Defect states and defect modes
in 1D Photonic Crystals

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Chapter 1

Introduction

1.1 Surprises from light in periodic media

Imagine shining a light through a layer of glass. As we learn from elementary physics, when light hits the interface, some of the light will reflect and some of it will continue propagating through the glass. Imagine now two layers of glass from different materials attached together. As before, the light will reflect and refract from both layers, and this time in a more intricate interaction than before. Next, suppose we duplicate the two layers thousands of times, and attached all of them together, making a periodic arrangements of these layers. Actually, the way to predict the behaviour of light in this case is not much different than the case of two layers, except now it will be a very cumbersome procedure. If you are lucky, you can see through this structure, or on the contrary, you might also see nothing at all.

It goes back over a century ago in the time of Rayleigh in 1887, that it was the first time a purely periodic system extending to infinity in one direction was investigated. He found out at that time that such type of structure exhibits a range of wavelengths such that waves having those wavelengths are forbidden to propagate inside this periodic arrangements. Nowadays this periodic arrangements of layers having different materials is called a Photonic Crystal. It is called a crystal, because of its periodicity, and photonic because it acts on light. If this periodic arrangement is on the order of the wavelength of light, then for some range of wavelengths light can not go through the crystal. This range of wavelength is called the Photonic Band Gap.

From mathematical point of view, this periodic system is well described by the Bloch-Floquet theorem. It tells that for wavelengths inside the band gap, there can be two possibilities. The amplitude of light can decay or grow exponentially inside the periodic system. Usually people say, that the exponential growth of the amplitude of light is not physical, so this solution inside the periodic system only exist mathematically.

What happens if the symmetry of the structure is broken by an anomalous defect layer, say having different material or thickness? When this happens then it is possible to glue the exponential growing solution with the other one
which is decaying. In this case we say that light is localized in the vicinity of the
anomalous defect layer. We call this state as the defect state.

In the spirit of the short introduction above, this thesis is about defect states
and defect modes in 1D Photonic Crystals with a defect layer. It is organized
as follows: Chapter 1 is about general introduction and Maxwell’s equation,
Chapter 2 is about 1D Photonic Crystal, and transfer matrix technique for 1D
Photonic Crystals. Then Chapter 3 is about light defect states and defect modes
in 1D Photonic Crystals. Due to a defect layer in the 1D Photonic Crystal a
localized state exist within the band gap. Using a combination of transfer matrix
technique and variational methods the defect frequency can be obtained. Also
in this Chapter the relation between defect states and defect modes arising from
a finite 1D Photonic Crystals will be given. Chapter 4 is a little bit different
in contents. It is about the experience using a commercial software package
called Femlab, some features, usefulness and weaknesses, and some examples
in optics solved with Femlab. Mainly, the investigation will be on the use of
boundary conditions that are available in the package. Chapter 5 concludes this
thesis.

1.2 Maxwell’s equation

As a natural starting point, all macroscopic electromagnetic phenomena are
governed by the Maxwell’s equations

\[ \nabla \times \mathcal{H} = \mathcal{J} + \frac{\partial}{\partial t} \mathcal{D} \]  
(1.1)

\[ \nabla \times \mathcal{E} = -\frac{\partial}{\partial t} \mathcal{B} \]  
(1.2)

\[ \nabla \cdot \mathcal{D} = \rho \]  
(1.3)

\[ \nabla \cdot \mathcal{B} = 0 \]  
(1.4)

with \( \mathcal{D} = \varepsilon \mathcal{E} + \mathcal{P} \) and \( \mathcal{B} = \mu_0 \mathcal{M} + \mu_0 \mathcal{H} \). Here \( \mathcal{E} \) and \( \mathcal{H} \) are the electric and
magnetic fields, \( \mathcal{D} \) is the electrical displacement, \( \mathcal{P} \) is the polarization density,
\( \mathcal{J} \) is the free current density, and \( \rho \) is the free charge density.

The configuration or structure of an optical device described by the dielectric
function \( \varepsilon \), which is a function of position in space. Throughout this thesis,
dielectric materials are considered that are linear (\( \mathcal{P} = 0 \)), independent of \( \mathcal{E} \),
non magnetic (\( \mathcal{M} = 0 \)) and also, absorption of light by the material is neglected,
\( \varepsilon \) is real valued.

Furthermore, a common interest in optics is in cases where no free charges
and no free currents are included, \( \mathcal{J} \) and \( \rho \) are zero. If the electric field \( \mathcal{E} \)
and the magnetic field \( \mathcal{H} \) are written as product of a function which depends
only on the position and a function which depends only on time, then this
separation of variable leads to time harmonic fields in the form of \( \mathcal{E} = \mathcal{E}e^{-i\omega t} \).
1.3 Scaling properties of the Helmholtz equation

and \( \mathcal{H} = \mathbf{H}e^{-i\omega t} \). Hence for Maxwell’s equations

\[
\frac{\partial}{\partial t} \leftrightarrow -i\omega
\]

and (1.1), (1.2) simplifies to

\[
\nabla \times \mathbf{H} = -i\omega \varepsilon \mathbf{E} \tag{1.6}
\]

\[
\nabla \times \mathbf{E} = i\omega \mu_0 \mathbf{H} \tag{1.7}
\]

In this thesis TE mode for 1D and 2D photonic crystal structures will be considered. For both cases the electric field component of the TE mode is perpendicular to the plane of propagation. Hence the consequence for equation (1.3)

\[
\nabla \cdot \mathbf{D} = (\nabla \varepsilon \cdot \mathbf{E} + \varepsilon \nabla \cdot \mathbf{E})e^{-i\omega t} = \varepsilon \nabla \cdot \mathbf{E}e^{-i\omega t} = 0
\]

and equations (1.3) and (1.4) simplify to

\[
\nabla \cdot \mathbf{E} = 0 \tag{1.9}
\]

\[
\nabla \cdot \mathbf{H} = 0 \tag{1.10}
\]

An equation only for \( \mathbf{E} \) can be obtained by taking the cross product of equation (1.7) and combining with equation (1.6), giving

\[
\nabla \times \nabla \times \mathbf{E} = \omega^2 \mu_0 \varepsilon \mathbf{E} \tag{1.11}
\]

and using the identity for the vector operation \( \nabla \times \nabla \times \mathbf{E} = \nabla(\nabla \cdot \mathbf{E}) - \nabla^2 \mathbf{E} \) leads to the equation for \( \mathbf{E} \)

\[
\nabla^2 \mathbf{E} + \frac{\omega^2}{c^2} \varepsilon_r \mathbf{E} = 0 \tag{1.12}
\]

where \( c^2 = 1/\sqrt{\mu_0 \varepsilon_0} \), \( \varepsilon_r = \varepsilon/\varepsilon_0 \). Further in this thesis we shall call this equation (1.12) the Helmholtz equation and omit the subscript \( r \) in \( \varepsilon_r \) for the sake of simplicity.

The Helmholtz equation (1.12) is the governing equation of all the phenomena that will be considered in this thesis. This applies also for the 1D photonic crystals structures (the grating) and the 2D photonic crystals.

### 1.3 Scaling properties of the Helmholtz equation

The Helmholtz equation (1.12) governs the electromagnetic phenomena for the electric field macroscopically. An interesting feature of electromagnetics phenomena in dielectric medium is that there is no fundamental length scale. The coefficients of the equation don’t have length as its dimension, so electromagnetic
problems that differ only by an expansion or a contraction can be considered to be the same problem. This suggest that the equation with its coefficients can be normalized with respect to a reference (length) parameter. Later in this thesis this normalization will be applied.

