Optical properties of anisotropic photonic crystals

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Optical Properties of Anisotropic Photonic Crystals

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**I DEDICATE THIS THESIS TO MY BELOVED PARENTS,
GANDHI AND PARVATHY**

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Abstract

A photonic crystal can be simply viewed as a lattice with a motif attached to each lattice point. If the re-orientation of the motif causes changes in the optical properties of the photonic crystal then the corresponding photonic crystal is an anisotropic photonic crystal. Anisotropic photonic crystals can be classified as materially and geometrically anisotropic photonic crystals. The study so far in the field of anisotropic photonic crystal was concentrated mainly in optimizing and tuning the photonic bandgaps. This thesis aims to provide a unified understanding of anisotropic photonic crystals using proper symmetrical tools. Apart from this, the thesis also examines the properties of anisotropic photonic crystals that remain unexplored.

Basic equations and operators that describe light propagation in one, two, and three dimensional anisotropic photonic crystals are formulated. The decoupling of the two independent polarizations of light in the case of a materially anisotropic photonic crystal is analyzed in detail. The symmetrical properties of the defined operator are investigated in detail using group theory, and novel concepts such as orientational group and fundamental zone of orientation are introduced. We have revealed a standard solution method based on plane wave expansion technique in order to solve the basic equations. In addition, a powerful approximation technique that leads to analytical equations to the evolution of the states in a two-dimensional photonic crystal is proposed.

Equal frequency surface of the anisotropic crystal is analyzed. We propose one-plane-wave and two-plane-waves approximation techniques for calculating equal frequency surfaces in the photonic crystals with a small spatial modulation. When the modulation is large, it is found that the equal frequency surfaces can be defined using a set of negative principal refractive indices. The properties of such anisotropic negative index states were analyzed in detail, and the tuning of negative principal refractive indices and the phenomena of accidental isotropy in the anisotropic states are reported. Equal frequency surfaces are also used in predicting conduction properties of light in the anisotropic photonic crystals. Controllable conduction devices such as tunable superprism and polarization splitters are proposed, based on two-dimensional anisotropic photonic crystals, with electrically re-orientable motif. We have shown both switching action and continuous tunability in these devices.

Apart from the conduction properties, bandgap engineering in materially anisotropic one- and two-dimensional photonic crystals is also investigated. In particular, we have shown how polarization dependent partial and full bandgaps are being created in a materially anisotropic square lattice photonic crystal. With the use of anisotropic materials and the flexibility of arranging the principal axes, the requirement on filling ratio, refractive index and anisotropy to achieve the largest bandgap is greatly alleviated.

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List of Abbreviations

PC	Photonic crystal
LC	Liquid crystal
1D	One-dimensional
2D	Two-dimensional
3D	Two-dimensional
EFS	Equal-frequency surface
<i>E</i> -polarization	Polarization for which the electric field is perpendicular to the periodic plane of a 2D PC
<i>H</i> -polarization	Polarization for which the magnetic field is perpendicular to the periodic plane of a 2D PC
<i>o</i> -polarization	Polarization in an 1D anisotropic PC for which the optical properties remain unaltered, when the optic axis of the anisotropic material is varied
<i>e</i> -polarization	Polarization in an 1D anisotropic PC for which the optical properties vary, when the optic axis of the anisotropic material is varied
IR	Irreducible representation
BZ	Brillouin zone
IBZ	Irreducible Brillouin zone
FZO	Fondamental zone of orientation
PWM	Plane wave expansion method
FDTD	Finite difference time domain
FEM	Finite element method
TMM	Transfer matrix method

List of Symbols

$\mathbf{r}$	Position vector
$\mathbf{k}$	Wavevector
$\mathbf{G}$	Reciprocal lattice vector
$\mathbf{H}$	Magnetic field
$\mathbf{E}$	Electric field
t	Time
μ_0	Permeability of the vacuum
ϵ_0	Permittivity of the vacuum
$\tilde{\epsilon}(\mathbf{r})$	Position dependant dielectric tensor
$\tilde{\epsilon}_a$	Dielectric tensor of the anisotropic material
$\tilde{\epsilon}_b$	Dielectric tensor of the isotropic material
c	Speed of light in the vacuum
λ	Free space wavelength
f	Filling ratio
f_{min}	Minimum filling ratio for existence of a band gap in a materially anisotropic photonic crystal
f_{max}	Maximum filling ratio for existence of a band gap in a materially anisotropic photonic crystal
f_c	Minimum filling ratio for existence of a band gap in an isotropic photonic crystal
a	Period of the photonic crystal
r_c	Radius of the circular motif
A_c	Area of the motif
ω	Normalized frequency (i.e., a/λ).
$\tilde{\epsilon}_m$	Average dielectric tensor [i.e., $\tilde{\epsilon}_m = \tilde{\epsilon}_b f + \tilde{\epsilon}_a (1 - f)$]
θ	Orientation of the motif

M	Differential operator that describes the dispersion of light in the photonic crystal
Ω	Eigenvalue of M
(x,y,z)	Coordinate system of the photonic crystal
(x_P,y_P,z_P)	Coordinate system of the anisotropic material (i.e., principal axes)
Q	Rotational operator from (x,y,z) to (x_P,y_P,z_P) .
α, β, γ	Eulerian angles to describe the orientations of the principal axes with respect to the coordinate system of the photonic crystal
α	Optic axes orientation in the two-dimensional periodic plane (Chap. 8); Angle between periodicity axis and optic axis in a one-dimensional photonic crystal (Sec. 7.3 of Chap. 7)
n	Refractive index
(n_x, n_y, n_z)	Principal refractive indices
r_n	n_y/n_x
Δn	$n_x - n_y$
n_o	Ordinary refractive index of the uniaxial material
n_e	Extra-ordinary refractive index of the uniaxial material
(n_1, n_2)	Pair of integers
(k_x, k_y)	Two independent axes of the two-dimensional reciprocal space
Γ	Symmetrical $\mathbf{k}$ vector with $(k_x, k_y) = (0, 0)$ in both square and hexagonal lattice
K	Symmetrical $\mathbf{k}$ vector with $(k_x, k_y) = (4/3, 0)\pi/a$ in a hexagonal lattice
M	Symmetrical $\mathbf{k}$ vector of a hexagonal lattice with $(k_x, k_y) = (1, -1/\sqrt{3})\pi/a$; Symmetrical $\mathbf{k}$ vector of a square lattice with $(k_x, k_y) = (1, -1)\pi/a$;
X	Symmetrical $\mathbf{k}$ vector of with $(k_x, k_y) = (1, 0)\pi/a$ in a square lattice
$\overline{T}$	Translational group
$\overline{G}$	Space group of the lattice
$\overline{G}_M$	Space group of the photonic crystal
$\overline{R}$	Point group of the lattice
$\overline{R}_M$	Point group of the photonic crystal

$\overline{R}_B$	Point group of the motif
$\overline{R}_\theta$	Orientational group
$\overline{G}(\mathbf{k})$	Subgroup of $\overline{G}$ consists of symmetry elements that transform $\mathbf{k}$ to $\mathbf{k}$ added with multiples of $\mathbf{G}$
$\overline{G}_M(\mathbf{k})$	Subgroup of $\overline{G}_M$ consists of symmetry elements that transform $\mathbf{k}$ to $\mathbf{k}$ added with multiples of $\mathbf{G}$
$\overline{R}(\mathbf{k})$	Subgroup of $\overline{R}$ consists of symmetry elements that transform $\mathbf{k}$ to $\mathbf{k}$ added with multiples of $\mathbf{G}$
$\overline{R}_M(\mathbf{k})$	Subgroup of $\overline{R}_M$ consists of symmetry elements that transform $\mathbf{k}$ to $\mathbf{k}$ added with multiples of $\mathbf{G}$
r	Number of elements in $\overline{R}$
r_m	Number of elements in $\overline{R}_M$
$r_m(\mathbf{k})$	Number of elements in $\overline{R}_M(\mathbf{k})$
g	Number of elements in $\overline{G}$
g_m	Number of elements in $\overline{G}_M$
$g_m(\mathbf{k})$	Number of elements in $\overline{G}_M(\mathbf{k})$
$\tilde{\kappa}(\mathbf{G})$	General Fourier transform coefficient of the inverse dielectric tensor
$\tilde{\kappa}_H(\mathbf{G})$	Fourier transform coefficient of the inverse dielectric tensor for H -polarization
$\kappa_E(\mathbf{G})$	Fourier transform coefficient of the inverse dielectric constant for E -polarization
m_{is}	Integer label of a state in the absence of refractive index modulation and material anisotropy [Chap. 3]
m_{anis}	Integer label of a state in the absence of refractive index modulation and however with a presence of material anisotropy [Chap. 3]
ϵ_{is}	Homogenous dielectric constant in the absence of refractive index modulation and anisotropy
$m_{\mathbf{k}}$	Integer label of a state in the absence of refractive index modulation and with a homogenous dielectric constant ϵ_{is} . [Chap. 5]

$n(m_{\mathbf{k}})$	Degeneracy of the state with label $m_{\mathbf{k}}$.
$(\mathbf{b}_1, \mathbf{b}_2)$	primitive real lattice vectors of a two-dimensional lattice
$\alpha_{\mathbf{k}}$	Angle between $\mathbf{k}$ and $\mathbf{k}+\mathbf{G}$.
$\alpha_{\mathbf{b}_i}$	Angle between k_x - axis of the reciprocal space and $\mathbf{b}_i$.
$p_{\mathbf{k}}, q$	Factors of $m_{\mathbf{k}}$
$h_{\mathbf{k}}$	$p_{\mathbf{k}}$ for hexagonal lattice
θ_i	Incident angle
θ_0	Propagation angle
θ_s	Polarization splitting angle

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Chapter 1

Introduction

This chapter presents an overview of the entire thesis. Firstly, we introduce the concept of the photonic crystal (PC) and its applications. Then, anisotropic PCs are defined and their applications are highlighted. Finally, the organization and the contributions of the thesis are presented.

1.1 Photonic Crystal

1.1.1 Introduction

PC is a class of materials with a periodic dielectric modulation that controls the propagations of light (photon).

Fig. 1.1 PCs in one, two and three dimension. The first 1D structure is a multilayer structure, which could be fabricated using the conventional crystal growth techniques [1-3]. The other two 1D structures, can be fabricated employing a mask similar to a fabrication of integrated electronic chips [4-6]. The first 2D structure resembles a

structure that is very close to an ideal 2D PC as the ratio of cylinder diameter to the depth is very small. The other 2D structures are in the slab form [7]. The first 3D PC is a structure fabricated from the self-assembly method [8-9]. The second 3D structure is a woodpile structure [10-11] while the third is an auto-cloned structure [12]. Comprehensive details on fabrication of 2D and 3D PCs can be found in Ref. 5, 6 and 13.

Fig. 1.2 Natural PCs – Photonic band gap (selective reflection of visible wavelength) is used as a coloring mechanism in biological/natural objects. (a) Peacock feather [14-16] (b) Butterfly wing [17-18] (c) Bristle of a polychete worm [18]

Such control is analogous to the control of electron propagations in a solid crystal which exhibits a periodic modulation in the electrical potential. The periodic dielectric modulation in the PC can be one-, two- or three-dimensional (1D, 2D, or 3D) and the corresponding structure is consistently named as 1D, 2D and 3D PC. Examples of artificially made PCs are shown in Figure 1.1 [1-13]. Meanwhile, Figure

1.2 shows several naturally existing PCs [14-18]. In these natural structures, a periodic variation in the dielectric property exists. This can be easily observed from Fig. 1.2 where we can see structures with repeating air hole. Depending on the period of this repetition, a selective wavelength of the visible light is reflected. This naturally gives the color for the structures in Fig. 1.2.

The history of a 1D PC, can be traced back to year 1887, when Lord Rayleigh [19] firstly studied a multilayer media. He found light with frequencies that fall within the 1D photonic band gap (incident angle dependent) cannot propagate through the multilayer media. In 1977, Yeh [20] showed that light can be localized within a defective 1D PC. Exploration of PCs with higher dimension started in 1979 where Othaka [21-22] introduced the vector-spherical wave expansion method to calculate the dispersion of a 3D PC made of dielectric spheres with a large dielectric modulation. However, active research pertaining to 2D and 3D PCs was only started after the year 1987. In this year, two milestone papers by Yablonavitch [23] and John [24] proposed the idea of Anderson localization and inhibition of spontaneous emission based on band gaps in the PC. Subsequently, many papers proposing structures with complete 2D [25-35] and 3D [36-44] photonic band gaps were published.

The action of a PC, prohibiting photons from propagating via the photonic band gap identifies PC as an insulator for photons. During the years 1996-1998, the behavior of light propagation with frequencies outside the photonic band gap had been studied and the propagation (i.e., conduction) was found to be totally different from that of photons in bulk homogenous media [45-46]. Snell's law fails to explain

the conduction behavior in PCs, but Kosaka *et al.*, [46] successfully explained the conduction of light in PCs using the concept of an equal frequency surface (EFS).

1.1.2 Applications

Thus far, PC has revolutionized the entire field of optics, enabling enormous applications in the field. Though the range of applications continues to expand since the work of Yablonavitch [23] and John [24], a partial list covering the important applications would be:

- Waveguides [47-50] – By introducing a line defect in the PC, light that falls within the frequency of photonic band gap can be guided through the defect line. High efficiency and low loss waveguides with sharp bends can be created.
- High quality factor microcavities and ultra small lasers [51-54] – By introducing a point defect in the PC, a cavity can be constructed. The quality factor of the cavity can be up to tens of thousands. A laser based on PC microcavities can have a very effective suppression of the spontaneous emission and this consequently minimizes the threshold voltage of the laser.
- Holy fibers [55-57] – This is a fiber with air core and 2D PC cladding layer. Holy fiber is a revolution in the fiber technology as light is guided in air layer which was classically thought to be impossible. It offers several advantages over the conventional fiber such as removal of chromatic dispersions.
- Light emitting diodes (LEDs) with high extraction efficiency [58-60] – The extraction efficiency of a conventional LED is bounded by the total internal reflection (TIR) at the device-air interface. Introduction of a PC in the LED

structure, engineers the light cone and subsequently overcomes the TIR problem.

Fig. 1.3 Applications of PCs (a) Waveguide with a sharp bend [6,50] (b) High quality factor nanocavity [53] (c) Wide angle splitter [49] (d) Holy Fiber [55] (e) Channel drop filter [82] (f) Superprism effect [61] (g) Polarization splitter [64-65] (h) Negative refraction in a PC [67], and (i) Flat lens [70].

- Superprism [45-46,61-64] – An action of prism is to spatially separate light with different wavelengths. Superprism is a PC structure that could spatially separate the wavelengths 50-500 times more effectively compared to an ordinary prism.
- Polarization splitters [64-65] – 2D PCs can be used to split the two independent polarizations of light with a large separation angle. In this application; normally each polarization will experience a different sign of refraction (i.e., positive and negative) and therefore in principle the separation angle can be more than 90° .
- Flat lens with a very high resolution [66-70] – PC exhibits negative refraction [66-75]. This negative refraction can be used to make a flat lens with a capability of amplifying the evanescent fields. Such a lens shows an ultra-high resolution that is beyond the classical diffraction limit.
- Supercolimators [76-78], beam splitters [78], beam-shapers [79], interferometers [80], planar antennas [81], channel add drop filters [82] and so on.

1.2 Anisotropic Photonic Crystals

A PC may be simply viewed as a lattice with a motif attached to each lattice point. If the re-orientation of the motif causes the symmetry elements of the PC to change, then the corresponding PC can be defined as an anisotropic PC, as opposed to an isotropic PC where the orientation of the motif is irrelevant to the symmetry of the PC. A PC made of only isotropic media with a circular motif in a 2D lattice is an example of a 2D isotropic PC.

Anisotropic PCs can be geometrically anisotropic or materially anisotropic. Figure 1.4(a) shows the geometry of a 2D hexagonal lattice PC with a square motif. The orientation of the square motif with respect to the underlying lattice plays a crucial role in determining the optical properties of the 2D PC. In Fig. 1.4(b), instead of a square motif, we have a circular motif for which the corresponding orientation is irrelevant. If all materials are isotropic, then the geometries in Figs. 1.4(a) and (b) represent examples of a geometrically anisotropic and isotropic PCs respectively. In the presence of an anisotropic material, the optical properties of a PC will vary in accordance to the orientation of the anisotropic material (i.e., the orientation of the principal axes with respect to the lattice) and therefore the corresponding PC is defined as a materially anisotropic PC. A PC with a geometry in Fig. 1.4(b) constitutes a materially anisotropic PC, if either the matrix or circular cylinders is an anisotropic medium. On the other hand, in the presence of an anisotropic material, a PC with a geometry as shown in Fig. 1.4(a) has a mixed anisotropy (i.e., both geometrical and material' anisotropy exist).

Fig. 1.4 Examples of geometries of a 2D hexagonal lattice PC. (a) square motif (b) circular motif

Geometrically anisotropic PCs have been widely used in exploring 2D and 3D photonic band gaps [10-12, 26, 29-35, 83-84]. Particularly in 2D PCs which are important in realizing integrated optical chips, motifs with various geometry have been used to improve the photonic band gap [29-34, 83]. On the other hand, materially anisotropic PCs, are found to be extremely useful in realizing tunable photonic crystals [85-99]. Liquid crystal (LC), a well-known anisotropic medium [100-101] with tunable optical properties, was firstly proposed by Kurt and John [96] to infiltrate the void regions of a 3D inverted opal PC [Figure 1.5(a)]. The first LC infiltrated 2D PC was shown by S. W. Leonard *et al.* [91]. They infiltrated LC in a 2D PC made of macroporous silicon [Figure 1.5(b)]. Apart from LC, other anisotropic media such as strontium barium niobate, lithium niobate, and tellurium have been used to investigate materially anisotropic PCs [102-107]. Detailed reviews on the applications of the anisotropic PCs are presented in Chapter 7 and Chapter 8 of the thesis.

Fig. 1.5 Examples of materially anisotropic PCs – (a) A LC (yellow) infiltrated 3D PC (blue) [96] (b) A 2D PC made of macroporous silicon. The holes are infiltrated with LCs [91].

1.3 Organization and Contributions

This thesis presents the theory (Chap. 2-5), characteristics (Chap. 6) and applications (Chap. 7 – 8) of an anisotropic PC. The basic Maxwell's equations and the operators are formulated in Chapter 2. Chapter 3 develops important symmetrical tools for a general anisotropic PC based on the operator defined in Chap. 2 using the language of symmetry (i.e., group theory). A review of a standard numerical method to solve the equations presented in Chap. 2 appears in Chapter 4. Chapter 5 is meant for the same task as in Chap. 4, but the chapter introduces an approximation technique that can be applied for any 2D PC (including isotropic PCs). Chapter 6 presents the details of an equal frequency surface and introduces the concept of negative principal refractive indices in anisotropic PC. Finally, the applications of anisotropic PCs are given in Chapter 7 and 8.

Most of the chapters in this thesis are organized to be self-contained and normally an introductory knowledge in linear algebra [108-109] and electromagnetic theory that includes optics of an anisotropic media [110-111] will be sufficient in order to grasp the materials presented. Additional proofs, theories and tables that support, however disturb the main flow, are separated from the chapters and presented in Appendix. Understanding of materials presented in Chapter 2 requires the reader to have knowledge in group theory and representations. Though many references are available for group theory, a fairly relevant and easy to read references include Ref. 112-116.

The presentations of the original contributions of the thesis are divided into six chapters. The details of the contribution are highlighted in the introduction

section of each chapter. Nevertheless, a very short summary of original contributions of the chapters is highlighted below:

1.3.1 Chapter 2

- Analyses of polarization decoupling in a 2D PC made of anisotropic materials
- Formulation of eigen-equations in a 1D PC with an anisotropic material. In particular, it is shown if the material is uniaxial, then regardless of optic axis orientations, we can always decouple the polarizations into ordinary and extraordinary polarizations.

1.3.2 Chapter 3

- Description of an irreducible Brillouin zone (IBZ) in an anisotropic PC using coset decompositions.
- Formulation of the orientational group and fundamental zone of orientations to describe the motif orientations in an anisotropic PC.
- A system for labeling states in anisotropic PC in the absence of a spatial modulation.
- Analyses of symmetry representation in anisotropic PC, in the absence and the presence of a spatial modulation and material's anisotropy.

1.3.3 Chapter 5

- Classification of degenerate states in the absence of spatial modulation.

- Approximation technique to describe the states in the presence of modulation and material anisotropy. Analytical equations will be shown.

1.2.4 Chapter 6

- One plane wave and two plane waves approximation techniques for calculation of equal frequency surfaces.
- States with negative principal refractive indices and the accidental isotropy in an anisotropic PC of large spatial modulation. Tunability of the negative principal refractive indices.

1.3.5 Chapter 7

- Band gap engineering in a 2D PC utilizing anisotropic materials. Opening of band gap for low refractive index materials and for a wide range of filling ratios.
- Tunable band gaps in 1D anisotropic PCs infiltrated with LC and Pockel materials.

1.3.6 Chapter 8

- Demonstration of switching effect of superprism and polarization in a 2D anisotropic PC.
- Demonstration of continuous tunability of conduction in a 2D anisotropic PC.

Chapter 2

Maxwell's Equations

2.1 Introduction

Maxwell equations are considered as the most fundamental formulation of electromagnetics [110-111]. In this chapter, we review Maxwell's equations in the context of a PC. The second section of the chapter presents general equations to model a PC with arbitrary dimension made of two materials of general anisotropy. In Sections 2.3 and 2.4, we discuss polarization decoupling and the corresponding wave equations for 2D and 1D structures respectively.

2.2 General Equations

In the absence of electric current and free charges, Maxwell's equations for a non-magnetic media can be written as [110-111],

$$\nabla \times \mathbf{E}(\mathbf{r}, t) = -\mu_o \frac{\partial \mathbf{H}(\mathbf{r}, t)}{\partial t}, \quad [2.1]$$

$$\nabla \times \mathbf{H}(\mathbf{r}, t) = \epsilon_o \tilde{\epsilon}(\mathbf{r}) \frac{\partial \mathbf{E}(\mathbf{r}, t)}{\partial t}, \quad [2.2]$$

where $\mathbf{r}$ is the position vector, $\tilde{\epsilon}(\mathbf{r})$ is the position dependent dielectric tensor, ϵ_o and μ_o are permittivity and permeability of the vacuum respectively, while $\mathbf{E}$ and $\mathbf{H}$ respectively represent the electric field and the magnetic field vectors. By eliminating either $\mathbf{E}$ or $\mathbf{H}$ in these equations, we can obtain the wave equation for a light propagating in the inhomogeneous medium. For example, elimination of $\mathbf{E}$ leads to

$$\nabla \times \frac{1}{\tilde{\epsilon}(\mathbf{r})} \nabla \times \mathbf{H}(\mathbf{r}, t) + \frac{1}{c^2} \frac{\partial^2 \mathbf{H}(\mathbf{r}, t)}{\partial t^2} = 0 \quad [2.3]$$

where c is the speed of light. Assuming a harmonic time dependence to the field with an angular frequency in the form of $c\sqrt{\Omega}$, we have,

$$\mathbf{H}(\mathbf{r}, t) = \mathbf{H}(\mathbf{r}) e^{-jc\sqrt{\Omega}t} . \quad [2.4]$$

Substituting Eqn. 2.4 into Eqn. 2.3, we obtain

$$\nabla \times \frac{1}{\tilde{\epsilon}(\mathbf{r})} \nabla \times \mathbf{H}(\mathbf{r}) = \Omega \mathbf{H}(\mathbf{r}) . \quad [2.5]$$

This is an eigen-equation with the operator, $M = \nabla \times \{1/\tilde{\epsilon}(\mathbf{r})\} \nabla \times$, and eigenvalue, Ω .

In order to model a PC with the unit cell defined by two materials of dielectric tensors $\tilde{\epsilon}_a$ and $\tilde{\epsilon}_b$, we assume $\tilde{\epsilon}(\mathbf{r})$ as,

$$\tilde{\epsilon}(\mathbf{r}) = \begin{pmatrix} \epsilon_{11}(\mathbf{r}) & \epsilon_{12}(\mathbf{r}) & \epsilon_{13}(\mathbf{r}) \\ \epsilon_{21}(\mathbf{r}) & \epsilon_{22}(\mathbf{r}) & \epsilon_{23}(\mathbf{r}) \\ \epsilon_{31}(\mathbf{r}) & \epsilon_{32}(\mathbf{r}) & \epsilon_{33}(\mathbf{r}) \end{pmatrix}, \quad [2.6]$$

where,

$$\epsilon_{ij}(\mathbf{r}) = \epsilon_{bij} + (\epsilon_{aij} - \epsilon_{bij}) p(\mathbf{r}) . \quad [2.7]$$

The subscript in Eqn. 2.7 denotes the tensor element of $\tilde{\epsilon}_a$ and $\tilde{\epsilon}_b$ with $i, j = 1, 2$ or 3

and the vector $\mathbf{r}$ is restricted to be pointing positions within the unit cell geometry.

The function, $p(\mathbf{r})$, becomes one if the $\mathbf{r}$ lies within the portion of unit cell, filled up by the material with the dielectric tensor $\tilde{\epsilon}_a$ and zero otherwise. If the medium is

isotropic, then the dielectric tensor ($\tilde{\epsilon}_a$ or $\tilde{\epsilon}_b$) can be written as a constant (square of

refractive index) multiplied by an identity matrix. If the medium is anisotropic then,

the dielectric tensor must take the orientation of the anisotropic material with respect

to the coordinate system of the PC into account.

For simplicity, among the two materials we assume, one is an isotropic material and in fact this is a typical (and practical) assumption[♥]. Specifically, we assume the material with the dielectric tensor $\tilde{\epsilon}_a$ and $\tilde{\epsilon}_b$ to be anisotropic and isotropic respectively. In the principal coordinate system of the anisotropic material, the dielectric tensor is given by $\tilde{\epsilon}_{ap} = \text{diag}(n_x^2, n_y^2, n_z^2)$, where n_x , n_y and n_z are the principal refractive indices. The coordinate system of the PC and the principal coordinate system of the anisotropic material are defined by (x, y, z) and (x_p, y_p, z_p) respectively. The general orientation of these principal axes is such that none of the principal axes is in the x - y , x - z , or y - z planes of the PC. Such an orientation can easily be represented with Eulerian angles [117]. The rotation operator Q from PC axes to principal axes can be written as $Q = R_z(\gamma)R_y(\beta)R_x(\alpha)$ [♦], where $R_p(\theta)$ is a 3 by 3 rotation matrix for planar rotation around the p -axis with a clock wise rotation angle of θ . The operator Q can be expressed as

$$Q = \begin{pmatrix} \cos \gamma \cos \beta \cos \alpha - \sin \gamma \sin \alpha & -\cos \gamma \cos \beta \sin \alpha - \sin \gamma \cos \alpha & -\cos \gamma \sin \beta \\ \sin \gamma \cos \beta \cos \alpha + \cos \gamma \sin \alpha & -\sin \gamma \cos \beta \sin \alpha + \cos \gamma \cos \alpha & -\sin \gamma \sin \beta \\ \sin \beta \cos \alpha & -\sin \beta \sin \alpha & \cos \beta \end{pmatrix}. [2.8]$$

Every row of Q is a unit vector representing the orientation of one of the principal axes relative to the PC-axes. For instance, the first row of Q is the unit vector along principal axis x_p . For general values of γ , β , and α , none of the elements of Q is zero, which means that none of the principal axes is in x - y , x - z , or y - z planes of the PC. The dielectric tensor of the anisotropic material in the principal axes, $\tilde{\epsilon}_{ap}$ can be

[♥] See the examples (and the cited references) of materially anisotropic PCs in Chap. 1.

[♦] This is a rotation using Eulerian angles. The first and the last operations of Q are rotations around the same axis. See Ref. 117 for more details.

expressed relative to the PC axes, $\tilde{\epsilon}_a$ by mean of an operation $\tilde{\epsilon}_a = Q^T \tilde{\epsilon}_{ap} Q$, where Q^T is the transposed matrix (also the inverse) of Q . This operation produces a symmetric tensor, which will not be represented here, because of the long expressions for the tensor elements. However, certain elements of $\tilde{\epsilon}_a$ will be given in later part of the chapter to illustrate the discussion.

Within this framework, the model for a PC with an arbitrary dimension made of two materials of general anisotropy is complete. Eqn. 2.3 (or Eqn 2.5) for a general $\tilde{\epsilon}(\mathbf{r})$ is basically a set of three coupled differential equations. These coupled equation can be decoupled into two equations corresponding to two independent polarizations of light in some cases. In the subsequent sections, we will analyze the decoupling of polarizations in a 2D and 1D structure.

2.3 Polarization decoupling in 2D PCs

Assuming the periodic dielectric modulation is in the x - and y -directions only, $\mathbf{r}$ can be written as $\mathbf{r} = x\hat{\mathbf{x}} + y\hat{\mathbf{y}}$. Hence for an in-plane propagation^{*}, the electromagnetic fields are spatially uniform along the z -direction. Writing $\mathbf{H}(\mathbf{r}, t) = H_x(\mathbf{r}, t)\hat{\mathbf{x}} + H_y(\mathbf{r}, t)\hat{\mathbf{y}} + H_z(\mathbf{r}, t)\hat{\mathbf{z}}$ and $\mathbf{E}(\mathbf{r}, t) = E_x(\mathbf{r}, t)\hat{\mathbf{x}} + E_y(\mathbf{r}, t)\hat{\mathbf{y}} + E_z(\mathbf{r}, t)\hat{\mathbf{z}}$, the Maxwell's equations (Eqn. 2.1-2.2) for the in-plane propagation in a 2D structure become,

$$\frac{\partial E_z}{\partial y} = -\mu_o \frac{\partial H_x}{\partial t}, \quad [2.9.1]$$

^{*} ALL discussions concerning 2D PCs in this thesis are limited to in-plane propagations only.

$$\frac{\partial E_z}{\partial x} = \mu_o \frac{\partial H_y}{\partial t}, \quad [2.9.2]$$

$$\frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} = -\mu_o \frac{\partial H_z}{\partial t}, \quad [2.9.3]$$

$$\frac{\partial H_z}{\partial y} = \epsilon_o \epsilon_{11}(\mathbf{r}) \frac{\partial E_x}{\partial t} + \epsilon_o \epsilon_{12}(\mathbf{r}) \frac{\partial E_y}{\partial t} + \epsilon_o \epsilon_{13}(\mathbf{r}) \frac{\partial E_z}{\partial t}, \quad [2.9.4]$$

$$\frac{\partial H_z}{\partial x} = -\epsilon_o \epsilon_{21}(\mathbf{r}) \frac{\partial E_x}{\partial t} - \epsilon_o \epsilon_{22}(\mathbf{r}) \frac{\partial E_y}{\partial t} - \epsilon_o \epsilon_{23}(\mathbf{r}) \frac{\partial E_z}{\partial t}, \quad [2.9.5]$$

$$\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} = \epsilon_o \epsilon_{31}(\mathbf{r}) \frac{\partial E_x}{\partial t} + \epsilon_o \epsilon_{32}(\mathbf{r}) \frac{\partial E_y}{\partial t} + \epsilon_o \epsilon_{33}(\mathbf{r}) \frac{\partial E_z}{\partial t}, \quad [2.9.6]$$

where the field notations are simplified as $A_i(\mathbf{r}, t) = A_i$.

As we can see from Eqn. 2.9.1-2.9.6, all field terms are coupled. Furthermore, classifications of E -polarization, corresponding to the set (H_x, H_y, E_z) , and H -polarization, corresponding to (E_x, E_y, H_z) , are only possible if the tensor elements $\epsilon_{13}(\mathbf{r})$, $\epsilon_{31}(\mathbf{r})$, $\epsilon_{23}(\mathbf{r})$ and $\epsilon_{32}(\mathbf{r})$ are zero. As can be seen from Eqn. 2.7, this requires the elements ϵ_{a13} , ϵ_{a31} , ϵ_{a23} and ϵ_{a32} to be zero. The expressions for these elements can be calculated by coordinate transformation in terms of the Eulerian angles as mentioned earlier. The elements $\epsilon_{a13} = \epsilon_{a31}$ and $\epsilon_{a23} = \epsilon_{a32}$ can be written as follows:

$$\epsilon_{a13} = \sin \beta \{ \cos \beta \cos \alpha (n_z^2 - n_x^2 \cos^2 \gamma - n_y^2 \sin^2 \gamma) + (n_x^2 - n_y^2) \sin \gamma \cos \gamma \sin \alpha \} \quad [2.10.1]$$

$$\epsilon_{a23} = \sin \beta \{ \cos \beta \cos \alpha (n_x^2 \cos^2 \gamma + n_y^2 \sin^2 \gamma - n_z^2) + (n_x^2 - n_y^2) \sin \gamma \cos \gamma \cos \alpha \}. \quad [2.10.2]$$

For isotropic material with $n_x = n_y = n_z$, obviously these components are zero regardless of γ , β , and α . Generally, for a 2D PC with an anisotropic material, the E - and H -polarizations can be decoupled as long as one of the principal axes is perpendicular to the periodic plane of the 2D PC (i.e. parallel to z). This is obvious

from Eqn. 2.10.1 and 2.10.2, where the tensor elements are zero as long as $\beta = 0$, which implies that the z_p axis coincides with z regardless the values of γ and α . The corresponding $\tilde{\epsilon}_a$ tensor, when $\beta = 0$, is given by,

$$\tilde{\epsilon}_a = \begin{pmatrix} n_x^2 \cos^2 \alpha' + n_y^2 \sin^2 \alpha' & (n_y^2 - n_x^2) \cos \alpha' \sin \alpha' & 0 \\ (n_y^2 - n_x^2) \cos \alpha' \sin \alpha' & n_x^2 \sin^2 \alpha' + n_y^2 \cos^2 \alpha' & 0 \\ 0 & 0 & n_z^2 \end{pmatrix}. \quad [2.11]$$

where $\alpha' = \gamma + \alpha$. When $\beta = 90^\circ$, which means that the z_p axis is in the x - y plane of the PC, the polarization decoupling requires either x_p or y_p to be parallel to z (i.e., $\gamma = 0$ or 90°). As can be seen from Eqn. 2.10.1 and 2.10.2, in a PC made of biaxial material ($n_x \neq n_y \neq n_z$), when $\gamma = 0$ or 90° , the elements ϵ_{a13} , ϵ_{a31} , ϵ_{a23} , and ϵ_{a32} are zero. The corresponding $\tilde{\epsilon}_a$ tensor for $\beta = 90^\circ$ and $\gamma = 0$ is as follows:

$$\tilde{\epsilon}_a = \begin{pmatrix} n_y^2 \sin^2 \alpha + n_z^2 \cos^2 \alpha & (n_y^2 - n_z^2) \cos \alpha \sin \alpha & 0 \\ (n_y^2 - n_z^2) \cos \alpha \sin \alpha & n_y^2 \cos^2 \alpha + n_z^2 \sin^2 \alpha & 0 \\ 0 & 0 & n_x^2 \end{pmatrix}, \quad [2.12]$$

and when $\gamma = 90^\circ$, the $\tilde{\epsilon}_a$ tensor is similar to the one of Eqn. 2.12, however, it requires interchanging of n_y and n_x . In a PC made of uniaxial material, we have $n_x = n_y = n_o \neq n_z = n_e$, and the principal axis along the n_e axis (z_p) is called the optic axis. The other two principal axes, x_p and y_p , can be chosen arbitrarily in the plane perpendicular to z_p . Thus the tensor elements in Eqn. 2.10.1 and 2.10.2, will vanish when $\beta = 90^\circ$, regardless of the value of γ in a PC made of uniaxial material, allowing decoupling of the E - and H -polarizations. The $\tilde{\epsilon}_a$ tensor for this case is similar to the one in Eqn. 2.12 with $n_x = n_y = n_o$ and $n_z = n_e$.

Assuming a configuration of principal axes, in which the polarizations can be decoupled, one can eliminate E_z from Eqn. 2.9.1, 2.9.2 and 2.9.6. Then assuming an

harmonic time dependence [Eqn. 2.4], we can write the following eigen equation for the E -polarization:

$$\nabla_{xy} \times \frac{1}{\epsilon_E(\mathbf{r})} \nabla_{xy} \times \{H_x(\mathbf{r})\hat{\mathbf{x}} + H_y(\mathbf{r})\hat{\mathbf{y}}\} = \Omega \{H_x(\mathbf{r})\hat{\mathbf{x}} + H_y(\mathbf{r})\hat{\mathbf{y}}\} \quad [2.13]$$

where, $\epsilon_E(\mathbf{r}) = \epsilon_{33}(\mathbf{r})$ and ∇_{xy} is a vector operator defined as $\hat{\mathbf{x}}(\partial/\partial x) + \hat{\mathbf{y}}(\partial/\partial y)$. The dielectric property of E -polarization is determined by $\epsilon_{33}(\mathbf{r})$. Thus for a given tensor orientation of the anisotropic material, the E -polarization finds itself in an isotropic configuration, i.e. it becomes independent of principal axes orientation in the 2D periodic plane.

By eliminating E_x and E_y from Eqn. 2.9.3, 2.9.4 and 2.9.5 and using Eqn. 2.4, the other group containing (E_x, E_y, H_z) for the H -polarization, can be simplified to,

$$\nabla_{xy} \times \frac{1}{\tilde{\epsilon}_H(\mathbf{r})} \nabla_{xy} \times H_z(\mathbf{r})\hat{\mathbf{z}} = \Omega H_z(\mathbf{r})\hat{\mathbf{z}}, \quad [2.14]$$

where $\tilde{\epsilon}_H(\mathbf{r})$ is given by

$$\tilde{\epsilon}_H(\mathbf{r}) = \begin{pmatrix} \epsilon_{11}(\mathbf{r}) & \epsilon_{12}(\mathbf{r}) \\ \epsilon_{21}(\mathbf{r}) & \epsilon_{22}(\mathbf{r}) \end{pmatrix}, \quad [2.15]$$

in which the elements can be evaluated from Eqn. 2.7, 2.11 and 2.12. For uniaxial material and $\beta = 0$, it follows from Eqn. 2.11 that $\epsilon_{11}(\mathbf{r}) = \epsilon_{22}(\mathbf{r})$ and $\epsilon_{12}(\mathbf{r}) = \epsilon_{21}(\mathbf{r}) = 0$. In this case, $\tilde{\epsilon}_H(\mathbf{r})$ is an isotropic tensor and generates an isotropic dielectric configuration. However, with $\beta = 90^\circ$, it can be seen from Eqn. 2.12 that none of the tensor elements in Eqn. 2.15 is zero, and they depend on the orientation of the optic axis relative to the periodic plane, α . Hence, for the H -polarization with $\beta = 90^\circ$, one obtains an anisotropic dielectric configuration. On the other hand, PCs made of biaxial materials always generate anisotropic configurations for both $\beta = 0$ and $\beta =$

90°. This can be concluded from the corresponding tensor expressions $\tilde{\epsilon}_a$ in Eqn. 2.11 and 2.12.

2.4 Polarization decoupling in 1D PCs

Assuming the periodic dielectric modulation is in the x direction only and restricting the light propagation direction along the periodicity direction (i.e., on-axis propagation)*, the derivatives with respect to y in Eqn 2.9.1-2.9.6 are zero and the vector $\mathbf{r}$ can be replaced with x . Following similar analyses as for the 2D structure it is found that decoupling of (H_x, H_y, E_z) and (E_x, E_y, H_z) requires one of the principal axes of the anisotropic material to be perpendicular to the periodicity axis (i.e., x -axis). If the anisotropic material is uniaxial, this condition is automatically satisfied. This is clarified using Figure 2.1 where the planes perpendicular to x -axis and the optic axis (assumed as z_p -axis) are shown. As the material is uniaxial, the two principal axes perpendicular to optic axis can be arbitrarily chosen in the plane perpendicular to the optic axis. Therefore, one of the principal axes of the uniaxial material can be chosen to be the intersection line (i.e., z axis) between the planes (x_p-y_p) and $(y-z)$, which is essentially perpendicular to x -axis.

Assuming polarizations can be decoupled, the differential equations for the set (H_x, H_y, E_z) are as follows:

$$\frac{\partial H_x}{\partial t} = 0 \quad [2.16.1]$$

$$\frac{\partial E_z}{\partial x} = \mu_o \frac{\partial H_y}{\partial t} \quad [2.16.2]$$

* ALL discussions concerning 1D PCs in this thesis are limited to on-axis propagations only.

$$\frac{\partial H_y}{\partial x} = \epsilon_o \epsilon_{33}(x) \frac{\partial E_z}{\partial t} \quad [2.16.3]$$

These equations can be reduced to a wave equation,

$$\left\{ \frac{\partial}{\partial x} \frac{1}{\epsilon_o(x)} \frac{\partial}{\partial x} \right\} H_y + \Omega H_y = 0, \quad [2.17]$$

where $\epsilon_o(x) = \epsilon_{33}(x)$. Note that in this set, we have both magnetic field and electric field perpendicular to the propagation axis (x -axis) and further $\epsilon_o(x)$ is independent of principal axes orientation [Eqn. 2.7, 2.11 and 2.12], therefore the polarization corresponding to the set (H_x, H_y, E_z) is termed as an ordinary polarization (o -polarization). Caution also has to be placed on the orientations of the fields when the material is uniaxial. For example, the electric field in this polarization lies along the z -axis (i.e., the intersection line between the planes x_p - y_p and y - z), and therefore rotates as optic axis (z_p -axis) rotates.

Fig. 2.1 – Two different orientations of the principal axes of the anisotropic material with respect to the coordinate system of the 1D PC.

For the set (E_x, E_y, H_z) , the differential equations are as follows:

$$\frac{\partial E_y}{\partial x} = -\mu_o \frac{\partial H_z}{\partial t} \quad [2.18.1]$$

$$\varepsilon_o \varepsilon_{11}(x) \frac{\partial E_x}{\partial t} + \varepsilon_o \varepsilon_{12}(x) \frac{\partial E_y}{\partial t} = 0 \quad [2.18.2]$$

$$\frac{\partial H_z}{\partial x} = -\varepsilon_o \varepsilon_{21}(x) \frac{\partial E_x}{\partial t} - \varepsilon_o \varepsilon_{22}(x) \frac{\partial E_y}{\partial t} \quad [2.18.3]$$

These equations can be reduced to

$$\left\{ \frac{\partial}{\partial x} \left(\varepsilon_{22}(x) - \frac{\varepsilon_{12}^2(x)}{\varepsilon_{11}(x)} \right)^{-1} \frac{\partial}{\partial x} \right\} H_z + \Omega H_z = 0. \quad [2.19]$$

For this set, we have magnetic field perpendicular to propagation axis, however there is a component of electric field parallel to the propagation axis. Further the definitions of $\varepsilon_{11}(x)$, $\varepsilon_{12}(x)$ and $\varepsilon_{22}(x)$ depend on the orientation of the principal axis [Eqn. 2.7, 2.11 and 2.12]. Fortunately, the portion of Eqn. 2.19, containing these terms can be simplified to be,

$$\left(\varepsilon_{22}(x) - \frac{\varepsilon_{12}^2(x)}{\varepsilon_{11}(x)} \right)^{-1} = \frac{1}{\varepsilon_{eff}(\alpha', x)}. \quad [2.20]$$

For $\beta = 0$, using Eqn. 2.7 and 2.11, we can show that,

$$\frac{1}{\varepsilon_{eff}(\alpha', x)} = \frac{\cos^2(\alpha')}{n_b^2 + p(x)(n_x^2 - n_b^2)} + \frac{\sin^2(\alpha')}{n_b^2 + p(x)(n_y^2 - n_b^2)}. \quad [2.21]$$

and for cases $(\beta, \gamma) = (90^\circ, 0)$ and $(0, 90^\circ)$, (n_x, n_y, α') in Eqn. 2.21 must be replaced with (n_y, n_z, α) and (n_x, n_z, α) respectively (see Eqn. 2.12). If the material is uniaxial ($n_x = n_y = n_o$ and $n_z = n_e$), then (n_x, n_y, α') in Eqn. 2.21 must be replaced with (n_o, n_e, α) . Note that α is the angle between x -axis and z_p (optic axis).^{*} As we can see from Eqn. 2.21, the expression for $\sqrt{\varepsilon_{eff}(\alpha', x)}$ resembles the definition of an extraordinary refractive index in a bulk anisotropic medium [111]. Therefore we define the polarization

^{*} See the discussion in the first paragraph of the section.

corresponding to the set (E_x, E_y, H_z) to be an extra ordinary polarization (e-polarization).

2.5 Summary

In summary we have presented formulation of basic equations [Eqn. 2.3, 2.5 2.13, 2.14, 2.17 and 2.19] starting from the fundamental Maxwell's equations. The details of decoupling of polarizations in 2D and 1D PCs are discussed. The decoupling of polarizations in 2D and 1D PC requires one of the principal axes of the anisotropic medium to be perpendicular to the 2D periodic plane and to the 1D periodicity axis respectively. If the anisotropic material is uniaxial then in the 1D structure the polarizations remain decoupled.

Chapter 3

Symmetrical Properties

3.1 Introduction

Before discussing the solution methods for the basic equations presented in the previous chapter, this chapter aims to develop a systematic understanding on the symmetrical properties of an anisotropic PC, based on the operator defined in Eqn. 2.5 of Chap. 2.

Although anisotropic PC occurs naturally in the design of PCs [see Chap. 1], adequate theoretical tools based on their symmetry are still lacking. Formal tools for such an analysis can be developed using group theory. Group theory has been proven to be highly valuable especially in understanding the symmetrical properties of an electronic energy band [118-119]. In the context of a PC, group theory has been employed in the investigations of mode couplings [120-123], existence of photonic band gaps [124], description of resonant modes in the defect state of a PC [125], the symmetrical properties of the eigenmodes of an opal [126] and a metallic PC [127] and very recently in the understandings of cutoff conditions of optical vortices in a 2D PC [128].

