tau\phi_2(\lambda, 0) - \phi_2(\lambda, p)]} \end{aligned} \tag{A.3b}$$

for $0 \le y < x \le p$. If $f(x - x_0) = \delta(x - x_0)$ we have $\psi(\lambda, x) = \mathcal{G}(x, x_0; \lambda) n(x_0)^2$.

Proof. To derive the Green's function we use the same method as used to derive the Green's function for the Sturm-Liouville problem. Let us assume that λ is not an eigenvalue of the differential equation (3.1) with boundary conditions (3.3). Let $\phi_1(\lambda, x)$ and $\phi_2(\lambda, x)$ stand for nontrivial solutions of (3.3) such that

$$\phi_1(\lambda, p) = \tau\phi_1(\lambda, 0), \qquad \phi_2'(\lambda, p) = \tau\phi_2'(\lambda, 0). \tag{A.4}$$

Then their (constant) Wronskian w is nonzero. We choose $\phi_1(\lambda, x)$ and $\phi_2(\lambda, x)$ as real functions under periodic ($\tau = 1$) and antiperiodic ($\tau = -1$) boundary conditions.

Let us solve the differential equation (A.1) under the boundary conditions (3.3) by the method of variation of parameters. Writing

$$\psi(\lambda, x) = c_1(x)\phi_1(\lambda, x) + c_2(x)\phi_2(\lambda, x),$$

we arrive at the linear system

$$\begin{pmatrix} \phi_1(\lambda, x) & \phi_2(\lambda, x) \\ \phi_1'(\lambda, x) & \phi_2'(\lambda, x) \end{pmatrix} \begin{pmatrix} c_1'(x) \\ c_2'(x) \end{pmatrix} = \begin{pmatrix} 0 \\ -n(x)^2 f(x) \end{pmatrix},$$

where the system determinant equals w. Then

$$\begin{aligned} \begin{pmatrix} c_1'(x) \\ c_2'(x) \end{pmatrix} &= \frac{1}{w} \begin{pmatrix} \phi_2'(\lambda, x) & -\phi_2(\lambda, x) \\ -\phi_1'(\lambda, x) & \phi_1(\lambda, x) \end{pmatrix} \begin{pmatrix} 0 \\ -n(x)^2 f(x) \end{pmatrix} \\ &= \frac{n(x)^2 f(x)}{w} \begin{pmatrix} \phi_2(\lambda, x) \\ -\phi_1(\lambda, x) \end{pmatrix}. \end{aligned}$$

Thus there exist constants c_1 and c_2 such that

$$c_1(x) = \frac{1}{w} \int_0^x \phi_2(\lambda, y) n(y)^2 f(y)\, dy + c_1,$$

and

$$c_2(x) = -\frac{1}{w} \int_0^x \phi_1(\lambda, y) n(y)^2 f(y)\, dy + c_2.$$

Then we can write

$$\begin{aligned} \psi(\lambda, x) &= c_1\phi_1(\lambda, x) + c_2\phi_2(\lambda, x) \\ &+ \frac{\phi_1(\lambda, x)}{w} \int_0^x \phi_2(\lambda, y) n(y)^2 f(y)\, dy - \frac{\phi_2(\lambda, x)}{w} \int_0^x \phi_1(\lambda, y) n(y)^2 f(y)\, dy. \end{aligned} \tag{A.5}$$

Differentiating with respect to x we get from (A.5)

$$\begin{aligned} \psi'(\lambda, x) &= c_1\phi_1'(\lambda, x) + c_2\phi_2'(\lambda, x) \\ &+ \frac{\phi_1'(\lambda, x)}{w} \int_0^x \phi_2(\lambda, y) n(y)^2 f(y)\, dy - \frac{\phi_2'(\lambda, x)}{w} \int_0^x \phi_1(\lambda, y) n(y)^2 f(y)\, dy. \end{aligned} \tag{A.6}$$

Substituting (3.2a) and using $\phi_1(\lambda,p) = \tau\phi_1(\lambda,0)$ in (A.5) we get

$$\tau c_2\phi_2(\lambda,0) = c_2\phi_2(\lambda,p) + \frac{\phi_1(\lambda,p)}{w}\int_0^p \phi_2(\lambda,y)n(y)^2 f(y)\,dy$$

$$-\frac{\phi_2(\lambda,p)}{w}\int_0^p \phi_1(\lambda,y)n(y)^2 f(y)\,dy.$$

Similarly using (3.3b) and $\phi_2'(\lambda,p) = \tau\phi_2'(\lambda,0)$ in (A.6) we get

$$\tau c_1\phi_1'(\lambda,0) = c_1\phi_1'(\lambda,p) + \frac{\phi_1'(\lambda,p)}{w}\int_0^p \phi_2(\lambda,y)n(y)^2 f(y)\,dy$$

$$-\frac{\phi_2'(\lambda,p)}{w}\int_0^p \phi_1(\lambda,y)n(y)^2 f(y)\,dy.$$

We now compute the constants c_1 and c_2 and substitute the resulting expressions in (A.5). We finally obtain

$$\psi(\lambda,x) = \phi_1(\lambda,x)\int_0^p \frac{\phi_1'(\lambda,p)\phi_2(\lambda,y) - \phi_2'(\lambda,p)\phi_1(\lambda,y)}{w[\tau\phi_1'(\lambda,0) - \phi_1'(\lambda,p)]}n(y)^2 f(y)\,dy$$