To see this, let’s consider the Helmholtz equation again, and say that a harmonic mode $E^*$ is a solution of the equation with frequency $\omega^*$ and dielectric function $\epsilon(x)$. Then its satisfies

$$\nabla^2 E^*(x) + \frac{\omega^*}{c^2} \epsilon(x) E^*(x) = 0 \quad (1.13)$$

Now suppose there is another dielectric function which is a scaling of the previous dielectric function $\tilde{\epsilon}(x) = \epsilon(dx)$ for some scaling parameter $d$. Then applying a change of variable in (1.13), using $x = x/d$ and $\tilde{\nabla} = d\nabla$

$$\frac{1}{d^2} \tilde{\nabla}^2 E^*(d\tilde{x}) + \frac{\omega^*}{c^2} \epsilon(dx) E^*(d\tilde{x}) = 0 \quad (1.14)$$

but since $\epsilon(dx) = \tilde{\epsilon}(\tilde{x})$ this equation above returns into

$$\tilde{\nabla}^2 E^*(d\tilde{x}) + \frac{\omega^*}{c^2} \tilde{\epsilon}(d\tilde{x}) E^*(d\tilde{x}) = 0 \quad (1.15)$$

This is nothing but the equation (1.13) again, but with the mode profile $E^*(d\tilde{x})$ and frequency $\omega^*d$. Simply stated in words, after scaling the physical system by a factor $d$, the mode profile and its frequency is the same as the old one but scaled with the factor $d$. 
Chapter 2

1-D photonic crystals

The simplest example of a photonic crystal, is the traditional multilayer film, which will further be called the grating. It is composed from alternating layers of high and low dielectric constants. A typical example is illustrated below. It is assumed that this structure extends to infinity in the $x$ axis direction. For each $z$ the medium is homogeneous in the $x$-axis direction, so an Ansatz is chosen in the form of

$$E(x, z) = E(z)e^{ik_x x}$$

(2.1)

where $k_x = \frac{\omega}{c}\sqrt{\epsilon}\sin(\theta)$, $\theta$ is the angle of incidence. Throughout this thesis, only normal incidence will be considered, hence for this typical structure of photonic crystal in 1D, the Helmholtz equation (1.12), reduces to only an equation for $E(z)$

$$\frac{\partial^2 E(z)}{\partial z^2} + \frac{\omega^2}{c^2}\epsilon(z)E(z) = 0$$

(2.2)

and further the dielectric constant $\epsilon(z)$ shall be defined as $\epsilon(z) = n^2(z)$, with $n(z)$ the refractive index function.
2.1 Normalized Helmholtz equation

To have light interact as much as possible with a structure, and giving interesting phenomena, the structure with which light interacts with should have changes of its properties in the order of the wavelength of light. Not much interesting things can be observed from light traveling in bulk media.

So, as motivated by the scaling properties of the Helmholtz equation explained in Section 1.3, it is favourable to scale / normalized the Helmholtz equation with a scaling which is in the order of the wavelength. Introduce a scaling as follows

\[ z = \lambda \hat{z}, \quad \Rightarrow \quad \partial_z = \lambda \partial_{\hat{z}} \]  

(2.3)

hence equation (2.2)

\[ \frac{1}{\lambda^2} \partial_{\hat{z}}^2 E(\lambda \hat{z}) + \frac{\omega^2}{c^2} n^2(\lambda \hat{z}) E(\lambda \hat{z}) = 0 \]  

(2.4)

or

\[ \partial_{\hat{z}}^2 \hat{E}(\hat{z}) + \hat{\omega}^2 n^2(\hat{z}) \hat{E}(\hat{z}) = 0 \]  

(2.5)

where \( \hat{E}(\hat{z}) = E(\lambda \hat{z}) \) and \( \hat{\omega} = \omega \lambda / c \). This normalized Helmholtz equation will be used further in this thesis to describe the grating, and for simplicity, the symbol “shall be omitted.

2.2 Transfer Matrix techniques for 1-D photonic crystals

The most simple way to describe the wave behaviour in 1D grating is by using the Transfer Matrix technique. Below the transfer matrix of one unit grating will be derived. As depicted in Figure 2.2 below, consider a periodic arrangement of multilayer films, with refractive indices \( n_1 \) and \( n_2 \), each with thicknesses \( d_1 \) and \( d_2 \) respectively. The solution for equation (2.5) will be a superposition of plane waves traveling to the right and to the left. Say, for layer with index \( n_1 \) the right going and left going plane waves have amplitudes \( A_1 \) and \( B_1 \) respectively,
and for layer with index $n_2$ the right going and left going plane waves have amplitudes $C_1$ and $D_1$ respectively. Hence for layer with index $n_1$ the solution of equation (2.5) is

$$E(z) = A_1 e^{ik_1 z} + B_1 e^{-ik_1 z}$$

(2.6)

and

$$E(z) = C_1 e^{ik_2 (z - d_1)} + D_1 e^{-ik_2 (z - d_1)}$$

(2.7)

for the layer with index $n_2$. The parameter $k_1$ and $k_2$ will be called the wavenumber, and the definition is given by $k_1 = \omega n_1$ and $k_2 = \omega n_2$. At the interface between layers ($z = d_1$), the solution and its derivative should be continuous. This gives a relation between plane waves amplitudes

$$A_1 B_1 = M_{12} A_1 B_1$$

(2.8)

with

$$M_{12} = \begin{bmatrix} \frac{1}{2} \left( 1 + \frac{k_1}{k_2} \right) e^{ik_1 d_1} & \frac{1}{2} \left( 1 - \frac{k_1}{k_2} \right) e^{-ik_1 d_1} \\ \frac{1}{2} \left( 1 - \frac{k_1}{k_2} \right) e^{ik_1 d_1} & \frac{1}{2} \left( 1 + \frac{k_1}{k_2} \right) e^{-ik_1 d_1} \end{bmatrix}$$

(2.9)

and also at $z = d$, the interface between layer with index $n_2$ and $n_1$, continuity of the plane waves and its derivative gives

$$A_2 B_2 = M_{21} A_1 B_1$$

(2.10)

where the matrix $M_{21}$ is the same as (2.9) but with interchanging the indices. Concluding from the two matrix equations above

$$A_2 B_2 = M A_1 B_1$$

(2.11)

where $M = M_{21} M_{12}$ with elements

$$M(1, 1) = e^{ik_1 d_1} \left[ \cos(k_2 d_2) + \frac{1}{2} i \left( \frac{k_2}{k_1} + \frac{k_1}{k_2} \right) \sin(k_2 d_2) \right]$$

$$M(1, 2) = e^{-ik_2 d_1} \left[ \frac{1}{2} i \left( \frac{k_2}{k_1} - \frac{k_1}{k_2} \right) \sin(k_2 d_2) \right]$$

$$M(2, 1) = e^{ik_1 d_1} \left[ -\frac{1}{2} i \left( \frac{k_2}{k_1} - \frac{k_1}{k_2} \right) \sin(k_2 d_2) \right]$$

$$M(2, 2) = e^{-ik_2 d_1} \left[ \cos(k_2 d_2) - \frac{1}{2} i \left( \frac{k_2}{k_1} + \frac{k_1}{k_2} \right) \sin(k_2 d_2) \right]$$

Further in this thesis, matrix $M$ shall be be called as the Transfer Matrix of one unit of grating. Observe that the matrix $M$ depends on the frequency $\omega$, and it is unimodular\(^1\). Hence for each $\omega$ the matrix $M$ defines a unique mapping for amplitudes of the plane waves in layer $n_1$ into the amplitude of the next layer

\(^1\)A unimodular matrix is a square matrix with its determinant equals to unity
2.3 Transmission experiment of gratings

In this section, a brief look at what is called a transmission experiment will be given. This experiment resembles a typical device which can function as a filter, or mirror for some interval of wavelength which lies in the band gap.  

The setting of the experiment is as follows, consider a periodic arrangement of multilayer films with index $n_1$ and $n_2$, and take $N$ unit of these cells, and stack them as depicted in Figure 2.3 below. At the left and right exterior

![Figure 2.3: Periodic arrangement of multilayer films of N unit, schematic illustration of a transmission experiment](image)

... (background), there is a homogeneous medium with index $n_0$. Light is incidence from the left exterior, say with unit amplitude and frequency $\omega$. Then light will interact within this structure, resulting into a right going plane wave with amplitude $t$ in the right exterior, and a reflected plane wave with amplitude $r$ to the left.