In this chapter, we develop necessary theoretical tools using group theory for symmetry analysis of the eigenstates in anisotropic PCs. By using coset decomposition of a group, we have drawn a relationship between isotropic and anisotropic PCs of the same lattice. We further use such a relationship to describe

the variation of the irreducible Brillouin zone (IBZ) of an anisotropic PC. Moreover, we have elaborated on the existence of a fundamental zone in the orientations of the motif with respect to the lattice. Taking 2D hexagonal lattice as an example, we first introduce an eigenstate classification scheme of degenerate states in the absence of a spatial modulation and in the absence of anisotropy, using a properly derived integer system. We then describe the splitting and the evolution of this states in the presence of the anisotropy and the spatial modulation. The rest of the chapter is organized as follows. In Section 3.2, we introduce relevant symmetry groups and cosets of anisotropic PC. In Section 3.3, we describe the use of cosets in identifying the IBZs of an anisotropic PC and outline the derivation of the orientational group that leads to the fundamental zone of orientations. In Section 3.4, we give the classification and the evolution of symmetry in an anisotropic 2D PC with an hexagonal lattice. Finally, Section 3.5 concludes the chapter.

3.2. Symmetry Groups

The symmetry of a PC is analyzed in terms of its symmetry elements. A collection of symmetry elements that satisfies the group axioms [113-114], is called a symmetry group. Throughout the thesis we denote a symmetry element of a group using a capital letter, U , the corresponding symmetry group using the same capital letter but with a bar on top, $\overline{U}$, and the order of the group using a small version of the same letter, u .

A PC is comprised of a lattice and a motif attached to each lattice point. The symmetry operation that leaves the lattice invariant is given by a space group, $\overline{G}$.

This group has a translational subgroup, $\bar{T}$, which contains all primitive translations of the lattice. As $\bar{T}$ is an Abelian group, it has only one-dimensional irreducible representations (IRs) with the corresponding basis function of each IR is a Bloch function of a wavevector, $\mathbf{k}$. Hence, a magnetic field distribution in a PC constitutes an example for a basis of $\bar{T}$. An action of $T \in \bar{T}$ on the magnetic field function, $\mathbf{H}_{\mathbf{k}}(\mathbf{r})$ can be illustrated as follows,

$$T\mathbf{H}_{\mathbf{k}}(\mathbf{r}) = e^{j\mathbf{k}\mathbf{t}}\mathbf{H}_{\mathbf{k}}(\mathbf{r}) \quad [3.1]$$

where $\mathbf{t}$ is a primitive real lattice vector and $e^{j\mathbf{k}\mathbf{t}}$ is a representation of T , identified with the wavevector, $\mathbf{k}$. Besides the translational symmetry, the lattice comes along with several compatible point group symmetries. The point group of a lattice can be denoted as, $\bar{R}$, and the action of R on T ($T \in \bar{T}$, $R \in \bar{R}$), leaves $\bar{T}$ invariant. Further, when R operates on a Bloch function of a wavevector- $\mathbf{k}$, it produces another Bloch function with a wavevector- $R\mathbf{k}$ [126,113-114],

$$R\mathbf{H}_{\mathbf{k}}(\mathbf{r}) = \mathbf{H}'_{R\mathbf{k}}(\mathbf{r}) \quad [3.2]$$

Assuming $\bar{G}$ is a symmorphic space group, any element of $\bar{G}$ can be expressed as a product of an element of $\bar{T}$ with an element of $\bar{R}$. That is $\bar{G} = \bar{T} \otimes \bar{R}$, where the sign $\otimes$ reminds the multiplication direction is from the left to right (i.e. semi-direct product).

On the other hand, the symmetry elements of a motif in general may be different from those of a lattice and depend on the geometry of the motif and the materials symmetry. The symmetry elements of the motif can be taken as $\overline{R_{geo}} \cap \overline{R_{mat}}$,

where $\overline{R_{geo}}$ and $\overline{R_{mat}}$ are respectively the geometrical and material point group of the motif. The intersection of two groups is always a group, thus the symmetry elements of the motif are also given by a point group, $\overline{R_B} = \overline{R_{geo}} \cap \overline{R_{mat}}$. If the material is isotropic then $\overline{R_B} = \overline{R_{geo}}$.

Further, an important group in determining the optical properties of a PC is a group of symmetry operations, $\overline{G_M}$. To define $\overline{G_M}$, we write the eigen-equation [Eqn. 2.5, 2.13, 2.14, 2.17 or 2.19] as,

$$M\mathbf{H}_k(\mathbf{r}) = \Omega(\mathbf{k})\mathbf{H}_k(\mathbf{r}) \quad [3.3]$$

where M is the differential operator [Chap. 2]. The group $\overline{G_M}$ is a subgroup of $\overline{G}$ and contains the symmetry operations, G_M , such that

$$G_M M G_M^{-1} = M. \quad [3.4]$$

Again, for a symmorphic $\overline{G}$, $\overline{G_M}$ can be expressed as $\overline{G_M} = \overline{T} \otimes \overline{R_M}$ where $\overline{R_M}$ is a point group of M . $\overline{R_M}$ is given by,

$$\overline{R_M} = \overline{R} \cap \overline{R_B} = \overline{R} \cap \overline{R_{geo}} \cap \overline{R_{mat}} \quad [3.5.1]$$

If the materials are assumed to be isotropic, then Eqn. 3.5.1 becomes

$$\overline{R_M} = \overline{R} \cap \overline{R_B} = \overline{R} \cap \overline{R_{geo}} \quad [3.5.2]$$

Table 3.1 shows some examples of $\overline{R_M}$ for various motifs in a 2D hexagonal lattice ($\overline{R} = C_{6v}$) and the corresponding definition of symmetry elements in the symmetry group can be found in Table A1 of Appendix-A1.

Table 3.1 - $\overline{R_M}$ for typical motifs in a 2D hexagonal lattice. Any two principal axes of the anisotropic material are assumed to be oriented in the 2D periodic plane. Key: *s.m.* – geometrical orientation of the motif (or orientation of the principal axes of the anisotropic media) is symmetrically matched with the lattice; *arb.* – arbitrary orientation with no symmetry matching.

Geometry ($\overline{R_{geom}}$)	Orientation	Materials		
		Isotropic	Anisotropic	
			<i>s.m.</i>	<i>arb.</i>
Circle (C_{6v})	-	C_{6v}	C_{2v}	C_2
Square (C_{4v})	<i>s.m.</i>	C_{2v}	C_{2v}	C_2
	<i>arb.</i>	C_2	C_2	C_2
Rectangle/Ellipse (C_{2v})	<i>s.m.</i>	C_{2v}	C_{2v}	C_2
	<i>arb.</i>	C_2	C_2	C_2
Triangle (C_{3v})	<i>s.m.</i>	C_{3v}	C_{1h}	C_1
	<i>arb.</i>	C_3	C_1	C_1
Hexagon (C_{6v})	<i>s.m.</i>	C_{6v}	C_{2v}	C_2
	<i>arb.</i>	C_6	C_2	C_2

In a 3D PC, Eqn. 3.3 is basically a set of coupled differential equations. But in a 2D PC, it is possible to decouple this set of coupled equations into two independent equations corresponding to *E*- and *H*-polarizations. Both polarizations satisfy Eqn. 3.3 with two different *M*'s [Eqn. 2.13 and 2.14]. It is worth mentioning that, if the 2D PC is made of isotropic materials, we can decouple the two polarizations and the corresponding two *M* operators will have the same symmetry group, $\overline{G_M}$, independent of polarizations [83, 115, 120]. On the other hand, if the 2D PC is made of an anisotropic material (i.e., uniaxial or biaxial), then in general the two polarizations are coupled and the point group of *M* is described by Eqn. 3.5.1. However, great simplification exists when one of the principal axes of the anisotropic material is perpendicular to the 2D periodic plane, where we can decouple the polarizations into *E*- and *H*-polarizations [see Sec. 2.3 of Chap. 2].

Furthermore in such cases, as the electric field in the E -polarization is parallel to the principal axis that is lying perpendicular to the 2D periodic plane, the symmetry of the E -polarization is therefore not affected by the anisotropy of the material (see Eqn. 2.13) and consequently the corresponding $\overline{G}_M$ is the same as if the 2D PC is constructed with isotropic materials (i.e., $\overline{R}_M$ is given by Eqn. 3.5.2), however for the H -polarization [Eqn. 2.14], $\overline{G}_M$ is obviously influenced by the material symmetry (i.e., $\overline{R}_M$ is given by Eqn. 3.5.1).

A subgroup of groups $\overline{G}$, $\overline{R}$, $\overline{G}_M$ and $\overline{R}_M$ can be formed for each wavevector $\mathbf{k}$, by considering the corresponding symmetries in the $\mathbf{k}$.

Fig. 3.1 Set relationships between $\overline{R}$, $\overline{R}_B$, $\overline{R}_M$, $\overline{R}(\mathbf{k})$ and $\overline{R}_M(\mathbf{k})$.

From Eqn. 3.1, each one-dimensional IR of $\overline{T}$ is given by $e^{j\mathbf{k}\cdot\mathbf{t}}$. Since, $e^{j\mathbf{G}\cdot\mathbf{t}} = 1$ ($\mathbf{G}$ is reciprocal lattice vector), two IRs of $\overline{T}$ identified by wavevectors, $\mathbf{k}$ and $\mathbf{k}+\mathbf{G}$, are essentially the same. Thus, the elements of $\overline{G}$ for which their action on $\mathbf{k}$ generates $\mathbf{k}$

added with multiples of $\mathbf{G}$, form a subgroup, $\overline{G}(\mathbf{k})$. Similarly we can form subgroups $\overline{R}(\mathbf{k})$, $\overline{G_M}(\mathbf{k})$ and $\overline{R_M}(\mathbf{k})$ from the main groups of $\overline{R}$, $\overline{G_M}$ and $\overline{R_M}$ respectively by considering the symmetries in $\mathbf{k}$. Figure 3.1 depicts the set relationship between the groups $\overline{R}$, $\overline{R_B}$, $\overline{R_M}$, $\overline{R}(\mathbf{k})$ and $\overline{R_M}(\mathbf{k})$. Any symmorphic space group can be written as a product of $\overline{T}$ and a point group. For groups of $\mathbf{k}$, this product is a direct product (i.e. the multiplication direction is irrelevant). For instance, $\overline{G} = \overline{T} \otimes \overline{R}$, is a semidirect product, but $\overline{G}(\mathbf{k}) = \overline{T} \times \overline{R}(\mathbf{k})$ is a direct product.

In discussing the properties of a group, a useful tool is a coset decomposition. When an element of a group acts on its subgroup, it produces a set of elements called coset. A group may have several (an integer number) distinct cosets depending on the size of the subgroup. Important subgroups and the corresponding cosets for groups C_{6v} and C_{4v} are tabulated in Table A3 and A4 of Appendix – A1. Based on the group properties, all cosets of a group (derived from the same subgroup) must be the same in size and must be either identical or totally a different set (i.e. no elements in common between any two cosets). Hence, a group can be decomposed into a sum of distinct cosets. For instance, a coset decomposition that will be useful in the later discussion, is given as

$$\overline{G_M} = \overline{G_M}(\mathbf{k})G_{M1} + \overline{G_M}(\mathbf{k})G_{M2} + \dots + \overline{G_M}(\mathbf{k})G_{M[r_m/r_m(\mathbf{k})]}. \quad [3.6.1]$$

In the above coset decomposition $G_{Mi} \in \overline{G_M}$ [$i = 1, 2, \dots, r_m/r_m(\mathbf{k})$], and $\overline{G_M}$ is decomposed with respect to its subgroup, $\overline{G_M}(\mathbf{k})$. $\overline{G_M}(\mathbf{k})G_{Mi}$ is said to be a “right coset” as the action of G_{Mi} is on the right to $\overline{G_M}(\mathbf{k})$. The number of cosets is given by the ratio of the orders of the group and the subgroup, $g_m/g_m(\mathbf{k})$ and it has to be an

integer. Since $\overline{G_M}$ and $\overline{G_M}(\mathbf{k})$ are products of $\overline{T}$ with $\overline{R_M}$ and $\overline{R_M}(\mathbf{k})$ respectively, $g_m/t = r_m/r_m(\mathbf{k})$. In addition, as the factor group $\overline{G_M}/\overline{T}$ is isomorphic to $\overline{R_M}$, Eqn. 3.6.1, can be equivalently written as

$$\overline{G_M} = \overline{T}R_{M1} + \overline{T}R_{M2} + \dots + \overline{T}R_{M[r_m/r_m(k)]} \quad [3.6.2]$$

where R_{Mi} is taken from each coset of $\overline{R_M}$ decomposed with respect to $\overline{R_M}(\mathbf{k})$.

An important property of a coset is that if $\phi(\mathbf{r})$ is a basis for an IR of a subgroup, the function, $U\phi(\mathbf{r})$ is a basis for a representation of the main group, $\overline{U}$, provided U is chosen from a coset of $\overline{U}$ expanded with respect to the same subgroup.

3.3. Symmetry in the Wave Equation

3.3.1. Irreducible Brillouin zones (IBZ)

Consider the symmetry operations that leave M invariant in Eqn. 3.3 at a particular $\mathbf{k}$ -vector. Such a symmetry operation comes from $\overline{G_M}(\mathbf{k})$. Operate $G_M(\mathbf{k})$, $G_M(\mathbf{k}) \in \overline{G_M}(\mathbf{k})$ on both sides of Eqn. 3.3 and as M commutes with $G_M(\mathbf{k})$ [Eqn. 3.4],

$$M[G_M(\mathbf{k})\mathbf{H}_k(\mathbf{r})] = \Omega(\mathbf{k})[G_M(\mathbf{k})\mathbf{H}_k(\mathbf{r})]. \quad [3.7]$$

Eqn. 3.7 shows that $G_M(\mathbf{k})\mathbf{H}_k(\mathbf{r})$ is an eigenfunction of M . Using group representation we can write $G_M(\mathbf{k})\mathbf{H}_k(\mathbf{r})$ as a sum of basis functions of an IR of $\overline{G_M}(\mathbf{k})$,

$$G_M(\mathbf{k})\mathbf{H}_k(\mathbf{r}) = \sum_{j=1}^d a_j \mathbf{H}_k^j(\mathbf{r}) \quad [3.8]$$

where $G_M(\mathbf{k}) \in \overline{G_M}(\mathbf{k})$, $\mathbf{H}_\mathbf{k}^j(\mathbf{r})$ with $j=1,\dots,d$, is a basis function of a d -dimensional IR of $\overline{G_M}(\mathbf{k})$ and a_j is a scalar coefficient.

A complete set of symmetry operations that leaves M invariant is given by the space group, $\overline{G_M}$. From Eqn. 3.3 and Eqn. 3.4 for any $G_M \in \overline{G_M}$,

$$M[G_M \mathbf{H}_\mathbf{k}(\mathbf{r})] = \Omega(\mathbf{k})[G_M \mathbf{H}_\mathbf{k}(\mathbf{r})]. \quad [3.9]$$

Clearly $G_M \mathbf{H}_\mathbf{k}(\mathbf{r})$ is an eigenfunction of M . Hence, as we did for $G_M(\mathbf{k})\mathbf{H}_\mathbf{k}(\mathbf{r})$, $G_M \mathbf{H}_\mathbf{k}(\mathbf{r})$ can be written as a linear combination of basis functions of an IR of $\overline{G_M}$. The basis function of its subgroup, $\overline{G_M}(\mathbf{k})$ is given by $\mathbf{H}_\mathbf{k}^i(\mathbf{r})$, $j=1,\dots,d$, thus from the coset decomposition [Eqn. 3.6.2], we know that $R_M \mathbf{H}_\mathbf{k}^i(\mathbf{r})$, ($R_M \in \overline{R_M}$) must be a basis function of a representation of $\overline{G_M}$. In this particular case it can be shown that, this representation is also irreducible [See pages 124-125 of Ref. 113]. As the coset decompositions have a number of $s = r_M / r_M(\mathbf{k})$ distinct cosets, the eigenspace described by Eqn. 3.9 thus has, sd -independent basis functions. Using Eqn. 3.2, $G_M \mathbf{H}_\mathbf{k}(\mathbf{r})$ can be written as,

$$G_M \mathbf{H}_\mathbf{k}(\mathbf{r}) = \sum_{i=1}^s \sum_{j=1}^d b_{i,j} \mathbf{H}_{R_M \mathbf{k}}^j(\mathbf{r}) \quad [3.10]$$

where $b_{i,j}$ is a scalar coefficient.

For a general wavevector, $\overline{R_M}(\mathbf{k})$ contains only the identity element and so only one one-dimensional IR (i.e. $d=1$) and $s = r_M$. Thus, the eigenvalue for a general wavevector is r_M -fold degenerate with r_M basis functions formed by r_M - $\mathbf{k}$ vectors in the first BZ. However it is sufficient to use only one of these vectors to obtain the

eigenvalue. So, among the zone of vectors defined in the first BZ only $1/r_M$ portion of wavevectors will have non-degenerate eigenvalue. That $1/r_M$ portion is the irreducible part of the BZ (IBZ).

Fig. 3.2 IBZs when $\overline{R_M}(\mathbf{k})$ equals to (a) C_{6v} (b) C_{3v} (c) C_{2v} (d) C_2 (e) C_1 (f) $C_{2v'}$. Symmetrical points of a 2D hexagonal lattice are labeled in (a).

For example, we illustrate the IBZs for a 2D hexagonal lattice PC in Figure 3.2 for various $\overline{R_M}$. In Fig. 3.2(a), we have $\overline{R_M} = \overline{R} = C_{6v}$, so $r_M = 12$ and the $1/r_M$ portion of the hexagonal BZ is a triangle as shown in the figure. Fig. 3.2(b), 3.2(c), 3.2(d), 3.2(e) and 3.2(f) show the IBZ for the case $\overline{R_M}$ equals to C_{3v} , C_{2v} , C_2 , C_1 and $C_{2v'}$ respectively. The definition of the first four groups can be found in the Table A1 of Appendix A1. The group $C_{2v'}$ is similar to C_{2v} , however the two mirror axes are σ_{-30° and σ_{60° .

As we described in the previous section, apart from the symmetry of the lattice, the definition of $\overline{G_M}$, is determined by the materials and the geometry of the motif. So the definition of the IBZ and the optical properties will vary when the elements of $\overline{G_M}$ vary. On the other hand, it is always possible to define an IBZ which is reduced from the BZ using the symmetries of the lattice, $\overline{G}$. Such an IBZ is that of the PC when $\overline{G_M} = \overline{G}$ and can be named as IBZ of the lattice. Given a lattice, $\overline{G}$ is fixed, however there could be many possibilities of its subgroup, $\overline{G_M}$. Thus, it is useful to draw a relationship between $\overline{G}$ and $\overline{G_M}$, so that the optical properties that belong to $\overline{G_M}$ can be obtained by means of $\overline{G}$. Such a relationship can be found using a coset decomposition of $\overline{G}$ with respect to its subgroup, $\overline{G_M}$,

$$\overline{G} = \overline{G_M}G_1 + \overline{G_M}G_2 + \dots + \overline{G_M}G_{g/g_m} \quad [3.11]$$

where $G_i \in \overline{G}$ and there are g/g_m distinct cosets. Since $\overline{G} = \overline{T} \otimes \overline{R}$, factor group $\overline{G}/\overline{T}$ is isomorphic to $\overline{R}$. Thus $g/g_m = r/r_m$ and for $R_i \in \overline{R}$, Eqn. 3.11 equivalently can be written as,

$$\overline{R} = \overline{R_M}R_1 + \overline{R_M}R_2 + \dots + \overline{R_M}R_{r/r_m}. \quad [3.12]$$

Any element R_j , of the same coset $\overline{R_M}R_i$ can be written as $R_{Mj}R_i$, $R_{Mj} \in \overline{R_M}$ without changing the coset representative R_i . Since $R_{Mj}^{-1}MR_{Mj} = M$, an operator defined as $R^{-1}MR$ remains unchanged for R belonging to the same coset. If R belongs to different cosets, $R^{-1}MR$ is essentially different. Hence, there are r/r_m different $R^{-1}MR$ operators with R chosen from each coset, $\overline{R_M}R_i$.

Consider a wavevector, $R\mathbf{k}$, with $R \in \overline{R}$, the corresponding eigenvalue is denoted as $\Omega(R\mathbf{k})$. From Eqn. 3.3,

$$M\mathbf{H}_{R\mathbf{k}}(\mathbf{r}) = \Omega(R\mathbf{k})\mathbf{H}_{R\mathbf{k}}(\mathbf{r}). \quad [3.13]$$

By writing $\mathbf{H}_{R\mathbf{k}}(\mathbf{r}) = R\mathbf{P}_{\mathbf{k}}(\mathbf{r})$, where $\mathbf{P}_{\mathbf{k}}$ is another Bloch function [Eqn. 3.2], Eqn. 3.13 can be rearranged for any R , ($R \in \overline{R}$),

$$R^{-1}MR[\mathbf{P}_{\mathbf{k}}(\mathbf{r})] = \Omega(R\mathbf{k})[\mathbf{P}_{\mathbf{k}}(\mathbf{r})]. \quad [3.14]$$

With the absence of the anisotropic motif (i.e. $\overline{R_M} = \overline{R}$), $R^{-1}MR = M$ for all R . Hence, $\Omega(R\mathbf{k}) = \Omega(\mathbf{k})$ for all R , $R \in \overline{R}$. However, with the presence of anisotropic motif, there will be r/r_M different eigenvalues since there are r/r_M distinct $R^{-1}MR$ operators. This also means that among r wavevectors, $R\mathbf{k}$ that are equivalent with the absence of the anisotropic motif, will split into r/r_M sets of non-equivalent $R\mathbf{k}$ wavevectors. Thus the IBZ size of the PC is bigger than the IBZ size of the lattice with a ratio of r/r_M . Further, from the coset decomposition, we know that r/r_M must be an integer and this means IBZ size of the PC is an integer multiples of the IBZ size of the lattice. Further, if the IBZ of the lattice is denoted as a collection of wavevectors $[\mathbf{k}_i]$, then the IBZ of the PC is a collection of $R_1[\mathbf{k}_i], \dots, R_{r/r_M}[\mathbf{k}_i]$, with R_i chosen each coset in Eqn. 3.13.

This result is very useful in identifying the IBZs of complicated 3D anisotropic PCs and a quick verification can be done using Fig. 3.2 for various $\overline{R_M}$ when $\overline{R} = C_{6v}$. For instance, when $\overline{R_M} = C_{2v}$, the IBZ of the PC is $r/r_M = 3$ times bigger than a IBZ of a lattice. IBZ of the lattice is a zone of wavevectors, $[\mathbf{k}_i]$ shown in a triangle of

Fig. 3.2(a). If $C_{2v} = [E, C_2, \sigma_0, \sigma_{90^\circ}]$ (App. A1, Table A1), the coset decomposition $\overline{R} = C_{6v}$ with respect to $\overline{R}_M = C_{2v}$ takes the form of $\overline{R} = C_{2v}E + C_{2v}R_2 + C_{2v}R_3$, where R_2 and R_3 are the coset representatives. Hence, the IBZ of the PC with $\overline{R}_M = C_{2v}$ is given by a collection of wavevectors, $E[\mathbf{k}_i]$, $\sigma_{30^\circ}[\mathbf{k}_i]$ and $C_6[\mathbf{k}_i]$, where E , σ_{30° , and C_6 are chosen from each coset of C_{2v} ($\overline{R}_M$) with respect to C_{6v} ($\overline{R}$) [App. A1, Table A4]. Such a collection of wavevectors forms the shaded region in Fig. 3.2(c). It has to be noted that the definition of an IBZ depends on the explicit definition of $\overline{R}_M$. For example if $C_{2v} = [E, C_2, \sigma_{-30^\circ}, \sigma_{60^\circ}]$ (i.e. $C_{2v'}$), the definition of cosets changes and this implies that the IBZ definition changes to a region, as shown in Fig. 3.2(f).

As we have shown, the definition of IBZ changes with the definition of $\overline{R}_M$, though the lattice group $\overline{R}$ does not change. This causes trouble in many cases especially for a 3D PC, where for a single $\overline{R}$ there are many possibilities of $\overline{R}_M$. In 2D PCs with anisotropic materials, if optical properties are to be monitored as a function of optic axis, the varying optic axis will require re-definition of IBZ for each orientation, and this may not be desired. An alternative way to such a redefinition can be obtained using Eqn. 3.14. Eigenvalue with a wavevector $R\mathbf{k}$, $\Omega(R\mathbf{k})$ can be obtained from a wavevector $\mathbf{k}$, but with a coordinate transformed M operator, $R^{-1}MR$. By selecting R from each coset of $\overline{R}$ expanded with respect to $\overline{R}_M$, we can find the eigenvalues at all non-equivalent $R\mathbf{k}$ vectors, from a single $\mathbf{k}$ vector. Thus, regardless of $\overline{R}_M$, we can fix the IBZ as the IBZ of the lattice, however, the

computations has to be repeated r/r_m times with each time using a $R^{-1}MR$ operator where R is chosen from one of the r/r_m distinct cosets.

3.3.2 Fundamental zone of orientations

The re-orientation of the motif with respect to a coordinate system of the lattice, will change the symmetry elements of $\overline{R_M}$. In this section, we analyze the consequence of such symmetry variation as a function of an orientational parameter. The orientational parameter, θ can be defined using the angle between two symmetry axis each from $\overline{R}$ and $\overline{R_M}$ respectively. As $\overline{R_M}$ is dependant on θ [Table 3.1], it will be useful to denote $\overline{R_M}$ as $\overline{R_M}(\theta)$. When the orientation of the motif is parallel to the symmetrical directions of the lattice, obviously $\overline{R_M}(\theta)$ is a larger group than $\overline{R_M}(\theta)$ of a general orientation for which none of the symmetrical axes overlaps [Table 3.1]. Further for a general orientation $\overline{R_M}(\theta)$ is an invariant subgroup of $\overline{R}$ (or a normal subgroup, [113-114]). For instance, in a 2D PC, the symmetrical axes are the mirror axes (in the periodic plane), and for a general orientation the entire elements in the class containing mirror elements are removed. If rotations exist in $\overline{R_M}(\theta)$, they should exist as a whole class and obviously are not disturbed by any orientation of the motif in the periodic plane as the rotational axis is perpendicular to the 2D periodic plane. For instance, considering a hexagonal lattice, $\overline{R} = C_{6v}$ and a motif with $\overline{R_B} = C_{2v}$ and defining the angle between σ_0 -axis in $\overline{R}$ and σ_0 -axis in $\overline{R_B}$ to be θ , when θ equals to the multiples of 30° (i.e. orientation of the motif matches symmetrical directions of hexagonal lattice) $\overline{R_M}(\theta) = C_{2v}$ and

for all the other angles we have a smaller group of $\overline{R_M}(\theta) = C_2$ [Table 3.1]. Thus the general orientation has $\overline{R_M}(\theta) = C_2$, which is obviously an invariant subgroup of $\overline{R}$.

Assuming that when $\theta = \alpha$, $M = M_\alpha$ with an eigenvalue of $\Omega_\alpha(\mathbf{k})$, Eqn. 3.3 becomes $M_\alpha \mathbf{H}_k(\mathbf{r}) = \Omega_\alpha(\mathbf{k}) \mathbf{H}_k(\mathbf{r})$. The re-orientation causes θ to change to a new value, $\theta = \beta$, M_α changes to M_β , $M_\beta = R_\theta^{-1} M_\alpha R_\theta$ and $\Omega_\alpha(\mathbf{k})$ changes to $\Omega_\beta(\mathbf{k})$. Thus when $\theta = \beta$, the eigen-equation becomes,

$$R_\theta^{-1} M_\alpha R_\theta [\mathbf{H}_k(\mathbf{r})] = \Omega_\beta(\mathbf{k}) [\mathbf{H}_k(\mathbf{r})]. \quad [3.15]$$

If $R_\theta \in \overline{R_M}(\alpha)$, then $R_\theta^{-1} M_\alpha R_\theta = M_\alpha$, and $\Omega_\beta(\mathbf{k}) = \Omega_\alpha(\mathbf{k})$. Furthermore, even if $R_\theta \notin \overline{R_M}(\alpha)$, however $R_\theta \in \overline{R}(\mathbf{k})$, following Eqn. 3.2, we have $\Omega_\beta(\mathbf{k}) = \Omega_\alpha(\mathbf{k})$ and in fact there could be more symmetries than just the symmetry elements of $\overline{R_M}(\alpha)$ and $\overline{R}(\mathbf{k})$. It can be easily shown a set of orientational operations, $[R_\theta]$, $R_\theta = R_M R$,[♥] where $R_\theta \in [R_\theta]$ (not necessarily belongs to $\overline{R_M}(\alpha)$ or $\overline{R}(\mathbf{k})$), $R_M \in \overline{R_M}(\alpha)$ and $R \in \overline{R}(\mathbf{k})$ for which Eqn. 3.15 is invariant and thus leads to the same eigenvalue. $[R_\theta]$ is a subset of $\overline{R}$ with the order of the set can be shown to be, $|r_\theta|$,

$$|r_\theta| = \frac{r(\mathbf{k}) r_m(\alpha)}{r_m(\mathbf{k})} \quad [3.16].$$

It is worth to note that, $\overline{R_M}(\mathbf{k}) = \overline{R}(\mathbf{k}) \cap \overline{R_M}(\alpha)$ [Fig. 3.1] and $\overline{R_M}(\mathbf{k}) \subset \overline{R}(\mathbf{k})$ [Fig. 3.1].

In Eqn. 3.16, $|r_\theta|$ is an integer as the division of the orders of the group and the subgroup must be an integer.

[♥] Note that the operation $R_\theta = R_M R$, also can be written as RR_M . For proof see Appendix – A2.

The set $[R_\theta]$ does not necessarily form a group though mostly it does. If $\overline{R_M}(\alpha)$ is a subgroup of $\overline{R}(\mathbf{k})$, then $\overline{R_M}(\mathbf{k}) = \overline{R_M}(\alpha)$, $|r_\theta| = r(\mathbf{k})$, and $[R_\theta] = \overline{R}(\mathbf{k})$. Inversely if $\overline{R}(\mathbf{k})$ is a subgroup of $\overline{R_M}(\alpha)$, then $\overline{R_M}(\mathbf{k}) = \overline{R}(\mathbf{k})$, $|r_\theta| = r_m(\alpha)$, and $[R_\theta] = \overline{R_M}(\alpha)$. If either $\overline{R}(\mathbf{k})$ or $\overline{R_M}(\alpha)$ is an invariant subgroup of $\overline{R}$, then it can be easily verified that they form a group with the order given by Eqn. 3.16, and further if $\overline{R_M}(\mathbf{k}) = E$ (i.e., identity element, see Table A1 in Appendix A), $[R_\theta]$ is a direct product group between $\overline{R}(\mathbf{k})$ and $\overline{R_M}(\alpha)$.

Table 3.2 – $\overline{R_\theta}$ at various $\mathbf{k}$ -vectors and for various $\overline{R_M}$ of general orientations in a 2D hexagonal lattice. The $\overline{R_\theta}$ groups formed by a direct product between $\overline{R}(\mathbf{k})$ and a $\overline{R_M}$ of a general orientation are underlined.

$\mathbf{k}$ points (π/a)	$\overline{R_M}$			
	C_6	C_3	C_2	C_1
$\Gamma (0,0)$	C_{6v}	C_{6v}	C_{6v}	C_{6v}
$K (4/3, 0)$	C_{6v}	C_{3v}	<u>C_{6v}</u>	C_{3v}
$M (1, -1/\sqrt{3})$	C_{6v}	<u>C_{6v}</u>	C_{2v}	C_{2v}
J (along MK)	<u>C_{6v}</u>	<u>C_{3v}</u>	<u>C_{2v}</u>	C_{1h}
T (along ΓK)	<u>C_{6v}</u>	<u>C_{3v}</u>	<u>C_{2v}</u>	C_{1h}
Σ (along ΓM)	<u>C_{6v}</u>	<u>C_{3v}</u>	<u>C_{2v}</u>	C_{1h}
L (along ΓJ)	C_6	C_3	C_2	C_1

Hence for a general orientation for which $\overline{R_M}(\alpha)$ is an invariant subgroup of $\overline{R}$, $[R_\theta]$ is a group and can be denoted as a group of orientation, $\overline{R_\theta}$. This group of orientation is fundamentally important because all orientations have minimum symmetry of $\overline{R_\theta}$. The existence of symmetry in the orientations leads to a fundamental zone of orientations (FZO) in which the orientations within the zone have unique eigenvalues. Such a fundamental zone can be obtained by considering

the symmetry of $\overline{R_\theta}$. For example, the groups of $\overline{R_\theta}$ for various $\mathbf{k}$ vectors of a 2D hexagonal lattice and $\overline{R_M}$, are listed in Table 3.2. The respective definition of the FZO for $\overline{R_\theta}$ is presented in Table 3.3, based on the symmetry elements listed in Table A1 of the Appendix A1.

Table 3.3 – FZO for various $\overline{R_\theta}$ that are compatible with a 2D hexagonal lattice with γ being an arbitrary positive angle. The definitions are based on the symmetry elements of Table A1 in Appendix-A1.

$\overline{R_\theta}$	FZO
C_{6v}	$0 < \theta < 30^\circ$
C_{3v}	$0 < \theta < 60^\circ$
C_{2v}	$0 < \theta < 90^\circ$
C_6	$\gamma < \theta < \gamma + 60^\circ$
C_3	$\gamma < \theta < \gamma + 120^\circ$
C_{1h}	$0 < \theta < 180^\circ$
C_2	$\gamma < \theta < \gamma + 180^\circ$
C_1	$\gamma < \theta < \gamma + 360^\circ$

A clearer representation of a FZO can be accomplished using a diagram. Assuming the orientation of the motif to be a vector of a unit length, the FZO can be represented in a unit circle in the case of a 2D PC and using a unit sphere in the case of a 3D PC. The FZO of a 2D PC with $\overline{R_\theta} = C_{3v}, C_{2v}, C_{2v'}$ and C_6 is shown in Figure 3.3(a), 3.3(b), 3.3(c), and 3.3(d) respectively. The shaded region in each circle represents the corresponding FZO. Such a sketch of FZO is advantageous as the symmetry operations of $\overline{R_\theta}$ can be highlighted in the diagram. For example, the thick lines in Fig. 3.3(a) to 3.3(c) represent the mirror operations in $\overline{R_\theta}$ whereas the centered ellipse, triangle and hexagon represent the two-, three- and six-fold

rotational operations of $\overline{R_\theta}$ respectively. Though C_{3v} and C_6 may have the same FZO [Fig. 3.3(a) and 3.3(d)], C_6 does not have any mirror operations and this makes the definition of equivalent orientations in both C_{3v} and C_6 different. The equivalent orientations in each case are shown in Fig. 3.3(a) and 3.3(d), respectively.

Fig. 3.3 FZO when $\overline{R_\theta}$ equals to (a) C_{3v} (b) C_{2v} (c) C_{2v} (d) C_6 . The thick lines represent the symmetrical axes of $\overline{R_\theta}$ whereas the ellipse, triangle and hexagon represent the two-, three- and six-fold rotational operations of $\overline{R_\theta}$. The red arrows in (a) and (d) denote the equivalent orientations in each case.

The concept of FZO is also applicable for 3D anisotropic PCs. All possible orientations of the motif in the 3D space can be represented in an unit sphere. Therefore, the existence of orientational symmetry (given by the group, $\overline{R_\theta}$) will reduce the sphere to a 3D FZO, for which the respective orientations produce unique eigenvalues for Eqn. 3.3. The corresponding orientational group for the 3D PC must consist of all symmetry operations, $R_\theta = R_M R$ with $R_M \in \overline{R_M}$ of general orientation of

the motif in the 3D space and $R \in \overline{R}(\mathbf{k})$. In 3D anisotropic PCs, instead of the whole 3D space, we could look for fundamental orientations of the motif within a particular plane of choice in the 3D space. In such case, the fundamental orientations of motif in the plane of choice can be obtained by constructing an orientational group consist of symmetry operations $R_\theta = R_M R$ with $R_M \in \overline{R}_M$ of general orientation in the plane of interest and $R \in \overline{R}(\mathbf{k})$. It is worth mentioning that in this case, instead of an unit sphere, we can use an unit circle to represent the FZO of the 3D anisotropic PC in the plane of interest.

The effect of the orientation to an eigenfunction is straightforward. To see this, re-arrange Eqn. 3.15 to $M_\alpha[R_\theta \mathbf{H}_\mathbf{k}(\mathbf{r})] = \Omega_\beta(\mathbf{k})[R_\theta \mathbf{H}_\mathbf{k}(\mathbf{r})]$ which shows that when $R_\theta \in \overline{R}_\theta$, but $R_\theta \notin \overline{R}_M(\mathbf{k})$, the eigenfunction at $\theta = \beta$ is a rotated version of the one at $\theta = \alpha$. If $R_\theta \in \overline{R}_M(\mathbf{k})$, the eigenfunctions at $\theta = \beta$ and $\theta = \alpha$ remain unaltered. Applications and examples of FZO appear in Sec. 3.4.2.3.

3.4. Symmetry of the Eigenvalues and the Eigenmodes

The complete set of basis functions that gives the same eigenvalue, Ω in Eqn. 3.3 is given by Eqn. 3.10. Hence, the corresponding eigenvalue can be labeled using an IR of $\overline{G}_M$. However, it will be useful and easy if we can identify the symmetry of an eigenmode using a point group representation. Since $\overline{G}_M$ is a semi-direct product between $\overline{T}$ and $\overline{R}_M$, the corresponding IR of $\overline{G}_M$ cannot be simply associated with those of $\overline{R}_M$.

If we concentrate on a particular $\mathbf{k}$, then the assignment of an IR to the eigenvalue becomes more apparent and simple. Such a representation is called a small representation [114]. The complete set of basis functions at a particular $\mathbf{k}$ that gives the same eigenvalue is given by Eqn. 3.8. As $\overline{G_M}(\mathbf{k}) = \overline{T} \times \overline{R_M}(\mathbf{k})$ is a direct product, by group theoretical arguments [113] we have,

$$\Gamma(G_M) = \Gamma(T)\Gamma[R_M(\mathbf{k})] = e^{j\mathbf{k}\cdot\mathbf{t}}\Gamma[R_M(\mathbf{k})] \quad [3.17]$$

where $T \in \overline{T}$, $R_M(\mathbf{k}) \in \overline{R_M}(\mathbf{k})$ and $\Gamma(U)$ denote a representation of a symmetry element, U . The dimension of $\Gamma(T)$ is one, thus the dimension of $\Gamma(G_M)$ is determined by the dimension of $\Gamma[R_M(\mathbf{k})]$. The eigenmode symmetry then can be identified with an IR of $\overline{R_M}(\mathbf{k})$, which is a point group and the corresponding IRs can be readily obtained from the standard literatures of crystallographic group theory [113-114]. The IRs of the group C_{6v} and the IRs of the compatible subgroups are listed in the Appendix – A1 (Table A1).

Degeneracy of a state is determined by the dimension of the IR of $\overline{R_M}(\mathbf{k})$, d , that labels the eigenvalue. This can be seen from Eqn. 3.8 and 3.17, where at a particular $\mathbf{k}$ -vector, the eigenspace is spanned by d -number of basis functions. Therefore the degeneracy of the state with a d -dimensional IR of $\overline{R_M}(\mathbf{k})$ must be d . However, there could be additional degeneracy, resulted from to the crossing of bands or the absence of spatial modulation. Such a degeneracy which cannot be explained using the IR dimension is termed as an accidental degeneracy [113-114]. A systematical method to determine accidental degeneracy in the absence of spatial

modulation will be shown in Sec. 3.4.1 for the symmetrical $\mathbf{k}$ -vectors of the hexagonal lattice.

Table 3.4 – $\overline{R_M}(\mathbf{k})$ for various θ and Δn in a 2D hexagonal lattice. θ_o represents an arbitrary orientation that does not coincide with any symmetrical directions of the lattice. The definition of the $\mathbf{k}$ -vectors is similar to that of Table 3.3.

$\mathbf{k}$	$\Delta n = 0$	$\Delta n \neq 0$		
		$\theta = 0$	$\theta = 60^\circ$	$\theta = \theta_o$
Γ	C_{6v}	C_{2v}	C_{2v}	C_2
K	C_{3v}	C_{1h}	C_{1h}	C_1
M	C_{2v}	C_2	C_{2v}	C_2
J	C_{1h}	C_1	C_{1h}	C_1
T	C_{1h}	C_{1h}	C_1	C_1
Σ	C_{1h}	C_1	C_{1h}	C_1
L	C_1	C_1	C_1	C_1

In order to illustrate the symmetry of the eigenmodes and the eigenvalues in an anisotropic PC, we use an example of a 2D PC with a hexagonal lattice and circular cylinders with a radius to period ratio of r_c . We assume the cylinders to be isotropic with a refractive index of 3.5 (silicon) and the matrix medium to be uniaxially anisotropic with an ordinary refractive index, n of 1.6 and a birefringence of Δn . Such a uniaxial medium can be a wide range of materials including organic materials [129] or liquid crystals with Δn ranging from 0.02 to 0.8 [97, 100-101, 130]. The optic axis of the uniaxial medium is assumed to be oriented parallel to the 2D periodic plane at an angle θ with respect to Γ -K axis of the hexagonal lattice [Fig. 3.2(a)]. The definition of $\overline{R_M}(\mathbf{k})$ for an hexagonal lattice for $\Delta n = 0$ and $\Delta n \neq 0$ is given in Table 3.4.

In the following we shall analyze the symmetry when the spatial modulation is switched off ($\Delta n = 0$) and switched on ($\Delta n \neq 0$). Though, we choose a materially anisotropic PC to study, the conclusion also applies for geometrically anisotropic PCs. In the geometrical anisotropic PC, the geometrical orientation of the motif is equivalent to the optic axis orientation.

3.4.1 Symmetry in the absence of a spatial modulation

In the absence of a spatial modulation (i.e. with a vanishingly small refractive index modulation), the photonic band structure must reduce to a free photon dispersion with the band folding effect taken into account. Assuming $\mathbf{k}=[k_x, k_y]$ and $\mathbf{G}=[G_x, G_y]$, Eqn. 3.3 for H -polarization in the absence of a spatial modulation and $\theta = 0$ reduces to*

$$\frac{(k_x + G_x)^2}{n_x^2} + \frac{(k_y + G_y)^2}{n_y^2} = \left(\frac{2\pi}{a} \omega \right)^2 \quad [3.18]$$

where $n_x = n + \Delta n$, $n_y = n$, with (x, y) being the periodic plane, a is the period of the PC and $\omega = a/\lambda$. For E -polarization, Eqn. 3.3 reduces to $(k_x + G_x)^2 + (k_y + G_y)^2 = (2\pi n_z \omega / a)^2$ with $n_z = n$.

* The dispersion relation for a bulk anisotropic medium is $\omega^2 = (k_x/n_x)^2 + (k_y/n_y)^2$ [normalized form, H -polarization]. For a PC in the absence of the spatial modulation, the dispersion relationship is the same as the bulk but the band folding effect of the PC must be taken into account. Therefore k_x (k_y) must be replaced with $k_x + G_x$ ($k_y + G_y$). Formal proof for Eqn. 3.18 requires knowledge of plane wave expansion, which will be covered in Chap. 4 and 5. See Sec. 4.2.2 (Chap. 4) and 5.2.1 (Chap. 5).

Using $\mathbf{G} = (2\pi n_1/a)(1, -1/\sqrt{3}) + (2\pi n_2/a)(0, 2/\sqrt{3})$, where (n_1, n_2) is a pair of integer that indexes the reciprocal lattice point, the dispersion of a free photon with H -polarization can be deduced from Eqn. 3.18 to be,

$$n_x \omega^2 = C_1 M_{is} + C_2 (r_n^2 - 1) M_{anis} + C_3 k_x M_{k_x} + C_4 k_y M_{k_y} + C_5 (r_n^2 - 1) k_x M_{anis-k_x} + C_6 \quad [3.19]$$

where $r_n = n_y/n_x$ whereas, C_1, C_2, C_3, C_4, C_5 and C_6 , are $\mathbf{k}$ -dependent constants with $M_{is}, M_{anis}, M_{k_y}, M_{k_x}$ and M_{anis-k_x} are discrete integers, that are independent of r_n and $\mathbf{k}$. For E -polarization, the dispersion is also governed by an equation similar to Eqn. 3.19, but in a simpler form with $M_{anis} = M_{anis-k_x} = 0$. Without losing generality, we shall consider only the H -polarization in the rest of the paper. Nevertheless, the discussion for E -polarization can be managed in a similar manner by setting $r_n = 1$.

As degenerate states occur only at the symmetrical points of the lattice, Eqn. 3.19 for the symmetrical points of the hexagonal lattice can be simplified to be

$$3n_x \omega^2 = c_1 m_{is} + c_2 (r_n^2 - 1) m_{anis} + \omega_c \quad [3.20]$$

where c_1, c_2 , and ω_c , are constants whereas m_{is} and m_{anis} are discrete integers.

Table 3.5 - Definitions of $c_1, m_{is}, c_2, m_{anis}$, and ω_c , in Eqn. 3.20 with $m = n_1^2 + n_2^2 - n_1 n_2$.

$\mathbf{k}$	c_1	m_{is}	c_2	m_{anis}	ω_c
Γ	4	m	3	n_1^2	0
K, K'	4	$m + n_1$	$\frac{1}{3}$	$(3n_1 + 2)^2 [K]$ $(3n_1 + 1)^2 [K']$	$\frac{4}{3}$
M, M'	2	$2(m + n_2) - n_1$	$\frac{3}{4}$	$(2n_1 + 1)^2 [M]$ $n_1^2 [M']$	1

The expressions c_1 , c_2 , ω , m_{is} and m_{anis} at the symmetrical points of the 2D hexagonal lattice [Γ , K, K', M, and M', Fig. 3.2(a)] are tabulated in Table 3.5. As we can see from Table 3.5, the distinction between K and K' as well as M and M' only occurs in their expression for m_{anis} . In the absence of the anisotropy, K and K' (M and M') are essentially equivalent points. On the other hand, it is worth mentioning that, the free photon relationship of a 2D square lattice with H -polarization is also governed by an equation similar to Eqn. 3.20 and the corresponding details are given in Appendix-B.