$$+\phi_2(\lambda,x)\int_0^p \frac{\phi_1(\lambda,p)\phi_2(\lambda,y) - \phi_2(\lambda,p)\phi_1(\lambda,y)}{w[\tau\phi_2(\lambda,0) - \phi_2(\lambda,p)]}n(y)^2 f(y)\,dy$$

$$+\frac{\phi_1(\lambda,x)}{w}\int_0^x \phi_2(\lambda,y)n(y)^2 f(y)\,dy - \frac{\phi_2(\lambda,x)}{w}\int_0^x \phi_1(\lambda,y)n(y)^2 f(y)\,dy.$$

If we use the Heaviside's function[10] $H(x-y)$ we can write all integrals as integrals on $[0,p]$:

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[10] Heaviside's function or step function $\delta_{-1}(x)$ is defined as:

$$H(x) = \delta_{-1}(x) = \begin{cases} 0 & x < 0, \\ 1 & x \geq 0. \end{cases}$$

$$\psi(\lambda,x)=\phi_1(\lambda,x)\int_0^p\frac{\phi_1'(\lambda,p)\phi_2(\lambda,y)-\phi_2'(\lambda,p)\phi_1(\lambda,y)}{w[\tau\phi_1'(\lambda,0)-\phi_1'(\lambda,p)]}n(y)^2f(y)\,dy$$

$$+\phi_2(\lambda,x)\int_0^p\frac{\phi_1(\lambda,p)\phi_2(\lambda,y)-\phi_2(\lambda,p)\phi_1(\lambda,y)}{w[\tau\phi_2(\lambda,0)-\phi_2(\lambda,p)]}n(y)^2f(y)\,dy$$

$$+\int_0^p\frac{\phi_1(\lambda,x)\phi_2(\lambda,y)-\phi_2(\lambda,x)\phi_1(\lambda,y)}{w}n(y)^2f(y)H(x-y)\,dy.$$

Hence, introducing the Green's function, we obtain the equation (A.2). □

A.1 - *Selfadjointness property*

The Green's function also satisfies the selfadjointness property[11]

$$\mathcal{G}(x,y;\lambda)=\overline{\mathcal{G}(y,x;\lambda)}\ . \tag{A.7}$$

Let us now differentiate $\mathcal{G}(x,y;\lambda)$ with respect to x. We get

$$\begin{aligned}\frac{\partial\mathcal{G}}{\partial x}&=\frac{\phi_1'(\lambda,p)\phi_1'(\lambda,x)\phi_2(\lambda,y)-\phi_2'(\lambda,p)\phi_1'(\lambda,x)\phi_1(\lambda,y)}{w[\tau\phi_1'(\lambda,0)-\phi_1'(\lambda,p)]}\\&\quad+\frac{\phi_1(\lambda,p)\phi_2'(\lambda,x)\phi_2(\lambda,y)-\phi_2(\lambda,p)\phi_2'(\lambda,x)\phi_1(\lambda,y)}{w[\tau\phi_2(\lambda,0)-\phi_2(\lambda,p)]}\end{aligned} \tag{A.8a}$$

for $0\le x<y\le p$, and

$$\begin{aligned}\frac{\partial\mathcal{G}}{\partial x}&=\frac{\tau\phi_1'(\lambda,0)\phi_1'(\lambda,x)\phi_2(\lambda,y)-\phi_2'(\lambda,p)\phi_1'(\lambda,x)\phi_1(\lambda,y)}{w[\tau\phi_1'(\lambda,0)-\phi_1'(\lambda,p)]}\\&\quad+\frac{\phi_1(\lambda,p)\phi_2'(\lambda,x)\phi_2(\lambda,y)-\tau\phi_2(\lambda,0)\phi_2'(\lambda,x)\phi_1(\lambda,y)}{w[\tau\phi_2(\lambda,0)-\phi_2(\lambda,p)]}.\end{aligned} \tag{A.8b}$$

For $0\le y<x\le p$. Then

$$\frac{\partial\mathcal{G}}{\partial x}(x,x^+;\lambda)-\frac{\partial\mathcal{G}}{\partial x}(x,x^-;\lambda)=1. \tag{A.9}$$

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[11] This property holds, because for $\lambda\in\mathbb{R}$ the Green's function $\mathcal{G}(x,y;\lambda)n(y)^2$ is the real integral kernel of an integral operator that is the inverse of a selfadjoint operator on $L^2((0,p);n(x)^2dx)$. A general direct proof can be found in [**16**].

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Abstract

In this article we introduce a mathematical model to describe light propagation in a mono-dimensional photonic crystal under the hypothesis of a linear, stationary, isotropic and lossless medium. We study the typical band structure and spectral properties. In addition, we analyse a crystal with an impurity confined to a bounded region and study the change in its spectrum as a result of introducing the impurity. The asymptotic expressions for the solution of the Helmholtz-Schrödinger model equation with impurity are analysed to derive the scattering matrix. We introduce the period map matrix and derive it from the scattering matrix. We pay particular attention to a photonic crystal with a piecewise constant index of refraction and recover it from the scattering matrix in a few important special cases.

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