Using the transfer matrix technique, it can be shown easily that the relation between the plane waves amplitudes in the left and right exterior is as follows

$$
\begin{pmatrix}
t \\
r
\end{pmatrix} = M
\begin{pmatrix}
1 \\
r
\end{pmatrix}
$$

(2.12)

where

$$
M = \begin{bmatrix}
\frac{1}{2}(1 + \frac{k_0}{k_1}) & \frac{1}{2}(1 - \frac{k_0}{k_1}) \\
\frac{1}{2}(1 - \frac{k_0}{k_1}) & \frac{1}{2}(1 + \frac{k_0}{k_1})
\end{bmatrix}
M^N
\begin{bmatrix}
\frac{1}{2}(1 + \frac{k_0}{k_2}) & \frac{1}{2}(1 - \frac{k_0}{k_2}) \\
\frac{1}{2}(1 - \frac{k_0}{k_2}) & \frac{1}{2}(1 + \frac{k_0}{k_2})
\end{bmatrix}
$$

(2.13)

with $M$ given in equation (2.11).

---

2For a precise definition of band gap for multilayer stacks of films see [8]
2.3 Transmission experiment of gratings

2.3.1 Quarter wave stack structure example

A specific case of a grating, called a quarter wave structure, is a case where for each layer of films, the optical path length is equal to a quarter of the wavelength. Take for example 8 units of grating with indices $n_1 = 1.25$ and $n_2 = 2.5$, the corresponding thicknesses of each layer are $d_1 = \lambda/(4n_1) = \lambda/5$ and $d_4 = \lambda/(4n_2) = \lambda/10$. Performing the transmission experiment for this structure, one can calculate the power transfer of light incidence on this grating for any frequency $\omega$. The power transfer is given by a quantity called the transmittance, defined as

$$T = |t|^2$$ (2.14)

Below is the transmittance curve as a function of frequency. Observe there is a region near frequency $= 1$, with vanishing transmittance. This region is called the band gap.

![Transmittance curve](image)

Figure 2.4: Transmittance curve as a function of frequency, for 8 units of grating with indices $n_1 = 1.25$ and $n_2 = 2.5$.

---

3 Optical path length is the product of the refractive index with the distance of which a light travels, $OPL = nd$. 

Chapter 3

Defect states and defect modes in 1D photonic crystals with a defect layer

The study of localized electromagnetic waves with frequencies arising in the middle of the forbidden gap due to an isolated defect in the periodic structure has been studied in recent years ([2]-[6]). Various techniques has been used to study this, such as with transfer matrix method ([4]-[6]), finite elements ([2],[3]), plane wave expansion method ([6]), etc. In this Chapter, defect states are to be calculated by using a combination of variational method and transfer matrix method. Further, the defect mode which exists in a transmission experiment of a finite grating with a defect layer can be constructed from the defect states.

3.1 Bloch waves

For an infinite grating extending on the whole $z$-axis, the solution of the Helmholtz equation (2.5) can be written in term of Bloch waves

$$E(z) = u(z)e^{iK(\omega)z} \quad (3.1)$$

where $u(z)$ is a complex valued periodic function with the period of the grating, $u(z) = u(z + d)$. The parameter $K(\omega)$ is called the Bloch wave number, where for a periodic grating with indices $n_1$ and $n_2$ there is an explicit expression for $K(\omega)$ as follows

$$K(\omega) = \frac{1}{d} \cos^{-1}\left(\frac{1}{2} \text{Trace}[M]\right) \quad (3.2)$$

with $M$ given in (2.11). The behaviour of the Bloch wave is characterized by this Bloch wave number. Generally, the behaviour of the Bloch wave can be divided into three cases.

- For $K(\omega)$ real which lie in the first Brillouin zone $[0, \pi/d]$, $E(z)$ is a periodic and traveling wave function. In this case it is said that $\omega$ is outside of the
3.2 Defect states for 1D photonic crystal with defect

For $\omega$ imaginary, defined by $K(\omega) = \pi/d + ip(\omega)$, $E(z)$ is a standing wave function, a product of $2d$ periodic function with an exponential increasing or decreasing function, depending on the sign of $\rho(\omega)$. In this case it is said that $\omega$ is inside the band gap.

- For $K(\omega) = \pi/d$, $E(z)$ is a periodic function with period $2d$, with special properties that it is $d$-shift skew symmetric, $E(z + d) = -E(z)$\(^1\).

Figure 3.1 below illustrates a typical graph of the Bloch wave number. This graph originated from an infinite Quarter Wave Stack structure with indices $n_1 = 1.25$ and $n_2 = 2.5$.

\begin{figure}[h]
  \centering
  \includegraphics[width=0.5\textwidth]{figure3_1.png}
  \caption{Graph of the Bloch wave number $K(\omega)$ as a function of $\omega$}
\end{figure}

3.2 Defect states for 1D photonic crystal with defect

For an infinite grating, solutions with frequency inside the band gap will have only an increasing and decreasing state. When the grating is 'broken up' by a defect layer, then it is possible to have a confined state. Below in Figure 3.2 is a typical example of a finite grating with a defect layer. The existence of a defect layer makes it possible to glue an exponential increasing state from the left with an exponential decreasing state to the right to make a confined (defect) state. For this state, light is trapped in the vicinity of the defect and can not escape anywhere. Not physical, but still it exists, is the other defect state which is not confined near the defect. This defect state is an exponential decreasing state from the left of the defect glued with an exponential increasing state to the right. As said before, from the physical point of view, this state is not interesting since

\(^1\)The terminology $d$-shift skew symmetric is introduced in [8].
3.2 Defect states for 1D photonic crystal with defect

3.2.1 Defect state calculation for infinite grating

Consider an infinite grating with a defect layer of width $2L$ placed in the center of the grating, as depicted in Figure 3.2 above, and consider frequencies inside the band gap. The general idea of how to calculate the defect state is by confining the domain of the problem on the positive real line to only the defect region $\Omega = [0, L]$. The motivation comes from the fact that for the half infinite grating region ($\Omega^c = (L, \infty)$), the solution can be written down explicitly and the frequency dependent behavior of the solution is well describe from Bloch theorem. From this information, value function for $\Omega^c$ can be calculated precisely, hence reducing the domain of the problem only to $\Omega$.

Value function for $\Omega^c$

Below the value function on $\Omega^c$ is to be calculated. Assume $E(z)$ is a solution of (2.5), then:

$$V(E) = \int_{\Omega^c} |\partial_z E|^2 - k^2(z)|E|^2 \, dz$$

$$= \frac{1}{2} \left[ \int_{\Omega^c} \partial_z E \overline{\partial_z \overline{E}} \, dz - \int_{\Omega^c} k^2(z)E\overline{E} \, dz \right] + c.c.$$  \hspace{1cm} (3.3)

For region $\Omega^c$:

$$= \frac{1}{2} \left[ \int_{\Omega^c} \partial_z E \overline{\partial_z \overline{E}} \, dz - \int_{\Omega^c} k^2(z)E\overline{E} \, dz \right] + c.c.$$  \hspace{1cm} (3.3)
Using the Bloch theorem, the solution of (2.5) for $z > L$ is of the form

$$E(z) = u(z)e^{iK(z-L)} \quad (3.4)$$

where

$$K = \pi/d + i\rho, \quad \rho > 0 \quad (3.5)$$

This solution vanishes when $z$ approaches infinity, hence the value function (3.3) simplifies to

$$V(E(L)) = -\frac{1}{2} \partial_z E(L)E(L) + c.c. \quad (3.6)$$

and let’s write this quadratic value function as

$$V(E(L)) \equiv \kappa(\omega) |E(L)|^2 \quad (3.7)$$

for some function $\kappa(\omega)$ that is to be determined later.

Now consider a functional on $\Omega \cup \Omega^c$:

$$F(E) = \int_{\Omega \cup \Omega^c} |\partial_z E|^2 - k^2(z) |E|^2 \, dz \quad (3.8)$$

$$= \int_{\Omega \cup \Omega^c} |\partial_z E|^2 - k^2(z) |E|^2 \, dz + V(E(L)) \quad (3.9)$$

The first variation of $F(E)$, for a variation $\eta$, is given by

$$\delta F(E; \eta) = \delta G(E; \eta) + \delta V(E(L); \eta(L))$$

$$= \int_{\Omega} \delta E G(E) \eta \cdot dz + \partial_z E \eta_{|\Omega}$$

$$+ \kappa(\omega) E(L)\eta(L) + c.c. \quad (3.10)$$

and requiring it to vanish (with free variation at $z = L$) results into the Euler-Lagrange equation $\delta E G(E) = 0$, which is

$$\partial_z^2 E(z) + k_0^2 E(z) = 0, \quad k_0^2 = \omega^2 n_0^2 \quad (3.11)$$

with a boundary condition at $z = L$

$$\partial_z E + \kappa(\omega) E = 0 \quad (3.12)$$

and symmetry condition at $z = 0$, $\partial_z E(0) = 0$, or antisymmetry condition at $z = 0$, $E(0) = 0$.