In Eqn. 3.20, both m_{is} and m_{anis} are discrete integers that are independent of r_n . Each state, at the symmetrical points can be labeled with these integers. In the absence of an anisotropy, i.e. $\Delta n = 0$ ($r_n = 1$ in Eqn. 3.20), ω [Eqn. 3.20] only depends on m_{is} and thus the corresponding frequency levels can be labeled by only using m_{is} . As a small anisotropy is introduced (i.e. $\Delta n \neq 0$ and hence $r_n \neq 1$), each state with distinct m_{is} label, will split into states with different m_{anis} . Thus in the presence of the anisotropy each state has to be identified by a pair of indices, (m_{is}, m_{anis}) . The degeneracy of a state, n_s with a frequency of ω [Eqn. 3.20] can be determined by finding the number of possible combinations of n_1 and n_2 that leads to the same (m_{is}, m_{anis}) . As we can see from Table 3.5, m_{anis} is a square integer. Thus we can equivalently use $(m_{is}, \sqrt{m_{anis}})$ to identify a state in the presence of the anisotropy. The possible values of m_{is} and m_{anis} and the corresponding degeneracy are listed in Table 3.6.1, Table 3.6.2, and Table 3.6.3 for $\mathbf{k}$ vectors Γ , K and M respectively. For instance at Γ point $m_{is} = n_2^2 + n_1^2 - n_1 n_2$ (Table 3.5) is an integer with the first six values of 0, 1, 3, 4, 7 and 9. The degeneracy (n_s) for the first six states is 6 except for $m_{is} = 0$ and $m_{is} =$

7, where we have $n_s = 1$ and $n_s = 12$ respectively (Table 3.6.1). Other possible values of n_s at Γ must be in the multiples of 6. As a small anisotropy is introduced, each m_{is} state will split into states with different $m_{anis} = n_1^2$ (Table 3.5). For $m_{is} = 1$, the possible values of m_{anis} are 0 and 1 (Table 3.6.1). Hence the corresponding state with $m_{is} = 1$ ($n_s = 6$) splits into two states labeled by $m_{anis} = 0$ ($n_s = 2$) and $m_{anis} = 1$ ($n_s = 4$) (Table 3.6.1) as an anisotropy is introduced. If $m_{is} = 7$, the degeneracy is 12 when $\Delta n = 0$. When $\Delta n \neq 0$, the state $m_{is} = 7$ splits into three states, each with degeneracy of 4 and $\sqrt{m_{anis}}$ of 1, 2 and 3, respectively (Table 3.6.1).

Table 3.6.1 – The discrete values of m_{is} and the corresponding allowed values of m_{anis} [Eqn. 3.20] at Γ point. The integer in the bracket indicates n_s of the state.

Γ											
m_{is}	0 (1)		1 (6)		3 (6)		4 (6)		7(12)		9 (6)
$\sqrt{m_{anis}} = n_I $	0 (1)	0 (2)	1 (4)	1 (4)	2 (2)	0 (2)	2 (4)	1 (4)	2 (4)	3(4)	0 (2) 3 (4)

Table 3.6.2 – The discrete values of m_{is} and the corresponding allowed values of m_{anis} [Eqn. 3.20] at K point. The integer in the bracket denotes n_s of the state.

K											
m_{is}	0 (3)		1 (3)		2 (6)		4 (6)		5 (3)		
$\sqrt{m_{anis}} = 3n_I + 2 $	1 (2)	2 (1)	2 (2)	4 (1)	1 (2)	4 (2)	5 (2)	2 (2)	5 (2)	7 (2)	4 (2) 8 (1)

Table 3.6.3 – The discrete values of m_{is} and the corresponding allowed values of m_{anis} [Eqn. 3.20] at M point. The integer in the bracket denotes n_s of the state.

M									
m_{is}	0 (2)		1 (2)	3 (4)		4 (2)	6 (4)		9 (4)
$\sqrt{m_{anis}} = 2n_I + 1 $	1 (2)	1 (2)	1 (2)	3 (2)	3 (2)	1 (2)	3 (2)	3 (2)	5 (2)

If ω is varied with regards to a parameter p such that $\omega(p)$ is a continuous function, then instead of a single state, we have a continuum of states. A band index for $\omega_1(p)$ is lower than $\omega_2(p)$ provided that $\omega_1(p) < \omega_2(p)$. If $p = \Delta n$, the corresponding $\omega(p)$ given by Eqn. 3.19, can be verified to be a continuous and a differentiable function of Δn , for all real values of Δn . The $\omega(\Delta n)$ functions ($n = 1.6$)

with the corresponding $(m_{is}, \sqrt{m_{anis}})$ labels are plotted at Γ point and K point in Figure 3.4(a) and 3.4(b), respectively.

Fig. 3.4 Splitting of degenerate states in the absence of a spatial modulation (H -polarization). ω versus Δn relationship at (a) Γ -point (b) K-point. The states are labeled by a pair of indices $(m_{is}, \sqrt{m_{anis}})$. Each different color represents a different m_{is} .

As we can see from the figure, in the absence of the anisotropy, a lower band essentially have a lower value of m_{is} . However when an anisotropy is introduced, such a correspondence is generally invalid. For instance in Fig. 3.4(a) when Δn is between -0.4 and 0, the states (4,2) have larger frequency than (3,1). When $\Delta n = 0.4$, the two states have a common frequency and when $\Delta n < -0.4$, the frequency of (3,1) leads the frequency of (4,2). The exact value of r_n^2 (or Δn), where any two state with $(m_{is}, \sqrt{m_{anis}})$ labels, $(a_{is}, \sqrt{a_{anis}})$ and $(b_{is}, \sqrt{b_{anis}})$ will meet at a common frequency can be obtained from Eqn. 3.20 to be,

$$r_n^2 = 1 - \frac{c_1(a_{is} - b_{is})}{c_2(a_{anis} - b_{anis})}. \quad [3.21]$$

It is clear from Eqn. 3.21 that, states with the same m_{is} will not cross unless $r_n = 1$ and crossing between states with the same m_{anis} is not allowed.

Table 3.7 – Representations of degenerate states of a 2D hexagonal lattice in the absence of spatial modulation

$\mathbf{k}$	m_{is}	Representation	$\sqrt{m_{anis}}$	Representation
Γ	0	A_I	0	A_I
	1	$A_I + B_2 + E_I + E_2$	0	$A_I + B_2$
			1	$A_I + A_2 + B_I + B_2$
	3	$A_I + B_I + E_I + E_2$	1	$A_I + A_2 + B_I + B_2$
			2	$A_I + B_I$
K	0	$A_I + E$	1	$A + B$
			2	A
	1	$A_I + E$	2	$A + B$
			4	A
	2	$A_I + A_2 + 2E$	1	$A + B$
			4	$A + B$
M			5	$A + B$
	0	$A_I + B_I$	1	$A + B$
	1	$A_I + B_2$	1	$A + B$
	3	$A_I + A_2 + B_I + B_2$	1	$A + B$
			3	$A + B$

The eigenmode symmetry of each degenerate state, $(m_{is}, \sqrt{m_{anis}})$ is described by a reducible representation and the characters[♥] of such representations are independent of r_n . The dimension of the representation in each state is given by n_s of the state and the corresponding characters of the representation can be found from the procedure outlined in Ref. 115 and 120. Using a standard group theory reduction procedure [112-114], the representation can be reduced as a direct sum of IR of

[♥] This is a group theoretical term, referring to the trace of a representation matrix [112-114].

$\overline{R_M}(\mathbf{k})$ [see Table 3.4 for definitions of $\overline{R_M}(\mathbf{k})$]. The result of such an analysis is presented in Table 3.7.

3.4.2 Symmetry in the presence of spatial modulation

As the spatial modulation is switched on, the degenerate states in Table 3.6 and 3.7 split into states which can be further labeled by an IR of $\overline{R_M}(\mathbf{k})$. If the modulation is increased such that the symmetry of $\overline{R_M}(\mathbf{k})$ in the absence of the spatial modulation is retained, then the corresponding state will split according to the IRs of $\overline{R_M}(\mathbf{k})$ in the absence of spatial modulation. If the increase in the modulation lowers, the symmetry of $\overline{R_M}(\mathbf{k})$, (i.e. $\overline{R_M}(\mathbf{k})$ in presence of the modulation is a subgroup of the one in the absence of the modulation), then the corresponding IRs has to be subdued[♦] from the IRs of $\overline{R_M}(\mathbf{k})$ in the absence of the modulation.

In the presence of the spatial modulation, the solutions to Eqn. 3.3 can be obtained by means of a plane wave expansion [Chap. 4 and 5] in which the eigenfunction is expanded into a set of basis functions, i.e. plane waves. Eigenvalues with a particular IR then can be obtained by only selecting the basis functions of this IR [113-114,124,131]. If the dispersion relation, $\omega(p)$ is a continuous and differentiable function of p and the group $\overline{R_M}(\mathbf{k})$ does not change as p changes, a small change in p

[♦] In group theory, the IR of a group is generally a reducible representation of its subgroup and called as a subdued representation. The subdued representation can be written as a sum of IRs of the subgroup using the standard group theory reduction procedure. More detailed information, can be found in any group theory textbooks (i.e., For example, 113-114).

then only causes a small change in the value of ω and has no effect on the symmetry of the eigenmode. Thus the eigenmodes along the $\omega(p)$ function with the same $\overline{R_M(\mathbf{k})}$ will have the same IR.

3.4.2.1 Symmetry as a function of modulation

The plot of $\omega(r_c)$ at Γ point, with $n = 1.6$, $\Delta n = 0.6$ and $\theta = 0$ is given in Figure

3.5.

Fig. 3.5 Splitting of states at Γ point, in the presence of a spatial modulation as a function of r_c , in a PC made of an isotropic circular cylinders of refractive index 3.5 in an uniaxial matrix medium (H – polarization, $\Delta n = 0.6$, $n = 1.6$ and $\theta = 0$).

The figure shows the splitting of degenerate states ($m_{is} = 1, \sqrt{m_{anis}} = 0$) and ($m_{is} = 1, \sqrt{m_{anis}} = 1$) as a function of r_c . The first degenerate state ($m_{is} = 1, \sqrt{m_{anis}} = 0$) in Fig. 3.5 has a representation $A_1 \oplus B_2$ [Table 3.7]. The symbol $\oplus$ indicates that the representation is a reducible and composes two IRs, A_1 and B_2 . As the spatial modulation is switched on, the state splits into two states and they form two differentiable $\omega(r_c)$ functions as r_c is varied continuously. The symmetry of the

eigenmodes at any r_c along the same function is the same and hence, these two functions can be written as $\omega_{A_1}(r_c)$ and $\omega_{B_2}(r_c)$ with the symmetry of the eigenmodes at any r_c is given by the IR, A_1 and B_2 respectively.

Fig. 3.6 Eigenmodes of the first band (with non-zero frequency) at Γ point of a PC made of an isotropic circular cylinders of refractive 3.5 in an uniaxial matrix medium (H – polarization, $\Delta n = 0.6$, $n = 1.6$ and $\theta = 0$) when r_c equals to (a) 0.1 (b) 0.25.

The definition of a band that indexes a lower frequency with a lower index and an higher frequency with an higher index causes a little confusion. That is, when $\omega_{A_1}(r_c)$ and $\omega_{B_2}(r_c)$ cross, the two bands interchange the symmetry. For instance, in Fig. 3.5, these two functions cross at $r_c = 0.18$ and the respective symmetry to the left and the right to the intersection point for band 1 is B_2 and A_1 , respectively. This can be further verified by examining the symmetries of the numerically computed eigenmodes in Figure 3.6(a) and 3.6(b) for $r_c = 0.1$ and $r_c = 0.25$ respectively. The intersection point at $r_c = 0.18$ has an accidental two-fold degeneracy with a 2D reducible representation, $A_1 \oplus B_2$.

The same analysis can be done for the second degenerate state when $r_c = 0$, ($m_{is} = 1, \sqrt{m_{anis}} = 1$). The representation of this state can be obtained from Table 3.7 to

be $A_1 \oplus A_2 \oplus B_1 \oplus B_2$, which contains four IRs. Hence there are four $\omega(r_c)$ functions with four different IRs originating from the second degenerate state ($m_{is}=1, \sqrt{m_{anis}}=1$). The $\omega(r_c)$ plot with the symmetry assignments at K point is given in Figure 3.7, for the same configuration of PC. The representation of the degenerate states ($r_c = 0$) can be obtained from Table 3.7 and note the state ($m_{is}=1, \sqrt{m_{anis}}=4$) has a larger frequency than the state ($m_{is}=2, \sqrt{m_{anis}}=1$) when $\Delta n = 0.6$ [Fig. 3.4(b)].

Fig. 3.7 Splitting of states at K point, in the presence of a spatial modulation as a function of r_c , in a PC made of an isotropic circular cylinders of refractive 3.5 in an uniaxial matrix medium (H -polarization, $\Delta n = 0.6$, $n = 1.6$ and $\theta = 0$).

As $\overline{R_M}(\Gamma) = C_{2v}$ for $\Delta n \neq 0$ and $\theta = 0$ [Table 3.4], all eigenmodes have only 1D IRs and all eigenvalues do not have any further degeneracy. If $\overline{R_M}(\Gamma)$ is a higher order group with 2D IRs, then we will have the two-fold degeneracy originating from the 2D IR retained. For example, when $\Delta n = 0$, $\overline{R_M}(\Gamma) = C_{6v}$ [Table 3.4], the state with $m_{is} = 1$ ($r_c = 0$) has a representation $A_1 \oplus B_2 \oplus E_1 \oplus E_2$ with a six-fold

degeneracy [Table 3.7] and there are four $\omega(r_c)$ functions originating from this state, as shown in Figure 3.8. The representation at $r_c = 0$, contains two 2D IRs and as the increase in r_c does not disturb $\overline{R}_M(\Gamma)$, these two-fold degeneracy is retained when r_c is varied. Fig. 3.8 also shows that as modulation increases, the symmetry at a particular band changes, and more specifically the occurrence of degenerate band could shift. Such a shift is easily predicted using plots like in Fig. 3.8. For instance in Fig. 3.8, until $r_c = 0.13$ the degenerate bands (at Γ point) are band 1 and 3, however for r_c values thereafter till $r_c = 0.46$ the degenerate bands shifts to be band 2 and 3.

Fig. 3.8 Splitting of states at Γ point, in the presence of a spatial modulation as a function of r_c , in a PC made of an isotropic circular cylinders of refractive 3.5 in an isotropic matrix medium of refractive 1.6 (H - polarization). The ω functions corresponds to A_1 , E_1 , E_2 and B_2 respectively have degeneracy of 1, 2, 2 and 1. The degeneracy in the ω functions of E_1 and E_2 could be removed by a material's anisotropy (see Fig. 3.10).

The ω versus r_c relationship for an inverse structure in which the matrix media is isotropic and the cylinders are uniaxially anisotropic, is different with the direct structure in which the matrix is anisotropic and the cylinders are isotropic.

The $\omega(r_c)$ plot at Γ point is shown in Figure 3.9 for the inverse structure with $\Delta n = 0.6$ and $\theta = 0$, which can be compared with Fig. 3.5 (direct structure). Unlike the direct structure where we do not have any six-fold degenerate points for $r_c = 0$, the inverse structure has a six-fold degenerate point when $r_c = 0$. This is because the inverse structure has $\overline{R_M}(\Gamma) = C_{6v}$ in the limit of zero modulation. Thus, its dispersion in the absence of a spatial modulation is similar to that of an isotropic medium, and hence the corresponding degenerate states in the limit $r_c \rightarrow 0$, can be labeled only using m_{is} . A small increase in r_c lowers the symmetry of $\overline{R_M}(\Gamma)$ from C_{6v} to its subgroup C_{2v} and as a consequence the IRs of C_{6v} becomes reducible representations for a nonzero r_c . From Table 3.7, when $m_{is} = 1$ ($r_c \rightarrow 0$), we have a representation $A_1 \oplus B_2 \oplus E_1 \oplus E_2$, for a very small however a nonzero r_c , this representation can be further reduced to $2A_1 \oplus 2B_2 \oplus A_2 \oplus B_1$. Thus there are six $\omega(r_c)$ functions [$2\omega_{A_1}(r_c)$, $2\omega_{B_2}(r_c)$, $\omega_{A_2}(r_c)$ and $\omega_{B_1}(r_c)$] in Fig. 3.9.

Fig. 3.9 Splitting of states at Γ point, in the presence of a spatial modulation as a function of r_c , in a PC made of uniaxial circular cylinders (H – polarization, $\Delta n = 0.6$, $n = 1.6$ and $\theta = 0$) in an isotropic matrix medium of refractive 3.5.

It is worth mentioning that, for a geometrically anisotropic 2D PC with no material anisotropy (i.e., isotropic material), the splitting of the states will be similar to the one in Fig. 3.9 as long as their $\overline{R_M}(\Gamma)$ in the presence and absence of a spatial modulation is C_{6v} and C_{2v} respectively. For example, let's consider a square motif with an area, A_c , in an hexagonal lattice PC with the orientation of the motif matches the symmetrical axes of the lattice (Table 3.1). If we assume the background is an isotropic material, then in the limit $A_c \rightarrow 0$, $\overline{R_M}(\Gamma) = C_{6v}$. For a very small but a nonzero A_c , we have $\overline{R_M}(\Gamma) = C_{2v}$ and therefore resembles a symmetry configuration as for Fig. 3.9. We could apply similar principles for other symmetrical $\mathbf{k}$ -points and other lattices as well.

3.4.2.2 Symmetry as a function of the anisotropy

It can be easily verified that the compatibility of the symmetry between Fig. 3.5 [$\overline{R_M}(\Gamma) = C_{2v}$] and Fig. 3.8 [$\overline{R_M}(\Gamma) = C_{6v}$] is somehow missing. For instance when $r_c = 0.25$, the first doubly degenerate band has an IR, E_1 in Fig. 3.8. From the compatibility relation between groups C_{6v} and C_{2v} [App. A1, Table A2], E_1 (IR of C_{6v}) is only compatible with B_1 and B_2 (IRs of C_{2v}). This means that the degenerate band, E_1 for $\overline{R_M}(\Gamma) = C_{6v}$ will split into bands with IRs B_1 and B_2 for $\overline{R_M}(\Gamma) = C_{2v}$. However the degenerate band, E_1 in Fig. 3.8, seems to be splitted into bands with IR B_2 (band 2) and A_1 (band 3) in Fig. 3.5. Such a non-compatibility is a consequence of a drastic change in the anisotropy [i.e. $\Delta n = 0$ in Fig. 3.8 and $\Delta n = 0.6$ in Fig. 3.5]. In order to monitor the symmetry evolution, a plot of $\omega(\Delta n)$ with a continuous variation of Δn , such as one in Figure 3.10 is required. From Fig. 3.10, we can see

that, E_1 (IR of C_{6v}) splits into the corresponding compatible IRs of C_{2v} (B_1 and B_2).

However, the crossing at $\Delta n = 0.45$ causes the change of the symmetry of the third band from B_1 to A_1 .

Fig. 3.10 Splitting of states at Γ point as a function of $|\Delta n|$, in a PC made of a isotropic circular cylinders ($r_c = 0.25$ and refractive index = 3.5) in an uniaxial matrix medium of birefringence Δn (H – polarization, $n = 1.6$ and $\theta = 0$).

3.4.2.3 Symmetry as a function of the orientation of the motif

The symmetry of the eigenmodes and the eigenvalues varies with the orientations of the motif. As an example, the relationship between ω and θ , $\omega(\theta)$ for $\Delta n = 0.6$ and $r_c = 0.25$ is shown in Figure 3.11(a), (b), (c) and (d), respectively, for Γ , T, Σ and L points. [The definitions of these $\mathbf{k}$ vectors can be found in Table 3.2]

The symmetries of the eigenvalues in Fig. 3.11(a) to 3.11(d) are governed by Eqn. 3.15 and the corresponding symmetries are given by the group, $\overline{R_\theta}$. The group of $\overline{R_M}$ for a general orientation is given by the group C_2 [Table 3.1], and hence the

corresponding definition of $\overline{R_\theta}$ can be found from Table 3.2 to be C_{6v}, C_{2v}, C_{2v} and C_2 , respectively, for Γ , T, Σ and L points (the elements of these groups can be found from App. A1, except for Σ point the group C_{2v} have mirror elements σ_{-30° and σ_{60° , i.e. $C_{2v'}$). The FZO of these $\overline{R_\theta}$ groups can be identified from Fig. 3.3 and Table 3.3. As we mentioned in Sec. 3.2, only eigenvalues within a FZO are unique and this can be readily verified from $\omega(\theta)$ plots in Fig. 3.11(a) to 3.11(d).

Fig. 3.11 ω as a function of θ , in a PC made of isotropic circular cylinders ($r_c = 0.25$ and refractive index = 3.5) in an uniaxial matrix medium (H -polarization, $\Delta n = 0.6$ and $\theta = 0$) at $\mathbf{k}$ -vectors (a) Γ (b) T (mid of ΓK) (c) Σ (mid of ΓM) (d) L (mid of ΓJ).

Similarly, the eigenfunctions remain distinct only for the orientations within a FZO. The corresponding assignment of IRs to the eigenmodes within a FZO is shown in Fig. 3.11(a) to 3.11(d).

As θ variation is continuous, the assignment of IR of $\overline{R_M}(\mathbf{k})$ to the eigenmodes of $\omega(\theta)$ can be done using compatibility relations. Compatibility relations between groups C_{6v} , C_{2v} and C_2 are given in Table A2 of App. A1 and the complete tables of compatibility relationships between crystallographic point groups can be obtained from Refs. 113-114.

In Fig. 3.11(a) (Γ point) when $\theta = 0$, $\overline{R_M}(\Gamma) = C_{2v}$ and the corresponding symmetry assignments at each band can be obtained from Fig. 3.5 at $r_c = 0.25$. For a small change in θ , $\overline{R_M}(\Gamma) = C_2$, the corresponding symmetry assignment can be done with the aid of compatibility relation between C_{2v} and C_2 [App. A1, Table A2]. Thereafter, a continuous variation of θ in $0 < \theta < 30^\circ$ causes the whole function of $\omega(\theta)$ ($0 < \theta < 30^\circ$) to possess the same IR, as such a variation of θ does not alter the group, $\overline{R_M}(\Gamma)$. As observed in Fig. 3.5 for $\omega(r_c)$ functions, if two $\omega(\theta)$ functions of different IRs cross, the bands exchange the symmetry at the intersection point. When $\theta = 30^\circ$, $\overline{R_M}(\Gamma) = C_{2v}$, the compatibility relations [App. A1, Table A2] show that a single IR of a group C_2 is compatible with more than one element of C_{2v} . Thus a numerical examination of the eigenfunction is also necessary in this case. The IR assignment of the other $\mathbf{k}$ -vector follows a similar approach and is presented within a FZO in Fig. 3.11(c) and 3.11(d). In Fig. 3.11(d), as $\overline{R_M}(L) = C_1$, all eigenmodes have an IR, A .

As we have mentioned in the last paragraph of Sec. 3.2, the equivalent orientations have rotated version of the eigenfunctions although the eigenmodes at equivalent orientations necessarily have the same characters. For instance, the eigenmodes of the band 3 at the equivalent orientations, $\theta = 0, 60^\circ$ and 120° are shown in Figure 3.12(a), (b) and (c) respectively. As we can see from these figures, all equivalent orientations have A_1 symmetry, but the eigenfunctions are rotated. When $\theta = 180^\circ$, $R_\theta = C_2 \in \overline{R_M}(\mathbf{k})$, $R_\theta \mathbf{H}_k(\mathbf{r}) = \mathbf{H}_k(\mathbf{r})$ and hence we have the same eigenfunction as when $\theta = 0$.

Fig. 3.12 Eigenmodes of equivalent orientations at the third band in a PC made of isotropic circular cylinders ($r_c = 0.25$ and refractive index = 3.5) in an uniaxial matrix medium (H – polarization, $\Delta n = 0.6$ and $\theta = 0$) at Γ point. (a) $\theta = 0$ and 180° (b) $\theta = 60^\circ$ (c) $\theta = 120^\circ$.

3.5. Summary and Discussion

This section summarizes the important results of the chapter and discusses how these results can be applied in the design of anisotropic PCs.

In Sec. 3.2, important symmetry groups that are relevant to anisotropic PCs were defined. The collection of all symmetry elements of the operator M in an

anisotropic PC with symmorphic space group, $\overline{G}_M$, can be expressed as $\overline{G}_M = \overline{T} \otimes \overline{R}_M$, where $\overline{R}_M$ is a subgroup of $\overline{R}$ ($\overline{R}_M = \overline{R} \cap \overline{R}_B$).

Sec. 3.3 discusses the symmetries in the wave equation and contains subsections devoted to theoretical formulations of IBZ and FZO of anisotropic PCs. Sec. 3.3.1 describes the IBZ of an anisotropic PC. The symmetry elements of group, $\overline{R}$ reduces the BZ to an IBZ. This IBZ is defined as the IBZ of the lattice. On the other hand, the symmetry elements of group $\overline{R}_M$ reduces BZ to the IBZ of the anisotropic PC. The relationship between IBZ of the lattice and IBZ of the anisotropic PC is defined through the coset expansion of $\overline{R}$ with respect to $\overline{R}_M$ and it is shown that the ratio of the size of the IBZ of the lattice to the size of the IBZ of the anisotropic PC must be an integer and equals to r/r_m . The IBZ of the lattice is fixed for a given lattice and can be found in the standard literatures and textbooks [113-114]. Once the IBZ of a lattice is known, we can obtain the IBZ of the anisotropic PC by transforming the wavevectors in the IBZ of the lattice using the r/r_m number of symmetry operations, R , where R is chosen from each coset of $\overline{R}$ expanded with respect to $\overline{R}_M$. The usefulness of an IBZ is well known as it defines the smallest zone of $\mathbf{k}$ -vectors in the reciprocal space for which the eigenvalues are unique. The complete information regarding photonic band gaps and EFSs can be obtained by only manipulating $\mathbf{k}$ -vectors within the IBZ. Therefore, the presented method to identify the IBZ of an anisotropic PC will be useful in the calculation of the photonic band gap [Chaps. 4 and 7] and EFS [Chaps. 6 and 8] of the anisotropic PC.

Sec. 3.3.2 introduced the concepts of orientational group and FZO. Orientational group, $\overline{R_\theta}$ consists of orientational symmetry operations, $R_\theta = R_M R$ with $R_M \in \overline{R_M}$ of general orientation and $R \in \overline{R(\mathbf{k})}$. If all possible orientations of motif are represented as a zone (an unit circle for a 2D PC and an unit sphere for a 3D PC), the existence of orientational symmetry reduces the zone to a FZO, where only the orientations within the FZO have unique eigenvalues [Eqn. 3.3]. The difference (and similarity) between IBZ and FZO of an anisotropic PC is that the IBZ of an anisotropic PC is a reduced zone of $\mathbf{k}$ -vectors (because of the symmetries in the $\overline{R_M}$), for which the eigenvalue of Eqn. 3.3 remain unique at a particular orientation of the motif, whereas FZO is a reduced zone of orientations (because of the symmetries in the $\overline{R_\theta}$), for which the eigenvalue of Eqn. 3.3 remain unique at a particular $\mathbf{k}$ -vector.

In the design of anisotropic PC's, FZO plays an important role. For example, optical properties such as curvatures of equal frequency surface near a particular $\mathbf{k}$ vector (important for dispersive effect such as superprism) and direction dependent band gaps (i.e. $\mathbf{k}$ – dependant) varies with the motif orientations, and therefore the range of orientations for which the optical properties remain unique is essentially governed by FZO. Hence, in applications like optimizing the band gap with respect to orientations of the anisotropic motif [30, 83, 96, Chap.7], FZO limits the unique orientations that could be explored for optimization. FZO also governs the symmetry seen in the EFS of an anisotropic for various orientation of motif. EFS of the anisotropic PC, centered at a particular $\mathbf{k}$ -point in the reciprocal space remains unique only for orientations within the FZO [see Sec. 8.3 of Chap. 8].

Sec. 3.4 discusses the symmetry of the eigenmodes in a 2D anisotropic PC with hexagonal lattice. In particular, we choose a structure with the matrix medium being uniaxially anisotropic with $\theta = 0$. We started with the discussion of labeling the system and symmetry representation in the absence of spatial modulation. Using Eqn. 3.20, the degenerate states at symmetrical $\mathbf{k}$ can be labeled using an integer m_{is} in the absence of spatial modulation and material's anisotropy. If material's anisotropy is present, the state with the label, m_{is} , will split into states that can be further identified with a label of $\sqrt{m_{anis}}$. Symmetry representation of each state labeled by a pair of integers $(m_{is}, \sqrt{m_{anis}})$ is described by a reducible representation which is independent of the strength of material's anisotropy (i.e. independent of r_n). The definition of m_{is} , m_{anis} and the possible values are described in Table 3.5 and 3.6 respectively.

The labeling system provides an analytical guideline in determining the degeneracy, explicit frequency levels, crossings between states, effect of material anisotropy to the splitting of degenerate states, and the representation of a degenerate state in the absence of spatial modulation. Apart from this, the labeling system and the integers (m_{is} and m_{anis}) help in getting analytical description for the evolution of the states in the presence of spatial modulation [Chap.5]. Furthermore, these integers derived from the free photon relationship of a PC and the corresponding degeneracy allow us to predict diffraction conditions and the number of diffracted spots (equals to degeneracy of the state) of a very weakly modulated anisotropic PC (i.e., diffraction grating) as the dispersion in such a structure is essentially free photon dispersion with the band folding effect taken into account. In

weakly modulated isotropic PC's, every m_{is} corresponds to a diffraction order. Following Eqn. 3.20, we can show that for isotropic PC ($r_n = 1$), the condition for the first order diffraction ($m_{is} = 1$) at the symmetrical $\mathbf{k}$ -point of hexagonal lattice is $3n^2\omega^2 > 2/3$, and there will be six diffracted spots (since the degeneracy of the state $m_{is} = 1$ is 6). The details of diffraction and the experiment for weakly modulated isotropic PCs have been presented previously based on Γ point [79]. In a weakly anisotropic PC [with uniaxial anisotropic matrix ($\theta = 0$)], the diffraction order must be identified with $(m_{is}, \sqrt{m_{anis}})$, and the corresponding diffraction condition will be $3n_y^2\omega^2 > c_1 m_{is} + c_2 (r_n^2 - 1)m_{anis} + \omega_c$ [Eqn. 3.20], and the degeneracy of the state $(m_{is}, \sqrt{m_{anis}})$ [Table 3.61 – 3.6.3] will be equal to the number of diffracted spots.

As the spatial modulation is switched on, the degenerate states in the absence of spatial modulation split into states which can be further labeled by the IRs of $\overline{R_M}(\mathbf{k})$. The degeneracy in the presence of spatial modulation is determined by the dimension of the IR that labels the eigenvalue. In this chapter we have presented the details of symmetry representation and the degeneracy for a 2D PC with circular air holes in the uniaxial matrix medium for a continuous variation of spatial modulation (i.e., r_c), material's anisotropy (i.e., Δn), and the orientation of the motif (i.e., θ). Understandings of symmetry representations of the eigenmodes of a PC have great importance as the coupling efficiency of light from an external source to the PC essentially depends on the eigenmode symmetry of the PC [120, 122-123]. The degeneracy in the presence of spatial modulation is very useful in engineering the band gap of an anisotropic PC [103-104, 106]. In Sec. 7.2 [Chap. 7], we will shall

present, how a removal of degeneracy can lead to opening of a large band gap in a materially anisotropic 2D PC.

Chapter 4

Solution Method I

4.1 Introduction

In Chap. 2, we have formulated the basic equations [Eqns. 2.3, 2.5, 2.13, 2.14, 2.17 and 2.19] for a PC from the fundamental Maxwell's equations. The next two chapters account for solution methods for the basic equations.

Various existing methods such as plane wave expansion method (PWM) [115,132-134], finite difference time domain (FDTD) [135-137], transfer matrix method (TMM) [138-141], finite element method (FEM) [57], scattering matrix method [142-144], multipole expansion method [145-147] and compact finite-difference frequency-domain method [147] were used to solve Eqns. 2.3, 2.5, 2.13, 2.14, 2.17 and 2.19 (i.e., basic equations) for the case of a PC with all isotropic materials. In this case, the tensor, $\tilde{\epsilon}_a$ [see Eqn. 2.7 of Chap. 2], reduces to an identity matrix multiplied by a dielectric constant. For PCs with anisotropic materials, the tensor, $\tilde{\epsilon}_a$ is generally not isotropic (i.e., cannot be reduced to a constant times an identity matrix) and therefore adds a complexity to the solution method.

Principally all method used for PCs with isotropic material can be extended for PCs with anisotropic materials as well. So far in the literature, PCs with anisotropic materials were studied using TMM [139], FDTD [107], FEM [148], and PWM [102, 106]. The TMM codes developed by Ming *et al.* [139] can handle 2D and 3D PCs with the principal axes of the anisotropic material is matched with the

coordinate system of the PC [i.e., a diagonal $\tilde{\epsilon}_a$]. More general orientations of the principal axes of the anisotropic material with non-diagonal $\tilde{\epsilon}_a$ were studied using FEM [148], FDTD [107] and PWM [106].

Though calculations based on FDTD shows good agreement with experiments [69-72], it is extremely time consuming. On the other hand PWM is computationally more efficient and has been widely used to study optical properties of a PC [115]. PWM has been used in computation of photonic band gaps [25-44], equal frequency surfaces for light refraction [67,150-151] and diffraction [152], Bragg transmittance and reflectance [153-154] and in the quantum optical calculations of a PC [155-156]. Further, experiments using PCs also showed good agreements with calculations based on the PWM [46, 61-62, 68, 97].

This chapter presents the PWM for a general anisotropic PC. In the second section of the chapter, the eigen-equations for PCs in three, two and one dimensions are formulated in the Fourier space. The third section illustrates the use of group theory in implementing the PWM and the fourth section discusses several numerical issues such as convergence and computation time in PWM. In the fifth section of the chapter, we present several case studies from literatures and compare the reported results with calculations based on the model established in this chapter.

4.2 Plane Wave Expansion

4.2.1 The general formulation

The solution for Eqn 2.5 (Chap. 2), can be obtained by formulating the eigen-equation in the Fourier space. The Fourier expansion for $\tilde{\kappa}(\mathbf{r}) = 1/\tilde{\epsilon}(\mathbf{r})$ is

$$\tilde{\kappa}(\mathbf{r}) = \sum_{\mathbf{G}} \tilde{\kappa}(\mathbf{G}) e^{j\mathbf{G}\cdot\mathbf{r}}, \quad [4.1]$$

in which $\tilde{\kappa}(\mathbf{G})$ takes the form,

$$\tilde{\kappa}(\mathbf{G}) = \begin{pmatrix} \kappa_{11}(\mathbf{G}) & \kappa_{12}(\mathbf{G}) & \kappa_{13}(\mathbf{G}) \\ \kappa_{21}(\mathbf{G}) & \kappa_{22}(\mathbf{G}) & \kappa_{23}(\mathbf{G}) \\ \kappa_{31}(\mathbf{G}) & \kappa_{32}(\mathbf{G}) & \kappa_{33}(\mathbf{G}) \end{pmatrix}. \quad [4.2]$$

If all the materials in the PC are isotropic then, $\kappa_{11}(\mathbf{G}) = \kappa_{22}(\mathbf{G}) = \kappa_{33}(\mathbf{G}) = \kappa(\mathbf{G})$ and $\kappa_{12}(\mathbf{G}) = \kappa_{21}(\mathbf{G}) = \kappa_{13}(\mathbf{G}) = \kappa_{31}(\mathbf{G}) = 0$. The magnetic field function which is a Bloch function of wavevector- $\mathbf{k}$, also can be expanded in terms of plane waves as

$$\mathbf{H}_{\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{G}} \mathbf{H}_{\mathbf{k}}(\mathbf{G}) e^{j(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}}, \quad [4.3]$$

where the plane wave condition is satisfied by a requirement $\mathbf{H}_{\mathbf{k}}(\mathbf{G}) \cdot (\mathbf{k} + \mathbf{G}) = 0$.

This enables us to write $\mathbf{H}_{\mathbf{k}}(\mathbf{G})$ as

$$\mathbf{H}_{\mathbf{k}}(\mathbf{G}) = h_{1,\mathbf{k}}(\mathbf{G}) \mathbf{e}_1 + h_{2,\mathbf{k}}(\mathbf{G}) \mathbf{e}_2, \quad [4.4]$$

where $\mathbf{e}_1$ and $\mathbf{e}_2$ are the unit vectors that define the plane perpendicular to $\mathbf{k}+\mathbf{G}$, and

$h_{1,\mathbf{k}}(\mathbf{G})$ and $h_{2,\mathbf{k}}(\mathbf{G})$ are the components along $\mathbf{e}_1$ and $\mathbf{e}_2$ respectively. Using Eqn. 4.1,

4.3 and 4.4, we can reformulate Eqn. 2.5 in the Fourier space as,

$$\sum_{\mathbf{G}'} M(\mathbf{G}, \mathbf{G}') \begin{bmatrix} h_{1,\mathbf{k}}(\mathbf{G}') \\ h_{2,\mathbf{k}}(\mathbf{G}') \end{bmatrix} = \Omega(\mathbf{k}) \begin{bmatrix} h_{1,\mathbf{k}}(\mathbf{G}) \\ h_{2,\mathbf{k}}(\mathbf{G}) \end{bmatrix} \quad [4.5]$$

with

$$M(\mathbf{G}, \mathbf{G}') = |\mathbf{k} + \mathbf{G}| |\mathbf{k} + \mathbf{G}'| \begin{bmatrix} \mathbf{e}_2 \cdot \tilde{\mathbf{K}}_H(\mathbf{G} - \mathbf{G}') \cdot \mathbf{e}'_2 & -\mathbf{e}_2 \cdot \tilde{\mathbf{K}}_H(\mathbf{G} - \mathbf{G}') \cdot \mathbf{e}'_1 \\ -\mathbf{e}_1 \cdot \tilde{\mathbf{K}}_H(\mathbf{G} - \mathbf{G}') \cdot \mathbf{e}'_2 & \mathbf{e}_1 \cdot \tilde{\mathbf{K}}_H(\mathbf{G} - \mathbf{G}') \cdot \mathbf{e}'_1 \end{bmatrix}. \quad [4.6]$$

We can normalize Eqn. 4.5 by dividing both sides of the equation with $2\pi/a$, where a is the period of the PC, to give,

$$\sum_{\mathbf{G}'} M(\mathbf{G}, \mathbf{G}') \begin{bmatrix} h_{1,\mathbf{k}}(\mathbf{G}) \\ h_{2,\mathbf{k}}(\mathbf{G}) \end{bmatrix} = \omega^2(\mathbf{k}) \begin{bmatrix} h_{1,\mathbf{k}}(\mathbf{G}) \\ h_{2,\mathbf{k}}(\mathbf{G}) \end{bmatrix}. \quad [4.7]$$

It is important to note that the vectors $\mathbf{k}$ and $\mathbf{G}$ in the formulation of $M(\mathbf{G}, \mathbf{G}')$ in Eqn. 4.7 have units $2\pi/a$ whereas ω is dimensionless and equals to a/λ , where λ is the free space wavelength.

4.2.2 Formulation for a 2D structure

The vectors $\mathbf{k} + \mathbf{G}$, $\mathbf{e}_1$ and $\mathbf{e}_2$ are shown in Figure 4.1 for an in-plane propagation in a 2D structure.

Fig. 4.1 The 2D periodic plane with the vectors $\mathbf{k} + \mathbf{G}$, $\mathbf{e}_1$ and $\mathbf{e}_2$.

The vector $\mathbf{k} + \mathbf{G}$ is confined to be in the x - y plane and hence, the unit vector $\mathbf{e}_1$ can be taken as oriented perpendicular to the x - y plane. Unit vector $\mathbf{e}_2$ is on the same plane with $\mathbf{k} + \mathbf{G}$ but orthogonal to it. Thus for E and H -polarization, $\mathbf{H}_{\mathbf{k}}(\mathbf{G})$ in Eqn. 4.4

simplifies to $h_{1,\mathbf{k}}(\mathbf{G})\mathbf{e}_1$ and $h_{2,\mathbf{k}}(\mathbf{G})\mathbf{e}_2$ respectively. Using this simplification, and employing Eqn. 4.1 and 4.3, we can write Eqn. 2.13 and 2.14 as

$$\sum_{\mathbf{G}'} M(\mathbf{G}, \mathbf{G}') h_{\mathbf{k}}(\mathbf{G}') = \omega^2(\mathbf{k}) h_{\mathbf{k}}(\mathbf{G}), \quad [4.8]$$

where we have neglected the subscripts (1, $\mathbf{k}$) and (2, $\mathbf{k}$) for easy notations. The definition of M in Eqn. 4.8 is

$$M(\mathbf{G}, \mathbf{G}') = \kappa_E(\mathbf{G} - \mathbf{G}') |\mathbf{k} + \mathbf{G}| |\mathbf{k} + \mathbf{G}'| \quad [4.9]$$

and

$$M(\mathbf{G}, \mathbf{G}') = |\mathbf{k} + \mathbf{G}| |\mathbf{k} + \mathbf{G}'| \{ \mathbf{e}_2 \cdot \tilde{\kappa}_H(\mathbf{G}_i - \mathbf{G}_j) \cdot \mathbf{e}'_2 \} \quad [4.10]$$

for E - and H -polarization respectively. In these equations, $\kappa_E(\mathbf{G}) = \kappa_{33}(\mathbf{G})$ and

$$\tilde{\kappa}_H(\mathbf{G}) = \begin{pmatrix} \kappa_{11}(\mathbf{G}) & \kappa_{12}(\mathbf{G}) \\ \kappa_{21}(\mathbf{G}) & \kappa_{22}(\mathbf{G}) \end{pmatrix} \quad [4.2a]$$

are the Fourier coefficients of $\kappa_E(\mathbf{r}) = 1/\varepsilon_E(\mathbf{r})$ and $\tilde{\kappa}_H(\mathbf{r}) = 1/\tilde{\varepsilon}_H(\mathbf{r})$ respectively [Sec. 2.3][▼]. If $\mathbf{G} = \mathbf{G}_i$ and $\mathbf{G}' = \mathbf{G}_j$, then Eqn. 4.9 and 4.10 can be written in terms of indices i and j as,

$$M_{ij} = \kappa_E(\mathbf{G}_i - \mathbf{G}_j) |\mathbf{k} + \mathbf{G}_i| |\mathbf{k} + \mathbf{G}_j| \quad [4.11]$$

and

$$M_{ij} = |\mathbf{k} + \mathbf{G}_i| |\mathbf{k} + \mathbf{G}_j| \{ \mathbf{e}_i \cdot \tilde{\kappa}_H(\mathbf{G}_i - \mathbf{G}_j) \cdot \mathbf{e}_j \} \quad [4.12]$$

respectively. Here, $\mathbf{e}_i$ ($\mathbf{e}_j$) is the $\mathbf{e}_2$ vector corresponds to $\mathbf{k} + \mathbf{G}_i$ ($\mathbf{k} + \mathbf{G}_j$). The use of i and j simplifies Eqn. 4.8 as

$$\sum_i M_{ij} h_i = \omega^2 h_j. \quad [4.13]$$

▼ If all the materials are isotropic, then we have $\kappa_E(\mathbf{G}) = \kappa(\mathbf{G})$ and Eqn. 4.2a becomes $\kappa(\mathbf{G})$ multiplies a two by two identity matrix.

4.2.2 Formulation for a 1D structure

Following similar procedures as for a 2D structure, it can be shown that both Eqn. 2.17 and 2.19 for an 1D structure can be formulated to a form of Eqn. 4.13 in the Fourier space. However the matrix element for the o and e -polarization of a 1D structure, are

$$M_{ij} = \kappa_o(\mathbf{G}_i - \mathbf{G}_j) \|\mathbf{k} + \mathbf{G}_i\| \|\mathbf{k} + \mathbf{G}_j\| \quad [4.14]$$

and

$$M_{ij} = \kappa_e(\mathbf{G}_i - \mathbf{G}_j) \|\mathbf{k} + \mathbf{G}_i\| \|\mathbf{k} + \mathbf{G}_j\| \quad [4.15]$$

respectively. In these equations $\kappa_o(\mathbf{G})$ and $\kappa_e(\mathbf{G})$ are the Fourier coefficients of $\kappa_o(x) = 1/\varepsilon_E(x)$ and $\kappa_e(x) = 1/\varepsilon_{eff}(\alpha, x)$ respectively [Sec. 2.4].

4.3 Photonic Band Structures

In order to plot a dispersion relation (i.e., ω versus $\mathbf{k}$), the eigen equations in the Fourier space must be solved for a range of $\mathbf{k}$ vectors, $[\mathbf{k}_i]$. For applications involving manipulations of band gap, it is typically sufficient to consider only the wavevectors along the boundary of the IBZ of a PC. In this case the dispersion can be plotted using 1D plot (i.e., 1D band structure) with the horizontal axis and vertical axis representing the path along the boundary of the IBZ and ω respectively. However, for computations of equal frequency surfaces, it is often required to have a full description of the dispersion. Therefore, it is necessary to have solutions with range of $\mathbf{k}$ -vectors covering the entire IBZ. The visualization of such a dispersion in a 2D PC requires a two-dimensional plot (i.e., 2D band structure) as the in-plane

problems involve 2D $\mathbf{k}$ -vectors. Examples of 2D band structures for a 2D PC appear in Chap. 6.

For a 3D PC, the representation of full description of the dispersion is more complicated as it involves 3D $\mathbf{k}$ -vectors. One way of visualizing a 3D dispersion is by having three axes for k_x , k_y and k_z with ω represented as a variation in color.

Group theory assisted calculations

As we have mentioned in Chap. 3, the orientation of motif changes the definition of the IBZ in an anisotropic PC, whereas in isotropic PC the orientation is irrelevant and therefore, we have a fixed IBZ. Assuming the ranges of $\mathbf{k}$ vectors in an isotropic PC and an anisotropic PC of a same lattice to be $[\mathbf{k}_i]_{is}$ and $[\mathbf{k}_i]$ respectively, from the discussion of Sec. 3.3.1, we know that

$$[\mathbf{k}_i] = R_1[\mathbf{k}_i]_{is} + R_2[\mathbf{k}_i]_{is} + \dots + R_{r/r_m}[\mathbf{k}_i]_{is} \quad [4.16]$$

Using Eqn. 4.16, we can implement a numerical scheme for manipulations of band gaps and photonic band structures. Figure 4.2 shows the flow chart for the implementation of a numerical scheme to solve the eigen-equations [Eqns. 4.6 and 4.8]. The first part of a numerical scheme contains the definitions of basic parameters which includes the lattice parameters, $\mathbf{G}$ vectors, dielectric tensor of the materials and the geometry of the unit cell. Loop 1 diagonalize the matrix M in order to obtain the eigenvalues and therefore the value of ω for all wavevectors, $\mathbf{k}_i \in [\mathbf{k}_i]_{is}$. Loop 1 includes a nested loop, Loop 2 where this loop evaluate ω for each $R_j \mathbf{k}_i$ [$j = 1, 2, \dots, r/r_m$]. Alternatively, in Loop 2 instead of finding the eigenvalues for each $R_j \mathbf{k}_i$, we can fix the wavevector to be $\mathbf{k}_i$, but diagonalize the matrix $R_j^{-1} M R_j$ for each R_j . The

second method has an advantage as it does not require the knowledge of group theory (cosets). A simple coding can accomplish the task to find all the distinct $R_i^{-1}MR_i$. The evaluation of $R_j^{-1}MR_j$ is straightforward, from the fact [see Ref. 115 for a proof]

$$R_j^{-1}MR_j = R_j^{-1}M[\tilde{\epsilon}(\mathbf{r})]R_j = M[R_j^{-1}\tilde{\epsilon}(\mathbf{r})R_j], \quad [4.17]$$

where $M[\tilde{\epsilon}(\mathbf{r})]$ and $M[R_j^{-1}\tilde{\epsilon}(\mathbf{r})R_j]$ represent M as a function of $\tilde{\epsilon}(\mathbf{r})$ and $R_j^{-1}\tilde{\epsilon}(\mathbf{r})R_j$ respectively. Hence, the task in Loop 2 is just performing diagonalizations of matrix M with distinct $R_j^{-1}\tilde{\epsilon}(\mathbf{r})R_j$. The task gets further simplified if the problems involves materially anisotropic PCs, where $R_j^{-1}\tilde{\epsilon}(\mathbf{r})R_j$ becomes $R_j^{-1}\tilde{\epsilon}_a R_j$.

Fig. 4.2 Numerical scheme for the calculations of photonic band structures in anisotropic PCs.

4.4 Numerical Issues

In general, the accuracy of PWM in evaluating the dispersion of PC is better with an increase in the number of plane waves. Structural parameters of a PC affect the rate of convergence in PWM and particularly the following:

- The shape of the unit cell - geometrical motif with a sharp edge requires more plane waves than the one with a smooth edge.
- Spatial modulation: The required number of plane waves for convergence increases with the strength of the spatial modulation (i.e., refractive index contrast and the filling ratio)

Apart from the structural parameters, the way of obtaining the coefficients $\tilde{\kappa}(\mathbf{G})$ significantly affects the convergence rate [133]. In a direct method [114,133-134], we first evaluate the inverse of $\tilde{\epsilon}(\mathbf{r})$, $\tilde{\kappa}(\mathbf{r})$ and then take their Fourier transform to find $\tilde{\kappa}(\mathbf{G})$. The alternate method (Ho's method) [36,133-134], reverses the inverse and Fourier transform operations in the direct method [i.e., evaluate $\tilde{\epsilon}(\mathbf{G})$ from $\tilde{\epsilon}(\mathbf{r})$ and invert it to obtain $\tilde{\kappa}(\mathbf{G})$]. Though the operations, inverse and Fourier transform commute for an ideal case with an infinite number of plane waves, the deviation in the results of these two methods is very significant for a finite and a small number of plane waves. The convergence rate of the direct and Ho's method can be seen from the specific example [133] presented in Figure 4.3 and as we can see readily from the figure, Ho's method provides a fast convergence compared to the direct method.

Besides, the convergence rate also depends on the $\mathbf{k}$ -vector and if polarizations can be decoupled, it also depends on the type of polarization. In 2D

structures where we can decouple the polarizations, H -polarization requires more plane waves than the E -polarization and this is due the vector nature of eigen equations of H -polarization [Eqn. 4.12].

Fig. 4.3 Convergence rate with Ho's and direct method. Relative error is defined to relative to converged value. Calculations were performed for-2D hexagonal lattice PC with other parameters as defined in [133].

Fig. 4.4 Computation time for a single $\mathbf{k}$ vector of a triangular lattice PC with air columns. Key: blue markers- computed result, red solid line – fitted result

Although the accuracy can be increased by increasing the number of plane waves, the increment enlarges the size of M and hence, consumes a considerable amount of time for diagonalization. The amount of time required for single

execution of loop 2 [Fig. 4.2] is presented in Figure 4.4^{♥*} as a function of n_{grid} {Number of plane waves = $(2n_{grid} + 1)^2$ [132]}. The computed time in Fig. 4.4 has an exponential dependence according to $a_1 \exp(a_2 n_{grid})$ with $a_1 = 0.124$ and $a_2 = 0.3868$. Thus, an increase in the number of plane waves increases the amount of computation time very significantly. The computation time becomes very expensive when the number of $\mathbf{k}$ -vectors is large.

As an example, we consider the typical procedure of obtaining an equal frequency surface (EFS). EFS in a 2D PC is obtained by projecting a 2D band structure onto the reciprocal plane (k_x, k_y) at a constant ω (i.e., contour in the reciprocal space with a constant frequency). Therefore, in order to numerically calculate the EFS, we need to have the details of the dispersion for a dense grid of $\mathbf{k}$ -vectors. For a grid with 10 000 $\mathbf{k}$ vectors the required computation time [based on Fig. 4.4] with $n_{grid} = 7, 10$ and 14 are 2.4, 14.7 and 79.5 hours respectively.

For all simulation in this thesis we have used $n_{grid} = 10$ (441 plane waves) [unless stated otherwise] and the convergence accuracy for the first six bands is estimated to be better than 1%. Similar accuracy values are also used in Refs. 29-33, 133 and 134.

[♥] The computations is performed using a computer with specifications: Intel Pentium 4, 3.2 GHz, RAM: 512MB Microsoft Windows XP. The program was written in MATLAB [132]. ^{*} The parameters of the PC is the same as in Fig. 4.3 [133].

4.5 Examples

In this section we compare the results obtained from the method presented in this chapter (i.e., PWM), with experimental results and results obtained using other methods.

4.4.1 Geometrically anisotropic PC

Moussa *et al.* [69] experimentally studied a geometrically anisotropic 2D PC as shown in Figure 4.5 for applications in microwaves regime (with frequencies around 6.5 GHz).

Fig 4.5 (left) The geometry of the 2D PC considered by Moussa *et al.* [69] (right) The 2D PC constructed by Moussa *et al.* using alumina bars

The 2D PC is made of rectangular alumina bars (dielectric constant = 9.61) in air and has specifications, $a = 1.59$, $r_x = 0.4a$ and $r_y = 0.8a$ with the length of the bar (in the axis perpendicular to the periodic plane) equals to 45.72 cm. The measured transmission spectrum for E -polarization, along the Γ -M direction is shown in Figure 4.6(a), whereas the result obtained from calculations based on the method presented

in the chapter (i.e., PWM) for the same configuration is shown in Fig. 4.6(b). As we can readily verify from the figure, the experimental result shares a good agreement with the calculated result.

Fig. 4.6 (a) Measured transmission spectrum (E -polarization) along the Γ -M direction [69] for the PC in Fig. 4.5. (b) The band structure for E -polarization along the Γ -M direction, calculated using the model presented in this chapter for the PC in Fig. 4.5. The text boxes in the figure indicate the band gap frequencies.

4.4.2 Materially anisotropic PC

Comparison with FEM

Hsu *et al.* [148] theoretically studied a materially anisotropic 2D PC using FEM. The studied PC consists of circular dielectric rods (dielectric constant = 11.56) in a LC ($n_o = 1.53$ and $n_e = 1.71$) background. Such a structure has a potential

application as a tunable filter [95]. The schematic of the considered structure is shown in Figure 4.7(a) with LC molecules are represented as ellipses.

Fig. 4.7 (a) Schematic of the structure considered by Hsu *et al.* [148] (b) Calculated photonic band structure of H -polarization (PWM) for the structure in (a) with $\alpha = 30^\circ$ and $r_c = 0.2a$ along $\Gamma(0,0) - X(0,\pi/a) - M(\pi/a,\pi/a) - \Gamma$ [orange lines], $\Gamma(0,0) - X(0,-\pi/a) - M(-\pi/a,-\pi/a) - \Gamma$ [blue lines].

The LC molecules is oriented parallel to the periodic plane, with an angle α with respect to the x -axis [see Fig. 4.7(a)]. We calculate the photonic band structure of H -polarization for the structure in Fig. 4.7(a) for $\alpha = 30^\circ$ and $r_c = 0.2a$, and the result is shown in Figure 4.7(b). This figure has a very good agreement with Figure 5(b)[♥] of Ref. 148 (authored by Hsu *et al.*) which was calculated using FEM.

Comparison with TMM

Bell *et al.* [137-138] developed a numerical method based on TMM for calculation of transmission spectrums of the PCs. The documentation of the numerical method and the source code can be downloaded from the program library of the journal of computer physics communication [137]. The method has been

[♥] The figure [Fig. 5(b) of Ref. 148] is not reproduced here as it has an exact match with Fig. 4.7(b).

There are no numerical values provided in Ref. 148 in order to compare the results quantitatively.

verified experimentally [see Ref. 14, 137, 138 and the references therein]. This method is used to simulate the structure studied by Hsu *et al.* [148] with specifications as in Fig. 4.7(b), but the orientations of the LC molecules were taken as being perpendicular to the 2D periodic plane[♣].

Fig. 4.8 (a)Band structure (Γ -X direction) of *E*-polarization calculated using PWM for the structure studied by Hsu *et al.* [148]. (b)The corresponding transmission spectrum for (a) calculated using TMM [137]. (c)Similar to (a) but for *H*-polarization. (d)Similar to (b) but for *H*-polarization

[♣] The software [137] only can handle this orientation of the anisotropic material.

The band structure [$\Gamma(0,0)$ - $X(\pi/a,0)$ direction] of E -polarization calculated using the model presented in this chapter is shown in Figure 4.8(a), whereas the transmission spectrum (Γ - X direction) of E -polarization calculated using the TMM [137] is shown in Figure 4.8(b). Results of similar PWM and TMM calculations for H -polarization are shown in Figures 4.8(c) and 4.8(d) respectively. In all TMM calculations we assumed 64 layers in the Γ - X direction and the transmissions were calculated for normalized frequencies from 0 to 0.81 in a step of 0.0027. As we can readily verify from Figs. 4.8(a)-4.8(d) results obtained from both FDTD and PWM share good agreements. For E -polarization, the mid values of the first band gap and the second band gap in Fig. 4.8(a) differ by only 0.65% and 0.75% respectively compared to the respective band gaps in Fig. 4.8(b). On the other hand, for H -polarization, the mid values of the first band gap and the second band gap in Fig. 4.8(c) differ by only 0.04% and 0.13% respectively compared to the respective band gaps in Fig. 4.8(d).

4.6 Summary

In this chapter, we have presented a solution method based on the PWM technique for the basic equations presented in Chap. 2. The numerical scheme and the use of group theory in the implementation were discussed in Secs. 8.2 and 8.3. The convergence of the PWM and the required time for computations were highlighted in Sec. 8.4. Sec. 8.5 of the chapter presented several case studies from the literatures and compared the reported results with calculations based on the model established in Secs. 8.2 and 8.3.

Chapter 5

Solution Method II

5.1 Introduction

In the photonic band structure calculation, the conventional PWM [13,114,132-134] is quite often modified (or extended) to handle specific PC structures or to increase the rate of convergence [149,157-160]. This includes the use of supercell techniques in modeling defects in PC [157-158], the extension to include the effect of the interface [159], augmented PWM for PCs with spherical and cylindrical motifs [160], and the use of fast factorization rules in PWM [149].

Unfortunately none of these modifications in PWM or those of other methods is simple, as they all involve numerical methods without any analytical details or a formula-like description. For example the solution in PWM is found by diagonalizing a very large matrix with the size determined by the number of plane waves. The typical number of plane waves used in PWM calculations for PCs with large modulation ranges from $\sim 10^2$ to $\sim 10^3$ [25-26,67,133-134]. For structures with small (but finite) spatial modulation, though they consume a slightly smaller number of plane waves the approach still fails to provide any useful analytical details.

To handle this main difficulty, in this chapter we present a systematic and generalized solution based on a PWM for 2D PCs. In order to illustrate the approach, the examples in the chapter have been specialized to a PC with an hexagonal lattice.

We first analyze the photonic states in the limit of zero modulation (i.e., free photon relationship) for a 2D PC with isotropic materials and we have introduced a systematic classification system based on integers for the states with distinct frequencies. These integers can be factored and states with the same factor can be categorized as they have the same form of solution when the spatial modulation or/and the material's anisotropy is switched on. As we shall show, such states can be easily solved with a reduced matrix size and typically lead to analytical equations within a small (however a finite) spatial modulation approximation.

The presented method is useful in the applications which exploit the unusual conducting properties of a PC, where properties such as superprisms, supercolimation, beam splitting etc. are only well pronounced in PCs with small spatial modulation [64,161-163]. Further in such PC structures, the method can be applied to obtain a fairly accurate solution for the insulating properties (i.e., band gaps). In a large refractive index contrast PC, the presented method likely leads to a deviated result, but the method surely serves a good approximation and produces necessary analytical details such as degeneracy of the state and the properties of a free photon behavior at the band edges.

5.2. States in the absence of spatial modulation

5.2.1 The general dispersion relation

In the absence of a spatial modulation, only the Fourier coefficient, $\tilde{\kappa}(0)$, $\tilde{\kappa}_H(0)$, and $\kappa_E(0)$ (Sec. 4.2) are nonzero. Therefore, Eqn. 4.10 and 4.9 (Chap. 4) reduce to

$$\omega^2 = (\mathbf{k} + \mathbf{G}) \cdot \tilde{\kappa}_H(0) \cdot (\mathbf{k} + \mathbf{G}) \quad [5.1]$$

and

$$\omega^2 = \kappa_{33}(0) |\mathbf{k} + \mathbf{G}|^2. \quad [5.2]$$

respectively. If the materials are isotropic, then for both E and H -polarizations, we have the same dispersion relation in the absence of the spatial modulation,

$$\omega^2 = \kappa_0 |\mathbf{k} + \mathbf{G}|^2 \quad [5.3]$$

where $\kappa_0 = \kappa(0)$.

A general form of $\tilde{\kappa}_H(0)$ requires a general orientation for the two orthogonal principal axes of the anisotropic material on the periodic plane (as mentioned earlier, another principal axis is assumed to be perpendicular to the periodic plane), and therefore $\tilde{\kappa}_H(0) = Q^T \tilde{\kappa}_p Q$ where $\tilde{\kappa}_p = \text{diag}(1/\varepsilon_x, 1/\varepsilon_y)$, Q is clockwise rotational operator at an angle β , Q^T is the transpose of Q , and ε_x and ε_y are the principal dielectric constants of the anisotropic material. Consequently, Eqn. 5.1 (H -polarization) in the rotated bases, can be written as $\omega^2 = (Q\mathbf{k} + Q\mathbf{G}) \cdot \tilde{\kappa}_p \cdot (Q\mathbf{k} + Q\mathbf{G})$. Assuming $\mathbf{k} = k[\cos(\theta), \sin(\theta)]$, in the coordinate system, (k_x, k_y) , Eqn. 5.1 can be further reformulated to [Appendix C1],

$$\varepsilon_x \omega^2 = G^2 + k(k + 2G \cos(\theta - \alpha_T)) + (r_\varepsilon - 1)(k \sin(\theta + \beta) + G \sin(\alpha_T + \beta))^2 \quad [5.4]$$

where $r_\varepsilon = \varepsilon_x / \varepsilon_y$, α_Γ is the angle between $\mathbf{G}$ vector and k_x – axis of the reciprocal plane, and k and G are the magnitude of $\mathbf{k}$ and $\mathbf{G}$ respectively. Eqn. 5.4 is a general form of the free photon dispersion relation in any two-dimensional lattice. Equation for E -polarization in the case of a 2D PC with an anisotropic material or for both polarizations in the case of a 2D PC with isotropic materials, can be obtained from Eqn. 5.4 by setting $r_\varepsilon = 1$,

$$\varepsilon_a \omega^2 = G^2 + k(k + 2G \cos(\theta - \alpha_\Gamma)) \quad [5.5].$$

where for the first case we have $\varepsilon_a = 1 / \kappa_{33}(0)$ (i.e., principal dielectric constant correspond to the principal axis that is lying perpendicular to the periodic plane) and for the latter we have $\varepsilon_a = \varepsilon_{is} = 1 / \kappa_0$.

The discretization of ω comes from the fact that G and α_Γ take discrete values. The degeneracy of the state for a specific ω , in the absence of the spatial modulation equals to the number of $\mathbf{G}$ vectors that produce the same value of ω (Eqns. 5.4-5.5). The reciprocal lattice vector, $\mathbf{G}$ of any two-dimensional lattice can be written in terms of unit vectors $\mathbf{b}_1$ and $\mathbf{b}_2$ as $\mathbf{G} = n_1 \mathbf{b}_1 + n_2 \mathbf{b}_2$, with n_1 and n_2 being any integers.

Fig. 5.1 Vectors $\mathbf{b}_1$, $\mathbf{b}_2$, $\mathbf{k}$, $\mathbf{G}$ and $\mathbf{k}+\mathbf{G}$ for an hexagonal lattice in the k_x - k_y axes. The pair (n_1, n_2) indexes each reciprocal lattice point as $\mathbf{G} = n_1 \mathbf{b}_1 + n_2 \mathbf{b}_2$.

The angle between $\mathbf{k}+\mathbf{G}$ vector and k_x – axis of the reciprocal space is denoted as $\alpha_{\mathbf{k}}$, whereas the angle between $\mathbf{b}_1$ ($\mathbf{b}_2$) vector with k_x – axis is denoted as α_{b_1} (α_{b_2}). The vectors for hexagonal lattice, $\mathbf{b}_1 = (1, -1/\sqrt{3})$, $\mathbf{b}_2 = (0, 2/\sqrt{3})$, $\mathbf{k}$, $\mathbf{G}$ and $\mathbf{k}+\mathbf{G}$ together with the k_x - k_y axes are shown in Figure 5.1 (all vectors have unit $2\pi/a$).

5.2.2 Dispersion relation at symmetrical points

Eqns. 5.4-5.5 often can be simplified for symmetrical $\mathbf{k}$ vectors and symmetrical orientations of principal axes of the anisotropic material. In this section, we discuss such simplifications for PCs with isotropic materials either in a square or an hexagonal lattice. For symmetrical points of such lattice, we can always write Eqn. 5.5 as,

$$\varepsilon_{is} \omega^2 = |\mathbf{k} + \mathbf{G}|^2 = c_{\mathbf{k}} m_{\mathbf{k}} \quad [5.6]$$

where $m_{\mathbf{k}}$ is an integer and $c_{\mathbf{k}}$ is a constant. The expressions for symmetrical points of an hexagonal lattice, $\mathbf{k}(k, \theta) = \Gamma(0,0)$, $K(2/3, 0)$ and $M(1/\sqrt{3}, 90^\circ)$ are tabulated in Table 5.1. The integer $m_{\mathbf{k}}$ in Eqn. 5.6 takes only specific values and allows us to label the state of a distinct ω with an integer label, $m_{\mathbf{k}}$.[♥] The degeneracy of the state, $n(m_{\mathbf{k}})$ can then be taken as the number of possible combinations of n_1 and n_2 that lead to the same $m_{\mathbf{k}}$. Using the angle, $\alpha_{\mathbf{k}}$, we can write $m_{\mathbf{k}}$ either in n_1 or n_2 alone. As such $m_{\mathbf{k}}$ decomposes into [Appendix C2],

[♥] This labeling system is consistent with the one introduced in Sec. 3.4.1. The consistency can be checked by comparing Table 3.5 (Chap. 3) with the Table 5.1. The m_{is} value in Table 3.5 for Γ , K and M points is respectively $m = n_1^2 + n_2^2 - n_1 n_2$, $m + n_1$, and $2m + 2n_2 - n_1$. These m_{is} expressions appear again in the expressions of m_{Γ} , m_K and m_M (Table 5.1). The additional linear coefficients in Table 5.1 are results of re-arrangement of Eqn. 3.20 (Chap. 3) and required for the factorization in Eqn. 5.7.

$$m_{\mathbf{k}} = q(\alpha_{\mathbf{k}}, \alpha_{bi}) p_{\mathbf{k}}(n_j) \quad [5.7]$$

where $i, j = 1, 2$ or $2, 1$, $p_{\mathbf{k}}$ is independent of $\alpha_{\mathbf{k}}$ but depends either on n_1 or n_2 , and

$$q(\alpha_{\mathbf{k}}, \alpha_{bi}) = \operatorname{cosec}^2(\alpha_{\mathbf{k}} - \alpha_{bi}), \quad \alpha_{\mathbf{k}} \neq \alpha_{bi} \quad [5.8]$$

in which $i = 1$ or 2 . Eqn. 5.7 allows us to categorize a set of parallel $\mathbf{k}+\mathbf{G}$ vectors with the same $\alpha_{\mathbf{k}}$ (and hence the same q). Therefore, the expressions for distinct $m_{\mathbf{k}}$ s of the same $\alpha_{\mathbf{k}}$ will be similar with the differences only in $p_{\mathbf{k}}$, representing the relative differences in the length of the $\mathbf{k}+\mathbf{G}$ vectors. If we define $p_{\mathbf{k},s}$ and $m_{\mathbf{k},s}$ to be the smallest value among the values of $p_{\mathbf{k}}$ and $m_{\mathbf{k}}$ of the same $\alpha_{\mathbf{k}}$, then we can define a useful ratio, $p_{\alpha_{\mathbf{k}}} = \sqrt{p_{\mathbf{k}} / p_{\mathbf{k},s}} = \sqrt{m_{\mathbf{k}} / m_{\mathbf{k},s}}$ to define any vector $\mathbf{k}+\mathbf{G}$ with angle $\alpha_{\mathbf{k}}$ as $\mathbf{k}+\mathbf{G} = p_{\alpha_{\mathbf{k}}}(\mathbf{k}+\mathbf{G})_s$, where $(\mathbf{k}+\mathbf{G})_s$ is the shortest among the $\mathbf{k}+\mathbf{G}$ vectors with an angle $\alpha_{\mathbf{k}}$.

For hexagonal lattice $\alpha_{b1} = -30^\circ$, $\alpha_{b2} = 90^\circ$ (Fig. 5.1), and the expressions for $\alpha_{\mathbf{k}}$, q and $p_{\mathbf{k}}$ are tabulated in Table 5.1.

Table 5.1 – The expressions $c_{\mathbf{k}}$, $m_{\mathbf{k}}$, $\alpha_{\mathbf{k}}$, and $p_{\mathbf{k}}$ for symmetrical $\mathbf{k}$ -points of an hexagonal lattice. Key: $m = n_1^2 + n_2^2 - n_1 n_2$

$\mathbf{k}$	$c_{\mathbf{k}}$	$m_{\mathbf{k}}$	$\sin(\alpha_{\mathbf{k}})$	$p_{\mathbf{k}}$	
				$p_{\mathbf{k}}(n_1)$	$p_{\mathbf{k}}(n_2)$
Γ	$\frac{4}{3}$	m	$\frac{2n_2 - n_1}{\sqrt{3c_{\Gamma}m_{\Gamma}}}$	$\frac{3}{4}n_1^2$	$\frac{3}{4}n_2^2$
K	$\frac{4}{9}$	$3(m + n_1) + 1$	$\frac{2n_2 - n_1}{\sqrt{3c_Km_K}}$	$\frac{1}{4}(2 + 3n_1)^2$	$\frac{1}{4}(1 + 3n_2)^2$
M	$\frac{1}{3}$	$2(2m + 2n_2 - n_1) + 1$	$\frac{2n_2 - n_1 + 1}{\sqrt{3c_Mm_M}}$	$3n_1^2$	$\frac{3}{4}(1 + 2n_2)^2$

Figure 5.2 give a visualization of the states [with indices m_k , $n(m_k)$, and α_k] using Eqn. 5.6 in the absence of a spatial modulation for Γ point of the hexagonal lattice. By multiplying p_k in Table 5.1 with the q , and forcing the result to be an integer, we could systematically rewrite the expressions for m_k of the same q in terms of a free integer, h_k (i.e., independent of n_1 and n_2).

Fig. 5.2 Degenerate states in the absence of the spatial modulation and material's anisotropy at the Γ -point of an hexagonal lattice. The states are indexed as $m_\Gamma[n(m_\Gamma)]$, α_Γ . Each state with the same α_Γ appears with the same color. The α_Γ is calculated based on Table 5.1 with an accuracy up to 1 decimal place.

The results of such analyses are presented in Table 5.2.1, 5.2.2 and 5.2.3 for Γ , M and K points respectively. Possible values of $\sin(\alpha_k)$ and α_k are calculated using the expressions in Table 5.1 and due to the symmetry of both lattice and the $\mathbf{k}$ -vector (i.e., point group of $\mathbf{k}$) [Chap. 3], the α_k angles in Table 5.2 are restricted between $0 \leq \alpha_\Gamma \leq 30^\circ$, $0 \leq \alpha_K \leq 60^\circ$ and $0 \leq \alpha_M \leq 90^\circ$ for Γ , K and M points respectively. Consider the state $\alpha_\Gamma = 10.9^\circ$, the results of $m_\Gamma = p_\Gamma(n_1)q(\alpha_{b_2})$ and $m_\Gamma = p_\Gamma(n_2)q(\alpha_{b_1})$ yields

$7n_1^2/9$ and $7n_2^2/4$ respectively. However by forcing $n_1 = 3h_\Gamma$ and $n_2 = 2h_\Gamma$, both $p_\Gamma(n_1)q(\alpha_{b2})$ and $p_\Gamma(n_2)q(\alpha_{b1})$ reduce to $7h_\Gamma^2$ (Table 5.2.1). Similar procedure was applied to obtain m_K for all other α_K states in Table 5.2.1-5.2.3.

Table 5.2.1 – The expressions for m_Γ in terms of a free integer, h_Γ ($h_\Gamma = 1, 2, 3, \dots$).

$\sin(\alpha_\Gamma)$	$\frac{1}{2}$	0	$\frac{1}{2\sqrt{7}}$	$\frac{1}{\sqrt{13}}$	$\frac{1}{2\sqrt{19}}$
α_Γ (°)	30	0	10.9	16.1	6.6
$q(\alpha_{b1})$	4/3	4	7/3	52/27	76/27
$q(\alpha_{b2})$	4/3	1	28/27	13/12	76/75
m_Γ	h_Γ^2	$3h_\Gamma^2$	$7h_\Gamma^2$	$13h_\Gamma^2$	$19h_\Gamma^2$

Table 5.2.2 – The expressions for m_M in terms of a free integer, h_M ($h_M = 1, 2, 3, \dots$). Key: ND – not defined.

$\sin(\alpha_M)$	1	0	$\frac{2}{\sqrt{7}}$	$\frac{1}{\sqrt{13}}$	$\frac{4}{\sqrt{19}}$
α_M (°)	90	0	49.1	16.1	66.6
$q(\alpha_{b1})$	4/3	4	28/27	52/27	76/75
$q(\alpha_{b2})$	ND	1	7/3	13/12	19/3
m_M	$(2h_M + 1)^2$	$3(2h_M + 1)^2$	$7(2h_M + 1)^2$	$13(2h_M + 1)^2$	$19(2h_M + 1)^2$

Table 5.2.3 – The expressions for m_K in terms of a free integer, h_K (or h'_K) ($h_K = 0, 1, 2, 3, \dots$, $h'_K = -1, -2, -3, \dots$).

$\sin(\alpha_K)$	0	$\frac{\sqrt{3}}{2}$	$\frac{1}{2}\sqrt{\frac{3}{7}}$	$\frac{3}{2}\sqrt{\frac{3}{13}}$	$\sqrt{\frac{3}{19}}$
α_K (°)	0	60	19.1	46.1	23.4
$q(\alpha_{b1})$	4	1	7/4	52/49	76/49
$q(\alpha_{b2})$	1	4	28/25	52/25	19/16
m_K	$(3h_K + 1)^2$	$(3h'_K + 1)^2$	$7(3h_K + 1)^2$	$13(3h_K + 1)^2$	$19(3h_K + 1)^2$

Fig. 5.3 $\mathbf{k}+\mathbf{G}$ vectors for the states at Γ , K and M -points of an hexagonal lattice. The states are labeled with the angle α_k [i.e., the angle made by the arrow with the k_x - axis in (a) to (f) and (h)]. The green marker is taken as

the origin of the reciprocal plane. (a),(b), and (c) – States for $\alpha_{\Gamma} = 30^{\circ}, 0$ and 10.9° respectively. (d), (e), and (f) States for $\alpha_K = 0, 60^{\circ}$ and 19.1° respectively. (g) States for $\alpha_M = 0$ (blue) and 90° (red). The markers circle, star and square respectively represents for $h_M = 0, 1$ and 2 respectively. (h) States for $\alpha_M = 40.1^{\circ}$.

Figures 5.3(a), (b) and (c) show $\mathbf{k}+\mathbf{G}$ vectors for the states of Γ -point with $\alpha_{\Gamma} = 30^{\circ}, 0$ and 10.9° respectively. The vectors connecting the origin (green marker) and the edges of each closed polygon in these figures represent the $\mathbf{k}+\mathbf{G}$ vectors. Edges of the same polygon necessarily have the same m_k (i.e., same length), and hence correspond to a single state. Within each figure, we have many isomorphic but scaled polygons, with different values of h_{Γ} (i.e., 1 to 6). Though each edge of the same polygon represents a symmetrical $\mathbf{k}+\mathbf{G}$ vector with different α_k , due to the symmetry of $\mathbf{k}$ -vector, we limit α_{Γ} to be $0 \leq \alpha_{\Gamma} \leq 30^{\circ}$. For example, in Fig. 5.3(a), the angle of $\mathbf{k}+\mathbf{G}$ vectors can be $30^{\circ}, 90^{\circ}, 150^{\circ}, 210^{\circ}, 270^{\circ}$ or 330° , but α_{Γ} is fixed as 30° .

Figures 5.3 (d), (e) and (f) show similar plots for K-point with $\alpha_K = 0, 60^{\circ}$ and 19.1° respectively. In Fig. 5.3(d) and (e), the expression for m_k is similar, as they have the same system of $\mathbf{k}+\mathbf{G}$ vectors. For instance, we have parallel vectors in both Fig. 5.3(d) and (e), with $\alpha_K = 0$ and $\alpha_K = 180^{\circ}$ respectively. The parameter that distinguishes the value of m_k for these two sets of states is h_K . For Fig. 5.3(d), h_K is positive while for Fig. 5.3(e), it is negative (Table 5.2). Figure 5.3(g) shows $\mathbf{k}+\mathbf{G}$ vectors for the states at M-point with $\alpha_M = 0$ (blue) and 90° (red) with different h_M identified with different marker. On the other hand, Figure 5.3(h) shows the plot for M-point with $\alpha_M = 40.1^{\circ}$.

On the other hand it is worth to note that, states with the same α_k will have the same symmetry system which means the symmetry representation of these states

is made up by an identical composition of irreducible representations [Sec. 3.4.1 of Chap. 3]. For example, the symmetry representation for the state $\alpha_{\Gamma} = 0$ and $\alpha_{\Gamma} = 30^\circ$ is $A_1 + B_2 + E_1 + E_2$ and $A_1 + B_1 + E_1 + E_2$ respectively. These representations can be obtained from Table 3.7 by considering $h_{\Gamma} = 1$ [i.e., corresponding to m_{Γ} (m_{is} at Γ -point) = 1 ($\alpha_{\Gamma} = 0$) and 3 ($\alpha_{\Gamma} = 30^\circ$)].

5.3. States in the presence of spatial modulation

5.3.1 Solution at symmetrical points

The solution at the symmetrical points are crucial as band gap openings and unusual conductions like superprism and negative refractions occur near the band edges (i.e., symmetrical points). The size of pseudo band gaps in PCs can be found only using the solutions at symmetrical $\mathbf{k}$ -points. Further, once the solution at a symmetrical $\mathbf{k}$ -point is known, then the solution for $\mathbf{k}$ -vectors in the neighborhood of the symmetrical point, can be easily obtained by mean of other methods such as perturbation theory [164-165]. In this section, we introduce a simple yet powerful method to approximate the solutions at symmetrical $\mathbf{k}$ – points of a 2D PC with isotropic materials and in the subsequent sections, the non symmetrical $\mathbf{k}$ – vectors will be handled and the influence of material's anisotropy will be considered.

From Eqn. 4.13 (Chap. 4) we write,

$$h_i = \frac{\sum_{i \neq j} M_{ij} h_j}{\{\omega^2 - M_{ii}\}} \quad [5.9]$$

where the size of matrix, M , is ideally infinity. For the 2D PC with all isotropic materials, we have,

$$h_i = \frac{\sum_{i \neq j} M_{ij} h_j}{\omega^2 - \kappa_0 |\mathbf{k} + \mathbf{G}_i|^2} = \frac{\varepsilon_o \sum_{i \neq j} M_{ij} h_j}{\{\varepsilon_o \omega^2 - c_{\mathbf{k}} m_{\mathbf{k}}\}} \quad [5.10]$$

At symmetrical $\mathbf{k}$ -points with small spatial modulation, $\varepsilon_o \omega^2 \approx c_{\mathbf{k}} m_{\mathbf{k}}$ [see Eqn. 5.6] and hence, only $n(m_{\mathbf{k}})$ – number of h_i will be dominant [since there are $n(m_{\mathbf{k}})$ combinations of $\mathbf{G}$ leading to the same $m_{\mathbf{k}}$], and therefore Eqn. 4.13 can be approximately written as

$$\sum_{j=1}^{n(m_{\mathbf{k}})} M_{ij} h_j = \omega^2 h_i \quad [5.11]$$

Eqn. 5.11 solves each state, $m_{\mathbf{k}}$ in Figs. 5.2 and 5.3, independently with a matrix size $n(m_{\mathbf{k}})$ by $n(m_{\mathbf{k}})$. In formulating the matrix elements of Eqn. 5.11, the vector $\mathbf{G}$ must be chosen such that they all have the same $m_{\mathbf{k}}$ (i.e., equal length of $\mathbf{k} + \mathbf{G}$). Eqn. 5.7 enables us to generalize the form of solution for Eqn. 5.11 with a particular $m_{\mathbf{k}}$, available for other states with the same $\alpha_{\mathbf{k}}$.

If we define, a set of $\mathbf{G}$ vectors as a set of fundamental vectors that lead to the smallest $m_{\mathbf{k}}$ within the states having the same $\alpha_{\mathbf{k}}$ (i.e., $p_{\mathbf{k}} = p_{\mathbf{k},s}$ and $m_{\mathbf{k}} = m_{\mathbf{k},s}$), then Eqn. 5.11 becomes,

$$\sum_{j=1}^{n(\alpha_{\mathbf{k}})} \overline{M}_{ij}^{\alpha_{\mathbf{k}}} h_j = \left(\frac{\omega_{\mathbf{k}}}{c_{\mathbf{k}} m_{\mathbf{k}}} \right)^2 h_i \quad [5.12.1]$$

where we have assumed states with the same $\alpha_{\mathbf{k}}$ have the same degeneracy $n(m_{\mathbf{k}}) = n(\alpha_{\mathbf{k}})$, and the definition of $\overline{M}_{ij}^{\alpha_{\mathbf{k}}}$ takes the forms of,

$$\overline{M}_{ij}^{\alpha_{\mathbf{k}}} = \begin{cases} \mathbf{e}_i \cdot \tilde{\mathbf{K}}_H \{p_{\alpha_{\mathbf{k}}} (\mathbf{G}_i - \mathbf{G}_j)\} \cdot \mathbf{e}_j, & H - \text{polarization} \\ \kappa_E \{p_{\alpha_{\mathbf{k}}} (\mathbf{G}_i - \mathbf{G}_j)\}, & E - \text{polarization} \end{cases} \quad [5.12.2]$$

where the vectors $\mathbf{G}_i$ with $i = 1, 2, \dots, n(\alpha_{\mathbf{k}})$ denotes a set of fundamental vectors with the smallest $m_{\mathbf{k}}$ among the set of vectors with the same $\alpha_{\mathbf{k}}$ and in the derivation,

the relationship between a general $\mathbf{k}+\mathbf{G}$ vector and the $\mathbf{k}+\mathbf{G}$ vector of the shortest length is used [see Figure 5.4]. For instance, the set of fundamental vectors for a state with $\alpha_\Gamma = 30^\circ$ will be the vectors indicated by the edges of the smallest polygon in Fig. 5.3(a). These vectors $\mathbf{G}_1, \mathbf{G}_2, \mathbf{G}_3, \mathbf{G}_4, \mathbf{G}_5$ and $\mathbf{G}_6$ have (n_1, n_2) indices (0,-1), (1,0), (1,1), (0,1), (-1,0) and (-1,-1). The solution to Eqn. 5.12.1 can be easily obtained and typical analytical solutions can be obtained for $n(\alpha_k) = 2, 3, 4$ or 6.

Fig. 5.4 Symmetrical $\mathbf{k}+\mathbf{G}$ vectors for the states of same α_k . The $\mathbf{g}_i$ and $\mathbf{g}_j$ denote unit vectors along $\mathbf{k}+\mathbf{G}_i$ and $\mathbf{k}+\mathbf{G}_j$ respectively.

For hexagonal lattice, we have $p_{\alpha_k} = h_\Gamma, 2h_M + 1$ and $3h_K + 1$ (Table 5.2) for Γ, M and K points respectively and the states with $n(\alpha_k) = 2, 3, 4$ and 6 are analytically solvable. Throughout this chapter we will use the state $\alpha_\Gamma = 30^\circ$ [$m_\Gamma = h_\Gamma^2, n(\alpha_\Gamma) = 6$] as an example unless otherwise stated. In the absence of modulation, these states are indicated as blue lines in Fig. 5.2 and they are the most occurring states in the first ten states at Γ point (see Fig. 5.2). The particular interest at Γ point is also due to the fact, that many interesting phenomena like circular equal frequency surface (i.e., the origin for negative refractive index) and cutoff conditions for diffractions at normal incidence are based on the solutions at this point. Nevertheless, similar analyses at

other symmetrical $\mathbf{k}$ -points can be handled in a similar manner and in fact the systems with $n(\alpha_k) = 2, 3$, and 4 (Table 5.2) at other $\mathbf{k}$ -points have smaller matrix sizes and therefore easier to handle.

For the state $\alpha_{\Gamma} = 30^\circ$, Eqns. 5.12.1-5.12.2 results in two 6 by 6 matrices corresponding to the two different polarizations. The matrix for E -polarization can be diagonalized [Appendix C3] to obtain normalized frequencies,

$$\omega_{o1}^2 = \frac{4}{3} h_{\Gamma}^2 (\kappa_0 - 2\kappa_1 + 2\kappa_2 - \kappa_3) \quad (1) \quad [5.13.1]$$

$$\omega_{o2}^2 = \frac{4}{3} h_{\Gamma}^2 (\kappa_0 + 2\kappa_1 + 2\kappa_2 + \kappa_3) \quad (1) \quad [5.13.2]$$

$$\omega_{o3}^2 = \frac{4}{3} h_{\Gamma}^2 (\kappa_0 - \kappa_1 - \kappa_2 + \kappa_3) \quad (2) \quad [5.13.3]$$

$$\omega_{o4}^2 = \frac{4}{3} h_{\Gamma}^2 (\kappa_0 + \kappa_1 - \kappa_2 - \kappa_3) \quad (2) \quad [5.13.4]$$

and similarly for H -polarization,

$$\omega_{o1}^2 = \frac{4}{3} h_{\Gamma}^2 (\kappa_0 + \kappa_1 - \kappa_2 - \kappa_3) \quad (1) \quad [5.14.1]$$

$$\omega_{o2}^2 = \frac{4}{3} h_{\Gamma}^2 (\kappa_0 - \kappa_1 - \kappa_2 + \kappa_3) \quad (1) \quad [5.14.2]$$

$$\omega_{o3}^2 = \frac{4}{3} h_{\Gamma}^2 \left\{ \kappa_0 - \frac{1}{2} (\kappa_1 - \kappa_2) - \kappa_3 \right\} \quad (2) \quad [5.14.3]$$

$$\omega_{o4}^2 = \frac{4}{3} h_{\Gamma}^2 \left\{ \kappa_0 + \frac{1}{2} (\kappa_1 + \kappa_2) + \kappa_3 \right\} \quad (2) \quad [5.14.4]$$

with the degeneracy in the presence of the spatial modulation indicated in the bracket. The degeneracy in the presence of the spatial modulation is a consequence of the symmetry possessed by the PC and has to be analyzed using group theoretical tools [115, 120-121]. In Eqns. 5.13-5.14, $\kappa_1 = \kappa\{h_{\Gamma}(\mathbf{G}_1 - \mathbf{G}_2)\}$, $\kappa_2 = \kappa\{h_{\Gamma}(\mathbf{G}_1 - \mathbf{G}_3)\}$, and

$\kappa_3 = \kappa\{h_T(\mathbf{G}_1 - \mathbf{G}_4)\}$. In the absence of the spatial modulation, $\kappa_1 = \kappa_2 = \kappa_3 = 0$ and only κ_0 is nonzero and hence all the four solutions for E and H -polarizations are equal.

In order to test the accuracy of Eqns. 5.13 and 5.14, the solutions for the state with $m_T = 1$ ($\alpha_T = 30^\circ$, $h_T = 1$) [Fig. 5.2] is analyzed for a 2D PC made of circular air holes of a filling ratio, f , in a matrix medium of refractive index n .

Fig. 5.5 The splitting of states in the presence of the spatial modulation for the state $\alpha_T = 30^\circ$ with $h_T = 1$ as a function of n . Key: solid lines - numerically evaluated using 361 plane waves, markers – analytically evaluated using Eqns. 5.13.1-5.13.4 and Eqns. 5.14.1 to 5.14.4. (a) E -polarization with $f = 0.15$ (b) E -polarization with $f = 0.23$. (c) H -polarization with $f = 0.15$.

Figures 5.5(a) and (b) show the result of numerical evaluation employing 361 plane waves and the result of analytical evaluation using Eqns. 5.13-5.14 as a function of n for the E polarization with $f = 15\%$ and 23% respectively.