Note that the periodic system plus defect depicted in Figure 3.2 possesses a reflection symmetry, i.e., the solution is either symmetric or antisymmetric with respect to reflection. From these results a confined problem formulation on $\Omega$
for the defect state can be formulated as

\[
\text{Crit}_E \{ G(E) + V(E(L)) \} \tag{3.13}
\]

for symmetric states, and

\[
\text{Crit}_E \{ G(E) + V(E(L)) \mid E(0) = 0 \} \tag{3.14}
\]

for antisymmetric states. Solutions of (3.11) in \( \Omega \) are given by

\[
E(z) = A \cos(k_dz), \quad \text{symmetric states,} \tag{3.15}
\]

\[
E(z) = B \sin(k_dz), \quad \text{antisymmetric states.} \tag{3.16}
\]

Substituting (3.15) and (3.16) above into (3.12) gives the relation for calculating the defect frequency

\[
k_d \tan(k_dL) = \kappa(\omega), \quad \text{for symmetric states,} \tag{3.17}
\]

and

\[
-k_d \cot(k_dL) = \kappa(\omega), \quad \text{for antisymmetric states.} \tag{3.18}
\]

Further on, \( \kappa(\omega) \) have to be calculated.

\( \kappa(\omega) \) calculation

Below \( \kappa(\omega) \) is calculated using transfer matrix method. Lets write the solution of the half infinite grating as a superposition of a right and left going monochromatic wave: \( E(z) = A_N e^{ik_1(z-L+(N-1)d)} + B_N e^{-ik_1(z-L+(N-1)d)} \) for the N-th layer with index \( n_1 \) and \( E(z) = C_N e^{ik_2(z-(L+(N-1)d+d_1))} + D_N e^{-ik_2(z-(L+(N-1)d+d_1))} \) for the N-th layer with index \( n_2 \). Then as explained in Section 2.2, there is a

![Figure 3.3: Defect layer and the first three layers of the grating](image)

relation for the plane wave amplitudes as follows

\[
\begin{bmatrix}
A_{N+1} \\
B_{N+1}
\end{bmatrix} = M \begin{bmatrix}
A_N \\
B_N
\end{bmatrix} \tag{3.19}
\]
3.2 Defect states for 1D photonic crystal with defect

with matrix \( \mathbf{M} \) define in (2.11). The matrix \( \mathbf{M} \) is unimodular hence the eigenvalue of \( \mathbf{M} \) is in the form of \( e^{iKd} \) and is given by

\[
e^{iKd} = \frac{1}{2} \text{Trace}(\mathbf{M}) \pm \left\{ \left[ \frac{1}{2} \text{Trace}(\mathbf{M}) \right]^{2} - 1 \right\}^{\frac{1}{2}}
\]

and remembering (3.5) gives

\[
-e^{-\rho d} = \frac{1}{2} \text{Trace}(\mathbf{M}) \pm \left\{ \left[ \frac{1}{2} \text{Trace}(\mathbf{M}) \right]^{2} - 1 \right\}^{\frac{1}{2}}
\]

The rhs of (3.21) will be automatically real since the frequencies considered are in the band gap, and the determination of the + or the − sign comes from the following argument:

Matrix \( \mathbf{M} \) is unimodular, the product of eigenvalues (both real and negative for the first band gap) equals to unity. This tells that \( \text{Trace}(\mathbf{M}) \) is negative, and to have the localized solution, the eigenvalue with the smaller magnitude has to be chosen. Hence

\[
-e^{-\rho d} = \frac{1}{2} \text{Trace}(\mathbf{M}) \pm \left\{ \left[ \frac{1}{2} \text{Trace}(\mathbf{M}) \right]^{2} - 1 \right\}^{\frac{1}{2}}
\]

Now from (3.4), (3.5), substituting \( z = L + d \) and using the periodicity property of \( u(z) \) gives

\[
E(L + d) = -E(L)e^{-\rho d}
\]

where in terms of the left and right going monochromatic wave, \( E(L + d) = A_2 + B_2 \) and \( E(L) = A_1 + B_1 \). But from matrix equation (3.19)

\[
\begin{align*}
A_2 &= \mathbf{M}(1, 1)A_1 + \mathbf{M}(1, 2)B_1 \\
B_2 &= \mathbf{M}(2, 1)A_1 + \mathbf{M}(2, 2)B_1
\end{align*}
\]

hence

\[
E(L + d) = (\mathbf{M}(1, 1) + \mathbf{M}(2, 1))A_1 + (\mathbf{M}(1, 2) + \mathbf{M}(2, 2))B_1 = -(A_1 + B_1)e^{-\rho d}
\]

Upon collecting the coefficients of \( A_1 \) and \( B_1 \) from the rhs of equations above, gives the relation

\[
B_1 = -\gamma A_1, \quad \gamma = \frac{\mathbf{M}(1, 1) + \mathbf{M}(2, 1) + e^{-\rho d}}{\mathbf{M}(1, 2) + \mathbf{M}(2, 2) + e^{-\rho d}}
\]

From this

\[
E(L) = (1 - \gamma)A_1 \Rightarrow A_1 = \frac{E(L)}{1 - \gamma}
\]
and it is easy to see that
\[
E_z(L) = i k_l (A_1 - B_1)
\]
\[
= i k_l (1 + \gamma) A_1
\]
\[
= i k_l \left( \frac{1 + \gamma}{1 - \gamma} \right) E(L)
\]  
(3.28)

From these result the value function (3.6) can be calculated
\[
V(E(L)) = -\frac{1}{2} \left[ E_z(L) \overline{U(L)} + E_z(L) E(L) \right]
\]
\[
= -\frac{1}{2} \left[ ik_l \frac{1 + \gamma}{1 - \gamma} |E(L)|^2 - ik_l \frac{1 + \gamma}{1 - \gamma} |E(L)|^2 \right]
\]
\[
= -\frac{1}{2} ik_l \left[ \frac{1 + \gamma}{1 - \gamma} - \frac{1 + \gamma}{1 - \gamma} \right] |E(L)|^2
\]
\[
= \kappa(\omega) |E(L)|^2, \kappa(\omega) = k_l \text{Im} \left( \frac{1 + \gamma}{1 - \gamma} \right)
\]  
(3.29)

As an example, a quarter wave stack structure is taken, with indices \( n_1 = 1.25 \) and \( n_2 = 2.5 \), and the defect layer with index \( n_d = 4.5 \). Calculating the defect frequency in the way that is describe above gives \( \omega = 2\pi \cdot 1.084071 \).

Figure 3.4 below \( \kappa \) is plotted together with \( h(\omega) = \omega n_d \tan(\omega n_d L) \). The intersection of the two curves gives the defect frequency \( \omega_d \) and the electric field profile is plotted in Figure 3.5 below.

![Graph of \( \kappa(\omega) \) and \( h(\omega) = \omega n_d \tan(\omega n_d L) \), for \( n_d = 4.5 \)]

Figure 3.4: Graph of \( \kappa(\omega) \) and \( h(\omega) = \omega n_d \tan(\omega n_d L) \), for \( n_d = 4.5 \)

What happens if the defect index \( n_d \) is increased / decreased? Qualitatively, it can be explained as follows. Consider the equation only for the defect layer
\[
\partial_z^2 E(z) + \omega^2 n_d^2 E(z) = 0
\]  
(3.30)

If \( n_d \) increases (decreases) very slightly, then the same solution \( E(z) \) can be
3.2 Defect states for 1D photonic crystal with defect

Figure 3.5: Symmetric state for infinite grating with defect, $\omega_d = 2\pi \cdot 1.084071$

recovered by compensating the value of $\omega$, decreasing (increasing) it. This
behaviour of the frequency shifting when the defect layer index $n_d$ changes can be
seen more precisely in Figure 3.6 below. It can be seen that if the defect

Figure 3.6: The defect frequencies as a function of the defect layer index $n_d$. The parameters of the underlying grating is $n_l = 1.25$ and $n_h = 2.5$

layer index increases for the same type of states, the defect frequency decreases until it merge with the lower edge of the band gap. But before this happens, a
different type of state emerge from the upper edge of the band gap.