Table 5.3.1 - Computed values using the numerical method (361 plane wave) and the analytical model for Fig. 5.5(a)

n	Band 1 (blue)		Band 2 (red)		Band 3 (green)		Band 4 (pink)	
	Numerical	Analytical	Numerical	Analytical	Numerical	Analytical	Numerical	Analytical
1.10	1.049858	1.049857	1.051137	1.051117	1.064683	1.064200	1.100233	1.100350
1.20	0.962460	0.962459	0.964528	0.964473	0.986788	0.985366	1.048608	1.048543
1.30	0.888490	0.888488	0.891043	0.890954	0.918895	0.916490	0.999985	0.999127
1.40	0.825074	0.825072	0.827921	0.827802	0.859306	0.856028	0.954388	0.952176
1.50	0.770106	0.770102	0.773122	0.772979	0.806660	0.802662	0.911750	0.907805
1.60	0.722002	0.721998	0.725106	0.724945	0.759861	0.755297	0.871947	0.866085
1.70	0.679553	0.679549	0.682690	0.682516	0.718022	0.713025	0.834823	0.827017
1.80	0.641817	0.641813	0.644951	0.644767	0.680420	0.675102	0.800207	0.790538
1.90	0.608051	0.608046	0.611157	0.610967	0.646460	0.640912	0.767922	0.756538
2.00	0.577659	0.577655	0.580721	0.580527	0.615651	0.609946	0.737794	0.724877
2.10	0.550161	0.550156	0.553168	0.552972	0.587584	0.581780	0.709656	0.695399
2.20	0.525161	0.525157	0.528107	0.527910	0.561916	0.556058	0.683351	0.667944
2.30	0.502334	0.502330	0.505216	0.505019	0.538357	0.532481	0.658732	0.642353
2.40	0.481409	0.481405	0.484223	0.484027	0.516662	0.510797	0.635662	0.618477
2.50	0.462157	0.462153	0.464904	0.464710	0.496623	0.490788	0.614017	0.596172
2.60	0.444386	0.444381	0.447065	0.446873	0.478058	0.472272	0.593683	0.575308
2.70	0.427930	0.427926	0.430543	0.430354	0.460814	0.455088	0.574555	0.555764
2.80	0.412650	0.412646	0.415198	0.415011	0.444756	0.439099	0.556539	0.537430
2.90	0.398423	0.398419	0.400908	0.400724	0.429767	0.424187	0.539548	0.520205
3.00	0.385144	0.385140	0.387568	0.387387	0.415745	0.410246	0.523503	0.504000

Table 5.3.2 - Computed values using the numerical method (361 plane wave) and the analytical model for Fig. 5.5(b)

n	Band 1 (blue)		Band 2 (red)		Band 3 (green)		Band 4 (pink)	
	Numerical	Analytical	Numerical	Analytical	Numerical	Analytical	Numerical	Analytical
1.10	1.050415	1.050408	1.054378	1.054245	1.080208	1.079047	1.110160	1.111743
1.20	0.963361	0.963339	0.969793	0.969417	1.013151	1.009541	1.066839	1.071782
1.30	0.889601	0.889566	0.897571	0.896953	0.952770	0.946401	1.025059	1.033695
1.40	0.826313	0.826266	0.835223	0.834400	0.898323	0.889350	0.985027	0.996877
1.50	0.771418	0.771361	0.780878	0.779892	0.849119	0.837887	0.946855	0.961067
1.60	0.723351	0.723288	0.733103	0.731993	0.804539	0.791438	0.910587	0.926219
1.70	0.680916	0.680847	0.690786	0.689584	0.764032	0.749439	0.876218	0.892400
1.80	0.643179	0.643106	0.653050	0.651783	0.727119	0.711365	0.843707	0.859724
1.90	0.609400	0.609325	0.619193	0.617883	0.693381	0.676749	0.812990	0.828303
2.00	0.578989	0.578913	0.588652	0.587314	0.662456	0.645180	0.783988	0.798222
2.10	0.551467	0.551389	0.560965	0.559611	0.634028	0.616300	0.756615	0.769534
2.20	0.526441	0.526363	0.535751	0.534392	0.607824	0.589799	0.730779	0.742258
2.30	0.503585	0.503508	0.512696	0.511338	0.583606	0.565409	0.706388	0.716383
2.40	0.482631	0.482554	0.491534	0.490184	0.561167	0.542898	0.683352	0.691875
2.50	0.463350	0.463273	0.472043	0.470704	0.540326	0.522065	0.661584	0.668687
2.60	0.445549	0.445473	0.454033	0.452709	0.520926	0.502734	0.641001	0.646757
2.70	0.429065	0.428990	0.437341	0.436034	0.502826	0.484754	0.621523	0.626023
2.80	0.413756	0.413682	0.421830	0.420542	0.485905	0.467991	0.603077	0.606415
2.90	0.399502	0.399429	0.407377	0.406109	0.470055	0.452328	0.585594	0.587866
3.00	0.386196	0.386125	0.393879	0.392632	0.455180	0.437663	0.569009	0.570309

Table 5.3.3 - Computed values using the numerical method (361 plane wave) and the analytical model for Fig. 5.5(c)

n	Band 1 (blue)		Band 2 (red)		Band 3 (green)		Band 4 (pink)	
	Numerical	Analytical	Numerical	Analytical	Numerical	Analytical	Numerical	Analytical
1.10	1.051137	1.051167	1.057297	1.057520	1.064683	1.064178	1.075965	1.076806
1.20	0.964528	0.964618	0.974700	0.975389	0.986788	0.985304	1.007445	1.010302
1.30	0.891043	0.891199	0.903820	0.905038	0.918895	0.916390	0.947082	0.952546
1.40	0.827921	0.828137	0.842364	0.844088	0.859306	0.855896	0.893395	0.901666
1.50	0.773122	0.773390	0.788594	0.790768	0.806660	0.802507	0.845283	0.856309
1.60	0.725106	0.725417	0.741173	0.743730	0.759861	0.755123	0.801895	0.815479
1.70	0.682690	0.683035	0.699052	0.701926	0.718022	0.712839	0.762560	0.778428
1.80	0.644951	0.645323	0.661400	0.664530	0.680420	0.674908	0.726737	0.744583
1.90	0.611157	0.611549	0.627550	0.630883	0.646460	0.640713	0.693980	0.713500
2.00	0.580721	0.581129	0.596958	0.600449	0.615651	0.609744	0.663919	0.684822
2.10	0.553168	0.553587	0.569180	0.572790	0.587584	0.581577	0.636242	0.658265
2.20	0.528107	0.528534	0.543849	0.547547	0.561916	0.555856	0.610682	0.633591
2.30	0.505216	0.505647	0.520657	0.524416	0.538357	0.532280	0.587014	0.610602
2.40	0.484223	0.484657	0.499347	0.503144	0.516662	0.510598	0.565039	0.589132
2.50	0.464904	0.465338	0.479700	0.483518	0.496623	0.490592	0.544588	0.569035
2.60	0.447065	0.447498	0.461529	0.465354	0.478058	0.472078	0.525512	0.550187
2.70	0.430543	0.430974	0.444676	0.448496	0.460814	0.454897	0.507682	0.532478
2.80	0.415198	0.415625	0.429003	0.432807	0.444756	0.438912	0.490981	0.515812
2.90	0.400908	0.401331	0.414392	0.418172	0.429767	0.424003	0.475310	0.500102
3.00	0.387568	0.387987	0.400737	0.404488	0.415745	0.410066	0.460578	0.485271

Figure 5.5(c) shows a similar plot with $f = 15\%$ for H -polarization. On the other hand, Tables 5.3.1, 5.3.2 and 5.3.3 present the actual computed values using the numerical and analytical model for Figs. 5.5(a), 5.5(b) and 5.5(c) respectively. As we can readily see from these figures and tables, Eqns. 5.13-5.14 provide good approximation for the values of ω_T for n even up to 3.0. The accuracy of the approximations reduces as the spatial modulation increases (i.e., when f or n is increased) and for a given set of the same parameters, the approximation is more accurate for E -polarization than H -polarization.

5.3.2. Solution for $\mathbf{k}$ -vectors in the neighborhood of symmetrical points

For $\mathbf{k}$ -vectors in the neighborhood of symmetrical points, we can assume

$$|\mathbf{k}_n + \mathbf{k} + \mathbf{G}_i| \approx |\mathbf{k} + \mathbf{G}_i|, \text{ where } \mathbf{k} \text{ and } \mathbf{k}_n \text{ stand for a symmetrical wavevector and a}$$

wavevector close to it (i.e., in the neighborhood region). As such, Eqn. 4.13 still can be approximated using Eqn. 5.12.1. The matrix elements, $\overline{M}_{ij}^{\alpha_k}$ take the form of

$$\overline{M}_{ij}^{\alpha_k} = \left\| \mathbf{k}_n + p_{\alpha_k} (\mathbf{k} + \mathbf{G}_i) \right\| \left\| \mathbf{k}_n + p_{\alpha_k} (\mathbf{k} + \mathbf{G}_j) \right\| \{ \mathbf{e}_i \cdot \kappa \{ p_{\alpha_k} (\mathbf{G}_i - \mathbf{G}_j) \} \cdot \mathbf{e}_j \} / (c_k m_k) \quad [5.15.1]$$

and

$$\overline{M}_{ij}^{\alpha_k} = \kappa \{ p_{\alpha_k} (\mathbf{G}_i - \mathbf{G}_j) \} \left\| \mathbf{k}_n + p_{\alpha_k} (\mathbf{k} + \mathbf{G}_i) \right\| \left\| \mathbf{k}_n + p_{\alpha_k} (\mathbf{k} + \mathbf{G}_j) \right\| / (c_k m_k) \quad [5.15.2]$$

for H and E -polarizations respectively. The size of the matrix defined by Eqns. 5.15.1-5.15.2 is $n(\alpha_k)$, and this significantly reduces the computational time required for diagonalizations. The result is particularly useful in calculations of an EFS, which typically involves dense $\mathbf{k}$ vectors. EFS is commonly employed in calculating the dispersive effects of a PC such as superprism, supercolimation, etc. Interestingly, these effects occur in PCs with a small (however a finite) spatial modulation, and as such the accuracy of the approximation provided by Eqns. 5.12.1, 5.15.1 and 5.15.2 will be fairly sufficient. Further, depending on $n(\alpha_k)$ and the $\mathbf{k}$ -vector, Eqns. 5.15.1-5.15.2 can be solved exactly. The full description of the solutions for states with $n(\alpha_k) = 2$ and the corresponding description of the EFS has been presented in detail in Sec. 6.3.2 (see Chap. 6).

Figures 5.6(a) and (b) show the approximated dispersion relation for E - and H -polarizations respectively for the state $m_\Gamma = 1$ ($\alpha_\Gamma = 30^\circ$, $h_\Gamma = 1$). The $\mathbf{k}_n$ was assumed to be along the Γ -K direction of the hexagonal lattice and the PC was assumed to have $n = 2$ with f being 15% and 23% for Figs. 5.5(a) and 5.5(b) respectively. For a comparison, the numerically evaluated dispersion curves using 361 plane waves are

also shown in these figures and as we can readily see the agreement is generally good especially for $\mathbf{k}_n$ vectors close to Γ point.

Fig. 5.6 The dispersion for wavevectors in the neighborhood of Γ point for the state $\alpha_\Gamma = 30^\circ$ ($h_\Gamma = 1$). The k_n vectors are along Γ -K direction. Key: solid lines - numerically evaluated using 361 plane waves, markers - approximated using Eqn. 5.12.1 with the matrix element given by Eqn 5.15.1 and 5.15.2 (a) E -polarization with $f = 0.15$. (b) H -polarization with $f = 0.23$.

The smaller matrix size, $n(\alpha_k)$ allows us to study any PC structure with in-depth analytical details. The time-independent perturbation theory [164-165] is particularly useful, and the application of the theory for states $m_\Gamma = h_\Gamma^2$ ($\alpha_\Gamma = 30^\circ$) in hexagonal lattice yields analytical solution for the dispersion of non-degenerate frequencies. Let the exact non-degenerate eigenvalue to the matrix in Eqn. 5.15.1-5.15.2 corresponding to the state $m_\Gamma = h_\Gamma^2$ ($\alpha_\Gamma = 30^\circ$) to be ω_i . If the unperturbed solution is taken as the solution when $\mathbf{k}_n = 0$, then for a small, $\mathbf{k}_n = [k_n \cos \theta, k_n \sin \theta]$, the results of perturbation provides an approximation to ω_i with accuracy up to the second order corrections, which can be written as [Appendix C4],

$$\omega_i^2 \approx \omega_{oi}^2 + k_n^2 \gamma_1 + k_n^2 \gamma_2 \quad [5.16]$$

where $i = 1$ or 2 (Eqn. 5.13-5.14), and $k_n^2 \gamma_1$ and $k_n^2 \gamma_2$ are the corrections due to first and second order perturbations respectively for any h_Γ . The coefficients γ_1 and γ_2 appear in Tables 5.4.1 and 5.4.2 for E and H -polarizations respectively. As suggested by Eqn. 5.16, the solution is isotropic (i.e., independent of θ) and the corresponding equal frequency surface is therefore circular with an effective refractive index given by $1/\sqrt{\gamma_1 + \gamma_2}$. The validity of the isotropic model are depicted in Figures 5.7 and 5.8 for E and H -polarizations respectively for the state $h_\Gamma = 1$ ($\alpha_\Gamma = 30^\circ$).

Table 5.4.1 – The coefficients γ_1 and γ_2 for E -polarization. For ω_{0i} definitions see Eqns. 5.13.1 - 5.13.4

i	γ_1	γ_2
1	$\frac{3\omega_{o1}}{4h_\Gamma^2}$	$\frac{3\omega_{o1}\omega_{o3}}{2h_\Gamma^2(\omega_{o1} - \omega_{o3})}$
2	$\frac{3\omega_{o2}}{4h_\Gamma^2}$	$\frac{3\omega_{o2}\omega_{o4}}{2h_\Gamma^2(\omega_{o2} - \omega_{o4})}$

Table 5.4.2 – The coefficients γ_1 and γ_2 for H -polarization. For ω_{0i} definitions see Eqns. 5.14.1 - 5.14.4

i	γ_1	γ_2
1	$\frac{3(2\omega_{o4} - \omega_{o2})}{4h_\Gamma^2}$	$\frac{3(2\omega_{o4} - \omega_{o2} + \omega_{o1})^2}{8h_\Gamma^2(\omega_{o1} - \omega_{o4})}$
2	$\frac{3(2\omega_{o3} - \omega_{o1})}{4h_\Gamma^2}$	$\frac{3(2\omega_{o3} - \omega_{o1} + \omega_{o2})^2}{8h_\Gamma^2(\omega_{o2} - \omega_{o3})}$

Fig. 5.7 The isotropic model, ω_i [Eqn. 5.16] for the state $\alpha_i = 30^\circ$ ($h_\Gamma = 1$) as a function of k_n along Γ -K direction for E -polarization and $n = 3$. Key: solid line with asterisk - approximated using Eqn. 5.12.1 with the matrix element given by Eqn 5.15.2, circles – analytically evaluated using Eqn. 20, Triangle – numerical evaluation with 361 plane waves. (a) $f = 0.33$ (b) $f = 0.23$ (c) $f = 0.15$.

Fig. 5.8 The isotropic model, ω_i [Eqn. 5.16] for the state $\alpha_i = 30^\circ$ ($h_\Gamma = 1$) as a function of k_n along Γ -K direction for H -polarization and $n = 3$. Key: solid line with asterisk - approximated Eqn. 5.12.1 with the matrix element given by Eqn 5.15.1, circles – analytically evaluated using Eqn. 20, Triangle – numerical evaluation with 361 plane waves. (a) $f = 0.23$ (b) $f = 0.15$ (c) $f = 0.10$.

In each of these figures we have plotted, the dispersion for ω_i ($i = 1$) as a function of $\mathbf{k}_n$ vectors along Γ -K line, using the exact method (employing 361 plane waves), Eqn. 5.12.1 (with the matrix element described by Eqn. 5.15.1 and 5.15.2) and the isotropic

model (Eqn. 5.16) for various modulation levels (i.e., f). As we can readily verify from these figures, the isotropic model provides a good approximation for $\mathbf{k}_n$ vectors close to Γ point and more importantly, the length in $\mathbf{k}_n$ vectors (radius in the reciprocal plane) for which the isotropic model is valid increases with the modulation. This is consistent with the findings of Notomi [67] where the states with circular equal frequency surfaces (i.e., isotropic dispersion) are found to be well pronounced in PCs with strong refractive index modulation.

5.3.3 Influence of anisotropy

Recall that in the presence of a material's anisotropy, the matrix element in Eqn. 4.8 is given by Eqn. 4.10. If $\tilde{\kappa}_H$ is taken as a sum of an isotropic tensor with an anisotropic tensor of smaller tensor components then, then Eqn. 5.11 can be used to approximate the dispersion relation in the presence of both anisotropy and spatial modulation. Though any orientation of anisotropic material can be handled by Eqn. 5.11, in the following, we will assume a specific, yet typical orientation [64,95] for which the solutions can be analytically described.

Consider a 2D PC with alternating isotropic and anisotropic material in an hexagonal lattice. The coordinate system of the anisotropic material is assumed to be parallel with the coordinate system of the PC, and the principal refractive indices along x and y -axis of the PC and $n+\Delta n$ and n respectively. As such, the matrix $\tilde{\kappa}_H$ in Eqn 4.2 can be written as,

$$\tilde{\kappa}_H(\mathbf{G}) = \begin{pmatrix} \kappa(\mathbf{G}) + \tau(\mathbf{G}) & 0 \\ 0 & \kappa(\mathbf{G}) \end{pmatrix} \quad [5.17]$$

where the matrix $diag[\kappa(\mathbf{G}), \kappa(\mathbf{G})]$ is the corresponding $\tilde{\kappa}_H$ matrix for a PC with $\Delta n = 0$. It is easy to see that if $\tau(\mathbf{G})$ (the coefficient representing the anisotropy) is small, then Eqn. 5.1 approximately equals to Eqn. 5.3 and therefore the condition for Eqn. 5.11 is valid. For states $m_\Gamma = h_\Gamma^2$ ($\alpha_\Gamma = 30^\circ$), being consistent with the definitions of $\kappa_0, \kappa_1, \kappa_2$ and κ_3 , the coefficients τ_0, τ_1, τ_2 and τ_3 can be respectively defined as $\tau_0 = \tau(0)$, $\tau_1 = \tau\{h_\Gamma(\mathbf{G}_1 - \mathbf{G}_2)\}$, $\tau_2 = \tau\{h_\Gamma(\mathbf{G}_1 - \mathbf{G}_3)\}$, and $\tau_3 = \tau\{h_\Gamma(\mathbf{G}_1 - \mathbf{G}_4)\}$. In the absence of modulation only κ_0 and τ_0 are nonzero.

With Eqn. 5.17, Eqn 5.11 (or 5.12.1) for the H -polarization[♥] can be exactly solved and the solutions for states $\alpha_\Gamma = 30^\circ$,

$$\omega_{a1} = \omega_{o1} + \frac{1}{2}(\tau_0 + \tau_m^1) - \kappa_{12} + \frac{1}{6}\sqrt{32\kappa_{12}^2 + [3(\tau_0 + \tau_m^1) + 2\kappa_{12}]^2} \quad [5.18.1]$$

$$\omega_{a2} = \omega_{o2} + \frac{1}{2}(\tau_0 + \tau_m^2) + \kappa'_{12} - \frac{1}{6}\sqrt{32\kappa'_{12}^2 + [3(\tau_0 + \tau_m^2) - 2\kappa'_{12}]^2} \quad [5.18.2]$$

$$\omega_{a3} = \omega_{o3} + \tau_0 + \tau_m^3 \quad [5.18.3]$$

$$\omega_{a4} = \omega_{o3} + \frac{1}{2}(\tau_0 + \tau_m^1) + \kappa_{12} - \frac{1}{6}\sqrt{32\kappa_{12}^2 + [3(\tau_0 + \tau_m^1) + 2\kappa_{12}]^2} \quad [5.18.4]$$

$$\omega_{a5} = \omega_{o4} + \tau_0 + \tau_m^4 \quad [5.18.5]$$

$$\omega_{a6} = \omega_{o4} + \frac{1}{2}(\tau_0 + \tau_m^2) - \kappa'_{12} + \frac{1}{6}\sqrt{32\kappa'_{12}^2 + [3(\tau_0 + \tau_m^2) - 2\kappa'_{12}]^2} \quad [5.18.6]$$

with $\kappa'_{12} = \kappa_1 + \kappa_2$, $\kappa_{12} = \kappa_1 - \kappa_2$ and the modulation terms resulting from the anisotropy were summed together as τ_m^i ($i = 1, 2, 3$ or 4),

[♥] The dispersion for the E -polarization is similar to an isotropic PC (see Sec. 2.3 of Chap. 2).

$$\begin{aligned}
\tau_m^1 &= \tau_1 - \tau_2 - \tau_3 \\
\tau_m^2 &= -\tau_1 - \tau_2 + \tau_3 \\
\tau_m^3 &= -\tau_1 + \tau_2 - \tau_3 \\
\tau_m^4 &= \tau_1 + \tau_2 + \tau_3
\end{aligned} \tag{5.19}$$

Eqns. 5.18.1-5.18.6, being a generalized version of Eqns. 5.14.1-5.14.4 apply for states of $\alpha_{\Gamma} = 30^\circ$ with any h_{Γ} . The equations provide an in-depth perspective towards the understanding of the splitting of states in the presence of anisotropy and in the presence of modulation. When we switch off the materials' anisotropy, Eqns. 5.18.1-5.18.6 accurately reproduce Eqns. 5.14.1-5.14.4 (*H*-polarization) with two non degenerate states and two doubly degenerate states. This can be seen by setting $\tau_0 = \tau_m^i = 0$, which consequently leads to $\omega_{a1} = \omega_{o1}$, $\omega_{a2} = \omega_{o2}$, $\omega_{a3} = \omega_{a4} = \omega_{o3}$ and $\omega_{a5} = \omega_{a6} = \omega_{o4}$. On the other hand, if the spatial modulation is switched off completely, (i.e., $\kappa_1 = \kappa_2 = \kappa_3 = \kappa'_{12} = \kappa_{12} = \tau_m^i = 0$), then we have ω_{oi} ($i = 1, 2, 3$, and 4) = ω_o (Eqns.5.14.1-5.14.4) and consequently, Eqn. 5.18.1, 5.18.3, 5.18.4 and 5.18.5 reduces to $\omega_{a1} = \omega_{a3} = \omega_{a5} = \omega_{a6} = \omega_o + \tau_o$ and Eqn. 5.18.2 and 5.18.6 reduces to $\omega_{a2} = \omega_{a4} = \omega_o$.

Figure 5.9* illustrates the results of Eqns. 5.18.1 – 5.18.6 and the numerical method (using 361 plane waves) for the state $h_{\Gamma} = 1$ ($\alpha_{\Gamma} = 30^\circ$) in the hexagonal lattice PC made of circular cylinders of refractive index 2.5 in an anisotropic matrix medium of $n = 1.4$. Horizontal axis in the figure represents the variation in Δn and f . At point A, we have, $f = 0.25$ and $\Delta n = 0.6$ and due to the large anisotropy, we have a

* Also refer to see Fig. 3.5 (Sec. 3.4.3.1, Chap. 3) which is obtained using a numerical computation. The part of figures with small r_c values can be compared to the one in Fig. 5.9 (left to A).

deviation between the analytical approximation and the numerically evaluated curves. This deviation reduces when f (left to the point A) and Δn (right to the point A) are reduced. As we can see from the figure, when the material's anisotropy is reduced from $\Delta n = 0.6$ (at point A) to $\Delta n = 0$, the six non-degenerate states at A transform to four states composed of two non-degenerate states and two doubly degenerate states. On the other hand, when the spatial modulation is reduced from $f = 0.25$ (at point A) to $f = 0$, the six non-degenerate states transform two states with degeneracy one and two (Fig. 5.9).

Fig. 5.9 The splitting of states in the presence of modulation and in the presence of material's anisotropy for the state $\alpha_T = 30^\circ$ ($h_T = 1$) for H -polarization and $n = 1.4$. Point A represents a configuration with $f = 0.25$ and $\Delta n = 0.6$. Key: solid lines - numerically evaluated using 361 plane waves, markers - analytically evaluated using Eqns. 5.18.1-5.18.6.

5.4. Summary and Remarks

This chapter presented a systematic and generalized method of getting analytical descriptions for 2D PCs. The photonic states in the limit of zero modulation were analyzed and a systematic classification system based on integers was introduced for the states with distinct frequencies. The integers can be factored

and states with the same factor can be categorized as they have the same form of solution when the spatial modulation is switched on. As it was shown in the chapter, such states can be easily solved and typically lead to analytical solutions.

With the presented work, it is now made possible to have an analytical description or formulas for many optical properties of PC explored previously using numerical methods such as band gaps, refractions, group velocities and density of states. This in turn, may enable researchers to engineer PCs and PC based devices analytically. An example of the application of the presented method to analytically describe the EFS of a PC appears in Section 6.3.2.

Chapter 6

Equal Frequency Surface

6.1 Introduction

PC forbids propagation of photons in a spectral range called photonic band gap and within this frequency gap PC behaves like an insulator for photons. The insulating properties of a PC have been widely used in the developments of waveguides, fibers and cavities [Chap. 1]. For frequencies outside the photonic band gaps, though photons can propagate, their propagation properties (i.e. conducting properties) are very different compared to propagation through a homogenous medium. The unusual conducting properties of a PC have led to invention of many novel devices, such as superprisms, beam splitters, negative lenses and optical cloaking devices [Chap. 1]. The applications based on insulating and conducting abilities of anisotropic PCs are presented in Chap. 7 and 8 respectively.

An essential tool for analyzing the conducting properties of a PC is the EFS method [46,67]. The gradient of the EFS plays a major role in determining the group velocity direction and hence, the propagation direction of the photons in the PC. EFS can be obtained by a numerical calculation employing a plane wave expansion methodology [Chap. 4]. If the dielectric contrast of the PC is large, then a large number of plane waves is required to obtain EFSs with good accuracy. However, as mentioned previously, dispersion properties like superprism and beam splitting are normally well-pronounced in PCs with a small dielectric modulation [64,161-163] for

which, the requirement on the large number of plane waves to obtain EFS can be relaxed.

In Section 6.2, we define the EFS of a general 2D PC in terms of plane waves. Then in Section 6.3, using one plane wave and two plane waves approximations, we obtain the analytical expressions of the EFS. It is worth mentioning that in electronic energy band theory, the one plane wave technique is used to approximate Fermi surfaces of a metal and it is known in the name of Harrison's principles [166-167]. We address the use of one plane wave method for PCs constructed using materials of general anisotropy with arbitrary orientations of principal axes.[♥] Though one plane wave approximation presented in this chapter succeeds to a large extent in predicting the EFS of a PC with a weak dielectric modulation, the approximation is inaccurate for wavevectors near the boundary of the BZ. Furthermore, the one plane wave approach often predicts a very sharp edge to an EFS. Though sharp edges are important for dispersive effect like superprism, the curvatures have to be predicted accurately. As we shall show that, the deficiencies in the one plane wave approximation are successfully removed in the two plane waves approach.

Section 6.4 of the chapter presents the properties of an EFS in an anisotropic PC of a large spatial modulation. Such a PC behaves similar to a bulk anisotropic medium in the vicinity of a photonic band gap with a set of effective negative principal refractive indices. In particular, we studied a 2D geometrically anisotropic PC with a rectangular basis in a hexagonal lattice, which forms states with elliptical

[♥] The one plane wave approximation technique, in the graphical form was first introduced by Notomi [67] for isotropic PCs.

EFSs near the band edge frequencies. By varying the filling ratio, it is possible to force such an anisotropic state to an accidental isotropic state. Further, by re-orienting the basis and continuously varying the filling ratio, the orientation of the elliptical states can be continuously tuned.

6.2 Formulation

Assuming the polarizations can be decoupled [Chap. 2], the photonic band structure of E - or H -polarization can be found by solving the eigen-equation, Eqn. 3.3 (also see Eqn 2.13 and Eqn. 2.14). Using bra-ket notation* Eqn 3.3 can be written as,

$$M|H_{\mathbf{k}}\rangle = \{2\pi\omega(\mathbf{k})/a\}^2 |H_{\mathbf{k}}\rangle, \quad [6.1]$$

where $|H_{\mathbf{k}}\rangle = \mathbf{H}_{\mathbf{k}}(\mathbf{r})$ and $\Omega(\mathbf{k}) = \{2\pi\omega(\mathbf{k})/a\}^2$. Ignoring $\mathbf{k}$ (for an easy notation) and assuming $|H\rangle$ is normalized, we can rewrite Eqn. 6.1 as $\Omega = \langle H|M|H\rangle$. In the reciprocal space (i.e. Fourier space), Ω can be written as,

$$\Omega = \sum_i \sum_j \langle H|G_i\rangle \langle G_i|M|G_j\rangle \langle G_j|H\rangle \quad [6.2]$$

where we have made use of the closure relation $\sum_i |G_i\rangle \langle G_i| = 1$ with $|G_i\rangle$ as a basis for the reciprocal space.

In Eqn. 6.2, $\langle G_i|M|G_j\rangle$ is a matrix element of M whereas $\langle G_j|H\rangle$ is the j -th component of the vector $|H\rangle = [\langle G_1|H\rangle \quad \langle G_2|H\rangle \quad \dots]$ and $\langle H|G_i\rangle = \langle G_i|H\rangle^*$. By

* Throughout this chapter we employ bra-ket notations [164-165] for a convenience of discussion and presenting equations.

writing $\langle H|G_i\rangle$, $\langle G_j|H\rangle$ and $\langle G|M|G\rangle$ as H_i^* , H_j and M_{ij} respectively, Eqn. 6.2 becomes,

$$\Omega = \sum_i \sum_j H_j H_i^* M_{ij}. \quad [6.3]$$

The matrix element, M_{ij} for H -polarization [Eqn. 4.12] in the bra-ket notation is given by,

$$M_{ij} = \langle k_i | \tilde{\kappa}_H(i-j) | k_j \rangle \quad [6.4]$$

where $\tilde{\kappa}_H(i) = \tilde{\kappa}_H(\mathbf{G}_i)$, $|k_i\rangle = \mathbf{k} - \mathbf{G}_i$, $\mathbf{k} = [k_x \ k_y]'$ and $\mathbf{G}_i = [G_{ix} \ G_{iy}]'$. For E -polarization, M_{ij} [Eqn. 4.13] using bra-ket notation is

$$M_{ij} = |k_i| |k_j| \kappa_E(i-j) \quad [6.5]$$

where $\kappa_E(i) = \kappa_E(\mathbf{G}_i)$, $|k_i| = \sqrt{\langle k_i | k_i \rangle}$ and $|k_j| = \sqrt{\langle k_j | k_j \rangle}$. If all the materials in the PC are isotropic then, Eqns. 6.4 and 6.5 become $M_{ij} = \langle k_i | k_j \rangle \kappa(i-j)$ and $M_{ij} = |k_i| |k_j| \kappa(i-j)$ respectively with $\kappa(i) = \kappa(\mathbf{G}_i)$.

6.3. Approximation Methods

Eqn. 6.2 (or 6.3) completely defines an EFS for a given frequency and has to be evaluated using the entire basis (i.e. plane waves) of the reciprocal space which is infinite in number. Numerical calculation of the EFS involves a finite number of bases and the number is often limited in accordance with a required degree of accuracy.[♥] In general, the larger is the dielectric modulation, the larger is the number

[♥] Numerical calculation of EFS was outlined in the last paragraph of Sec. 4.4 (Chap. 4).

of plane waves required. For PCs with a weak dielectric modulation which are the favorites for the dispersive effects, the number of plane waves can be significantly less.

In the following sections, we will use one plane wave and two plane waves to approximate the EFS and as we shall see, such approximations lead to meaningful analytical expressions.

6.3.1. One plane wave approximation

Assume a PC made of two materials with dielectric tensors $\tilde{\epsilon}_a$ and $\tilde{\epsilon}_b$ and the filling ratio of the material with the dielectric tensor $\tilde{\epsilon}_b$ is f , the one plane wave approximation assumes $\tilde{\kappa}_H(i-j) = \delta_{ij} \tilde{\epsilon}_m^{-1}$ [Ho's Method, Sec.4.4] with $\tilde{\epsilon}_m$ given by,

$$\tilde{\epsilon}_m = \tilde{\epsilon}_b f + (1-f)\tilde{\epsilon}_a \quad [6.6]$$

Consequently matrix, M is diagonal and Eqn. 6.3 becomes, $\Omega = \sum_i H_i H_i^* M_{ii} = \sum_i H_i^2 \langle k_i | \tilde{\epsilon}_m^{-1} | k_i \rangle$ for the H -polarization. By selecting an eigenvector $|H\rangle = [0 \dots 1 \dots 0]^T$ with 1 at the i -th position,

$$\langle k_i | \tilde{\epsilon}_m^{-1} | k_i \rangle = \Omega \quad [6.7]$$

which must be true for every i . The tensor $\tilde{\epsilon}_m$ in general can be written as $\tilde{\epsilon}_m = Q^T \tilde{\epsilon}_{mp} Q$ [Chap. 2] where $\tilde{\epsilon}_{mp}$ is the dielectric tensor in the principal coordinate system of the anisotropic material, Q is a rotational operator (an orthogonal operator) and Q^T is the transpose of Q . Thus, Eqn. 6.7 can be rewritten using the inner product properties [108] to,

$$\Omega = \langle k_i | Q^T \tilde{\epsilon}_{mp}^{-1} Q | k_i \rangle = \langle Qk_i | \tilde{\epsilon}_{mp}^{-1} | Qk_i \rangle \quad [6.8]$$

where $|Qk_i\rangle = [k_{x'} - G_{ix'}, k_{y'} - G_{iy'}]$ is a rotated vector of $|k_i\rangle = [k_x - G_{ix}, k_y - G_{iy}]$. If one of the materials is assumed to be isotropic and the other is assumed to be anisotropic which is often the case [Chap. 2], then using Eqn. 6.6 we have,

$$\tilde{\epsilon}_{mp}^{-1} = \begin{pmatrix} 1/\{\epsilon_b f + \epsilon_{a1}[1-f]\} & 0 \\ 0 & 1/\{\epsilon_b f + \epsilon_{a2}[1-f]\} \end{pmatrix} \quad [6.9]$$

where $\tilde{\epsilon}_b$ is taken as an identity matrix multiplied by a constant, $\epsilon_b = n_b^2$ and $\tilde{\epsilon}_a$ is assumed as the dielectric tensor of the anisotropic material in the principal coordinate system, with ϵ_{a1} and ϵ_{a2} being the principal dielectric constants. Substituting the expressions for $|Qk_i\rangle$ and $\tilde{\epsilon}_{mp}^{-1}$ in Eqn. 6.7, we obtain the following equation to define an EFS of the H -polarization in the rotated frame,

$$\frac{(k_{x'} - G_{ix'})^2}{\epsilon_b f + \epsilon_{a1}[1-f]} + \frac{(k_{y'} - G_{iy'})^2}{\epsilon_b f + \epsilon_{a2}[1-f]} = \Omega. \quad [6.10]$$

Eqn. 6.10 basically describes an ellipse in the rotated frame $(k_{x'}, k_{y'})$ with the origin located at $(k_{x'}, k_{y'}) = (G_{ix'}, G_{iy'})$. As the equation is true for every i , there will be repetitions of the same ellipse for each i . EFS is then simply an ensemble of these ellipses within a BZ.

Similarly for E -polarization it can be shown that, the one plane wave approximation leads to $|k_i|^2 = \Omega \epsilon_m$ where $\kappa_E(i-j) = \delta_{ij} / \epsilon_m$ has been used for Eqn. 6.5. Assuming $|k_i\rangle = [k_{x'} - G_{ix'}, k_{y'} - G_{iy'}]$, we will arrive at the same equation as Eqn. 6.10, however the denominators at the left hand side of the Eqn. 6.10 are replaced

with $\epsilon_m = \epsilon_b f + \epsilon_{a3}[1 - f]$, where ϵ_{a3} is the principal dielectric constant of the anisotropic material experienced by the E -polarization.

To illustrate the EFS construction, let's first assume both materials are isotropic (i.e. $\epsilon_{a1} = \epsilon_{a2} = \epsilon_{a3} = n_a^2$) and consider a PC with a square lattice, $n_b = 1.6$, $f = 0.4$ and a very small modulation (i.e. $n_a \rightarrow n_b$). For example, considering $\omega = 0.5$ and using the radius given by Eqn. 6.10, we draw circles at each reciprocal lattice point as shown in Figure 6.1(a).

Fig. 6.1 EFS constructions of a square lattice PC with $f = 0.4$, $n_b = 1.6$ and $n_a \rightarrow n_b$. Band indices: band 2 – blue, band 3 – red, band 4 – pink, band 5 – yellow. The thin lines indicate boundaries of the square lattice BZ (a) EFS construction with the band index for $\omega = 0.5$ (b) EFS for $\omega = 0.5$ (c) EFS for $\omega = 0.36$ (d) EFS for $\omega = 0.67$.

Each closed contour forms a band or part of a band and due to the band folding effect, if the contour encloses an area which is an intersection of n circles, then the band index is n [166-167]. Following this principle, we can index each closed contour with the corresponding band index as shown in Fig. 6.1(b) where the bands are indexed with different colors. The EFS construction with the band assignment for $\omega = 0.36$ and 0.67 are shown in Fig. 6.1(c) and 6.1(d) respectively. It is worth to note that the area enclosed by black lines in Fig. 6.1(c) is not an intersection of many circles but only involves the first band and thus, the band index is 1.

Now let's demonstrate the validity of the EFS obtained from the one plane wave approximation by comparing with those of numerically evaluated using large number of plane waves. In Figure 6.2(a) and 6.2(b) we plot EFSs ($\omega = 0.5$) for $n_a = 2.0$ and 2.6 respectively and the other parameters are kept to be the same as for Fig. 6.1. The one plane wave construction is shown using dotted lines whereas the EFS obtained from the numerical calculation employing 361 plane waves is highlighted in color. As it is clear from the Fig. 6.2(a) for low modulation, the construction agrees well with the numerically calculated EFS. When the modulation increases, the degree of disagreement increases [Fig. 6.2(b)]. In PCs with a large dielectric modulation, the one plane wave approximation can be used to gain a rough idea on the band shape for an ω that is far away from a photonic band gap and it is important to note that the EFS construction using one plane wave fails if ω lies close to the photonic band gap [67].

Finally we provide a construction example for H -polarization using one plane wave approximation at $\omega = 0.5$ for a square lattice PC with anisotropic material

($\sqrt{\epsilon_{a1}} = 1.6$, $\sqrt{\epsilon_{a2}} = 2.0$), $n_b = 1.8$ and $f = 0.2$. The principal axis with the smaller principal dielectric constant is oriented 45° with respect to the k_x - axis of the PC as shown Figure 6.3(a).

Fig. 6.2 EFS constructions (dotted black line) and the numerically calculated EFS (color) of a square lattice PC with $f = 0.4$, $n_b = 1.6$ and $\omega = 0.5$. Band indices: band 3 – red, band 4 – pink, band 5 – yellow. The thin lines indicate boundaries of the square lattice BZ (a) EFS for $n_a = 2.0$ (b) EFS $n_a = 2.6$.

Fig. 6.3 EFS constructions for H -polarization (dotted black line) and the numerically calculated EFS (color) of a square lattice PC with anisotropic materials ($f = 0.2$, $n_b = 1.8$, $\sqrt{\epsilon_{a1}} = 1.6$, $\sqrt{\epsilon_{a2}} = 2.0$, $\omega = 0.5$) band 2 – blue, band 3 – red, band 4 – pink. (a) EFS construction (b) EFS with the band index.

The Q operator in Eqn. 6.8 is a 45° anticlockwise rotational operator and hence, following Eqn. 6.8 and Eqn. 6.10 we draw ellipse at each reciprocal lattice point in the rotated coordinate system as shown in Fig. 6.3(a). The numerically calculated EFS plot is shown in Fig. 6.3(b) and as we can readily verify from the figure that, both the construction and numerical evaluation share a good agreement.

Though one plane wave approximation seems to be good in approximating an EFS of a PC with a weak modulation, a magnified diagram of the EFS will show that, this approach is unable to approximate the edges of the EFS accurately. This problem will be addressed in the following.

6.3.2 Two plane waves approximation

In this section, we will demonstrate a two plane waves* approximation to obtain EFS of a 2D PC. We assume the modulation is finite and weak such that only the first two Fourier coefficients of $\kappa(i)$ [i.e. $\kappa(0)$ and $\kappa(1)$], $\tilde{\kappa}_H(i)$ or $\kappa_E(i)$ are significant. Then we can approximate Eqn. 6.3 as,

$$\Omega = H_i M_{i,i} H_i + H_i M_{i,i+1} H_{i+1} + H_{i+1} M_{i+1,i} H_i + H_{i+1} M_{i+1,i+1} H_{i+1} \quad [6.11]$$

which has to be true for every i . We can choose $i = 1$ and the eigenvalues, Ω of the resulting M can be obtained by finding the determinant of the matrix,

* The method of two plane waves approximation is indeed an application of the method presented in Chap. 5, (see Sec. 5.2.2) to find the dispersion relation for the wavevectors in the neighborhood of symmetrical points of a PC with $n(m_k) = 2$. Therefore, the matrix in Eqn. 6.12 has dimension of 2 by 2 and in general; we need a matrix with dimension $n(m_k)$ by $n(m_k)$ [i.e., a $n(m_k)$ plane waves approximation] in order to describe the EFS around a symmetrical point of a label m_k (see Sec. 2 and 3 of Chap. 5), using a small spatial modulation approximation.

$$M = \begin{bmatrix} M_{11} - \Omega & M_{12} \\ M_{21} & M_{22} - \Omega \end{bmatrix}. \quad [6.12]$$

Using the fact $M_{ij} = M_{ji}^*$ we can show that

$$2\Omega = \langle k_0 | \tilde{\mathbf{K}}_H(0) | k_0 \rangle + \langle k_1 | \tilde{\mathbf{K}}_H(0) | k_1 \rangle \pm \sqrt{\left\{ \langle k_0 | \tilde{\mathbf{K}}_H(0) | k_0 \rangle - \langle k_1 | \tilde{\mathbf{K}}_H(0) | k_1 \rangle \right\}^2 + 4 \langle k_0 | \tilde{\mathbf{K}}_H(1) | k_1 \rangle^2} \quad [6.13.1]$$

for H -polarization. For E -polarization we have,

$$2\Omega = \kappa_0 (k_0^2 + k_1^2) \pm \sqrt{\kappa_0^2 (k_0^2 - k_1^2)^2 + (2\kappa_1 k_0 k_1)^2}, \quad [6.13.2]$$

where $k_i k_j$, κ_0 and κ_1 represent $|k_i| |k_j|$, $\kappa_E(0)$ and $\kappa_E(1)$ respectively. If all the materials in the PC are isotropic, then for both H - and E -polarizations, the two plane waves approximation yields similar result as in Eqn. 6.13.2 but now $k_i k_j$ represents $\langle k_i | k_j \rangle$ and $|k_i| |k_j|$ for H - and E -polarization respectively. Further in this case, we have to replace $\kappa_E(0)$ and $\kappa_E(1)$ in Eqn. 6.13.2 with $\kappa(0)$ and $\kappa(1)$ respectively.

Eqn. 6.13.1 and 6.13.2 can be evaluated using specific choices of the wavevectors and reciprocal lattice vectors. For example, we consider the EFS's near the first band gap of a square lattice PC around $X(-\pi/a, 0)$ point of E -polarization with all isotropic materials. To examine such EFS's, we assume $\kappa(0) = \kappa_0$, $\kappa(1) = \kappa_1$, $\mathbf{k} = [k_x \ k_y]'$, $\mathbf{G}_0 = [0 \ 0]'$ and $\mathbf{G}_1 = [-g \ 0]'$ with $g = 2\pi/a$, and consequently the terms in Eqn. 6.13 become,

$$\kappa_0 (k_0^2 + k_1^2) = 2\kappa_0 [(k_x + g/2)^2 + k_y^2 + g^2/4] \quad [6.14.1]$$

$$\kappa_0^2 (k_0^2 - k_1^2)^2 = [2\kappa_0 g (k_x + g/2)]^2 \quad [6.14.2]$$

$$(2\kappa_1 k_0 k_1)^2 = 4\kappa_1^2 [(k_x + g/2)^2 + k_y^2 + g^2/4]^2 - [2\kappa_1 (k_x + g/2)]^2 \quad [6.14.3]$$

We move the origin of the reciprocal space from (0,0) to the X point by writing $k_x = k_x + g/2$ and therefore Ω transforms to,

$$\Omega = \kappa_0 (k_x^2 + k_y^2 + g^2/4) \pm \sqrt{(\kappa_0 k_x g)^2 + \kappa_1^2 (k_x^2 + k_y^2 + g^2/4)^2 - (\kappa_1 k_x g)^2} \quad [6.15]$$

Eqn. 6.15 does not provide any insight to the EFS. More useful information can be obtained if we can transform the equation to a simpler form. To do this, we first seek an approximation to the square root term in Eqn. 6.15 for a small k_x . The square root term for a small k_x can be written as $y = \sqrt{P^2 + Q^2}$, where $P = |\kappa_0 k_x g|$ and $Q = |\kappa_1| (k_x^2 + k_y^2 + g^2/4)$. We can expand y using binomial expansion as $y \approx Q + \frac{P^2}{2Q}$ however, this requires $Q > P$ and this assumption will be justified later in the discussion. Using the binomial expansion of y and assuming a small k_x and k_y , Eqn. 6.15 can be simplified and after some algebra we arrive at the following set of equations,

$$\left[\Omega_1 - \frac{g^2}{4} (\kappa_0 - |\kappa_1|) \right] = k_x^2 \left(\kappa_0 - |\kappa_1| - \frac{2\kappa_0^2}{|\kappa_1|} \right) + k_y^2 (\kappa_0 - |\kappa_1|) \quad [6.16.1]$$

$$\left[\Omega_2 - \frac{g^2}{4} (\kappa_0 + |\kappa_1|) \right] = k_x^2 \left(\kappa_0 + |\kappa_1| + \frac{2\kappa_0^2}{|\kappa_1|} \right) + k_y^2 (\kappa_0 + |\kappa_1|) \quad [6.16.2]$$

where the two solutions of Eqn. 6.15 are denoted as Ω_1 and Ω_2 and these equations provide meaningful representations of the EFS. It can be shown that in Eqns. 6.16.1

(band 1) and 6.16.2 (band 2), $\kappa_0 + |\kappa_1| + 2\kappa_0^2 / |\kappa_1| > 0$ and $\kappa_0 - |\kappa_1| - 2\kappa_0^2 / |\kappa_1| < 0$ for all κ_0 and κ_1 with $\kappa_0 > |\kappa_1|$ and hence, Eqn. 6.16.2 gives EFS's of an elliptical shape with the length of the semi-major and -minor proportional to the reciprocals of $\sqrt{\kappa_0 + |\kappa_1| + 2\kappa_0^2 / |\kappa_1|}$ and $\sqrt{\kappa_0 - |\kappa_1| - 2\kappa_0^2 / |\kappa_1|}$ respectively.

Now let's examine the validity of the assumption $Q > P$ in deriving Eqns. 6.16.1 and 6.16.2. The expressions P and Q are linear and quadratic functions of k_x respectively and the minimum point of Q is $f(k_y) = |\kappa_1|(k_y^2 + g^2/4)$. Hence, a sufficient condition for $Q > P$ is then simply $f(k_y) > P$. Thus, the sufficient condition on k_x can be shown to be,

$$-\frac{|\kappa_1|}{\kappa_0 g}(k_y^2 + g^2/4) < k_x < \frac{|\kappa_1|}{\kappa_0 g}(k_y^2 + g^2/4). \quad [6.17]$$

The conditions on k_x and k_y also can be solved by solving the quadratic in-equality $Q - P > 0$, and again we will encounter square roots in the solutions. If the square root term produces an imaginary value, then Q will never cross P and hence, $Q > P$ for all k_x . The corresponding condition on k_y is,

$$k_y > \frac{g}{2|\kappa_1|} \sqrt{\kappa_0^2 - \kappa_1^2}. \quad [6.18]$$

To illustrate the EFS construction using the two plane waves approximation, consider a square lattice PC with $n_a = 1.8$, $n_b = 1.6$ and $f = 0.2$. The numerically calculated EFS and the approximated EFS (using Eqn 6.13-6.14) for frequencies in the first and second band are shown in Figures 6.4(a) and 6.4(b) respectively. In both figures, we have evaluated Eqn. 6.13 for wavevectors in the ranges $-\pi/a < k_y < \pi/a$

and $-2\pi/a < k_x < 0$, and the result shares a good agreement with those of numerically evaluated around the $X(-\pi/a, 0)$ point. As Eqn 6.11 has to be true for every i , we can translate the EFS approximated for $i = 1$ by a vector $\mathbf{G}_i$.

Fig. 6.4 EFS approximations using two plane waves for a square lattice PC with $n_b = 1.6$, $n_a = 1.8$ and $f = 0.2$. The numerically calculated EFS (thin black lines) and the approximated EFS (thick blue lines) for frequencies in the (a) first band (b) second band.

Furthermore the EFS in the neighborhood at the other symmetrical X points [i.e. $(\pi/a, 0)$, $(0, \pi/a)$ and $(0, -\pi/a)$] can be reproduced using the EFS approximated in the neighborhood of $X(-\pi/a, 0)$ by point group – symmetry operations [from group $\overline{R}_M$, see Chap. 3].