These defect states are standing states, do not propagate to the left or right of the grating. In such an idealized one dimensional structure, light is trapped forever in the neighborhood of the defect layer. This is the simplest case of light trapping.
3.2 Defect states for 1D photonic crystal with defect

3.2.2 Defect state calculation for finite grating

In this section, a finite grating with a defect will be considered, and the objective is to calculate the defect states. The situation is illustrated in Figure 3.7 below. Let's start by writing the solution of the finite grating as a superposition of a right and left going monochromatic wave:

\[ E(z) = A_N e^{ik_1(z-(L+(N-1)d))} + B_N e^{-ik_1(z-(L+(N-1)d))} \]

for the N-th layer with index \(n_1\) and

\[ E(z) = C_N e^{ik_2(z-(L+(N-1)d+d_1))} + D_N e^{-ik_2(z-(L+(N-1)d+d_1))} \]

for the N-th layer with index \(n_2\). In the same way as explained in Section 3.2.1, a matrix relation between field amplitudes at \(z = L + Nd\) and \(z = L\) is obtained as follows

\[
\begin{bmatrix}
A_{N+1} \\
B_{N+1}
\end{bmatrix} = N
\begin{bmatrix}
A_1 \\
B_1
\end{bmatrix}
\]

(3.31)

where \(N = M^N\), with elements of matrix \(M\) given in (2.11). To obtain the standing states, it must be required that

\[
B_{N+1} = A_{N+1}
\]

(3.32)

and consider the inverse of system (3.31)

\[
\begin{bmatrix}
A_1 \\
B_1
\end{bmatrix} = N^{-1}
\begin{bmatrix}
A_{N+1} \\
B_{N+1}
\end{bmatrix}
\]

(3.33)

which gives

\[
A_1 = (N(2,2) - N(1,2))A_{N+1}
\]

\[
B_1 = (N(1,1) - N(2,1))A_{N+1}
\]

(3.34)

and upon simplifying, this results in a relation between \(B_1\) and \(A_1\)

\[
B_1 = -\gamma_N A_1, \quad \gamma_N = \frac{N(1,1) - N(2,1)}{N(2,2) - N(1,2)}
\]

(3.35)

Value function (3.3) can be calculated further in the same way as explained in Section 3.2.1, except now the symbol \(\gamma\) is replaced with \(\gamma_N\), and infinity is replaced with \(L + Nd\). The value function at \(z = L + Nd\) is precisely zero since

Figure 3.7: Finite grating with a defect layer, for positive z axis. The number of units in the grating is \(N\).
3.2 Defect states for 1D photonic crystal with defect

\( B_{N+1} = A_{N+1} \) is required. The value function has the form

\[
V(U(L)) = \kappa_N(\omega) |U(L)|^2
\]

with

\[
\kappa_N(\omega) = k_l \text{Im} \left( \frac{1 + \gamma_N}{1 - \gamma_N} \right)
\]

Example

As an example, take \( N = 4 \), with parameters the same as given in Section 3.2.1. In Figure 3.8 \( \kappa_N \) is plotted for \( N=2,4 \). It can be seen that already for a small number of units of grating, \( \kappa_N \) is very close to \( \kappa \). Figure 3.9 shows the variation of the defect frequencies (first antisymmetric) which respect to changes in \( n_d \), plotted together with the one for the infinite case. For \( n_d = 2.5 \), the defect frequency is 1 and the field is depicted in Figure 3.10. It can be seen that the field is amplified inside the grating, and for this reason this state will be called the amplified state.

For this set of parameters and defect frequency, actually there exist another state which decays inside the grating. If the requirement

\[
B_{N+1} = -A_{N+1}
\]

is chosen instead of the one given in (3.32), the electric field profile will look like the one in Figure 3.11. Lets call this state as the attenuated state.
3.2 Defect states for 1D photonic crystal with defect

Figure 3.9: Comparison of defect frequencies for $N = 4$ and the infinite case. The solid curve is the defect frequencies for infinite grating while dashed curve is for the finite grating.

Figure 3.10: Field profile for a finite grating with $N = 4$, $n_I = 1.25$, $n_H = 2.5$, and the defect layer index $n_d = 2.5$, with $\omega = 2\pi f = 2\pi$

Figure 3.11: The attenuated field for a finite grating with $N = 4$, $n_I = 1.25$, $n_H = 2.5$, and the defect layer index $n_d = 2.5$, with $\omega = 2\pi f = 2\pi$
3.3 From defect states to defect modes

In this section, a relation for defect states and defect modes will be given. A defect mode is the electric field with the defect frequency for a transmission experiment. So consider a finite grating (quarter wave stack) with a defect layer, 4 units of grating on the left and right of it, as illustrated in Figure 3.12 below. The thickness of the defect layer is chosen to be twice the thickness of the high index layer. The defect index is chosen to be $n_d = 2.5$ and the indices

\[
\begin{align*}
&n_0 = 1.25, \\
n_1 = 2.5, \\
n_d = 2.5
\end{align*}
\]

Figure 3.12: Transmission experiment of a finite grating. The indices of the grating are $n_1 = 1.25$, $n_2 = 2.5$ and the defect index $n_d = 2.5$ of the grating $n_1 = 1.25$, $n_2 = 2.5$. For this structure the transmittance curve is as shown below in Figure 3.13. Unlike the transmittance of a uniform grating (shown in Figure 2.4), there is a frequency with transmittance one in the middle of the band gap. So the introduction of a defect layer makes an extra resonance peak in the transmittance. For this set of parameters, the defect frequency is $\omega = 2\pi f = 2\pi$. Like the defect states, these defect modes for the transmission

\[
\begin{align*}
&n_0 = 1.25, \\
n_1 = 2.5, \\
n_d = 2.5
\end{align*}
\]

Figure 3.13: Transmittance curve for a grating with defect illustrated in Figure 3.12

experiment will also shift if the defect layer index is changed. This behaviour is illustrated in Figure 3.14 below. One must underline the fundamental difference between defect modes and defect states is that the defect modes are traveling

\[\text{A resonant frequency is a frequency having unit transmittance}\]
waves unlike the defect states which are standing waves.

![Figure 3.14: Resonant modes of the transmission experiment. The dark region in the middle is the band gap, and the white curve in it is the defect frequencies.](image)

3.3 From defect states to defect modes

Definition

The Poynting quantity describes the amount and direction of light that is propagated. For an arbitrary domain $\Omega$, the Poynting quantity can be found easily by multiplying the Helmholtz equation (2.5) with the complex conjugate of $E$ and integrate over $\Omega$ giving

$$\int_\Omega [\partial_z^2 E + \omega^2 n^2(z)E]E^* dz = \left[\partial_z E E^*\right]_{\partial \Omega} + \int_\Omega [-|\partial_z E|^2 + \omega^2 n^2(z)|E|^2]dz = 0 \quad (3.39)$$

Separating real and imaginary part leads to the condition $P(E)|_{\partial \Omega} = 0$ where $P$ is the Poynting quantity, $P(E) = \text{Im}(\partial_z E E^*)$. The condition $P(E)|_{\partial \Omega} = 0$ means that for 1D structures $P$ is independent of $z$.