In order to appreciate the ability and inability of the two plane waves approximation, we plot EFS's (band 2, $\omega = 0.3$) obtained from the one plane wave approximation, two plane waves approximation and numerical calculation in Figures 6.5(a) and 6.5(b) for $n_a = 1.8$ and $n_a = 2.0$ respectively. The one plane wave-EFS is constructed using two circles originated from $(0, 0)$ and $(-g, 0)$ points. Thus it always predicts sharp edges for the EFS [see band 2 in Fig. 6.1(c), 6.5(a) and 6.5(b)]. The sharp edges do not appear in the numerically calculated EFS which is the

accurate EFS. The failure of one plane wave method is corrected in the two plane waves approximation and the approximation perfectly matches the numerical counterpart when the dielectric modulation is small [Fig. 6.5(a)]. As expected, when the dielectric modulation becomes large, the two plane waves approximation becomes poorer [Fig. 6.5(b)], however the approach still exhibits a better accuracy compared to the one plane wave approach.

Fig. 6.5 The merit of two plane waves – EFS approximation for a square lattice PC with $n_a = 1.6$, $f = 0.2$. EFS ($\omega = 0.31$) obtained from the one plane wave approximation (dashed black line), two plane waves approximation (thick blue line) and numerical calculation (thin red line) for (a) $n_a = 1.8$ (b) $n_a = 2.0$.

6.4 Negative principal refractive indices and accidental isotropy

The periodic dielectric modulation in a PC is similar to a periodic modulation of the electronic potential in an electronic crystal (i.e. a semiconductor). Hence, it is natural to have similar phenomena, for example band gaps in both PCs and semiconductors. The behavior of an electron near the band edges of a semiconductor can be approximated as that of a free electron with an effective mass. The analogous concept in a PC was shown by Notomi [67], that, in the vicinity of a photonic band gap, PC behaves like an isotropic bulk medium with an effective refractive index. Furthermore, this effective refractive index could be negative and hence, could give rise to the properties similar to those of a negative index material [66,72]. In this part of the chapter, we study the formation and the properties of anisotropic negative index materials based on an anisotropic 2D PC, whose effective principal refractive indices are negative in the vicinity of the photonic band gap.

The EFS of a 2D isotropic PC is circular for a frequency near the bottom edge of the first band (i.e. in the long wavelength limit) and hence, the PC behaves like a bulk isotropic medium with an effective refractive index [168-169]. This effective index is positive since the first band has a positive sign of $\nabla_{\mathbf{k}}\omega$. It is also reported that in such 2D PCs when the modulation of the refractive index become stronger, the EFSs become circular for frequencies near the edge of the higher order bands. Thus for the corresponding range of frequencies, the 2D PC can be homogenized to an isotropic bulk medium with an effective refractive index. However, this effective index can be negative if the sign of $\nabla_{\mathbf{k}}\omega$ of the particular band is negative [67]. Similar analysis can be envisioned for a 2D anisotropic PC. In this case, if the

anisotropic PC has no rotational axes with order larger than two[♥], the EFSs in the long wavelength limit become elliptical [168-169]. As we shall show, near the photonic band gaps, such anisotropic PCs do behave like bulk media, with an anisotropy and thus, a set of effective principal refractive indices can be defined.

In order to investigate this, we consider a 2D PC made of isotropic materials and a geometry as shown in Figure 6.6. Recall in Chap. 3, that the point group of a PC, which can be defined as a group of symmetry elements, R_M such that $R_M M R_M^{-1} = M$ can be expressed as $\overline{R_M} = \overline{R} \cap \overline{R_B}$, where $\overline{R}$ and $\overline{R_B}$ are the point group of the lattice and basis respectively.

Fig.6.6 The geometry of the 2D PC.

[♥] Regardless of lattice, most of 2D anisotropic PCs have no rotational axes of order larger than 2. For example, see the symmetry elements in Table 3.1 for the hexagonal lattice. If the 2D anisotropic PC has a rotational axes of order larger than 2, then the EFS becomes circular in the long wavelength limit [168-169].

For a rectangular basis using Schonflies notations, $\overline{R_B} = [E, C_2, \sigma_\theta, \sigma_{\theta+90^\circ}]$, where E is an identity element, C_2 is a two-fold rotational operation, σ_θ and $\sigma_{\theta+90^\circ}$ are mirror operations along the axes defined by θ and $\theta + 90^\circ$ [See Fig. 6.6 for the definition of θ]. Hence for $\theta = 0$, $\overline{R_M} = C_{2v} = [E, C_2, \sigma_0, \sigma_{90^\circ}]$ ($\overline{R} = C_{6v}$, $\overline{R_B} = C_{2v}$). The same symmetry can be found in many PC configurations with different choices of lattices and bases. For instance, a square basis in a 2D hexagonal lattice and a rectangular basis in a 2D square lattice lead to the same $\overline{R_M}$, when their symmetry axes coincide in both cases. Besides geometrically anisotropic PCs, the same symmetry also can be found in materially anisotropic PCs. For instance, a PC with uniaxially anisotropic circular cylinders in the 2D hexagonal lattice will have the same symmetry ($\overline{R_M} = C_{2v}$) if the optic axis of the anisotropic material is aligned parallel to any of the symmetrical directions of the hexagonal lattice. When $R_M \in \overline{R_M}$, using Eqn. 6.1,

$$\begin{aligned} \Omega(R_M \mathbf{k}) &= \langle \mathbf{H}_{R_M \mathbf{k}} | M | \mathbf{H}_{R_M \mathbf{k}} \rangle \\ &= \langle R_M \mathbf{H}_\mathbf{k} | M | R_M \mathbf{H}_\mathbf{k} \rangle = \langle \mathbf{H}_\mathbf{k} | R_M^{-1} M R_M | \mathbf{H}_\mathbf{k} \rangle = \langle \mathbf{H}_\mathbf{k} | M | \mathbf{H}_\mathbf{k} \rangle = \Omega(\mathbf{k}) \end{aligned} \quad [6.20]$$

where we have made use of Eqn. 3.2 and 3.4 of Chap. 3. From Eqn. 6.20 we conclude that EFSs at any frequency are invariant under the symmetry operations of $\overline{R_M}$.

The 2D band structure of the PC with a geometry as shown in Fig. 6.6 is computed for the H -polarization, using PWM [Ho's approach, Chap. 4] and the result is shown in Figure 6.7(a) with the vertical axis representing the normalized frequency, ω . In the calculation, we used 361 plane waves and the convergence accuracy for the first three bands was better than 1%. Moreover, we used $p = q = 0.8a$, $\theta = 0$ (Fig. 6.6) with the dielectric constants of the matrix and the rectangular basis

taken as 12.96 (silicon) and 1 (air) respectively. Fig. 6.7(a) was obtained by firstly solving the eigen-equation for $\mathbf{k}$ -vectors within the IBZ (Chap. 3). Then, by means of symmetry operations in $\overline{R_M}$, the band structure corresponding to the whole BZ was obtained.

Fig. 6.7 (a) 2D band diagram with $p = q = 0.8a$ and $\theta = 0$. (b) Contour plot of the second band within the first BZ of a hexagonal lattice. The IBZ is the region confined by Γ -K-M-K'-M'- Γ .

As we can see from Fig. 6.7(a), there is a band gap between the second and the third band with a width of 5% of the midgap frequency. Fig. 6.7(b) also shows a contour plot of the second band in Fig. 6.7(a). As we can see from Fig. 6.7(b), when we move from the bottom edge frequency to the top edge frequency of the second band, the EFS clearly transforms from more complex shape to an elliptical one and for any frequency, the EFS clearly possesses the full point group symmetry, $\overline{R_M}$. Furthermore, for the frequencies in the second band, the EFS moves inward when ω increases, which indicates a negative sign of $\nabla_{\mathbf{k}}\omega$. Thus, for the photonic states near

the edge of the second band, a set of effective negative principal refractive indices and hence an elliptical EFS can be defined (similar to the principal indices used to define elliptical EFSs in a bulk anisotropic medium [110-111]). The effective negative principal refractive index along k_x and k_y direction can be respectively written as

$$n_x = \frac{p_x a}{2\pi\omega} \text{ and } n_y = \frac{p_y a}{2\pi\omega} \text{ with } p_x \text{ and } p_y \text{ are the lengths (in } a^{-1}) \text{ of the semi-major and}$$

semi-minor axes of the ellipse. These indices can be found by fitting the numerically

computed EFS to the equation of $\omega^2 = \frac{a^2}{4\pi^2} \left(\frac{k_x^2}{n_x^2} + \frac{k_y^2}{n_y^2} \right)$, using a method of least

square [109]. Using the usual definition, a fitting parameter, R^2 is defined to evaluate

the accuracy of the fitting; $R^2 = 1$, indicates a perfect fitting. Figure 6.8(a) shows R^2

plotted against the frequencies of the second band and it is obvious that R^2 increases

to 1 for frequencies closer to the top edge of the second band. The computed

effective principal indices and the anisotropy, $\Delta n = n_x - n_y$ are shown in Fig. 6.8(b) for

frequencies in the second band with $R^2 > 0.98$. The value of Δn remains fairly at a

constant value of 0.2, for a frequency range of $0.31 < \omega < 0.36$. As the frequencies

approach the band gap [inset of Fig. 6.8(b)], both principal indices and Δn reduce to

zero, which agree with the fact that the group velocity approaches zero near the

band gap frequency. The obtained principal indices can be used to analytically

approximate the gradients of the EFS and hence to predict the light propagation

directions in the PC.

The investigation of the effect of filling ratio on these anisotropic negative index states produces a very surprising result. For instance, we vary p while keeping the remaining parameters the same as before ($q = 0.8a$ and $\theta = 0$). The band edge

frequency as a function of p is shown in Figure 6.9(a). The bottom edge of third band touches the top edge of the second band when $p = 0.74a$. For $p < 0.74a$, we have overlapping of two bands which means that, it is possible to have two states for a given frequency. For $p > 0.74a$, the two bands split and a band gap opens. In order to keep a single state for a given frequency, we choose an ω that is 10% below the top edge of the second band [indicated as triangles in Fig. 6.9(a)].

Fig. 6.8 (a) R^2 as a function of ω ($p = q = 0.8a$ and $\theta = 0$). (b) n_x , n_y and Δn as a function of ω ($p = q = 0.8a$ and $\theta = 0$). The inset in (b) shows similar relationships for frequencies near the top edge of the band 2.

Fig. 6.9 (a) The maximum ω of band 2 and the minimum ω of band 3 as a function of p ($q = 0.8a$ and $\theta = 0$).

Pink triangles identifies an ω that is 10% below the maximum of band 2. (b) n_x , n_y and Δn as a function of p ($q = 0.8a$ and $\theta = 0$) for ω 's shown as pink triangles in (a).

The corresponding principal refractive indices and the Δn as a function of p are plotted in Figure 6.9(b). The R^2 parameter for all values of p is greater than $0.98a$. As we can see from Fig. 6.9(b), n_x reduces as p is increased. However, the similar change in n_y is at a slower rate compared to that in n_x . This is expected since, when p is increased the corresponding Fourier expansion of the dielectric constant rises faster along k_x – direction, than k_y – direction. The different rates of $\partial n_y / \partial p$ and $\partial n_x / \partial p$, force n_y and n_x to cross at $p = 0.7a$, $\Delta n = 0$ (i.e. an isotropic state with a circular EFS). Apparently, EFSs at all values of p , are invariant under the symmetry operations of $\overline{R_M}$. However, such an isotropic state at $p = 0.7a$, is accidental since the corresponding EFS exhibits higher order symmetries that are not in the group of $\overline{R_M}$. Further, the formation of the anisotropic negative index states and the accidental isotropic states can also be observed for other q 's. For instance, when q is changed from $0.8a$ to $0.68a$, we found that the isotropic state is moved from $p = 0.7a$ to $0.6a$.

Though Δn varies as a function of filling ratio when $\theta = 0$, the orientation of elliptical EFSs remains the same for all filling ratios. Such a fixed orientation is a consequence of the symmetry requirement for $\theta = 0$, where we have $\overline{R_M} = C_{2v}$. The presence of mirror symmetries along k_x and k_y axes in $\overline{R_M}$ keeps the orientation of ellipse to be the same for all values of filling ratios. If $\overline{R_M}$ does not have such mirror symmetries, the orientational requirement is relaxed and the orientation is found to be varying with the change in filling ratio.

For instance, instead of varying p at $\theta = 0$, we can vary p at $\theta = 45^\circ$. In general, when $\theta = 45^\circ$, $\overline{R_M} = C_s = [E, C_2]$ which does not have any mirror axis. The EFS near

the top edge of the second band is still elliptical but the orientation of the ellipse is now changed. The orientation of the ellipse, ϕ , is taken as an angle between the semi-major axis and the k_y -axis of the reciprocal lattice. In Figure 6.10, we show the numerically computed ϕ as a function of p for $q = 0.68a$ and for an ω that is 15% below the top edge of the second band. Since the orientation of the ellipse is unknown, we cannot fit the numerically computed data to an elliptical equation as we did for $\theta = 0$. Hence a more general fitting technique of an ellipse is employed to obtain ϕ [170] and the values of principal refractive indices.

Fig. 6.10 ϕ versus p ($q = 0.8a$, $\theta = 45^\circ$ and for an ω that is 10% below the top edge of the second band). The inset shows the definition of ϕ .

As we can see from Fig. 6.10, as p is changed from $0.3a$ to $0.8a$, ϕ changes from 54° to -37° (nearly 90°). As $\phi \neq 0$, the EFS at any p does not have any mirror symmetries along k_x and k_y axes which agree with the fact that $\overline{R_M} = C_S$ for $\theta = 45^\circ$, with an exception at $p = 0.68a$. When $p = 0.68a$, we have $\phi = 0$ and thus the EFS exhibits mirror symmetries along k_x and k_y axes. This is not accidental, because when $p =$

$0.68a$ (i.e. $p = q$), we have a square basis ($\theta = 45^\circ$) with a point group $\overline{R}_B = C_{4v} = [E, C_2, C_4, C_4^{-1}, \sigma_0, \sigma_{90^\circ}, \sigma_{45^\circ}, \sigma_{135^\circ}]$, and hence, $\overline{R}_M = \overline{R} \cap \overline{R}_B = C_{2v}$. So the presence of mirror symmetries along k_x and k_y axes, when $p = 0.68$, forces ϕ to be zero. On the other hand, it is worth mentioning that the variation of Δn with respect to p , when $\theta = 45^\circ$, is small (0.11-0.14) compared to a large variation of Δn when $\theta = 0$.

6.5 Summary

In this chapter we have presented the formulations, approximations and characteristics of EFSs of an anisotropic PC.

In Sec. 6.2, a general description of an EFS was given. Sec. 6.3 presented an analytical approach to the EFS of a 2D PC made of materials of general anisotropy using one and two plane waves approximations. The analytical expression of the EFS can be used to directly predict the refraction angles and hence the superprism effect of PCs with a weak modulation, analytically. The analytical description of EFS also overcomes the problem of computational efficiency in the existing numerical method to calculate EFS which needs a large computational time [see Chap. 4].

Sec. 6.4 of the chapter described an EFS based phenomena in an anisotropic PC with a large refractive index modulation. In particular, we studied a PC with a rectangular basis in a 2D hexagonal lattice and showed that the EFS near the band edge frequency is elliptical similar to the EFS of a bulk anisotropic medium. A set of effective negative principal refractive indices was defined to describe the photonic states with elliptical EFSs (i.e., anisotropic states). By varying the filling ratio, it is possible to force such an anisotropic state to an accidental isotropic state (i.e., states

with circular EFS). Further, by re-orienting the motif and continuously varying the filling ratio, the orientation of the elliptical EFS can be continuously tuned.

Chapter 7

Insulating Properties

7.1 Introduction

In the next two chapters, applications of anisotropic PCs will be presented. The applications can be classified into two main groups based on the two distinct properties, namely insulating (if the light wavelength falls within the band gap) and conducting (if the light wavelength falls outside the band gap) properties. This chapter focuses on the applications of the anisotropic PCs based on the insulating capabilities, and the applications based on their ability of conducting photons appear in Chap. 8.

Applications of insulating properties of anisotropic PCs can be categorized into two main categories namely band gap engineering and band gap tuning.

7.1.1 Applications for band gap engineering

Since PC was firstly introduced in 1987 till now, construction of PCs with large and full band gaps is one of the major goals of the field [25–44]. This is because; many applications require a large photonic band gap. For instance, if there is a large band gap then the spontaneous emission can be inhibited for a wide range of frequencies [52–54], and in the case of a laser, this could lead to a substantial reduction in the threshold voltage for lasing.

Geometrically anisotropic PCs have been widely used in the explorations of 2D and 3D photonic band gaps [10-12, 26, 29-35, 83-84]. Particularly in 2D PCs,

motifs with various geometry have been used to improve the photonic band gap [29-34, 83]. Importantly, it was shown that geometries like square [26], rotated square [30-31] and ellipse [29] produce very large and complete 2D photonic band gaps for both polarizations of light. A comprehensive study with detailed specifications on the effect of various motifs and their orientations to the photonic band gap can be found in Ref. 83. In this thesis, we study materially anisotropic PCs, to investigate their role in engineering the band gap of a PC.

For a 3D materially anisotropic PC, Zhi-Yuan Li *et al.* [103] and Zabel *et al.* [102] have shown how the anisotropy of the material opens and closes the band gap. For 2D structures, Li *et al.* [33] have shown previously, that a complete gap can be achieved, using uniaxial materials with optic axis along the extension direction of the cylinders. In Li's approach, *E*- and *H*-polarizations experience different refractive indices and therefore the band structure for both polarizations can be adjusted to match each other. As the optic axis is along the extension direction of the cylinders, these refractive indices are direction independent (i.e. isotropic). A more general case of arranging the principal axis of the birefringent material in the 2D periodic plane was not considered where the *H*-polarization will experience direction dependent refractive index. By optimizing the optic axis direction in the periodic plane of a 2D PC, the photonic band gap can be tailored along a wide range of directions, which is useful in a variety of applications. Such a 2D PC is more practical, because the refractive index can be chosen in a range, for example, n_e (extraordinary refractive index) and n_o (ordinary refractive index) for uniaxial materials, to adjust the band gap along a particular wave propagation direction.

In the first section of the chapter, we consider a 2D materially anisotropic PC with the principal axis of the birefringent material in the 2D periodic plane. The anisotropic material can be either uniaxial or biaxial. Without losing generality, the optic axis of an uniaxial material or any two principal axes of a biaxial material is placed in the 2D periodic plane. For a square lattice with a circular motif, the band gap for E -polarization exists for quite a wide range of filling ratios. However, the band gap for H -polarization exists at very high filling ratio or for large refractive index contrast, which makes such a PC difficult to be realized. By re-orienting the optic axis (principal axes) in the 2D periodic plane, we shall show that the band gap for H -polarization can be engineered so that a large band gaps can be opened. The gap is observed for a wide range of filling ratio and low refractive index contrast in the square lattice, which makes it easy in fabrication and in choosing materials. With our proposed technique to tailor the band gap of H -polarization, aided by the band gap matching technique for different polarizations proposed by Li *et al* [33], comprehensive band gap design of 2D PC can be realized.

7.1.2 Applications for band gap tuning

Materially anisotropic PCs, are found to be extremely useful in realizing tunable band gaps [85-99]. Tunable PCs are extremely important as they provide external controls to the optical properties of a PC, and therefore, beneficial in many applications like optical computers, switches and modulators. LC is a well-known anisotropic medium [100-101] with attractive thermo-optic and electro-optic properties. When LC is heated up to its phase transition temperature, a large refractive index change can be obtained. Further, by applying a small voltage that is

larger than the threshold voltage for Frederick's transition (about 1 V) [100-101], the optic axis of the LC can be aligned according to the orientation of the applied electric field. LC was firstly proposed by Kurt and John [96] to infiltrate the void regions of a 3D inverted opal PC [Fig. 1.5(a) of Chap. 1]. They showed that, 2% of the 3D photonic band gap can be completely opened and closed by controlling the LC's optic axis orientation. Their findings motivated many researchers to explore tunable band gaps in 1D [85-90], 2D [91-95], and 3D [96-99] LC infiltrated PCs. Apart from LC, Pockel materials also have been employed in tunable band gap applications [171-172]. However, Pockel materials require a large electric field in order to induce a notable change in the principal refractive indices and hence in the band gap. In the following we shall analysis in more detail, the previous works on the applications of 2D and 1D anisotropic PCs based on band gap tuning.

The first experimental realization of a LC infiltrated 2D PC [Fig. 1.5(b) of Chap. 1] made of porous silicon was shown by S. W. Leonard *et al.* [91]. In particular they showed that the transmission of the *H*-polarization can be tuned about 70 nm around the wavelength of 4.4 μm by heating the sample to the nematic-isotropic phase transition temperature of the LC. They used a LC with $n_o=1.49$, $n_e=1.69$ and phase transition temperature of 59°C.

Theoretical model for tuning of band gaps using the optic axis re-orientation was proposed by Liu *et. al* [95]. They studied silicon rods arranged in a LC ($n_o=1.52$ and $n_e=1.71$) background. Figure 7.1(a) shows the schematic of their proposal for applications in optical communications. The calculated band gap as a function of

optic axis orientation, α , is shown in Figure 7.1(b) for both square and hexagonal patterns of silicon rods.

Fig. 7.1(a) Structure considered by Liu *et al.*[95] to design a tunable band pass filter for operation around the communication wavelength, 1.55 μm . The optic axis orientation is denoted as α . (b) Calculated band gap as a function of α for square and triangular array of silicon rods with $f = 0.15$.

If a point defect is introduced in a LC infiltrated 2D PC, then a tunable cavity can be constructed. The wavelength of light that falls within the band gap will be localized in the cavity.

Fig. 7.2 Tunable LC – PC laser [173]. (a) Scanning electron micrograph of the fabricated 2D PC laser. Period of the PC is 500 nm. The radius of the periodic hole is 320 nm. The radius of the defect hole is 100 nm. (b) Laser spectra as a function of applied voltage. The electric field direction is perpendicular to the 2D periodic plane.

This cavity is then can be used to a construct a tunable PC laser. Maune *et al.* [173] constructed such a laser, based on a 2D PC using Indium Gallium Arsenide

Phosphide (InGaAsP) as an active material. The geometry of the cavity is shown in Figure 7.2(a). LC with $n_o=1.47$ and $n_e=1.52$ is infiltrated into the holes of 2D PC and a tuning about of 1.2 nm in the lasing wavelength is demonstrated when an external voltage (0 – 20V) is applied [Figure 7.2(b)].

If a line defect is introduced in the LC infiltrated 2D PC, then a tunable waveguide can be constructed. This was demonstrated by Schuller *et al.* [93] using a 2D PC slab made of Gallium Arsenide (GaAs) [Figure 7.3(a)].

Fig. 7.3 Tunable LC – PC waveguide [93]. (a) Scanning electron micrograph of the fabricated 2D PC waveguides. Period of the PC is 300 nm and $f=0.4$. (b) Transmission peak (E -polarization) with LC and without LC. The type of LC used is E7 with phase transition temperature of 60°.

Specifically they showed that by varying the periods of the sample, the normalized frequency (i.e., period to wavelength ratio) of the transmission peak of the E -polarization can be tuned from 0.27 to 0.28 (about 4%) when the LC is heated to his phase transition temperature [Figure 7.3(b)]. Based on similar line defects in the 2D LC infiltrated PC, other tunable applications such as tunable Mach Zehnder interferometers [174] and tunable light propagations in Y-shaped waveguides [175] have also been investigated.

Apart from 2D PCs, 1D PCs also have many interesting applications such as dielectric mirrors, optical limiter [176-177], second harmonic generation devices [178], filters [88] and phase modulators [179]. In all these applications, it is always desirable to have some tunability, and this can be realized by mean of an 1D anisotropic PC. Previously, 1D anisotropic PCs have been studied for band gap tuning applications. Wavelength switchable Bragg grating, an example of 1D PC, was experimentally demonstrated using polymer dispersed LCs [89]. Cholesteric LC which naturally behaves like 1D PC is used to construct tunable PC lasers [90]. Besides, Perova *et al.* [180] experimentally demonstrated band gap tuning in 1D LC infiltrated PC made of silicon by heating the LC to its phase transition temperature. On the other hand, Young *et al.* [85] theoretically analyzed tunable omni-directional band gaps as a function of applied voltage (below threshold voltage for Frederick's transition [100-101]), in a 1D PC made of alternating layers of LC and an isotropic dielectric material.

As we have shown above there are numerous studies pertaining to the band gap tuning in 2D PCs. In the case of 1D PCs, though there are several works pertaining to the 1D materially anisotropic PCs, the dependence of band gap on a general orientation of the optic axis (i.e., in the 3D space) has not been addressed yet. Therefore, in the second section of this chapter, we shall present the details of the band gap tunability of the 1D materially anisotropic PC obtained by varying the optic axis orientation of the anisotropic media. Specifically, the study will focus on 1D PCs infiltrated with LC and Pockel materials.

7.2 Engineering the band gap of a 2D PC

7.2.1 Formulation

The 2D PC is assumed to have circular cylinders in a homogenous matrix medium with either the matrix or the cylinder being anisotropic. In order to decouple the two independent polarizations, the principal axis, z_p , of the anisotropic material is assumed to be perpendicular to the 2D periodic plane [Chap. 2]. The orientations of the other two principal axes (x_p, y_p) with respect to the (x, y) axes of a square lattice PC is shown in Figure 7.4(a). The results in this section were obtained using PWM [Ho's method, Chap. 4] and in particular we used 361 plane waves to calculate the photonic band structures. The convergence accuracy for the first six bands is estimated to be better than 1%.

The band structure of E -polarization is solely dependent on the principal refractive index n_z and therefore Γ -X-M- Γ vectors [Fig. 7.4(a)] in the reciprocal space define the IBZ similar to a PC with isotropic materials. For H -polarization, the IBZ varies with the principal axes orientation (i.e., motif orientation) [Chap. 3]. When (x, y) coincides with (x_p, y_p) , the IBZ is a square region defined by Γ -X-M-X'- Γ vectors [Fig. 7.4(a)]. This definition of IBZ will change as x_p - y_p rotates away from x - y . For example, if x_p - y_p rotates 45° anticlockwise around z -axis, the corresponding IBZ becomes Γ -M-X-M'- Γ [Fig. 7.4(a)]. This region composes of two IBZs that correspond to an isotropic PCs. In fact, for any such planar rotation with an angle in multiples of 45° , the size of the IBZ remains as two isotropic IBZs. However, for other angles of

rotation, the IBZ of square lattice anisotropic PC increases to four isotropic IBZs.*

The IBZ for a PC made of uniaxial material with its optical axis along z-axis is polarization independent[♥], it remains in a triangle, M-X- Γ , as for an isotropic PC.

Fig. 7.4 (a) The first BZ of a square lattice and the coordinate system. The coordinates of Γ , X, M, X' and M' are (0, 0), (π/a , 0), (π/a , π/a), (0, π/a) and (π/a , $-\pi/a$) respectively. Principal axes: (x_p, y_p) PC axes: (x, y) (b) Band structure of H -polarization in Γ -X-M- Γ region for a PC with isotropic pillars of refractive index 3.8 in air background and with $f = 0.5$.

7.2.2 Two-dimensional PCs made of high refractive index materials

Figure 7.4(b) shows the band structure of H -polarization, for a 2D square lattice PC with isotropic circular pillars of refractive index of 3.8 in air background and $f = 0.5$. Degeneracy of dispersion lines at M point (between second and third

* The size of the IBZ for an anisotropic PC is r/r_m times bigger than the size of the IBZ of an isotropic PC of the same lattice [see Sec. 3.3.1]. For square lattice $\bar{R} = C_{4v}$ and hence $r = 8$. By consulting Table 3.1 [Chap. 3], $\bar{R}_M = C_2$ ($r_m = 2$) and C_{2v} ($r_m = 4$) for an arbitrary θ and θ equals to multiple of 45° respectively.

♥ The in-plane band structure for this orientation of optic axis is similar to an isotropic 2D PC. See Sec. 2.3 of Chap. 2.

band) prevents this structure from having a full gap (i.e., a common band gap for all wavevectors) in Γ -X-M- Γ region. This structure can be engineered to achieve full gap in Γ -X-M- Γ region if an anisotropic material is used. For instance, consider a PC with the same configuration as before but with an anisotropic material, antimony sulfide ($SbSI$)[♥] as pillars. $SbSI$ is a biaxial material with principal refractive indices $n_x = 2.7$, $n_y = 3.8$ and $n_z = 3.2$ [111, 181-182]. In order to introduce larger anisotropy in x - y plane, we aligned the principal axis, z_p to be along extension axis of the cylinders. This will guarantee the other two principal axes are in the periodic plane with the largest index variation ($n_y - n_x$) for H -polarization. The band structure of H -polarization is then controlled by the orientation of the two principal axes. Figure 7.5(a) shows the gap to mid gap ratio along Γ -M direction, as a function of θ , where θ denotes the orientation, x_p with respect to x [Fig. 7.4(a)]. As we can see from Fig. 7.5(a), band gap of H -polarization along Γ -M, which is closed for the isotropic case [Fig. 7.4(b)], opens in the anisotropic case for any θ , and large optimized gap is obtained when $\theta = 45^\circ$.^{♦♦} Figure 7.5(b) shows band structures of E - and H -polarizations for such a configuration of PC with $\theta = 45^\circ$. It can be seen from Fig.

♥ Previously $SbSI$ has been grown as a large single crystal (with thickness 9 cm) [181] and as a thin film (with thickness ranging from 100 nm to 1.5 μ m) [182]. The material is transparent in the near IR range [181-182] and therefore can be used for applications in the field of optical communications.

* The doubly degenerate ω in Fig. 7.4(b) at the M-point [$\overline{R}_M(\mathbf{k}) = C_{4v}$] has a 2D IR [Chap. 3]. As a consequence of the change in $\overline{R}_M(\mathbf{k})$, this state splits into two states with each labeled by an 1D IR in Fig. 7.2(b) [$\overline{R}_M(\mathbf{k})$ at M point in Fig. 7.5(b) is C_{2v}]. Note that, all IRs of C_{2v} are 1D.

♦ From the discussion in Sec. 3.3.2, we can easily show the FZO of M point is $0 < \theta < 45^\circ$ and this formally explains the symmetry seen in Fig. 7.5(a).

7.2(b) that an overlapping band gap for both polarizations exists, in Γ -X-M- Γ region.

With no rotation of principal axes, light entering along Γ -M direction will experience refractive index between 2.7 and 3.8.

Fig. 7.5 (a) Gap to mid gap ratio of the pseudo band gap of H -polarization at Γ -M direction for a PC with $SbSI$ pillars in air background, as a function of θ ($f = 0.5$). (b) Band structures of E - and H -polarization in Γ -X-M- Γ for a PC with the same configuration as in (a) but $\theta = 45^\circ$. (c) Two dimensional band structure of the second band for a PC with the same configuration as in (a) but with $\theta = 45^\circ$. (d) Two dimensional band structure of the third band for a PC with the same configuration as in (a) but with $\theta = 45^\circ$. (e) Gap to mid gap ratio of the partial

band gap of H -polarization (between second and third bands) as a function of f for a PC with the same configuration as in (a).

However, with the lowest refractive index principal axis (x_p of $SbSI$), pointing along M point ($\theta = 45^\circ$), H polarized light entering this direction will see the highest refractive index (n_y of $SbSI$), which equals to 3.8. The high refractive index at Γ -M direction leads to larger band gap for H -polarization with $\theta = 45^\circ$. In Figures 7.5(c) and 7.5(d) we plot the normalized frequencies, ω of the second and third bands respectively, in the entire BZ, for the same PC configuration as in Fig. 7.5(b). In a PC with isotropic materials, the band structure in Γ -X-M- Γ region is symmetrical with the one in Γ -X-M'- Γ region. However, as we can see from Fig. 7.5(c) and 7.5(d), this symmetry is destroyed for a PC made of anisotropic materials. For a PC with configurations as in Fig. 7.5(b), the minima of the third band [Fig. 7.5(d)] are below the maximum of the second band [Fig. 7.5(c)] along Γ -M', and hence, the band gap in Γ -X-M'- Γ region is closed. The band gap exists only in (Γ -X-M- Γ region (half of IBZ), for a PC with configurations as in Fig. 7.5(b).

Figure 7.5(e) shows the gap to mid gap ratio, $\Delta\omega/\omega$, for the band gap between the second and the third bands of H -polarization in Γ -X-M- Γ region [Fig. 7.5(c) and 7.5(d)], as a function of filling ratio for $\theta = 0$ and $\theta = 45^\circ$. The gap to mid gap ratio is always larger for the case of anisotropic PC with $\theta = 45^\circ$, compared to the anisotropic PC without any rotation of principal axes. It is worth mentioning that, $\Delta\omega/\omega$ of such a gap is much smaller (close to zero), i.e. almost no gap, for all filling ratio, for an isotropic PC with pillars of refractive index 3.8.

Band gap of H -polarization exists in an isotropic PC with air hole structure. However, their presence is only at higher filling ratios. If anisotropic materials with re-orientation of principal axes as we described above, are used instead, the existence of band gap of H -polarization is observed for quite a wide of range of filling ratios. Importantly, in air hole structures the band gap is observed for the entire IBZ, unlike half of the IBZ in the pillar type anisotropic PC.

Fig. 7.6(a) Gap to mid gap ratio of the full band gap of H -polarization (between first and second bands) as a function of f for PCs with air hole structures. Open circles refer to $SbSI$ case with $\theta = 45^\circ$. Closed circles refer to isotropic case with refractive index of 3.8. The inset shows gap to mid gap ratio as a function of f for $\Delta n = 0$ (solid), 0.7 (dashed), and 1.1 (solid) respectively. (b) Two dimensional band structure of the first band for an anisotropic PC with the same configuration as in (a) but with $f = 0.5$. (c) Two dimensional band structure of the second band for an anisotropic PC with the same configuration as in (a) but with $f = 0.5$.

Figure 7.6(a) shows the gap to mid gap ratio for the full gap between the first and second bands of H -polarization, for a PC with air hole structure in $SbSI$ matrix ($\theta = 45^\circ$) as a function of filling ratio (open circles). In the same figure, the gap to mid gap ratio for a PC with isotropic matrix of refractive index 3.8 is also plotted as closed circles. It is clear from Fig. 7.6(a) that larger band gap exists in anisotropic PCs for a wider range of filling ratio as compared to the isotropic PC. The inset in the Fig. 7.6(a) will be explained in the later part of discussion. In Figures 7.6(b) and 7.6(c), we plot the normalized frequencies of the first and second bands respectively, in the entire BZ, for the same anisotropic PC configuration, as in Fig. 7.6(a), but with $f = 0.5$. The maxima of the first band (along Γ -M) are lower than the minimum of the second band (at X), and hence a full band gap is created.

In our discussion so far we fix the Δn ($\Delta n = n_y - n_x$) to 1.1 using $SbSI$. It is worth mentioning that a band gap of H -polarization with re-orientation of principal axes, exists even for materials of smaller anisotropy. In the following, we analyze how the band gap varies with Δn and to see this, we fix $\theta = 45^\circ$, $n_y = 3.8$ and vary n_x from 2.7 (maximum Δn , equals to the anisotropy of $SbSI$) to 3.8 ($\Delta n = 0$, isotropic case). Figure 7.7(a) shows $\Delta\omega/\omega$ for the partial band gap of H -polarization in a pillar type PC, as a function of Δn for $f = 0.28, 0.38$ and 0.50 , corresponding to r_c of $0.3a$, $0.35a$ and $0.4a$ respectively. The partial band gap in a pillar type PC is completely closed for all the three filling ratios when $\Delta n = 0$, and it opens when a small anisotropy is introduced. The gap to mid gap ratio of the partial band gap in pillar type PC increases as Δn increases.

Fig. 7.7 Gap to mid gap ratio as a function of Δn for a PC with anisotropic materials, with $n_y = 3.8$ and $\theta = 45^\circ$, for (a) partial band gap of H -polarization (in half an IBZ) between the second and third bands in pillar type PC, and (b) full band gap of H -polarization between the first and second bands for a PC with air hole structures. f_{min} (open circle) as a function of Δn is also shown in (b).

On the other hand, for the full band gap of H -polarization in a PC with air hole structures [Figure 7.7(b)], the variation with respect to Δn , follows a similar trend, however, the band gap variation with respect to f is significantly different. To understand this we recall Fig. 7.6(a), in which $\Delta\omega/\omega$ as a function of f is plotted for both for $\Delta n = 1.1$ and $\Delta n = 0$. By examining this figure, we found that there are two limits of filling ratio, f_{min} and f_{max} for which no band gap is observed for $f > f_{max}$ and $f < f_{min}$. It is worth mentioning that, $\Delta\omega/\omega$ versus f curve for the other values of Δn is similar to those in Fig. 7.6(a), with a similar f_{max} , but different f_{min} . For instance, the curve of $\Delta n = 0.7$ is shown as dashed line in the inset of Fig. 7.6(a). Largest value of f_{min} is f_c , occurs when $\Delta n = 0$ and f_c is indicated in the inset of Fig. 7.6(a). The value of f_{min} decreases as Δn increases [open circles in Fig. 7.7(b)]. As Δn increases, the effect of anisotropy becomes stronger, this in turn causes band gap to exist even at smaller filling ratios, and in turn forces band gap to exist for a wider range of f . If $\Delta\omega/\omega$ is

plotted as a function of Δn for a fixed f , with $f < f_c$, then there is a threshold Δn , required to open the band gap. This threshold Δn goes to zero as f reaches f_c .

7.2.3 Two-dimensional PCs made of low refractive index materials

The phenomena of opening up a band gap, shown in Fig. 7.5(b), can be even observed with PCs made from low refractive index materials. In the study, we keep $n_x = 1.5$ and $n_y = n_x + \Delta n$. The anisotropy, Δn is varied from 0 to 1.2, and materials with such a range of principal indices are available [100-101, 129-130, 183-184]*. The corresponding band structures (H -polarization) for various values of n_y are analyzed, and for a comparison, the band structures of isotropic PCs with refractive index that equals to n_y are also analyzed. Due to the lower value of n_x the band gap of PC with anisotropic materials, does not persist in the entire IBZ, however large pseudo band gaps at particular direction and large partial band gaps in half of the IBZ are observed.

Figures 7.8(a) and 7.8(b) show the first gap (the gap between the first and the second bands of H -polarization) at Γ -X and Γ -M directions for a square lattice PC in air matrix ($f = 0.64$), as a function of n_y for both isotropic and anisotropic ($\theta = 45^\circ$) pillars respectively. As we can see from Fig. 7.8(b) that, the gap at Γ -M direction is larger than the isotropic PC's [Fig. 7.8(a)] for any value of n_y , except for $n_y = n_x$,

* Typical LCs have Δn ranging from 0.02-0.3 [100-101]. Gauza *et al.* [130] synthesized LCs with Δn ranging from 0.5 to 0.8 for potential applications in optical communications. Besides, organic salts such as 4-dimethyl-aminobenzaldehyde-4-nitrophenyl-hydrazone (DANPH) with $\Delta n = 0.9$ (at $\lambda = 700\text{nm}$) [184] and 4-N, N-dimethylamino-4'-N'-methyl-stilbazolium tosylate (DAST) [129, 183] with $\Delta n = 1.2$ (at $\lambda = 632\text{nm}$) also have been synthesized and used for fabrication of waveguides [183].

where both have the same band gap. Furthermore in Fig. 7.8(b), the two pseudo band gaps at Γ -M and Γ -X directions start to overlap each other as n_y reaches 2.7 (i.e. corresponds to Δn of 1.2) to form a large partial band gap in Γ -X-M- Γ region. This required value of anisotropy to cause overlapping between Γ -X and Γ -M direction decreases with the increase in filling ratio. For $f = 0.72$, the required Δn is 0.9.

Fig. 7.8 Variation of pseudo band gaps as a function of refractive index (H -polarization). (a) The first gap of a PC with $f = 0.64$, for isotropic pillars of refractive index n_y . (b) The first gap of a PC with $f = 0.64$ and $\theta = 45^\circ$, for anisotropic pillars as a function of n_y . Refractive index, n_x , is kept at 1.5. (c) The first gap of a PC with $f = 0.28$ and air holes in isotropic matrix of refractive index n_y . (d) The first gap of a PC with $f = 0.28$, $\theta = 45^\circ$ and air holes in anisotropic matrix as a function of n_y . Refractive index, n_x , is kept at 1.5.

Figures 7.8(c) and 7.8(d) show the first gap (the gap between the first and the second bands of H -polarization) at Γ -X and Γ -M directions as a function of n_y for PCs with air holes in isotropic and anisotropic ($\theta = 45^\circ$) PCs respectively, with $f = 0.28$. In

fact for any filling ratio with such a low refractive index, no overlapping band gap for H -polarization is observed for isotropic matrix and the gap at Γ -M direction is very small especially when n_y is small [Fig. 7.8(c)]. However, for PCs with anisotropic matrix with $\theta = 45^\circ$, the pseudo-gap at Γ -M direction is relatively larger than the corresponding pseudo-gap for an isotropic PC, even for smaller anisotropies [Fig. 7.8(d)]. Furthermore, as we show above, the gap at Γ -M direction starts to overlap with gap at Γ -X direction as anisotropy increases and thus leads to a large partial band gap in Γ -X-M- Γ region.

It is worth mentioning that, for the structure with air holes the required anisotropy to have a band gap in Γ -X-M- Γ region decreases as f is decreased. For example, the required Δn are 1.1 and 0.7 for $f = 0.64$ and $f = 0.28$ respectively. Both the increment of f in a pillar type PC and the decrement of f in a PC with air hole structures, cause the filling fraction of the anisotropic medium to increase, consequently the anisotropic effect becomes stronger and thus there is a decreases in the minimum Δn to cause overlapping.

7.2.4 Summary and Discussion

In this section, photonic band structures of 2D square lattice PCs made of anisotropic materials with one of the principal axes oriented along the extension direction of cylinders were studied. By re-orienting the principal axes in periodicity plane, we showed that the band structure of H -polarization can be improved to achieve large partial band gap for a pillar type PC and full band gap for a PC with air hole structures. Both band gaps exist for a wider range of filling ratios compared to a PC with isotropic materials and exist even for a small value of anisotropy.

Besides, it is also demonstrated how the pseudo-gap of H -polarization opens and overlaps each other in anisotropic PCs with lower value of refractive indices.

This analysis serves as a guide to enlarge photonic band gaps using anisotropic materials. Such a materially anisotropic PC can be realized with optical materials of low refractive index and for a wide range of filling ratios. The presented study is expected to have potential impact in the applications that demands large photonic band gaps such as broad band mirrors, filters and low threshold lasers [Chap. 1 and the references therein].

7.3 1D PC with a tunable band gap

In this section of the chapter, we used the 1D model presented in Secs. 2.4 and 4.2.2 to study 1D PCs made of an anisotropic materials. Specifically, 1D PCs infiltrated with LC and Pockel materials are investigated. We shall present the details of the band gap tunability (along the 1D periodic direction) obtained by varying the optic axis (or principal axes) orientation of the anisotropic media.

For conventional PCs with alternating isotropic layers, the refractive index difference between the two alternating materials, is the same regardless of polarization. However for PCs with alternating anisotropic and isotropic media, the refractive index difference is polarization dependent. The refractive index difference, for e -polarization and o -polarization are $n_e(\alpha) - n$ and $n_o - n$ respectively, where n is the refractive index of the isotropic layer and α is the angle between optic axis (z_p -axis) and periodicity axis (x -axis) [see Sec. 2.4]. These refractive index differences lead to polarization dependent band gap. Hence, the band structure, which

originally degenerates for isotropic case, will split for anisotropic case. The amount of splitting is strongly dependent on optical anisotropy of the anisotropic medium, Δn ($\Delta n = n_e - n_o$), and the width of the anisotropic layer.

Figure 7.9 (a) shows the band structure for a silicon – LC 1D PC. The type of LC is E7 with $n_o = 1.52$ and $n_e = 1.74$ [101].

Fig. 7.9 (a) Band diagram for the 1D PC with *Si-LC* configuration. The width of the *LC* layer is $0.68a$. The band structures of o - and e -polarizations are represented as dashed and solid lines, respectively. (b) Transmission spectrum of e -polarization for the same 1D PC configuration in (a), computed with transfer matrix method. (c) Gap to mid gap ratio for the first order gap of a 1D PC with *Si-LC* configuration for two kinds of LCs, E7 and phenylacetylene.

Band structures are computed using PWM [Eqn. 4.13, 4.14 and 4.15] with optic axis perpendicular to periodicity direction, x . When optic axis is perpendicular to x , which is also the light propagation direction, the refractive index experienced by o and e polarization are n_o and n_e , respectively, irrespective to optic axis orientation in the y - z plane. In the simulation, the width of the LC layer, w , is $0.68a$ (quarter wavelength thickness), which is computed by,

$$w = (\lambda/4n_{LC})/(\lambda/4n_{LC} + \lambda/4n_{Si}) a \quad [7.1]$$

where n_{Si} is the refractive index of silicon, n_{LC} is taken as the average of n_e and n_o of the LC. We used 301 plane waves in calculation. The mid values, ω_c , for the first ten

band gaps, differ at most by 0.00046 when the number of plane waves is further increased from 301 to 401 (i.e. $|\omega_{e,401} - \omega_{e,301}| \leq 0.00046$). The band structure computed using PWM is also compared to the transmission spectrum obtained by transfer matrix method [140-141]. The transmission spectrum of *e*-polarization calculated for 50 periods of PC is given in Figure 7.9(b). It is clear from the figure that, the plane wave result is in good agreement with the one obtained from transfer matrix method.

Figure 7.9(c) shows the gap to mid gap ratio of the first order gap for LC – Si PC as a function of the LC's normalized thickness, d/a , where d is thickness of the LC layer, for two kinds of LCs, E7 and phenylacetylene types ($n_o = 1.59$, $n_e = 2.22$ [97]). The normalized thickness, at the peak of gap to mid gap ratio, obeys Eqn. 7.1 with n_{LC} taken as n_e and n_o for *e* and *o* polarizations, respectively. The peak occurs at normalized quarter wavelength thickness of both layers, because the Bragg reflection is the strongest at quarter wavelength thickness, which results in the largest gap and hence, the largest gap to mid gap ratio [185]. It can be seen from Fig. 7.9(c) that, the gap to mid gap ratio of the two polarizations deviates significantly and the amount of splitting differs with d/a . The splitting increases until it reaches the maximum at normalized quarter wavelength thickness, thereafter the deviation between the two gaps reduces again. The effect of anisotropy on the splitting, can also be seen by comparing the curves for the two kinds of LC. It can be seen from Fig. 7.9(c) that, the splitting between the two polarizations is larger for PC with phenylacetylene-Si configuration, compared to the E7-Si configuration, as phenylacetylene type LC has larger anisotropy than E7.

7.3.1 Tunable LC infiltrated 1D PC

The optic axis orientation of LC can be easily varied by applying external electric field, and by doing so, the band gap becomes electro-optically tunable.

The on-axis band structure of the *e*-polarization changes as the optic axis orientation varies. However, for *o*-polarization, the band structure remains unchanged [Sec. 2.4]. Hence, shifts in band gaps occur only for the case of *e*-polarization. As the optic axis is tuned to be parallel with the periodicity direction, the band structure for both polarizations is the same. However, when optic axis is tuned to be perpendicular to the periodicity direction, the band structure of *e*-polarization shifts down for positive uniaxial material (i.e. $n_e > n_o$) due to the higher refractive index experienced by *e*-polarization in the LC layer. For a negative uniaxial material (i.e. $n_o > n_e$), the band structure shifts up for a similar re-orientation of optic axis. In any case, the band shifts lead to mismatch in the band gap of *e* and *o* polarizations, and hence, affect the overall band gap for both polarizations.

Referring to Fig. 7.9(a), band structure of *e*-polarization, originally is the same as the *o*-polarization when optic axis is along the *x*-axis of *Si*-LC (E7) PC. However, when optic axis is tuned to be perpendicular to the *x*-axis, the band structure of *e*-polarization shifts down as E7 is a positive uniaxial material. These band shifts differ with band order. It can be seen from Fig. 7.9(a) that, at the edge of the Brillion zone ($|\mathbf{k}| = \pm \pi/a$) where the reflections are the strongest [185], the overall band gap for both polarizations reduces as the gap order increases, and starting from the fifth order gap, the overall band gap for both polarizations is completely closed.

The band shifting with re-orientation of optic axis can be used to tune the band gap of a PC. In the following, we shall illustrate the electro-optic tunability of 1D PC made of silicon, infiltrated with E7 LC. The width of LC layer is the same as in Fig. 7.6(a). Figure 7.10 displays the general optic axis orientation of the LC (i.e., the z_p axis, see Sec. 2.4) and propagation direction, $\mathbf{k}$, which is assumed along the x -axis.

Fig. 7.10 The laboratory coordinate system of 1D PC used in calculation. Optic axis is represented as $\mathbf{s}$, and $\mathbf{k}$ is the propagation direction. The x -axis is the 1D periodicity axis.

The coordinate system is in laboratory arrangement and it is different from principal coordinate system of the LC. The angle between optic axis and x -axis is the angle, α and can be computed using,

$$\alpha = \cos^{-1}(\cos \theta \sin \phi) \quad [7.2]$$

where θ and ϕ are defined in Fig. 7.10. As mentioned in Sec. 2.4, the orientation of the polarizations will vary with respect to the fixed laboratory frame (x_L, y_L, z_L) , when the optic axis is varied [see Fig. 2.1, Chap. 2]. The angle between o -polarization and the laboratory axis, z_L , can be manipulated as $\tan^{-1}(\cos \phi / \tan \theta)$.

The refractive indices of the e -polarization in the LC layer are n_o and n_e when the optic axis is parallel and perpendicular to periodicity axis (x -axis) respectively. Hence, when optic axis is varied in a plane containing periodicity axis, the largest

refractive index variation for e -polarization is obtained. For simplicity, this plane is assumed as $\phi = 90^\circ$ (x_L - y_L) plane. Referring to Fig. 7.10, when optic axis is varied in $\phi = 90^\circ$ plane, from $\theta = 0^\circ$ to $\theta = 90^\circ$, the refractive index of e -polarization varies from 1.52 to 1.74 (LC layer). However, when the optic axis is varied in the other planes, i.e. for other values of ϕ , the variation is smaller. For example when optic axis is varied in plane $\phi = 45^\circ$, the refractive index variation in the LC layer is just 0.1, and this variation equals to zero for $\phi = 0^\circ$.

1D PC may have infinite number of gaps [185], however, the first order gap is the largest, centered at the shortest wavelength. Hence, the gap to mid gap ratio is the largest for the first order gap. However, for applications like tunable narrow band pass filters, higher order gaps are probably good candidates since they have small gaps for fixed design wavelength (i.e. smaller gap to mid gap ratio). The first order gap of LC-Si PC with a LC layer width of $0.68a$ is shown in Figure 7.11(a) as a function of θ in x_L - y_L plane ($\phi = 90^\circ$).

Fig. 7.11 (a) The first order gap of LC-Si 1D PC (with a LC layer thickness of $0.68a$) as a function of θ in x_L - z plane ($\phi = 90^\circ$). (b) The first gap to mid gap ratio for the overall band gap (both polarizations), of LC-Si 1D PC (with a LC layer thickness of $0.68a$) as a function of θ in x_L - y_L plane ($\phi = 90^\circ$). (c) Tunability of e -polarization, as a function of ϕ .

The figure displays the gaps for both e and o polarizations. The overall band gap for unpolarized light, which is an overlap between the gaps of o and e polarizations in Fig. 7.11(a), reduces as the value of θ increases. Figure 7.11(b) shows the gap to mid gap ratio, for the overall band gap for both polarizations, based on the first order gap.

For both o -and e -polarization, with optic axis along x -axis ($\theta = 0$) of PC, the gap is at the range of normalized frequency, 0.173 - 0.291. When the optic axis is parallel to y_L -axis, the gap for e -polarized light narrows to 0.171 - 0.267, whereas, for o -polarization regardless of optic axis position the gap remains at 0.173 - 0.291. Thus, mismatch occurs between the band structures of o and e polarizations as optic axis moved from x to y_L [Fig. 7.11(a)]. This results in the reduction of overall band gap for both polarizations. As we can see from Fig. 7.11(b) that the gap to mid gap ratio for overall band gap (first order gap) reduces, as the value of θ increases. Gap to mid gap ratio decreases 16% from 0.509 when θ is varied from 0 to 90° in the $\phi = 90^\circ$ plane. When ϕ reduces (i.e., different plane), the tunability (changes in the gap to mid gap ratio when θ is varied from 0 to 90°) reduces too. When $\phi = 45^\circ$, the tunable range is only 7.8%. Figure 7.11(c) displays the tunability of e -polarization, when optic axis is varied in planes with different ϕ . This may be useful in applications, where the device requires different tuning range.

The presented tunable LC infiltrated 1D PC can be used for many practical applications. For instance, we can design tunable band pass filters and tunable band edge lasers based on the presented LC-PC structure.

When the optic axis of LC is varied from $\theta = 0$ to 90° in the plane $\phi = 90^\circ$, the center frequency of the first band gap (e -polarization) shifts from 0.232 to 0.219 [Fig. 7.11(a)]. Assuming the first bad gap for $\theta = 0$ (i.e., optic axis along the x -axis) is centered at the communication wavelength, $1.55 \mu\text{m}$, the required pitch for the tunable PC can be designed to be $0.232 \times 1.55 \mu\text{m} = 0.36 \mu\text{m}$. If the optic axis is re-oriented from $\theta = 0$ to 90° in the plane $\phi = 90^\circ$, the center wavelength will be tuned about 90 nm from $1.55 \mu\text{m}$ ($\theta = 0$) to $1.64 \mu\text{m}$ ($\theta = 90^\circ$). This tuning range will reduce if the optic axis is varied in other planes with different ϕ [see Fig. 7.11(c)]. For instance if $\phi = 45^\circ$, the tuning is only 40 nm compared to 90 nm for $\phi = 0$. Hence, tunable band pass filters with different band sizes can be designed by controlling the value of ϕ .

For tunable band edge lasers, the studied LC-PC structure can be doped with a suitable gain medium. Previously dye-doped LCs were used in lasing applications [186]. If the period of the PC is fixed as 267 nm, then the upper band edge wavelength (i.e., the lasing wavelength [186]) of the e -polarization will shift from 1561 nm to 1543 nm[▼]. Note that the period is designed such that the center of the tuning range is 1550 nm. If the center wavelength of the tuning range is greater than 1550 nm, the pitch value will be greater than 267nm.

The optic axis of LC can be varied by mean of an external electric filed. For instance, LC can be aligned parallel to a direction with a desired value of ϕ in the x - y plane (see Fig. 7.10), before an electric field is applied. An electric field along x

[▼] Note that the wavelength is inversely proportional to the normalized frequency. Therefore, lower band edge frequency must be used to obtain the upper band edge wavelength.

direction, could be applied to re-orient the optic axis towards x direction of PC (i.e., varying θ with a fixed ϕ). The initial alignment (without field) of optic axis can be induced by an alignment layer [187-190]. For wavelength of 1.55 μm , considering the gap centered at a normalized frequency of 0.232, the thickness of 10 nm alignment layer [188] is just 3% of the period. This fraction will further decrease with the decrease of alignment layer thickness. The alignment layer can be as thin as 25Å [187]. Hence, we can expect a small change in the band gap and thus, the alignment layer thickness was ignored in our calculations.

7.3.2 Pockel effect in 1D PC

Pockel effect [111,191-192] can be used as a refractive index changing medium in PC. Not all materials exhibit Pockel effect. Only material with non-centrosymmetric structure exhibits this effect. In the presence of Pockel effect, the higher order effect like quadratic electro-optic effect is negligible since the corresponding electro-optic coefficient is typically small. In this chapter, we consider 1D PC with alternate layers of Pockel medium and non-Pockel isotropic medium. Pockel medium can be isotropic, uniaxial anisotropic, or biaxial anisotropic, before an electric field is applied. In general, the isotropy and anisotropy of the Pockel medium may change after electric field is applied.

Assume all the principal axes of the Pockel media coincide with the PC axes. Before an electric field is applied, the index ellipsoid of a biaxial Pockel material (for a general discussion) can be written as

$$\frac{x'^2}{n_x'^2} + \frac{y'^2}{n_y'^2} + \frac{z'^2}{n_z'^2} = 1 \quad [7.3]$$

where n_x' , n_y' and n_z' are the principal refractive indices. The on-axis propagation direction, x (PC axis), is assumed to be along one of the principal axes. If an electric field, $\mathbf{E} = (E_x', E_y', E_z')$, with respect to principal axes is applied to a medium with the initial principal refractive indices of n_x' , n_y' and n_z' , the index ellipsoid of the medium will be modified to

$$\frac{x''^2}{n_x''^2} + \frac{y''^2}{n_y''^2} + \frac{z''^2}{n_z''^2} = 1 \quad [7.4]$$

where n_x'' , n_y'' and n_z'' are the new principal indices and can be calculated with the help of Pockel tensor, which contains all Pockel coefficients r_{ij} . The new principal coordinate system is (x'', y'', z'') .*

As mentioned before, the on-axis propagation direction, x (PC axis), is assumed to be along one of the principal axes. In general, the applied electric field will rotate the principal axes from x' , y' and z' to x'' , y'' and z'' . If the applied electric field, causes a rotation of principle axis which is initially along the periodicity direction, x of PC then, there will be a significant reduction in the electro-optic efficiency. However, depending on the symmetry of the Pockel medium and electric field direction, it is possible to avoid such a rotation of principal axis along x , under an electric field. Table 7.1 summarizes some of these cases [111, 191-192]. We shall discuss, in the following, the band gap tunability for non-rotated and rotated, principle axis along x .

* Note that in order to distinguish principal axes before and after an electric field is applied, (x', y', z') [before an electric field is applied] and (x'', y'', z'') [after an electric field is applied] are used instead of (x_p, y_p, z_p) .

Table 7.1 Point group and the electric field direction, under which the principal axis along the periodicity direction (z) of the 1D PC does not rotate. The point groups are denoted using the Schoenflies Notation [113].

Point group	Electric field	Unrotating principal axis along the periodicity direction of 1D PC		Remarks
$C_4, C_6, C_{2v}, C_{3v}, C_{4v}$ and C_{6v}	$E_{z'}$ only	x', y 'or z'		No rotation of principle axes
C_{2v}	$E_{x'}$ only	y'		Only $x'z'$ plane rotates
D_{3h}	$E_{y'}$ only	z'		No rotation of principle axes
D_{3h}	$E_{x'}$ only	z'		Only $x'y'$ plane rotates
C_{4v} and C_{6v}	$E_{x'}$ only	y'		Only $x'z'$ plane rotates
D_{2d} and T_d	$E_{z'}$ only	z'		Only $x'y'$ plane rotates

For 1D PC with Pockel material from point group $C_4, C_6, C_{2v}, C_{3v}, C_{4v}$ or C_{6v} , the index ellipsoid for only non-zero $E_{z'}$ can be written as.

$$\left(\frac{1}{n_o^2} + r_{13} E_{z'} \right) x'^2 + \left(\frac{1}{n_o^2} + r_{13} E_{z'} \right) y'^2 + \left(\frac{1}{n_e^2} + r_{33} E_{z'} \right) z'^2 = 1. \quad [7.5]$$

Clearly, there are no diagonal terms involving $y'z'$, $x'z'$, and $x'y'$, and hence, there is no rotation of principal axes. The new principal refractive indices are as follow:

$$n_{x'}'' \approx n_o - \frac{1}{2} r_{13} n_o^3 E_{z'} \quad [7.6.1]$$

$$n_{y'}'' \approx n_o - \frac{1}{2} r_{13} n_o^3 E_{z'} \quad [7.6.2]$$

$$n_{z'}'' \approx n_e - \frac{1}{2} r_{33} n_e^3 E_{z'} \quad [7.6.3]$$

The material remains uniaxially anisotropic. The propagation direction is taken as y' (i.e. y' is along x -axis of PC). The refractive indices (experienced in the layer Pockel material) of o - and e -polarizations, after an electric field applied in z' direction, are n_x'' and n_z'' respectively, and they are tunable with electric field. The electro-optic efficiency differs with polarizations and the efficiency can be determined from the value of $r_{13}n_o^3$ and $r_{33}n_e^3$. $LiNbO_3$, from the point group, C_{3v} , has $r_{13}n_o^3=104.25pm/V$ and $r_{33}n_e^3=302.25pm/V$ at wavelength $1.55 \mu m$ [111, 192]. The breakdown field of $LiNbO_3$ is about $7 \times 10^7 V/m$ [193] and this imposes the limit on the range of electric field that can be applied. For a $LiNbO_3$ -Si PC, with a width of $LiNbO_3$ layer of $0.27a$ (quarter wavelength thickness) the changes in mid value of the tenth band gap, when an electric field about $6.5 \times 10^7 V/m$ is applied, are 0.12% and 0.03%, for e and o polarizations respectively. In particular for e -polarization, the mid band gap changes from 1.617 to 1.619 when the electric field is applied. This corresponds to a tunability of 2 nm^* around communication wavelength, 1550 nm, and requires $44 \text{ V}^\heartsuit$ to be applied across $LiNbO_3$ layer. Even though the tunability is small, they are sufficient for tunable filter applications in WDM technology [194].

For a rotated symmetry axis system, let's consider a 1D PC with a Pockel material from point group of T_d [111]. Assume the principal axis, x' is parallel to the periodicity axis of the PC (i.e., x' is along the x -axis of the PC). Materials from this

* Setting $a/\lambda = 1.617$ with $\lambda = 1550 \text{ nm}$, yields $a = 2506.4 \text{ nm}$. When normalized frequency changes to 1.619, λ changes to 1548.1 nm.

♥ The thickness of $LiNbO_3$ layer is $0.27a$ and therefore the applied voltage can be calculated as $6.5 \times 10^7 V/m$ multiplied by $0.27a$.

point group, T_d change from isotropic to anisotropic when an electric field is applied.

Under an electric field, the index ellipsoid could be written as,

$$\frac{x'^2}{n_o^2} + \frac{y'^2}{n_o^2} + \frac{z'^2}{n_o^2} + 2r_{41}y'z'E_{x'} + 2r_{41}x'z'E_{y'} + 2r_{41}x'y'E_{z'} = 1. \quad [7.7]$$

The rotation of principal axes will occur regardless of the applied field direction.

When a field is applied along the y' direction, the principal refractive indices are as follows:

$$n_x'' \approx n_o \quad [7.8.1]$$

$$n_y'' \approx n_o + \frac{1}{2}r_{41}n_o^3E_{x'} \quad [7.8.2]$$

$$n_z'' \approx n_o - \frac{1}{2}r_{41}n_o^3E_{x'} \quad [7.8.3]$$

The principal refractive indices indicate that the index ellipsoid becomes slightly biaxial. The $x'z'$ plane rotates to $x''z''$ and the angle between x' (along the periodicity axis) and x'' (rotated x') is 45° . As we discussed in Sec. 2.4, due to the planar rotation, the resulting problem can be separated into two polarizations satisfying Eqn. 2.17 and 2.19 with o -polarization experiencing n_y'' and e -polarization experiencing $n(45^\circ)$,

$$\frac{1}{n^2(45^\circ)} = \frac{\cos^2(45^\circ)}{n_x''^2} + \frac{\sin^2(45^\circ)}{n_z''^2} \quad [7.9]$$

in the layer containing the anisotropic material.

With point group, T_d , $ZnTe$ has $r_{41}n_o^3=107.99\text{pm/V}$ and $n_o = 2.99$ at wavelength $0.633\mu\text{m}$ [111]. For an electric field about $1 \times 10^9\text{V/m}$, we have $n_x'' = 3.044$, $n_z'' = 2.936$ and $n(45^\circ) = 2.9885$. The difference of refractive indices for e -polarization with and without electric field is $n_o - n(45^\circ) = 0.0015$. Hence the refractive index change is very

small and only a small change in band diagram is expected. If the field direction is along x' , from Eqn. 7.7, the principal axis along the periodicity direction remains unrotated. In this case, the change of refractive index is the maximum which equals to $(1/2)r_{41}n_0^3E_{z'}$. Since both polarizations experience equal but opposite sign of refractive index change, the amount of shift is the same but in opposite directions. For a field of $1 \times 10^9 \text{V/m}$, the change is 0.054. The computed gap to mid gap ratio of the first gap for *ZnTe*-air PC is shown in Figure 7.12, for both rotated (with $E_{y'}$ only) and unrotated (with $E_{x'}$ only) systems that we discussed. It is clear from the figure that the electro-optic efficiency for unrotated system is much larger than the rotated system. High field values were used in our calculation, to clearly show the effect of principal axis (along x) rotation on the electro optic efficiency. In general, the conclusions remain unchanged if smaller field values are used.

Fig. 7.12 Gap to mid gap ratio of *ZnTe*-air PC, with a *ZnTe* layer width of $0.25a$ (normalized quarter wavelength thickness) as a function of applied field along y' -direction (rotated) and x' -direction (unrotated).

7.3.3 Section summary

In summary, the band structures of 1D PCs with alternating isotropic and anisotropic material were analyzed. Tunability in such structures can be obtained through the electro-optic effect of the anisotropic layer. In particular, we have presented the details of tunability in a LC infiltrated 1D PC, by considering various re-orientations of LC's optic axis. Furthermore, for a 1D PC with a Pockel material, the details of electro-optic efficiency in tuning the band gaps were analyzed in a principal axes rotated and not rotated system.

7.4 Summary

This chapter has presented applications of the anisotropic PCs based on their ability of providing band gaps. Sec. 7.2 described the role of the material's anisotropy in engineering the band gap of a 2D PC, while Sec. 7.3 elaborated 1D anisotropic PCs on their use for tuning of the band gaps. A separate section summary has also been given at the end of the Secs. 7.2 and 7.3.

Chapter 8

Conducting Properties

8.1 Introduction

Besides the insulating properties, PCs also exhibit various conducting (i.e., propagating) properties such as negative refractions, super-lensing, super-collimation, super-prism etc [Chap. 1]. This chapter presents the applications of anisotropic PCs based on their conducting properties.

Moussa *et al.* [69, Sec. 4.5 of Chap. 4] studied a geometrically anisotropic 2D PC for investigation of negative refractions using microwaves with frequencies around 6.5 GHz.

Fig. 8.1(a) Schematic of the experiment conducted by Moussa *et al.*[69] (b) Measured transmission spectrum at the first interface without the PC and at the second interface with the PC.

They considered a structure with rectangular alumina bars in air with a period of 1.59 cm (hexagonal lattice). In the experiment a Gaussian source (Gaussian in space

and highly monochromatic, $\lambda = 46.2$ mm) is launched at the incident angle of 30° as shown in Figure 8.1(a). The measured transmission as a function of position is shown in Figure 8.1(b) at the first interface (without the PC) and at the second interface (with the PC). The figure clearly shows how the center of the outgoing Gaussian beam is shifted toward left-handed side of the center of the incident beam. This is a clear indication of negative refractions in microwave regime using an anisotropic PC.

One of the important applications of the negative refraction is a flat lens [66-68]. Feng *et al.* [195] considered a geometrically anisotropic 2D PC with elliptical dielectric rods (dielectric constant = 14, $f = 0.28$) arranged in a square lattice in air. They showed that the image location of a point object in the image plane, can be tuned by tuning the orientation of the elliptical rod in the anisotropic PC.

Self-collimation is a phenomenon, where a diverging light beam becomes collimated after passing through a self-collimation medium. Self-collimation has been investigated in anisotropic PCs. Specifically, a materially anisotropic 2D PC made of DAST[♥] and circular air holes (square lattice with $f = 0.13$) was shown to exhibit self-collimation for an input incident angle range that is wider than that provided by an equivalent isotropic PC [196]. The equivalent PC was assumed to be made of an isotropic material with refractive index equals to the average of principal refractive indices of DAST.

Apart from geometrically anisotropic PCs, materially anisotropic PCs also have been studied for applications in conduction. Specifically anisotropic materials

[♥] DAST is an anisotropic material. The details of this material is given in Chap. 7 (page 148).

which exhibit Pockel effect have been used for tunable light propagations in 2D PCs [107, 197]. Jian *et al.* [107] proposed a square lattice PC with strontium barium niobate (SBN)[♦] rods in air, and showed that the refraction can be tuned from a positive refraction to a negative refraction by applying an electric field of $1.4 \text{ V}/\mu\text{m}$.

Fig. 8.2(a) Schematic of the structure and the formalism considered by Jian *et al.* [107] (b) Refraction angle as a function of applied electric field. Key: NR – negative refraction; PR – positive refraction.

They assumed a structure with a period of 170nm and a filling ratio of 0.64 and a setup as shown in Figure 8.2(a). The calculated refraction angle as a function of applied electric field is shown in Figure 8.2(b). As we can see from the figure, the refraction angle tunes about 26° when an electric field is applied from 0 to 1.4×10^7

[♦] SBN is an anisotropic Pockel material with large Pockel coefficients ($r_{33} = 1340 \text{ pm/V}$). SBN is transparent for light with frequencies in the visible range [107].

V/m. On the other hand, Amet *et al.* [197] studied a LiNbO_3 – air hole materially anisotropic PC with a hexagonal lattice and a filling ratio of 0.15, and showed that near the band edge frequency, the refraction angle of the anisotropic PC can be tuned about 60° if the electric field is varied from 0 to $660 \text{ V}/\mu\text{m}$.

In this chapter, we present tunable light propagations using LC infiltrated 2D anisotropic PCs. In Chap. 7, we showed the use of LC in tuning the band gaps of a PC, this chapter presents its use for tunable dispersions (i.e., tunable conductions) of a PC.

The second section of the chapter outlines a general method of finding light propagation directions in a PC based on their EFS. This section also highlights the fundamental conduction properties of light in the anisotropic 2D PC. The subsequent sections demonstrate two independent examples concerning the applications of 2D LC infiltrated PCs in tuning the conduction of light based on PWM [Chap. 4]. In particular, Section 8.3 presents a fully switchable superprism and polarization splitting effects based on the LC infiltrated 2D PC made of silicon oxynitride (SiON)[▼]. Section 8.4 presents a continuously tunable phenomenon in a similar structure, but with silicon as a matrix medium. The presented conducting properties are compared with simulations based on the FDTD method in Section 8.5 and finally potential applications are discussed in Section 8.6.

▼ SiON is a dielectric material with the refractive index can be tailored to be in between the refractive indices of silicon nitride ($n=2$) and silicon dioxide ($n = 1.45$). SiON has been used in fabrications of photonic devices. See for example Refs. 198 and 199.

8.2. Fundamental properties of conduction

This section reviews a well known method [46,67,187] of finding light propagation directions in a PC, based on its EFS (Chap. 6). In Figure 8.3, the EFSs for two media, m_1 and m_2 , are shown. One of the media, m_1 , is assumed to be a bulk isotropic material, hence the corresponding EFS is a circle. The other medium, m_2 , is considered to be uniform or an anisotropic PC. The interface orientation, ϕ , and the orientation of the anisotropic motif, α are also shown in the Fig. 8.3. The conservation of momentum requires the parallel component of the wave vector to be conserved across the interface. Hence a line of momentum conservation, being a vertical line parallel to the normal line (Fig. 8.3), determined by the incident angle, θ_i , and passing through the EFS of m_2 produces two intersection points. The direction of the normal vector at the intersection point between the EFS of m_2 and the line of momentum conservation gives the propagation direction in m_2 . The normal vector, with the same sign of vertical component as the vertical component of the incident wave vector is considered, as forward wave and the other, is considered as reverse wave (Fig. 8.3) [200]. If the forward wave travels with an angle of θ_p , then the reverse will travel with $-\theta_p$. This will only be true with the presence of mirror symmetry $\sigma_{\phi+90^\circ}$ in the EFS of m_2 . Besides the symmetry in the forward and reverse waves, another important symmetrical property is the equivalence of two propagating waves with incident angles, θ_i and $-\theta_i$. If there is a symmetry element, σ_ϕ (Fig. 8.3) in the EFS of m_2 , these two incident angles will excite two symmetrical waves with propagation angles θ_p and $-\theta_p$ in m_2 . If m_2 is a bulk isotropic material, then the corresponding EFS is a circle for any ω . Hence, the two symmetries $\sigma_{\phi+90^\circ}$ and σ_ϕ , always exist

independent of ϕ and ω . If m_2 is a bulk anisotropic material, the dispersion curve is elliptical and the symmetries exist for any ω , as long as one of the principal axes is aligned parallel to the normal line, $\alpha = \phi$.

Fig. 8.3 In-plane conduction of light from m_1 to m_2 . m_1 : isotropic medium, m_2 : arbitrary medium, e.g. PC

When the medium m_2 is a PC having lower values of ω (from the first band), then the corresponding EFS can be a circle or an ellipse [168-169]. Hence, it's refraction properties are similar to a bulk case. If m_2 is a PC and ω is from higher order bands, then there is a significant constraint, because of the presence of $\sigma_{\phi+90^\circ}$ and σ_ϕ , symmetries in the EFS. If the 2D PC is isotropic, then the EFS will show the

symmetry given by $\overline{R_M} = \overline{R}$ [see Secs. 3.2 and 6.4]. In a square lattice PC, $\overline{R} = C_{4v}$ has only four mirror symmetries and they are σ_{-45° , σ_0 , σ_{45° and σ_{90° . Hence, ϕ is restricted to multiples of 45° . In a hexagonal lattice PC ϕ must be a multiple of 30° , since the corresponding $\overline{R} = C_{6v}$ has only σ_{-60° , σ_{-30° , σ_0 , σ_{30° , σ_{60° and σ_{90° mirror symmetries.

For an anisotropic 2D PC, similar constraints apply, however, since $\overline{R_M} = \overline{R} \cap \overline{R_B}$ [Sec. 3.2], there is an additional constraint; i.e. the orientation of the motif, α has to be parallel to the normal line, $\alpha = \phi$.[♥] For example, the propagation angle of light with H -polarization in an anisotropic 2D PC, as a function of the incident angle for $\omega = 0.308$ has been plotted in Figure 8.4, by assigning m_1 to be air and m_2 to be a hexagonal lattice PC with circular cylinders ($r_c = 0.4a$) of LC ($n_o = 1.6$ and $n_e = 2.2$) in silicon (background medium).

Fig. 8.4 Propagation angle versus incident angle in an anisotropic PC. Solid line: forward wave, dotted line: reverse wave.

The optic axis of the LC (i.e., the motif) is aligned parallel to the normal line, $\phi = \alpha$ and Figs. 8.4(a), 8.4(b) and 8.4(c) correspond to the following set of α values ($0, 60^\circ$),

[♥] The motif is assumed to have $\sigma_{\alpha+90^\circ}$ and σ_α in the group $\overline{R_B}$. If $\overline{R_B}$ have no such symmetry elements, then the mentioned symmetries in the forward and reversed waves and in the positive and negative incident angles will be missing, although $\alpha = \phi$.

(30°,90°) and (15°,75°) respectively. The band structure for α values within the same set are identical, since the underlying lattice directions are the same. However, the orientations of the EFSs with respect to the interface are different and hence, the refraction properties can be expected to be different as well. However, the interface is aligned such that $\phi = \alpha$, and hence, the refraction properties are the same in this particular case, as shown in Fig. 8.4. For the first two sets of α values the corresponding EFSs possess σ_α and $\sigma_{\alpha+90^\circ}$ symmetries (for $\overline{R_M}$, see Table 3.1 with the orientation is *s.m.*). Due to these symmetries and for the incident angles θ_i and $-\theta_i$, the corresponding propagation angles for the forward waves are symmetric, being θ_0 and $-\theta_0$ respectively, as can be observed in Fig. 8.4(a) and 8.4(b). Similarly for reverse waves the propagation angles are also symmetric and they have the same values as the forward waves but reversed signs (i.e. $-\theta_0$ and θ_0). These symmetries are not observed in Fig. 8.4(c), corresponding to the set of α values (15°, 75°), because of the absence of σ_α and $\sigma_{\alpha+90^\circ}$ symmetries (for $\overline{R_M}$, see Table 3.1 with the orientation is *arb.*). This is a significant difference when compared with bulk anisotropic material, with $\overline{R_B} = \{E, C_2, \sigma_\alpha, \sigma_{\alpha+90^\circ}\}$, in which the mirror symmetries apply for any value of α . The symmetries σ_α and $\sigma_{\alpha+90^\circ}$ are lost if the same material (with α not equals to multiples of 30°) is used to construct a hexagonal lattice PC, since $\overline{R_M} = \overline{R} \cap \overline{R_B} = \{E, C_2\}$ does not have mirror symmetry. An incident wave with an incident angle of θ_i excites forward and reverse waves with different propagation angles given by θ_{01} and θ_{02} , as can be observed in Fig. 8.4(c). If the incident angle is reversed, i.e. $-\theta_i$, then the propagation angles of forward and reverse waves are interchanged. So, the propagation angles still exhibit symmetry and this is merely caused by the presence

of the C_2 symmetry element in the band structure. This C_2 symmetry is not disturbed by the optic axis orientation in the periodic plane and exists for any value of α since the operation $\overline{R_M} = \overline{R} \cap \overline{R_B}$, always produces C_2 independent of α .

8.3 Switching of superprism and polarization splitting in a LC infiltrated 2D PC

In this section, we shall present switchable superprism and polarization splitting effects based on a LC infiltrated 2D PC made of SiON.

A hexagonal lattice PC of circular cylindrical rods with $f = 0.58$ ($r_c = 0.4a$) is considered. The cylindrical rod is assumed to be uniaxially anisotropic LC with n_o and n_e of 1.6 and 2.2 respectively [97]. LCs with higher birefringence and smaller viscosities are also available [130, 201]. An isotropic material with a refractive index of 1.9 (the average of n_e and n_o) is used as the background material. We found that, such an assignment of refractive index to the background medium led to a larger polarization splitting and good tunable effects. The proposed PC structure can be constructed by etching holes in a matrix medium such as SiON, whose refractive index can be tailored to 1.9 by adjusting the oxygen and nitrogen ratio. The dispersion properties are calculated using PWM [Chaps. 4, 5 and 6], for two configurations of LC's optic axis, 1) perpendicular to the periodic plane (*s*-orientation) and 2) parallel to the periodic plane (*p*-orientation). These two configurations of optic axis allow decoupling of *E* and *H*-polarizations in the 2D anisotropic PC [Sec. 2.3, Chap. 2]. The interfacing media is assumed to be air and the

interfacing plane is assumed to be along Γ K - direction of the hexagonal lattice [Fig. 3.2(a) of Chap. 3].

For s -orientation of optic axis, the E - and H -polarizations will experience refractive indices of 2.2 and 1.6, respectively, in the LC layer. Comparing the refractive index of the background medium, both polarizations have similar refractive index differences of 0.3. However, the refractive index of E -polarization is higher than the background medium (direct configuration of PC) and for H -polarization it is lower than the refractive index of the background media (inverse configuration of PC).

Fig. 8.5 Band structure for both E - and H -polarizations with s -orientation of optic axis. Insets show EFSs at $\omega = 0.311$ (dashed line, black) for both E - (solid line, blue) and H - (dashed line, red) polarizations (a) s -orientation of optic axis (b) p -orientation of optic axis.

This difference in PC configuration substantially splits the band structure of the two polarizations, as shown in Figure 8.5, in which the band structure for the case of s -orientation of optic axis is plotted, for both E - and H -polarizations. The normalized frequency, ω , ranging from 0.308 to 0.327, lies in the first band of H -polarization, and

in the second of E -polarization. The dispersion curve for $\omega = 0.311$ is given in the inset (a) of Fig. 8.5, for s -orientation of optic axis. The EFS for H -polarization is circular in shape, which is a typical shape for the first band and hexagonal-like shape for E -polarization.

For p -orientation of optic axis, the E -polarization, which is perpendicular to the periodic plane, will experience refractive index of 1.6 in LC layer, and the PC configuration becomes an inverse configuration. Hence the band structure of E -polarization will be very close to the one for H -polarization in s -orientation of optic axis, as they have the same refractive index modulation and both are in inverse configuration. One can still expect distinct band structures for these two optic axis orientations since they correspond to different polarizations. However, the refractive index modulation is small and thus the band structure should be very close. This can be seen by comparing the dispersion curves of H -polarization with s -orientation of optic axis [inset (a) of Fig. 8.5] and E -polarization with p -orientation of optic axis [inset (b) of Fig. 8.5].

For H -polarization, with p -orientation of optic axis, the refractive index is anisotropic in LC layer (Eqns. 2.14 and 2.13 of Chap. 2). Hence, the dispersion curves will lose a few symmetry elements [inset (b) of Fig. 8.5]. Along Γ -M' direction, the refractive index in LC layer, experienced by H -polarization is 1.6 and along Γ -K is 2.2. With the p -orientation of optic axis, $\omega = 0.311$ lies in both first and second bands of H -polarization. As we can see from the inset (b) of Fig. 8.5, there are two distinct curves for H -polarization. The horizontal, longer curve is the contour caused by the first band and the vertical, shorter curve is the contour corresponding to the second

band. The shape of dispersion curve near ΓK direction is close to the one in E -polarization with s -orientation of optic axis and the shape near $\Gamma M'$ direction is close to the one for H -polarization with s -orientation of optic axis. As mentioned earlier, their similarity is due a small modulation of refractive index, the EFSs of the two polarizations with the same refractive index contrast between the background medium, should be very close.

The distinct EFSs for E - and H -polarization with s -orientation of optic axis, at $\omega = 0.311$ lead to substantial difference in the corresponding propagation angles for the two polarizations. For E -polarization, we have all angle negative refraction; for H -polarization, we have all angle positive refractions. This substantial difference is due to the opposite sign of $\nabla_{\mathbf{k}}\omega$ for the first band of H -polarization and second band for E -polarization. As a result, an unpolarized light entering such a PC will propagate in PC with a large splitting angle between E - and H -polarizations. Figure 8.6 shows, the splitting angle for both s - and p -orientations of optic axis. For s -orientation of optic axis, the splitting angle is nearly 60° , for incident angle, θ_i between 15° and 90° . The splitting angle increases drastically, for $\theta_i < 15^\circ$. For instance, near $\theta_i = 11.5^\circ$ the splitting angle is 80° . When the optic axis re-oriented to p -configuration, both H - and E -polarization are positively refracted since the responsible EFSs are from the first band for both polarizations [inset (b) of Fig. 8.5]. As a result, the splitting angle is substantially reduced and varies between 0 and 11° for incident angle between 0 to 90° (Fig. 8.6).

Fig. 8.6 Splitting between E - and H -polarizations as a function of incident angle ($\omega = 0.311$).

Considering E -polarization, in which the EFS changes drastically when optic axis is re-oriented from s - to p -orientations, a fully switchable superprism effect is obtainable. This is vivid from the insets of Fig. 8.5, in which EFS at $\omega = 0.311$ for E -polarization, changes from circular to hexagonal-like shape upon transition of optic axis from p to s . In fact, such observation applies for a wider range of frequencies mentioned previously, from 0.308 to 0.327. The hexagonal-like shape of EFS for s -orientation at $\omega = 0.311$ is widely opened, especially at the high symmetrical corners. A more closed shape can be found at higher frequencies within the mentioned range. For $\omega = 0.321$, the propagation angle, θ_o versus θ_i curve is shown in Figure 8.7. A clear switching of superprism effect for E -polarization can be seen from the figure, when optic axis is varied from p - to s -orientation. For p -orientation, the responsible band is the first band with circular dispersion curve. The propagation angle can be well determined by using Snell's law and by assuming PC, as a bulk medium with an effective refractive index of $n_{eff} = 1.8$ ($n_{eff} = \sin(\theta_i)/\sin(\theta_o)$). For s -orientation of optic axis, the refraction deviates drastically from a bulk medium refractions. In

particular, θ_o swings from -80° to 80° , near $\theta_i = 0$. This large swing in the refraction completely disappears, instead, a bulk like refractions emerges when optic axis re-oriented to p -configuration. Furthermore, the refraction angle changes about 60° nearly for all incident angles except for a small range of incident angles near $\theta_i = 0$ for optic axis re-orientation from p - to s -orientation.

Fig. 8.7 Propagation angle versus incident angle curves for $\omega = 0.321$ (bottom axis), and propagation angle versus normalized frequency curves at $\theta_i = 75^\circ$ (top axis). The closed and open circles are used for propagation angle versus incident angle curves to enhance the visibility.

Besides the control over incident angle dependent superprism effect, switchable wavelength dependent superprism effect for E -polarization, can also be demonstrated. The band structure for E -polarization with s -orientation of optic axis, can be seen from Fig. 8.5. As mentioned earlier, the band structure of E -polarization with p -orientation of optic axis is very close to that of H -polarization with s -orientation, thus the corresponding band structure in Fig. 8.5 for H -polarization, can be used for E -polarization with p -orientation of optic axis. As we can see from Fig. 8.5, the frequency range 0.25-0.327 lies in the first band of E -polarization with p -

orientation. However, transition of band occurs near $\omega = 0.271$, for the case of s -orientation. Thus, large swing in the propagation angle can be observed around this frequency at a particular value of incident angle. This is clear from Fig. 8.5, in which the propagation angle as a function of frequency at incident angle of 75° is also plotted for both orientations of optic axis. The propagation angle swings from 24° to -34° (about 58°) upon a change of 5% in ω near $\omega = 0.271$, with s -orientation of optic axis. This large swing disappears when optic axis is re-oriented to p -configuration, demonstrating fully tunable wavelength dependent superprism effect.

8.4 Tunable dispersion properties of a LC infiltrated 2D PC

In the last section, we have presented a switching action provided by the effect of orienting optic axis from being perpendicular to the periodic plane to an orientation parallel to the periodic plane. In this section, we would like to describe a different tunable phenomena corresponding to the continuous variation of optic axis in the periodic plane of the PC. For such variation of optic axis, the polarization remains decoupled and a more convenient structure was found to be a structure with silicon as a matrix medium. Therefore, in this section, we shall present continuously tunable conducting properties of a LC infiltrated 2D PC made of silicon.

The structural parameters of the 2D PC remain to be the same as in the previous section except the matrix medium is replaced with silicon. For the interfacing medium, we used silica with a refractive index of 1.45 and the interface is aligned along the ΓK direction of the hexagonal lattice, as shown in Figure 8.8.

Fig. 8.8 Positive refraction with both incident angle, $\theta_i > 0$, and propagation angle, $\theta_o > 0$. The insets show the BZ of the hexagonal lattice (left) and the definition for the orientation of the optic axis (right). The interface of the PC is aligned along the ΓK direction.

The definitions of the incident angle, θ_i , the propagation angle, θ_o , and the optic axis orientation of the LC versus the periodic plane, α , are given in Fig. 8.8. Furthermore, Fig. 8.8 shows a positive refraction with $\theta_i > 0$ and $\theta_o > 0$. Both θ_i and θ_o are negative, if the incident and the propagation direction are right and left to the normal line, respectively. Positive refraction is defined when the signs of θ_i and θ_o are the same, whereas negative refraction is defined if the signs of θ_i and θ_o are opposite.

The two polarizations (E and H) of light can be decoupled as long as the optic axis of the LC is either parallel or perpendicular to the 2D periodic plane of the PC. When the optic axis is perpendicular to the periodic plane, the H - and E -polarized wave traveling in the periodic plane in the vicinity of the LC material experience constant refractive indices of n_o and n_e , respectively. In this case, the symmetry of the underlying lattice is not disturbed. However, when the optic axis is parallel to the

periodic plane, the refractive index of the H -polarization is strongly influenced by the optic axis orientation. Thus, the corresponding EFS of the H -polarization varies with α . The EFSs of the H -polarization for $\alpha = 0, 30^\circ, 60^\circ$ and 90° at a normalized frequency ω of 0.308 are plotted in Figures 8.9(a), (b), (c) and (d), respectively.

Fig. 8.9 EFSs at constant $\omega = 0.308$ of an LC infiltrated PC (thick dashed line) and bulk medium (thin solid line) (a) – (d) EFSs for the H -polarization where the optic axis is in the periodic plane at $\alpha = 0, 30^\circ, 60^\circ$ and 90° , respectively. The letters A, B, and C are used to label the sharp corners of the EFSs. Corners with identical labels have identical curvatures. (e) EFSs for the E -polarization with the optic axis in the periodic plane

The EFSs of the H -polarization for $\alpha = 0$ and 60° have the same shape, since the underlying lattice directions, Γ -M and Γ -M' (Fig. 8.8) are symmetric.[♣] The shapes

[♣] We can use the results obtained in Sec. 3.3.2 [Chap. 3] to explain the symmetry observed in the EFS for various optic axis orientation. All EFSs are centered at the Γ -point. For general orientation of optic

only differ by their orientations. Similar isomorphism applies to any set of EFSs with optic axes aligned along any pair of symmetry directions of the lattice. On the other hand, when the optic axis is in the periodic plane, the refractive index of the E -polarization in the LC layer is constant regardless of α and, hence, the EFS of the E -polarization is the same regardless of the optic axis orientations. Figure 8.9(e) shows the EFS of the E -polarization also at $\omega = 0.308$.

The vertical lines in Fig. 8.9(a) – 8.9(d) correspond to momentum conservation lines, determined by the incident angle. The curvature at the intersection point between such a line and the EFS of the PC determines the propagation angle ϕ in the PC. The propagation angle as a function of α is presented in Figure 8.10, for $\theta_i = -27^\circ$, -7° and 56° respectively. The reason for choosing these particular incident angles is to present three representative curves of θ_o versus α . For $\theta_i = -27^\circ$, the propagation angle is continuously tunable from negative to positive as α increases, since the curvatures of the EFSs are almost linearly dependent on α (Fig. 8.9). As can be seen from Fig. 8.10, at $\theta_i = -27^\circ$, the propagation angle changes about 90° when α is varied from 0 to 90° . For $\theta_i = -7^\circ$, the propagation angle becomes less sensitive to α , which can be understood from the similar curvatures of the EFSs at various α 's in Fig. 8.9(a) – 8.9(d). For $\theta_i = 56^\circ$, the propagation angle becomes highly sensitive at $\alpha \approx 30^\circ$. The angle swings from -50° to 25° (about 75°) upon a change of α from 20° to 30° , and then decreases from 25° to -65° (about 90°) for another 10° change of α . The inset in Fig. 8.10 shows the EFSs and the momentum conservation line at $\theta_i = 56^\circ$ for $\alpha = 20^\circ$,

axis we have $\overline{R_M} = C_2$. Therefore from Table 3.2, we have $\overline{R_\theta} = C_{6v}$. The FZO for $\overline{R_\theta} = C_{6v}$ is defined in Table 3.3 as $0 < \alpha < 30^\circ$. Hence, only EFSs within the FZO ($0 < \alpha < 30^\circ$) are unique.

30°, and 45° respectively. As can be seen from the inset, the curvature of the EFS at $\alpha = 30^\circ$ is distinctly different from $\alpha = 20^\circ$ and 40° , and causes the extreme sensitivity of the propagation angle as a function of the optic axis orientation near $\alpha = 30^\circ$. The high sensitivity of the propagation angle versus the optic axis orientation (i.e. large $\Delta\theta_o/\Delta\alpha$) illustrates an α dependent superprism effect and implies tunable superprism by re-orienting the optic axis.

Fig. 8.10 The propagation angle of the H -polarization when optic axis is varied in the periodic plane as a function of the optic axis orientation $\theta_i = -27^\circ$, -7° and 56° . The inset shows the enlarged EFSs at $\theta_i = 56^\circ$, for $\alpha = 20^\circ$, 30° and 40° , respectively.

The EFS of the E -polarization shown in Fig. 8.9(e) is close to a circular shape and $\nabla_{\mathbf{k}}\omega < 0$, for $\omega = 0.308$, regardless of α . Hence, the E -polarization is negatively refracted for all incident angles and the propagation angles do not vary with α . Since the refraction of the H -polarization can be controlled from positive to negative, by varying α , the two polarizations can be splitted and the splitting angle θ_s between the E - and H -polarizations can be controlled to a large extent. The splitting angle θ_s as a function of α , is plotted in Figure 8.11 for various incident angles.

Fig. 8.11 Splitting angle between the H - and E -polarization as a function of the optic axis orientation in the periodic plane for $\theta_i = -7^\circ$, and -27° , respectively. The inset shows the direction of refracted beams at the interface for an incident angle of -27° . The refraction of the E -polarization is negative and remains the same for all α , whereas for the H -polarization the refraction angle depends on α .