Denote the defect states obtained in the previous Subsection 3.2.2 with $G^+$ for the amplified state and $G^-$ for the attenuated state. Then it is easy to see that $P(G^+) = P(G^-) = 0$ since both of them are standing states (real valued function). Below will be shown, that a complex superposition of these states will give a field with non zero Poynting quantity.
Nonzero Poynting from combined defect states

The condition $B_{N+1} = A_{N+1}$ in (3.32) is equivalent with saying that $E(z) = \cos(k_1(z - (L + Nd)))$ in the homogeneous background. Also, $B_{N+1} = -A_{N+1}$ in (3.38) is equivalent with saying that $E(z) = \sin(k_1(z - (L + Nd)))$ in the homogeneous background. This can also be seen clearly from Figures 3.11 and 3.10. If a complex superposition of these fields in the homogeneous background is taken, $E^* = \cos(k_1(z - (L + N d))) + i \sin(k_1(z - (L + N d)))$, this is precisely a right traveling wave ($e^{ik_1(z-(L+Nd))}$), with non vanishing Poynting quantity $P(E^*) = k_1$. So if a complex superposition of the amplified state $G^+$ and the attenuated state $G^-$ is taken:

$$E_m = G^+ + iG^- \quad (3.40)$$

then the Poynting quantity

$$P(E_m) = \text{Im}[\partial_z G^+ + i \partial_z G^-] (G^+ - iG^-)$$

$$= \partial_z G^- G^+ - \partial_z G^+ G^-$$

and since $P$ is independent of $z$

$$P(E_m) = P(E^*) = k_1$$

The field $E_m$ has the same frequency as the defect states $G^+$ and $G^-$, but

![Diagram showing construction of the defect mode from complex superposition of the defect states](image)

Figure 3.15: Construction of the defect mode from complex superposition of the defect states

has nonvanishing Poynting quantity. Hence this is the defect mode from the transmission experiment, which is a traveling wave.
Chapter 4

Numerical experiences using Femlab

Femlab\textsuperscript{1} is a software package built to solve physical problems numerically by using Finite Element Method. It can solve various physical phenomena, ranging from fluid dynamics, heat transfer, structural mechanics, electromagnetics, diffusion processes, etc. It is built as an interactive environment in a Graphical User Interface (GUI) to model and simulate physical and engineering problems based on partial differential equations (PDEs) - equations that are the basis for the laws of science. Femlab runs under the platform of Matlab\textsuperscript{2}, a programming language to do (quoting from their web page): numeric computation, technical graphics and visualization, and an intuitive programming language for applications in engineering and science.

The contents of this chapter is somewhat different from that of the previous chapters. The intention is to see and to investigate the usefulness, the advantages, and weaknesses, if there are any, of this commercial software package. The primary module that has been used is the Electromagnetics Module, since it is specially built to model and solve electromagnetic phenomena, which is the subject of interest. Mainly, the investigation will be on the use of different types of boundary condition that is already available in the software package.

In a nutshell, Femlab can be described as in the following diagram in Figure 4.1 below.

4.1 Reconstruction of 1D transmission experiment with defect

4.1.1 Calculating the Transmittance with Femlab

Let’s start by simulating the defect grating transmission experiment similar as in Section 3.3. This problem has a governing equation and boundary condition

\begin{footnotesize}
\textsuperscript{1}Femlab is a product of COMSOL AB, Sweden. www.femlab.com
\textsuperscript{2}Matlab is a product of The MathWorks, Inc. www.mathworks.com
\end{footnotesize}
4.1 Reconstruction of 1D transmission experiment with defect

Figure 4.1: Short description of \textit{Femlab}

as follows:

\[
\begin{align*}
\partial^2_z E(z) + \omega^2 n^2(z) E(z) &= 0, \quad z \in [-M, M] \\
\partial_n E + i\omega n_0 E &= 2i\omega n_0, \quad z = -M \\
\partial_n E + i\omega n_0 E &= 0, \quad z = M
\end{align*}
\]

(4.1)

where \(\partial_n E\) denotes the normal (outward) derivative at both boundaries, \(\partial_n E = \mp \partial_z E\) for \(z = \mp M\). In \textit{Femlab} the time dependence behaviour of the electric field is obtained via multiplying \(E(z)\) with \(e^{i\omega t}\), hence \(e^{-ik_0 z} (e^{ik_0 z})\) represents a forward (backward) traveling wave. So from here it is clear that the boundary condition at \(z = -M\) is transparent for the incoming wave (TIBC = Transparent Influx Boundary Condition) while the boundary condition at \(z = M\) represents transparency for outgoing wave from the grating structure. This type of boundary condition is standard in \textit{Femlab} and can be easily implemented.

For this transmission experiment the refractive index profile is depicted in Figure 4.2 below, and choosing the Helmholtz equation from the Model Navigator, the interval \([-M, M]\) is then meshed, with 10 elements for each layer. The mesh can be arranged such that the jump in the refractive index coincides with the grid points, and linear basis functions are used. Figure 4.2 (below) is the illustration of the discretization of the domain. Running this simulation for the frequency range \([0,2]\), with \(\Delta \omega = 2/200\), the Transmittance can be calculated and the result shows a very good agreement with the result calculated with the transfer matrix method. The transmittance curve is shown in Figure 4.3 below, and the defect mode in Figure 4.4.
4.1 Reconstruction of 1D transmission experiment with defect

Figure 4.2: Refractive index function for the transmission experiment (top), and mesh for 1D transmission experiment (below)

Figure 4.3: Transmittance curve obtained with Femlab

Figure 4.4: The defect mode calculated using Femlab
4.1 Reconstruction of 1D transmission experiment with defect

4.1.2 Finite Element discretization with linear basis functions

In this section, a brief explanation of the use of finite elements method with linear basis functions is presented. The intention is to give some background on how the method is used to solve the transmission experiment in the previous section. The basis function used is the linear basis "tent" function, and each element has the same size (uniform mesh).

The functional to be discretized is the following

\[ F(E) = Q(E) - \omega^2 P(E) + B(E) \]  \hspace{1cm} (4.2)

where

\[ Q(E) = \int_{-M}^{M} (\partial_z E)^2 dz, \quad P(E) = \int_{-M}^{M} n^2(z) E^2 dz \] \hspace{1cm} (4.3)

\[ B(E) = i \omega n_0 (E^2(M) + E^2(-M) - 2E(-M)) \]

with \( n(z) \) is the refractive index function depicted in Figure 4.2 (top). One can show easily that the critical point of \( F(E) \) will lead to system (4.1).

Let’s divide the interval \([-M, M]\) in to \( N \) subintervals with equal length, such that we have \( N + 1 \) nodal points \( z_j, j = 1, ..., N + 1 \). Then \( E(z) \) is approximated with

\[ \tilde{E}(z) = \sum_{j=1}^{N+1} c_j \varphi_j(z) \equiv \tilde{e} \cdot \tilde{\varphi} \]  \hspace{1cm} (4.4)

where the basis function \( \varphi_j \) is the linear 'tent function' at the nodal point \( z_j \) and its neighbour. To obtain a second order accurate scheme, the discretiza-

\[ \tilde{P}(\tilde{E}) = \frac{\Delta z}{3} \sum_{j=1}^{N+1} c_j \cdot (c_j^2 + c_j c_{j+1} + c_{j+1}^2), \quad c_j = n^2(z_j) \]  \hspace{1cm} (4.5)
and for $Q(E)$ and $B(E)$

$$Q(E) = \frac{1}{\Delta z} \sum_{j=1}^{N+1} e_j^2 - 2e_j e_{j+1} + e_{j+1}^2$$

$$B(E) = i\omega n_0 (e_{N+1}^2 + e_1^2 - 2e_1)$$

Looking for the critical point, the gradient of the discrete functional $\tilde{F}(E)$ should vanish

$$\nabla \tilde{F}(E) = \nabla [Q(E) - \omega^2 \tilde{P}(E) + B(E)] = 0 \quad (4.6)$$

and this leads to a matrix equation as follows

$$[M_1(\omega) - \omega^2 M_2] \tilde{e} = \tilde{v} \quad (4.7)$$

where

$$M_1(\omega) = \frac{1}{\Delta z} \begin{bmatrix} 2 + 2i\omega n_0 \Delta z & -2 & \cdots & 0 \\ -2 & 4 & -2 \\ 0 & -2 & 4 & \vdots \\ \vdots & \ddots & \ddots & \ddots \\ 0 & \cdots & 0 & -2 & 2 + 2i\omega n_0 \Delta z \end{bmatrix} \quad (4.8)$$

and

$$M_2 = \frac{\Delta z}{3} \begin{bmatrix} 2c_1 & c_1 & 0 & \cdots & 0 \\ c_1 & 2c_1 + 2c_2 & c_2 \\ 0 & c_2 & 2c_2 + 2c_3 & \vdots & \ddots \\ \vdots & \ddots & \ddots & \ddots & \cdots \\ 0 & \cdots & 2c_{N-1} + 2c_N & c_N & 0 \\ c_N & 2c_N + 2c_{N+1} & c_{N+1} & c_{N+1} \end{bmatrix} \quad (4.9)$$

and $\tilde{v} = [2i\omega n_0 \ 0 \ \cdots \ 0]^T$. This (sparse) matrix system can be solved easily using any matrix solver giving $\tilde{e}$ as the solution.
4.2 2D calculation, homogeneous domain

Starting this section, 2 dimensional problems will be considered. The polarization of light being considered is TE polarization, and let’s write it as $E_z(x, y)$, meaning that the domain is characterized by the variable $x$ and $y$ and the TE wave is pointing into the $z$ direction. The governing equation is the Helmholtz equation (1.12).

Let’s start by considering a rectangular domain $[0, 1] \times [0, 1]$ having refractive index $n = 1$. A plane wave with unit amplitude is incidence from the left boundary, denoted as boundary No.1, into the domain. The situation is illustrated below in Figure 4.6. The domain is then discretized automatically using the mesh generator giving a mesh as shown below with 120 elements on the boundary and 3088 elements in the interior.

Figure 4.6: The rectangular domain, with boundaries numbered from 1 to 4

Figure 4.7: Discretization of the domain, with 3088 elements in the interior and 120 elements along the boundary.
4.2 2D calculation, homogeneous domain

Boundary conditions

Below are three boundary conditions which are mostly used in this chapter

- Low-Reflecting (LR), in equation it is given by \( \mathbf{e}_z \cdot \mathbf{n} \times (\sqrt{\mu} \mathbf{H} + \sqrt{\varepsilon} \mathbf{E}_z) = 2\sqrt{\varepsilon} \mathbf{E}_0 \). Quoting from the module: This boundary condition is mainly intended to be used at boundaries in the model, which do not represent a physical boundary. The term low reflecting means that only a small part of the wave is reflected, and that the wave propagates through the boundary as if it was not present. The source term \( \mathbf{E}_0 \) is a source field which propagates inwards through the boundary.

- Matched boundary (MB), in equation it is given by \( \mathbf{e}_z \cdot \mathbf{n} \times (\nabla \times \mathbf{E}_z) = -ik \mathbf{E}_z = -2ik \mathbf{E}_0 \). The same as LR, this boundary conditions is intended to represent non physical boundaries. The value \( k \) in the boundary condition is determined by the user, inputed from the GUI, and it is defined as \( k = \frac{\omega}{c} \varepsilon_r \).

- Perfect Magnetic Conductor (PMC), in equation it is given by \( \mathbf{n} \times \mathbf{H} = 0 \), which sets the tangential component of the magnetic field to be zero at a boundary.

One has to note that the boundary conditions LR and MB are actually the same boundary condition. If the relation \( \mathbf{H} = -\frac{1}{\omega \varepsilon_0} \nabla \times \mathbf{E} \) is substituted in the LR boundary condition then it gives precisely the MB boundary condition.

Now the problem on the rectangular domain above is going to be solved. The frequency is \( \omega = 2\pi f = 8\pi \), for boundary No. 1 and 4, LR boundary condition is used with \( \mathbf{E}_0 \) = 1. For boundary No. 2 and 3 MB boundary condition is used. The result is as the following Figure below. And if boundary condition

![Figure 4.8: The solution given by Femlab for 3088 elements. LR for boundary 1 and 4, and MB for boundary 2 and 3.](image)

PMC is used for boundaries 2 and 3, the result shown in Figure 4.9 (left), and on the right is the result for periodic boundary condition for boundaries 2 and 3.
To see the quality of the solution of Femlab, the time average Poynting vector is calculated along boundary 1 and 4, and the result is shown in the following table below. The exact analytic time average Poynting vector is $P_{av} = \frac{1}{2} \text{Re}(E \times H) = \frac{1}{2} E_0^2 z = \frac{1}{2}$. Configuration 1 means LR on boundaries 1 and 4, MB on boundaries 2 and 3, Configuration 2 means LR on boundaries 1 and 4, PMC on boundaries 2 and 3, and Configuration 3 means LR on boundaries 1 and 4, periodic boundary condition on boundaries 2 and 3.

<table>
<thead>
<tr>
<th>No. of elements</th>
<th>Poynting Bound 1 ; Bound 4 Configuration 1</th>
<th>Poynting Bound 1 ; Bound 4 Configuration 2</th>
<th>Poynting Bound 1 ; Bound 4 Configuration 3</th>
</tr>
</thead>
<tbody>
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<td>772</td>
<td>-0.5532 ; 0.5514</td>
<td>-0.5532 ; 0.5514</td>
<td>-0.5532 ; 0.5514</td>
</tr>
<tr>
<td>3088</td>
<td>-0.5158 ; 0.5152</td>
<td>-0.5158 ; 0.5152</td>
<td>-0.5158 ; 0.5152</td>
</tr>
<tr>
<td>12352</td>
<td>-0.5041 ; 0.5039</td>
<td>-0.5041 ; 0.5039</td>
<td>-0.5041 ; 0.5039</td>
</tr>
</tbody>
</table>

The minus sign in the table above for boundary No. 1 is due to the orientation of the integration. It can be seen from the table above, that the numerical Poynting quantity approaches the exact result as the number of mesh increases.

If Low-Reflecting boundary condition is used also for boundary 2 and 3, the result is not good, and it can be seen from Figure 4.10 below. In Femlab, a plane wave incidence with an angle can also be implemented. Figure 4.11 below shows the implementation of an incoming plane wave with an angle $\frac{\pi}{4}$, and amplitude 1. All 4 boundaries uses the LR boundary condition, and the intention is to see the quality of the LR boundary condition representing a non physical boundary. It turns out that the reflection that the boundary condition gives is quite high. It can be seen from the Colorbar on the right of the figure, the maximum amplitude reached is 1.57.
Figure 4.10: The solution given by \textsc{Femlab} for 3088 elements. LR for boundary 1,2,3 and 4.

Figure 4.11: The solution given by \textsc{Femlab} for 3088 elements, of an incoming plane wave with an angle $\frac{\pi}{6}$, and amplitude 1. LR boundary condition is used for all boundaries.
4.3 Uniform Photonic Crystal

In this Section a uniform 2 dimensional Photonic Crystal will be considered. Uniform, meaning that the dielectric pillars forming the Photonic Crystal are all of the same size and material, and no defects. The Photonic Crystal is infinite into the $z$ direction, hence the dielectric function is characterized by the coordinates $(x,y)$. Consider now a transmission problem, of a Photonic Crystal having 11 pillars in the $x$ and $y$ direction. An incoming plane wave with amplitude 1 is incidence from the left, and the transmittance\(^3\) is to be calculated. The crystal is assumed to be infinite into the $y$ direction, so a good boundary condition has to be chosen. A more clear picture of the situation is illustrated in Figure 4.13 below. The distance between dielectric pillars is chosen to be $a = 1$, and the radius of the pillars is $r = \frac{1}{6}a = \frac{1}{6}$ with refractive

\[^3\text{The transmittance is defined in (4.10)}\]
index 2.5, and the refractive index of the background is 1.25. This domain is then discretized and a sample discretization with 15564 elements is shown in Figure 4.14.

\[ T = \frac{1}{L} \int_{\text{bound4}} E_z \overline{E_z} \]  

where \( L \) is the width of the domain, is calculated for the frequency range \([0, 0.6]\).

In Femlab the evaluation of this integration is simple, that is by inserting the integrand expression to the GUI, and then Femlab integrates it along the boundary. The discretization of the boundary for this integration is simply the discretization of the domain (shown is Figure 4.14) along the boundary. In Figure 4.15 below the transmittance \( T \) is plotted for the frequency range \([0, 0.6]\)^4. Figure 4.16 shows plots of the electric field profile for some frequencies.

The use of PMC and MB on boundary 2 and 3 also gives a good result for this case, and it is shown in Figure 4.17 for frequency 0.3039.

The last figure for the uniform Photonic Crystal is the use of LR on all 4 boundaries, in Figure 4.18 below. It can be seen that the result gives quite high reflections from boundary 2 and 3, and actually it does not make sense to use this boundary condition for boundary 2 and 3 since for a homogeneous domain, shown in Figure 4.10, this type of boundary condition already gives significant reflections.

\(^4\)It has to be admitted that until the time of writing this thesis, the Transmittance curve obtained with Femlab could not be verified yet. A comparation with the MIT Photonic Band Package has been done, and shows a discrepancy in the result. We will leave this for future investigation and research.
4.3 Uniform Photonic Crystal

Figure 4.15: Transmittance curve obtained from Femlab, with LR on boundaries 1 and 4 and periodic boundary condition for boundaries 2 and 3.

Figure 4.16: Electric field profile in the crystal for the frequency 0.3039 (left) and for the frequency 0.36 (right).

Figure 4.17: Electric field profile in the crystal for the frequency 0.3039. LR boundary condition is used for both cases on boundaries 1 and 4, with MB boundary condition for boundaries 2 and 3 (left) and PMC boundary condition for boundaries 2 and 3 (right).
In this Section a 2 dimensional Photonic Crystal with a point defect will be considered. A point defect, meaning that there is one dielectric pillar having a different size or material properties. The Photonic Crystal is infinite into the $z$ direction, and hence like the uniform Photonic Crystal the dielectric function is characterized by the coordinates $(x, y)$.

Consider again a transmission problem, of a Photonic Crystal with the point defect having 11 pillars in the $x$ and $y$ direction, with the point defect positioned in the middle. An incoming plane wave with amplitude 1 is incidence from the
left, and the transmittance is to be calculated. The crystal is assumed to be infinite into the $y$ direction, so a good boundary condition has to be chosen.

A more clear picture of the situation is illustrated in Figure 4.20 below. The distance between dielectric pillars is chosen to be $a = 1$, and the radius of the pillars is $r = \frac{\sqrt{2}}{6}a = \frac{1}{6}$ with refractive index 2.5, and the refractive index of the background is 1.25. The defect has a radius of twice of the pillars, $r_d = \frac{1}{3}$ and the refractive index is the same as the pillars, 2.5. This domain is then discretized and a sample discretization with 15532 elements is shown in Figure 4.21.

The existence of the point defect will act as an anomalous scatterer within the crystal. The scattering due to this defect can not be compensated by the neighbouring pillars like in the case of the uniform crystal, where the phenomena is ”almost” one dimensional. All the boundary conditions have been tested and
the only reasonable combination is to use LR on boundary 1 and 4, and periodic boundary condition on boundary 2 and 3. Other combinations of boundary conditions give more reflections. But by using this configuration of the boundary conditions, it has a drawback that the crystal is periodic in $y$ direction, thus the point defect is not really single. So implementing this, and using a mesh with 61784 elements, the transmittance is calculated for the frequency range $[0, 0.45]$. The transmittance curve is shown in Figure 4.22 below. For this experiment

![Transmittance curve](image)

Figure 4.22: Transmittance curve obtained with Femlab, with LR on boundaries 1 and 4, and periodic boundary condition for boundaries 2 and 3.

there are some interesting modes. In the transmittance curve above they are pointed with the blue and red circle. The first one to plot is the frequency pointed with the blue circle, which corresponds with frequency 0.3065. The electric field profile is on the left of Figure 4.23 and its absolute value on the right.

![Electric field profile](image)

Figure 4.23: The electric field profile in the crystal for the frequency 0.3065 (left), and its absolute value (right)

The second one is the frequency pointed with the red circle, which corresponds to frequency 0.3936. This mode is more interesting since it is localized
near the defect region, as shown in Figure 4.24. From the intensity plot it can be seen that near the defect, the amplitude increases with a factor of 12.1 compared with the input.

Figure 4.24: The electric field profile in the crystal for the frequency 0.3936 (left), and its absolute value (right)

4.5 Comments on Femlab

In this Section some general comments on Femlab will be given. It is shown in the previous sections in this Chapter, that Femlab can be used to model some electromagnetics problem. The construction of the geometry / domain of the problem is very easy, and its very similar like a CAD (Computer Aided Design) software.

Here are a few notes from the experience of using Femlab until the time of writing this thesis:

- For 1D problem (grating), the mesh growth rate, which is a ratio of an element and its neighbouring element is limited to a number between $1 < \text{growth} < 2$. If for example a grating is considered, built periodically from two layers, with one having a thickness twice of the other, then the domain can’t be discretized into a mesh with a uniform element size.

- For 2D problems, the Low-Reflecting boundary condition does not give a really small reflection, as it is shown from the homogeneous domain with oblique incidence.

- For some structures in 2D, it happens that the mesh generator fails to refine the mesh when a finer mesh is really required to get a better result.

- For parametric solving, (eg. when calculating the transmittance curve), Femlab had to solve the whole problem first for the whole parameters and stores the whole solution in the memory, and afterwards calculating the parameter of interest (eg. the transmittance). So it can not do the
4.5 Comments on Femlab

'parametric calculation' in every iteration, without having to store the solution (one step process from the GUI). This is not favourable since for 2D problems the computer often runs out of memory.

- It is not possible to insert our own boundary condition from the GUI, since there are only standard types of boundary conditions available from the GUI. Probably it can be done via the programing language\(^5\), but then Femlab would lose its strength as 'one click' solving software.

- The Femlab GUI is not connected to the Matlab command lines, meaning that the user can not invoke the Femlab GUI from writing Matlab command lines in the Matlab command window. But it is possible to insert data / information from the Matlab workspace.

- It is not possible to access the finite element matrix resulting from the discretization in Femlab.

- The numbering of the elements is not really clear, but experience tells that it always start from the boundary of the domain, then the boundary of the subdomains with different material properties, then after that the interior.

- When doing the 2D transmission problem with the iterative solver, sometimes the number of iterations until the solution converges (for a fixed frequency) is very different than for another frequency, although they are very small in difference. To overcome this we can choose as initial condition the solution from first frequency. But, this can only be done once (from the GUI), and can not be done simultaneously for solving a range of frequencies (as already explained in item number 3 above).

- To plot the results, Femlab uses patch objects to represents the triangular shape elements in space. This takes much more time to plot, and the size of the graphics is much larger (for vector format graphics such as eps, emf.) than a normal Matlab mesh or surf plotting function, since each patch contains its own information. The finer the mesh, the longer it will take to plot and the bigger the graphics size.

\(^5\)It is not known yet how to do this by the time of writing this thesis, so it needs further investigation.
Chapter 5

Conclusion

This thesis is mainly divided into two parts. The first part is about a grating with a defect layer. An infinite grating with a defect layer can have a state which is localized in the vicinity of the defect layer. The combined structure of the defect layer and the surrounding grating acts as a cavity plus a mirror, and as the resulting effect, light is trapped near the defect layer. Besides the localized state there also exists a state which is completely the opposite of localization. This state is a state which grows exponentially away from the grating, and this state is not interesting from the physics point of view. Nevertheless, for a finite grating, this state which decays towards the defect layer, plays an important role in understanding the construction of a defect mode from defect states.

In a finite grating with defect, there exist two defect states which has been called the amplified and the attenuated state. A complex superposition of these states results in the defect mode, which is the electric field with the defect frequency, for a transmission experiment. This superposition of two states having zero Poynting quantity resulted in a mode with non vanishing Poynting quantity.

In this thesis, the frequency of the defect state is calculated with a method which is a combination of variational method and transfer matrix method. The general idea is to introduce a suitable boundary condition in the interface of the defect layer, and hence the problem is localized only in the region of the defect layer. The result of this localization is a transcendental equation for the defect frequency, and further it is easy to solve with any root finding method.

The second part of the thesis is an investigation about the use of a commercial software package, Femlab. Femlab is a modeling tool with Finite Element Method in its core. It has been shown in this thesis that Femlab can be used to model some interesting electromagnetics problems. The construction of the domain of the problem is very easy, since it adopts a lot of the features of a CAD software. Types of boundary conditions available are only the standard types, so defining a more general boundary condition in Femlab (eg. for two or more frequencies) from the Graphical User Interface (GUI) is still not possible. Although probably it can be done via programing language, but then Femlab would loose its strength as a ‘one click’ solving software.
For the 1D grating case it has been shown that Femlab works perfectly. For 2-dimensional problems, the available boundary conditions still have weaknesses, and the result for the Photonic Crystal must be verified in the future with some other scientific software, or with a self-written code.
Bibliography