The inset in Fig. 8.11 shows the E - and H -polarized waves at an incident angle of -27° . For the E -polarization the propagation angle is 49° (negative refraction) regardless of α , at $\theta_i = -27^\circ$, whereas for the H -polarization the propagation angle depends on α (Fig. 8.10). For $\alpha = 0$ and $\theta_i = -27^\circ$, the refraction for H -polarization is positive with the smallest negative propagation angle (Fig. 8.10), which results in a maximum θ_s of 61° (Fig. 8.11). This splitting is substantially larger as compared to the conventional double refractions using bulk birefringent media, where the refractions of both polarizations are always positive. For comparison, if the same PC is considered to be a bulk birefringent medium, with effective ordinary and extraordinary refractive indices of $\sqrt{fn_{o,LC}^2 + (1-f)n_{Si}^2}$ and $\sqrt{fn_{e,LC}^2 + (1-f)n_{Si}^2}$ respectively [98], the maximum splitting angle is calculated to be below 3° , which is very small. With increasing α the propagation angle for H -polarization increases for

$\theta_i = -27^\circ$ (Fig. 8.10), causing a reduction in θ_s . When $\alpha = 45^\circ$, the propagation angle for both H - and E -polarization is 49° , hence, $\theta_s = 0$. With further increase of α , the propagation angle of H -polarization continuously increases and hence, the splitting angle increases again, as shown in Fig. 8.11. On the other hand, it is also possible to achieve a large polarization splitting that is less sensitive to α . For instance, the θ versus α curve of the H - polarization at $\theta_i = -7^\circ$ (Fig. 8.10), is less sensitive to α , and hence, the corresponding θ_s versus α curve at $\theta_i = -7^\circ$ shows a similar splitting angle of about 12° for nearly all α 's.

Besides the large control over refraction and polarization splitting, at particular incident angles, a large and controllable superprism effect can be obtained. This can be understood by examining the sharp corners of EFSs [Fig. 8.9], which are responsible for superprism effect, for various α 's. Figure 8.12 shows the incident angle at which the superprism effect occurs, θ_s , the swing of the propagation angle, $\Delta\theta_o$, the corresponding incident angle change, $\Delta\theta_i$, and the sensitivity of propagation angle to incident angle, $\Delta\theta_o/\Delta\theta_i$, as a function of α , for positive incident angles; the respective definitions are illustrated in the inset of Fig. 8.12. It can be seen from Fig. 8.9 that, the same sharp corners appear for both positive and negative incident angles in the EFSs in Figs. 8.9(a)-8.9(d). Thus, the sensitivities (i.e. $\Delta\theta_o/\Delta\theta_i$) and the tuning range are similar for both positive and negative incident angles. So, we devote the discussion for positive incident angle only in Fig. 8.12. The position of the sharp corner varies as α is varied, and hence, θ_s , changes with α (Fig. 8.12). The other parameters, $\Delta\theta_o$, $\Delta\theta_i$, and $\Delta\theta_o/\Delta\theta_i$, can directly be interpreted from the curvature of the sharp corners and the orientation of EFSs.

Fig. 8.12 θ_{is} , $\Delta\theta_o$, $\Delta\theta_i$, and $\Delta\theta_o/\Delta\theta_i$ as a function α for H -polarization. The inset shows the definitions of $\Delta\theta_o$ and $\Delta\theta_i$. θ_{is} is defined in the middle of $\Delta\theta_i$.

As can be seen from Fig. 8.9, the sharp corner transition is $A \rightarrow B \rightarrow C \rightarrow B$ when α is varied from $0 \rightarrow 30^\circ \rightarrow 60^\circ \rightarrow 90^\circ$ (Fig. 8.9(a)-8.9(d)). When α is increased from 0 to 30° , the curvature changes from smoother (A) to sharper (B), and hence, $\Delta\phi / \Delta\theta$ increases from 2.6 to 26.4. Thereafter, when α is increased from 30° to 60° , the curvature becomes smoother (C), causing a reduction in $\Delta\theta_o / \Delta\theta_i$ from 26.4 to 2.8. Finally, as α is increased from 60° to 90° , the curvature becomes sharper (B), causing a drastic increase of $\Delta\theta_o / \Delta\theta_i$ from 2.8 to 81.1. Although the value of $\Delta\theta_o / \Delta\theta_i$ is similar for all α 's except 30° and 90° , $\Delta\theta_o$ and $\Delta\theta_i$ differ significantly as a function of α , as shown in Fig. 8.12. It should also be noted that, even though the EFSs for $\alpha = 0$ and $\alpha = 60^\circ$ are the same, the points at which superprism occur (i.e. A and C) are different, thus $\Delta\theta_o$, are different for these two α 's. Whereas for both $\alpha = 30^\circ$ and 90° , $\Delta\theta_o = 113.5^\circ$, since the shape of both EFSs and the superprism point (i.e. B) are the same for both α 's. However, due to a fixed orientation of the interface, $\Delta\theta_i$ differs for $\alpha = 30^\circ$

and 90° , as shown in Fig. 8.12. When $\alpha = 30^\circ$, $\Delta\theta_i = 4.3^\circ$, and when $\alpha = 90^\circ$, $\Delta\theta_i = 1.4^\circ$. Thus, the corresponding $\Delta\theta_o/\Delta\theta_i$ differs significantly, as 26.4 for $\alpha = 30^\circ$ compared to 81.1 for $\alpha = 90^\circ$.

A wavelength dependent superprism effect is very useful, especially in realizing applications like wavelength demultiplexing for optical communications. In an LC infiltrated PC, this wavelength dependent superprism effect can be enhanced substantially and, thus, it can be controlled better. Figure 8.13 shows θ_o versus ω for various values of α at $\theta_i = -20^\circ$ for H -polarization.

Fig. 8.13 Propagation angle as a function of ω for various α , at $\theta_i = -20^\circ$, for H -polarization, showing the tunable wavelength dependent superprism effect ($f = 0.58$). The inset shows the sensitivity of propagation angle to wavelength in degree/nm as a function of α , near wavelength of 1550nm, at $\theta_i = -20^\circ$.

When $\alpha = 0$, the curvatures of the EFSs for $0.29 < \omega < 0.32$ are almost the same at an incident angle of -20° . This results in identical propagation angles at all ω . However, for $\alpha = 60^\circ$, at the same incident angle, the EFSs vary significantly with ω , causing wavelength dependent refraction. The propagation angle at $\alpha = 60^\circ$ swings from -5° to 56° (about 61°), when ω is changed from 0.29 to 0.32. The inset in Fig. 8.13 shows

the sensitivity of propagation angle versus wavelength at $\theta_i = -20^\circ$, as a function of α . It can be seen from the inset that the sensitivity can be tuned continuously from $0.01^\circ/\text{nm}$ to $0.4^\circ/\text{nm}$, as α changes from 0 to 60° at the optical communication wavelength, $1.55\mu\text{m}$.

It is worth mentioning that, tunability of the dispersion properties decreases as the cylindrical radius of the PC decreases. Taking the wavelength dependent tunable superprism effect as an example in Fig. 8.13, the effect is observed for a cylindrical radius of $0.4a$ (i.e. $f = 0.58$) in a normalized frequency range of 0.29 - 0.32 , which is located near the bottom edge of the third band in the photonic band structure.

Fig. 8.14 Propagation angle as a function of ω for various α , at $\theta_i = -20^\circ$, for H -polarization, showing the tunable wavelength dependent superprism effect ($f = 0.44$). The inset shows the sensitivity of propagation angle to wavelength in degree/nm as a function of α , near wavelength of 1550nm , at $\theta_i = -20^\circ$.

When the cylindrical radius is reduced to $0.35a$ (i.e. $f = 0.44$), the edge of the third band shifts down ($\alpha = 60^\circ$, the same as in Fig. 8.13). As a result, the tunable superprism effect is observable at lower frequencies ($0.27 - 0.3$), which is shown in

Figure 8.14. It can be seen from Fig. 8.12 that, the propagation angle swings about 33° from -8° to 25° , when ω is changed from 0.27 to 0.3. Similar to Fig. 8.11, the inset in Fig. 8.14 shows the sensitivity of propagation angle as a function of wavelength, for $f = 0.44$. It can be seen from the inset in Fig. 8.14 that the sensitivity can be tuned continuously, however the tuning range is smaller than that for $f = 0.58$ (inset in Fig. 8.13).

Thus, the tuning range is larger if the filling ratio of the tunable element (i.e. LC) is larger. On the other hand, a very high filling ratio is more challenging to realize [185]. So in both Sec. 8.3 and 8.4 we considered a reasonably high filling ratio but still amenable to fabrication in the chapter ($f = 0.58$). Moreover, PCs with a similar f , has been fabricated previously [202].

8.5. Comparison with results based on the finite difference time domain method

In this chapter all conducting properties were obtained using calculations based on the PWM [Chap. 4]. In this section, we verify the results by comparing the presented results with calculations based on the FDTD method. FDTD method has been previously employed to analyze light propagations and very good agreement between the theory and the experiments were reported [69-72]. However, as we have mentioned in Chap. 4, FDTD demand large computational time and computer memory. Therefore we only picked few of the presented results to verify using FDTD.

We used the FDTD software developed by Ward and Pendry [140] with a time step of 1.693×10^{-16} s and the space is discretized using a non-orthogonalized

coordinate system. The band structures are obtained using the fast Fourier transform method and the data were smoothened using a polynomial fitting. The refraction angles were calculated using the EFS produced by the FDTD calculations. More details on the employed FDTD method can be found in Ref. 140.

We picked the superprism effects presented in Fig. 8.7 and perform the required FDTD calculations. The FDTD results are displayed in Figures 8.15(a) and 8.15(b) as open circles. In the same figures, the results displayed in Fig. 8.7 (the one obtained using PWM) are re-plotted using solid lines.

Fig. 8.15 Comparison of calculated propagation angles using PWM (solid lines, re-plotted from Fig. 8.7) and FDTD (open circles, obtained using the software in Ref. 140) (a) as a function of incident angle (b) as a function of normalized frequency

As we can readily verify from Figs. 8.15(a) and 8.15(b), results of the FDTD method share good agreements with the results of the PWM. The largest deviation between the results of PWM and FDTD occurs for s -orientation, near the band gap frequency [PWM results deviate about 2° (in the propagation angle) from the corresponding FDTD result when the normalized frequency is 0.265, see Fig. 8.15(b)]. The observed good matching between results of PWM and FDTD is not surprising as the band

structure calculations based on PWM converges with an error less than 1% for the lower order bands (up to the sixth band) [Sec. 4.4 of Chap. 4, 29-33, 133 and 134]. In Secs. 8.3 and 8.4 we have the operational frequency that is either in the first band or near the bottom edge of the second band, and hence it can be expected all PWM results presented in Secs. 8.3 and 8.4 will have similar accuracies with the special case presented in this section.

8.6. Potential applications

The presented studies in Secs. 8.3 and 8.4 are useful for many practical applications such as tunable wavelength demultiplexers, polarization splitters, light deflection (i.e., bending) devices etc.

In WDM technology [203], several wavelength channels are multiplexed together in the same optical fiber. The standard wavelength separation between channels is 0.8 nm [61-62, 203]. At the end of the transmission the multiplexed wavelength channels must be separated in order to reach the users (i.e., demultiplexing). Based on the study we presented in Secs. 8.3 and 8.4, we can design compact and tunable demultiplexers. In Sec. 8.3 we have shown that, the propagation angle swings about 58° when normalized frequency is increased about 5% from the value 0.271 for the *s*-orientation of optic axis and this change is almost zero for the *p*-orientation of optic axis. If the period of the PC is fixed as $1550 \times 0.271 = 420$ nm, then the 58° swing in the refraction angle for 5% increment in the normalized frequency corresponds to a 0.78 degree/nm sensitivity at the wavelength 1550nm. Therefore, to separate two channels centered at 1550.0 and 1550.8 nm to a

distance of $3\text{ }\mu\text{m}$, we need a device length of $275\text{ }\mu\text{m}^{\star}$. This is very short compared to the conventional arrayed waveguide grating (AWG), which is typically few centimeters in length [61]. Note that the proposed device is indeed a switch. When the optic axis is in the s -orientation, the demultiplexer is in the “on” state and when the orientation is p -orientation the demultiplexer is in the “off” state. Similarly, by applying the results presented in Sec. 8.4 we can design demultiplexers with continuous tunabilities. Examples of tunable sensitivity curves appear in the insets of Figs. 8.13 and 8.14.

Apart from tunable demultiplexers, tunable polarization splitters also can be developed from the presented study. Most of the planar photonic devices such as waveguides, modulators couplers, and interferometers are polarization dependent [13, 185]. Therefore it is essential to split the polarization of light before light is coupled into these devices. Conventional polarizers [141] are large in size and exist as a separate optical component. However, using the polarization splitting mechanism presented in this chapter, compact and tunable polarization splitters can be made. For instance, in Sec. 8.3, we have shown that at the normalized frequency of 0.308, the splitting angle between the two polarizations of light, can be tuned in the range $0 < \theta_s < 60^\circ$, by controlling the optic axis orientation. This means for applications at the wavelength of 1550 nm, the required pitch of the PC is $0.308 \times 1550 = 477\text{ nm}$ and in order to split the polarizations to a distance, $d = 3\text{ }\mu\text{m}$ with

[★] The length is calculated as separation ($3\text{ }\mu\text{m}$) divide by the product of the sensitivity (0.78 degree/nm converted to rad/nm) with the channel spacing (0.8 nm) [61]. The $3\text{ }\mu\text{m}$ separation was used in Ref. 62.

$\theta_s=60^\circ$, the length of the device is $1.73 \mu\text{m}$ [i.e., $d/\tan(\theta_s)$]. If the length of the device is fixed at $1.73 \mu\text{m}$, then we can tune the separation distance from $d = 0$ to $3 \mu\text{m}$ by controlling the optic axis orientation.

8.7. Summary and remarks

In summary, we have presented the conducting properties of an anisotropic PC in this chapter. Sec. 8.2 outlined the general principles and the fundamental properties of the conduction in the anisotropic PC. In Secs. 8.3 and 8.4 specific anisotropic PCs with electro-optically tunable motifs were studied. These structures contain LC and provide controls when LC's optic axis is re-oriented. The re-orientation of the LC's optic axis can be done by applying an external electric field. Based on this mechanism, controllable refraction, controllable polarization splitting and controllable superprism effect have been investigated. In Sec. 8.5 we have compared the results of the chapter with simulations based on the FDTD method and good matchings were found. Finally, potential applications for the presented studies in Secs. 8.3 and 8.4 were discussed in Sec. 8.6.

It is worth mentioning that in our calculations, we have neglected the effect of finite beam width of the light source (i.e. the incident beam was assumed to be a plane wave). This assumption is valid provided the incident beam diameter is relatively larger compared to the period of the PC. Previous experiments on refraction, polarization splitting and superprism showed good agreement with simulations using such a plane wave assumption [46,61-62,162]. However, a more rigorous analysis is needed to take the finite beam width of the source into account [204-206]. Such an analysis is important especially in designing practical wavelength

division multiplexers, where analysis on crosstalk between adjacent wavelength channels is needed [205]. It is worth to note that that the effects of other practical issues in implementing PC devices have been discussed in Refs. 62, 204 and 206.

Conclusion

This chapter concludes the thesis, with a summary and recommendations for future work.

9.1 Summary of the thesis

In this thesis, we have defined a category of PC called anisotropic PC. Starting from the fundamental formulations of Maxwell, the basic equations describing an anisotropic PC (or generally a PC) were reviewed. In-depth analyses of the polarizations decouplings in 2D and 1D materially anisotropic PCs were presented. The decouplings of the polarizations in the 2D and 1D PCs require one of the principal axes of the anisotropic medium to be perpendicular to the 2D periodic plane and to the 1D periodicity axis respectively. If the anisotropic material is uniaxial then in the 1D structure the polarizations remain decoupled.

The symmetrical properties of the anisotropic PCs were investigated in detail using group theory. Particularly, the use of coset decomposition in identifying their IBZs was shown and novel concepts such as the orientational groups and fundamental zone of orientations were introduced. In the design of an anisotropic PC, fundamental zone of orientation plays an important role. The range of orientations for which the optical properties remain unique is essentially governed by the fundamental zone of orientation. Further, the symmetry representations and

the degeneracy of the eigenstates in anisotropic PCs were analyzed in detail. This will be useful in analyzing band crossings, opening and closing of band gaps in the anisotropic PC.

The photonic states in the limit of zero modulation were analyzed and a systematic classification system based on integers was introduced for the states with distinct frequencies. The integers can be factored and states with the same factor can be categorized as they have the same form of solution when the spatial modulation is switched on. As it was shown in Chap. 5, such states can be easily solved and typically lead to analytical solutions. With this work, it is now made possible to have an analytical description or formulas for many optical properties of PC explored previously using numerical methods such as band gaps, refractions, group velocities and density of states. This in turn, may enable researchers to engineer PC and PC based devices analytically.

EFS approximation techniques with one plane wave and two plane waves were proposed for PCs of a small refractive index modulation. The analytical expression of the EFS can be used to predict the refraction angles and hence the superprism effect of PCs with a weak dielectric modulation, analytically. When the modulation is large, it is found that the EFS of an anisotropic PC for the state near the band edge is elliptical similar to the EFS of a bulk anisotropic medium. A set of effective negative principal refractive indices was defined to describe such anisotropic states with elliptical EFSs. Further, by varying the filling ratio, it is possible to force such an anisotropic state to an accidental isotropic state (i.e., states

with circular EFS). In addition, by re-orienting the motif and continuously varying the filling ratio, the orientation of the elliptical EFS can be continuously tuned.

The thesis also presented band gap engineering of a 2D materially anisotropic PC. Specifically, photonic band structures of 2D square lattice PCs made of anisotropic materials with one of the principal axes oriented along the extension direction of cylinders were studied. By re-orienting the principal axes in the 2D periodic plane, we showed that the band structure of the *H*-polarization can be improved to achieve large partial band gap for a pillar type PC and full band gap for a PC with air hole structures. Both band gaps exist for a wide range of filling ratios and even for a small value of anisotropy. Besides, it was also demonstrated how the band gaps of *H*-polarization at various directions of the lattice open and overlap each other in the anisotropic PCs with lower value of refractive indices.

Apart from the insulating properties of the 2D anisotropic structures, the insulating properties of an 1D anisotropic structure were also investigated. In particular, we have presented the details of tunable band gaps in a LC infiltrated 1D PC, by considering various orientations of LC's optic axis. Furthermore, for the 1D PC with a Pockel material, the details of the electro-optic efficiency in tuning the band gaps were analyzed in principal axes rotated and not rotated systems.

Tunable conduction devices such as tunable superprism and polarization splitters were proposed based on the 2D materially anisotropic PC. These structures contain LC and provide tunability when LC's optic axis is re-oriented. Based on this mechanism, controllable refraction, controllable polarization splitting and controllable superprism effect have been demonstrated. The presented conducting

properties can be very useful in designing tunable optical components such as tunable wavelength de-multiplexers and tunable light deflection devices for WDM technology.

9.2 Recommendations for future works

The field of anisotropic PC is indeed an exciting area of research. Though, this thesis has contributed to the field, there are still many aspects of anisotropic PCs that are worth exploring. In the following, recommendations for future works are proposed.

9.2.1 Quantum optical properties of an anisotropic PC

Quantum optics in a PC is an exciting and a promising field of research. Several relevant resources includes Ref. 115 (see Chap. 10-11), 207 (Review Paper) and 208. So far, the research in this field is mainly based on isotropic PCs. The study of quantum optics in an anisotropic PC is very useful as it will allow us to study, the quantum properties (properties relevant to local density of states, fluorescence, lamb shift, entanglement etc.) as a function of an orientational parameter. This may lead to optimization of the corresponding quantum parameter or a tunable quantum device (i.e., with the use of LC).

9.2.2 Diffractions in isotropic and anisotropic PC

Diffraction in isotropic PCs have been explored previously [79,152,196-197]. In particular, we have shown deformations of circular rings into various shapes using a weakly modulated PC (WPC) [79,209] and a PC with a finite spatial modulation (FPC) [210]. The photonic band structure for a WPC is basically a free photon

relationship and therefore, we can label the diffracted rings (or the diffracted spots) of a WPC with the integer system introduced in Chap. 3 and 5. The number of diffracted rings and the shape can be predicted analytically. For a FPC, we could apply the approximation technique presented in Chap. 5 to analytically approximate the shape of the diffracted rings. Further, the effect of a material's or geometrical anisotropy to the number and the shape of the diffracted rings also can be investigated for both WPC and FPC.

9.2.3 Classification and description of photonic states in a 3D PC

In Chap. 3 and 5 we have demonstrated a scheme to label and classify the degenerate states of a 2D PC. This scheme allows to categorize states with the same kind of evolution when the spatial modulation or material's anisotropy is switched on. Further, it enables us to have an analytical description for the photonic states in a 2D PC. The techniques presented in Chap. 3 and 5 can be extended to a 3D anisotropic PC and this promises rich analytical results.

9.2.4 New type of materials

In Chap. 6, the concept of a negative anisotropic medium is presented for the H -polarization in an anisotropic PC. For frequencies near the edges of the higher order bands, the anisotropic PC behaves in a similar way as a bulk anisotropic medium, however with a set effective negative principal refractive indices. This concept also can be developed for the E -polarization. By including some degree of material's anisotropy in the structure presented in Sec. 6.4, we could substantially split the band structure for E - and H -polarization and engineer the band structure of

the E -polarization such that the corresponding frequency of light falls in the first band with a positive effective refractive index and a circular (or an elliptical) EFS.

Such a study will lead to a formation of new kind of material that resembles the properties of a bulk biaxial material but with a set of positive and negative effective principal refractive indices for the E and H -polarization respectively. This type of material will exhibit permanent and very large polarization splitting capability.

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Appendix

Appendix –A

A1 - Tables

Group	Order	Symmetry Elements	IRs
C_{6v}	12	$E, C_2, C_3, C_3^{-1}, C_6, C_6^{-1}, \sigma_{-60^\circ}, \sigma_{-30^\circ}, \sigma_0, \sigma_{30^\circ}, \sigma_{60^\circ}, \sigma_{90^\circ}$	$A_1, A_2, B_1, B_2, E_1, E_2$
C_{3v}	6	$E, C_3, C_3^{-1}, \sigma_{-60^\circ}, \sigma_0, \sigma_{60^\circ}$	A_1, A_2, E
C_{2v}	4	$E, C_2, \sigma_0, \sigma_{90^\circ}$	A_1, A_2, B_1, B_2
C_6	6	$E, C_2, C_3, C_3^{-1}, C_6, C_6^{-1}$	A, B, E', E''
C_3	3	E, C_3, C_3^{-1}	A, E
C_{1h}	2	E, σ_0	A, B
C_2	2	E, C_2	A, B
C_1	1	E	A

Table A1 – The order, symmetry elements and IRs of the symmetry groups compatible with the 2D hexagonal lattice. Notation of symmetry elements and IRs follows Schonflies's and Mulliken's, respectively [113-114]. Symmetry element, σ_ϕ , refers to a mirror operation along an axis $y = x \tan(\phi)$ [ϕ is defined along anticlockwise direction from $+x$ axis] and C_n in the symmetry element refers to n -fold rotation (anticlockwise rotation around the axis perpendicular to the 2D periodic plane).

C_{6v}	C_{2v}	C_2
A_1	A_1	A
A_2	A_2	A
B_1	B_1	B
B_2	B_2	B
E_1	$B_1 + B_2$	$2B$
E_2	$A_1 + A_2$	$2A$

Table A2 – Compatibility relation between groups C_{6v} , C_{2v} and C_2 .

$\bar{S}$	Elements	Cosets
C_{4v}	all elements of C_{4v}	C_{4v}
C_{2v}	$E, C_2, \sigma_0, \sigma_{90^\circ}$	$\{E, C_2, \sigma_0, \sigma_{90^\circ}\}, \{C_4, C_4^{-1}, \sigma_{-45^\circ}, \sigma_{45^\circ}\}$
$C_{2v'}$	$E, C_2, \sigma_{-45^\circ}, \sigma_{45^\circ}$	$\{E, C_2, \sigma_{-45^\circ}, \sigma_{45^\circ}\}, \{C_4, C_4^{-1}, \sigma_0, \sigma_{90^\circ}\}$
C_2	E, C_2	$\{E, C_2\}, \{C_4, C_4^{-1}\}, \{\sigma_0, \sigma_{90^\circ}\}, \{\sigma_{-45^\circ}, \sigma_{45^\circ}\}$

Table A3 – Invariant subgroups, $\bar{S}$ of C_{4v} . For invariant subgroups the right and left cosets of a particular subgroup are the same.

$\bar{S}$	Elements	Cosets
C_{6v}	all elements of C_{6v}	C_{6v}
C_{2v}	$E, C_2, \sigma_0, \sigma_{90^\circ}$	$\{E, C_2, \sigma_0, \sigma_{90^\circ}\}, \{C_3, C_6^{-1}, \sigma_{30^\circ}, \sigma_{-60^\circ}\}, \{C_3^{-1}, C_6, \sigma_{-30^\circ}, \sigma_{60^\circ}\}$
$C_{2v'}$	$E, C_2, \sigma_{30^\circ}, \sigma_{-60^\circ}$	$\{E, C_2, \sigma_{30^\circ}, \sigma_{-60^\circ}\}, \{C_3, C_6^{-1}, \sigma_{-30^\circ}, \sigma_{60^\circ}\}, \{C_3^{-1}, C_6, \sigma_0, \sigma_{90^\circ}\}$
$C_{2v''}$	$E, C_2, \sigma_{-30^\circ}, \sigma_{60^\circ}$	$\{E, C_2, \sigma_{-30^\circ}, \sigma_{60^\circ}\}, \{C_3, C_6^{-1}, \sigma_0, \sigma_{90^\circ}\}, \{C_3^{-1}, C_6, \sigma_{30^\circ}, \sigma_{-60^\circ}\}$
C_2	E, C_2	$\{E, C_2\}, \{C_6, C_3^{-1}\}, \{C_6^{-1}, C_3\}, \{\sigma_0, \sigma_{90^\circ}\}, \{\sigma_{30^\circ}, \sigma_{-60^\circ}\}, \{\sigma_{-30^\circ}, \sigma_{60^\circ}\}$

Table A4 – Invariant subgroups, $\bar{S}$ of C_{6v} . For invariant subgroups the right and left cosets of a particular subgroup are the same.

A2- Orinetational Group

Initially we have,

$$M_\alpha[\mathbf{H}_k(\mathbf{r})] = \Omega_\alpha(\mathbf{k})[\mathbf{H}_k(\mathbf{r})] \quad [\text{A2.1}]$$

After re-orinetation of motif we have [Eqn. 3.15],

$$R_\theta^{-1} M_\alpha R_\theta [\mathbf{H}_k(\mathbf{r})] = \Omega_\beta(\mathbf{k})[\mathbf{H}_k(\mathbf{r})] \quad [\text{A2.2}]$$

Case 1 - Let $R_\theta = R_M R$, where $R \in \bar{R}$ and $R_M \in \overline{R_M}$. Using Eqn. 3.4 and 3.2,

$$\begin{aligned} (R_M R)^{-1} M_\alpha R_M R [\mathbf{H}_k(\mathbf{r})] &= \Omega_\beta(\mathbf{k})[\mathbf{H}_k(\mathbf{r})] \\ \Rightarrow R^{-1} (R_M^{-1} M_\alpha R_M) R [\mathbf{H}_k(\mathbf{r})] &= \Omega_\beta(\mathbf{k})[\mathbf{H}_k(\mathbf{r})] \\ \Rightarrow M_\alpha [R \mathbf{H}_k(\mathbf{r})] &= \Omega_\beta(\mathbf{k})[R \mathbf{H}_k(\mathbf{r})] \\ \Rightarrow M_\alpha [\mathbf{H}'_{Rk}(\mathbf{r})] &= \Omega_\beta(\mathbf{k})[\mathbf{H}'_{Rk}(\mathbf{r})] \end{aligned} \quad [\text{A2.3}]$$

Therefore, by comparing the final result of A2.3 to A2.1, $\Omega_\alpha(\mathbf{k}) = \Omega_\beta(\mathbf{k})$.

Case 2 - Let $R_\theta = R R_M$, where $R \in \bar{R}$ and $R_M \in \overline{R_M}$. Since $R R_M \in \bar{R}$, we can apply Eqn.

3.2 to show,

$$\begin{aligned} (R R_M)^{-1} M_\alpha R R_M [\mathbf{H}_k(\mathbf{r})] &= \Omega_\beta(\mathbf{k})[\mathbf{H}_k(\mathbf{r})] \\ \Rightarrow M_\alpha [R R_M \mathbf{H}_k(\mathbf{r})] &= \Omega_\beta(\mathbf{k})[R R_M \mathbf{H}_k(\mathbf{r})] \\ \Rightarrow M_\alpha [\mathbf{H}_{R R_M k}(\mathbf{r})] &= \Omega_\beta(\mathbf{k})[\mathbf{H}_{R R_M k}(\mathbf{r})] \end{aligned} \quad [\text{A2.4}]$$

Using the property of a Bloch function, $\mathbf{H}_{R R_M k}(\mathbf{r}) = \mathbf{H}_{R_M^{-1} R k}(\mathbf{r})$ [see Chap. 7 of Ref.

113] we can further simplify the final results of A2.4 as,

$$\begin{aligned} \Rightarrow M_\alpha [\mathbf{H}_{R_M^{-1} R k}(\mathbf{r})] &= \Omega_\beta(\mathbf{k})[\mathbf{H}_{R_M^{-1} R k}(\mathbf{r})] \\ \Rightarrow M_\alpha [R_M^{-1} \mathbf{H}_{Rk}(\mathbf{r})] &= \Omega_\beta(\mathbf{k}) R_M^{-1} [\mathbf{H}_{Rk}(\mathbf{r})] \\ \Rightarrow R_M M_\alpha R_M^{-1} [\mathbf{H}_{Rk}(\mathbf{r})] &= \Omega_\beta(\mathbf{k})[\mathbf{H}_{Rk}(\mathbf{r})] \\ \Rightarrow M_\alpha [\mathbf{H}_{Rk}(\mathbf{r})] &= \Omega_\beta(\mathbf{k})[\mathbf{H}_{Rk}(\mathbf{r})] \end{aligned} \quad [\text{A2.5}]$$

Therefore, by comparing the final result of A2.5 to A2.1, $\Omega_\alpha(\mathbf{k}) = \Omega_\beta(\mathbf{k})$.

Appendix-B

The free photon dispersion in a 2D hexagonal lattice is described by Eqn. 3.20.

For a 2D square lattice, the equation takes a similar form,

$$\omega = \frac{1}{n_x} \sqrt{c_1 m_{is} + c_2 (r_n^2 - 1) m_{anis} + \omega_c} \quad (\text{B1})$$

where the expressions for the constants c_1 , c_2 , and ω_c , and the discrete integers m_{is} and m_{anis} are listed in the following table for the symmetrical points of a square lattice.

k	c_1	m_{is}	c_2	m_{anis}	ω_c
$\Gamma(0,0)$	1	$n_1^2 + n_2^2$	1	n_1^2	0
$M(\pi/a, \pi/a)$	1	$n_1^2 + n_2^2 + n_1 + n_2$	$\frac{1}{4}$	$(2n_1 + 1)^2$	$\frac{1}{2}$
$X(\pi/a, 0)$	1	$n_1^2 + n_2^2 + n_1$	$\frac{1}{4}$	$(2n_1 + 1)^2$	$\frac{1}{4}$

Table B1 - Definitions of c_1 , m_{is} , c_2 , m_{anis} , and ω_c , in Eqn. B1

Appendix C

C1 – Proof to Eqn. 5.4

Fig. C1 – Proof to Eqn. 5.4

Referring to Figure C1 we can write the following in the phasor notation:

$$\mathbf{k} = k \angle \theta \quad [\text{C1.1}]$$

$$\mathbf{G} = G \angle \alpha_r \quad [\text{C1.2}]$$

$$\mathbf{k} + \mathbf{G} = |\mathbf{k} + \mathbf{G}| \angle (\chi + \theta) \quad [\text{C1.3}]$$

Applying cosine and sine rules we have,

$$|\mathbf{k} + \mathbf{G}|^2 = k^2 + G^2 + 2kG \cos(\theta - \alpha_r), \quad [\text{C1.4}]$$

$$\sin(\chi) = \frac{G}{|\mathbf{k} + \mathbf{G}|} \sin(\alpha_r - \theta), \quad [\text{C1.5}]$$

$$\cos(\chi) = \frac{k + G \cos(\alpha_r - \theta)}{|\mathbf{k} + \mathbf{G}|}. \quad [\text{C1.6}]$$

Referring to Figure C1,

$$\mathbf{Q}(\mathbf{k} + \mathbf{G}) = |\mathbf{k} + \mathbf{G}| \angle (\theta + \beta + \chi) = |\mathbf{k} + \mathbf{G}| \begin{pmatrix} \cos(\theta + \beta + \chi) \\ \sin(\theta + \beta + \chi) \end{pmatrix}, \quad [\text{C1.7}]$$

and using $\omega^2 = Q(\mathbf{k} + \mathbf{G}) \cdot \tilde{\kappa}_H(0) \cdot Q(\mathbf{k} + \mathbf{G})$,

$$\omega^2 = \frac{|\mathbf{k} + \mathbf{G}|^2 \cos^2(\theta + \beta + \chi)}{\varepsilon_x} + \frac{|\mathbf{k} + \mathbf{G}|^2 \sin^2(\theta + \beta + \chi)}{\varepsilon_y}. \quad [\text{C1.8}]$$

Adding a dummy term and applying $\sin^2(\theta + \beta + \chi) + \cos^2(\theta + \beta + \chi) = 1$,

$$\begin{aligned} \Rightarrow \omega^2 &= \frac{|\mathbf{k} + \mathbf{G}|^2 \cos^2(\theta + \beta + \chi)}{\varepsilon_x} + \left\{ \frac{|\mathbf{k} + \mathbf{G}|^2 \sin^2(\theta + \beta + \chi)}{\varepsilon_x} - \frac{|\mathbf{k} + \mathbf{G}|^2 \sin^2(\theta + \beta + \chi)}{\varepsilon_x} \right\} \\ &+ \frac{|\mathbf{k} + \mathbf{G}|^2 \sin^2(\theta + \beta + \chi)}{\varepsilon_y} \\ \Rightarrow \omega^2 &= \frac{1}{\varepsilon_x} |\mathbf{k} + \mathbf{G}|^2 + \left(\frac{1}{\varepsilon_y} - \frac{1}{\varepsilon_x} \right) |\mathbf{k} + \mathbf{G}|^2 \sin^2(\theta + \beta + \chi) \end{aligned}$$

Finally we obtain,

$$\varepsilon_x \omega^2 = |\mathbf{k} + \mathbf{G}|^2 + (r_\varepsilon - 1) |\mathbf{k} + \mathbf{G}|^2 \sin^2(\theta + \beta + \chi) \quad [\text{C1.9}]$$

where $r_\varepsilon = \varepsilon_x / \varepsilon_y$. Expanding $\sin(\theta + \beta + \chi)$, and using Eqns. C1.5-C1.6, we can show

$$\begin{aligned} |\mathbf{k} + \mathbf{G}| \sin(\theta + \beta + \chi) &= k \sin(\theta + \beta) + G \{ \cos(\theta - \alpha_\Gamma) \sin(\theta + \beta) - \sin(\theta - \alpha_\Gamma) \cos(\theta + \beta) \} \\ &= k \sin(\theta + \beta) + G \sin(\alpha_\Gamma + \beta) \end{aligned} \quad [\text{C1.10}]$$

Therefore, Eqn. C9 becomes

$$\varepsilon_x \omega^2 = |\mathbf{k} + \mathbf{G}|^2 + (r_\varepsilon - 1) |\mathbf{k} + \mathbf{G}|^2 \{ k \sin(\theta + \beta) + G \sin(\alpha_\Gamma + \beta) \}^2 \quad [\text{C1.11}]$$

This completes the proof to Eqn. 5.4.

C2- Notes to Eqn. 5.7-5.8

Eqn. 11 can be derived for an arbitrary wavevector and a general 2D lattice.

To see this, we assume:

$$\mathbf{b}_1 = [b_{1x}, b_{1y}] \quad [\text{C2.1}]$$

$$\mathbf{b}_2 = [b_{2x}, b_{2y}] \quad [\text{C2.2}]$$

$$\mathbf{k} = [k_x, k_y]. \quad [\text{C2.3}]$$

Consequently

$$\mathbf{k} + \mathbf{G} = [k_x + n_1 b_{1x} + n_2 b_{2x}, k_y + n_1 b_{1y} + n_2 b_{2y}] \quad [\text{C2.4}]$$

$$\tan(\alpha_{\mathbf{k}}) = k_y + n_1 b_{1y} + n_2 b_{2y} / (k_x + n_1 b_{1x} + n_2 b_{2x}) \quad [\text{C2.5}].$$

Using Eqn. C2.5 we can write n_2 in terms of n_1 (or n_1 in terms of n_2). For example by eliminating n_2 ,

$$|\mathbf{k} + \mathbf{G}|^2 = \{k_x b_{2y} - k_y b_{2z} + n_1 (b_{1x} b_{2y} - b_{2x} b_{1y})\} \text{cosec}^2(\alpha_{\mathbf{k}} - \alpha_{b_2}) / |\mathbf{b}_2|^2. \quad [\text{C2.6}]$$

where

$$q(\alpha_{b_2}) = \text{cosec}^2(\alpha_{\mathbf{k}} - \alpha_{b_2}) \quad [\text{C2.7}]$$

$$c_{\mathbf{k}} p_{\mathbf{k}}(n_1) = \frac{\{k_x b_{2y} - k_y b_{2z} + n_1 (b_{1x} b_{2y} - b_{2x} b_{1y})\}}{|\mathbf{b}_2|^2} \quad [\text{C2.8}]$$

C3- Notes to Eqns. 5.13.1-5.13.4 and 5.14.1-5.14.4

Eqns. 5.13.1-5.13.4 and 5.14.1-5.14.4 can be obtained by diagonalizing the matrix in Eqn. 5.12.1-5.12.2. Following MAPLE* script is used to obtain the eigenvalues of the M matrices of E and H -polarization analytically.

```
> #-----MAPLE CODES-----
> restart:
with(LinearAlgebra):
> kappa:=Matrix([ [kappa0, kappa1, kappa2, kappa3, kappa2, kappa1],
                  [kappa1, kappa0, kappa1, kappa2, kappa3, kappa2],
                  [kappa2, kappa1, kappa0, kappa1, kappa2, kappa3],
                  [kappa3, kappa2, kappa1, kappa0, kappa1, kappa2],
                  [kappa2, kappa3, kappa2, kappa1, kappa0, kappa1],
                  [kappa1, kappa2, kappa3, kappa2, kappa1, kappa0] ]):
> n1:= [0, 1, 1, 0, -1, -1]: n2:= [-1, 0, 1, 1, 0, -1]:
b1:=Vector([1, -1/sqrt(3)]): b2:=Vector([0, 2/sqrt(3)]):
G1 := n1[1]*b1 + n2[1]*b2: G2 := n1[2]*b1 + n2[2]*b2: G3 :=
n1[3]*b1 + n2[3]*b2:
G4 := n1[4]*b1 + n2[4]*b2: G5 := n1[5]*b1 + n2[5]*b2: G6 :=
n1[6]*b1 + n2[6]*b2:
GM:=RandomMatrix(2, 6):
GM[1..2, 1]:=G1: GM[1..2, 2]:=G2: GM[1..2, 3]:=G3:
GM[1..2, 4]:=G4: GM[1..2, 5]:=G5: GM[1..2, 6]:=G6:
```

* For more information on MAPLE see: <http://www.maplesoft.com/>

```

> MH:=RandomMatrix(6,6):
for ii from 1 to 6 do
for ij from 1 to 6 do
vGii:=GM[1..2,ii]; vGij:=GM[1..2,ij];
Gii:=GM[1..2,ii]/sqrt(DotProduct(vGii,vGii));
Gij:=GM[1..2,ij]/sqrt(DotProduct(vGij,vGij));
MH[ii,ij]:=kappa[ii,ij]*DotProduct(Gii,Gij);
end do: end do:
> #-----E-Portization-----
> Eigenvalues(kappa);
      -k3 + k0 + 2 k2 - 2 k1
      k3 + k0 + 2 k2 + 2 k1
      k3 + k0 - k2 - k1
      -k3 + k0 - k2 + k1
      k3 + k0 - k2 - k1
      -k3 + k0 - k2 + k1

> #-----H-Portization-----
> Eigenvalues(MH);
      -k3 + k0 - k2 + k1
      k3 + k0 - k2 - k1
      k3 + k0 +  $\frac{1}{2}$  k2 +  $\frac{1}{2}$  k1
      -k3 +  $\frac{1}{2}$  k2 -  $\frac{1}{2}$  k1 + k0
      k3 + k0 +  $\frac{1}{2}$  k2 +  $\frac{1}{2}$  k1
      -k3 +  $\frac{1}{2}$  k2 -  $\frac{1}{2}$  k1 + k0

> #-----

```

Using the eigenvalues of the matrix M , the proofs to Eqns. 5.13.1-5.13.4 and 5.14.1-5.14.4 are obvious.

C4- Notes to Eqn. 5.16 – Perturbation Theory

Let M' to be,

$$M' = M + M_{per} \quad [C3.1],$$

Corrections in the eigenvalues of M' , due to the presence of M_{per} can be formulated using the time-independent perturbation theory [164]. The first order correction, ε_1 , to a nondegenerate eigenvalues, E_j reads

$$\varepsilon_1 = \langle E_j^1 | M_{per} | E_j^1 \rangle \quad [C3.2]$$

The corresponding second order correction for the nondegenerate eigenvalues, ε_2 , reads

$$\varepsilon_2 = \sum_{i=1}^n \sum_{p=1}^{n(E_j)} \frac{\langle E_j^1 | M_{per} | E_i^p \rangle \langle E_i^p | M_{per} | E_j^1 \rangle}{E_i - E_j} \quad [C3.3]$$

with $i \neq j$. The flow chart for calculation of C3.1 and C3.2 appears in Figure C3.

The maple codes to calculate ω_1 are given below. Note that $M' = M_{all}$ and $M = M_o$. The orthonormal eigenvectors, $|E_i^p\rangle$ are obtain using the Gram-Schmidt procedure [108]. The results in Table 5.3 are obtained, by reformulating the output of the program using Eqns. 5.13.1-5.13.4 and 5.14.1-5.14.4.

```
> restart;
> kappa:=Matrix([ [kappa0,kappa1,kappa2,kappa3,kappa2,kappa1],
                  [kappa1,kappa0,kappa1,kappa2,kappa3,kappa2],
                  [kappa2,kappa1,kappa0,kappa1,kappa2,kappa3],
                  [kappa3,kappa2,kappa1,kappa0,kappa1,kappa2],
                  [kappa2,kappa3,kappa2,kappa1,kappa0,kappa1],
                  [kappa1,kappa2,kappa3,kappa2,kappa1,kappa0] ]):
> with(LinearAlgebra):
> n1:= [0, 1, 1, 0, -1, -1]: n2:= [-1, 0, 1, 1, 0, -1]:
b1:=Vector([1,-1/sqrt(3)]): b2:=Vector([0,2/sqrt(3)]):
G1 := n1[1]*b1 + n2[1]*b2: G2 := n1[2]*b1 + n2[2]*b2: G3 :=
n1[3]*b1 + n2[3]*b2:
G4 := n1[4]*b1 + n2[4]*b2: G5 := n1[5]*b1 + n2[5]*b2: G6 :=
n1[6]*b1 + n2[6]*b2:
GM:=RandomMatrix(2,6):
GM[1..2,1]:=G1: GM[1..2,2]:=G2: GM[1..2,3]:=G3:
GM[1..2,4]:=G4: GM[1..2,5]:=G5: GM[1..2,6]:=G6:
> #-----Mall = M', Mor = Mo and Mper-----
> kv:=Vector([k*cos(theta),k*sin(theta)]):
Mall:=RandomMatrix(6,6):
for ii from 1 to 6 do
for ij from 1 to 6 do
Gii:=kv+GM[1..2,ii];
Gij:=kv+GM[1..2,ij];
Mall[ii,ij]:=kappa[ii,ij]*DotProduct(Gii,Gij);
end do: end do:
Mall:=simplify(Mall) assuming k>0, theta::real:
> Mo:=simplify(algsb(k=0,Mall)):
Mper:=simplify(Mall-Mor) assuming k>0, theta::real:
```

```

> #-----Eigenvectors of Mor-----
u:=Matrix([ [1, -1, -1, -1, 1, -1], [1, 1, 1, 0, 0, -1], [1, -1, 0,
1, -1, 0], [1, 1, -1, -1, -1, 1], [1, -1, 1, 0, 0, 1], [1, 1, 0, 1,
1, 0]]):
gs:=GramSchmidt([u[1..6,1],u[1..6,2],u[1..6,3],u[1..6,4],u[1..6,5]
,u[1..6,6]]):
um:=RandomMatrix(6,6):
ii:=1: um[1..6,ii]:=gs[ii]/sqrt(DotProduct(gs[ii],gs[ii])):
ii:=2: um[1..6,ii]:=gs[ii]/sqrt(DotProduct(gs[ii],gs[ii])):
ii:=3: um[1..6,ii]:=gs[ii]/sqrt(DotProduct(gs[ii],gs[ii])):
ii:=4: um[1..6,ii]:=gs[ii]/sqrt(DotProduct(gs[ii],gs[ii])):
ii:=5: um[1..6,ii]:=gs[ii]/sqrt(DotProduct(gs[ii],gs[ii])):
ii:=6: um[1..6,ii]:=gs[ii]/sqrt(DotProduct(gs[ii],gs[ii])):
Moru:=simplify(Transpose(um).Mor.um):
> #-----First order corrections-----
> Mperu:=Transpose(um).Mper.(um):
elc:=simplify(Mperu[1,1]):
e2c:=simplify(Mperu[2,2]):
> E1:=Moru[1,1]: E2:=Moru[2,2]: E3:=Moru[3,3]: E4:=Moru[5,5]:
> w3:=RandomMatrix(2,2): w4:=RandomMatrix(2,2):
> ev1:=um[1..6,1]:
ev2:=um[1..6,2]:
ev3a:=um[1..6,3]:
ev3b:=um[1..6,4]:
ev4a:=um[1..6,5]:
ev4b:=um[1..6,6]:
> #-----Second order corrections-----
evecs:=RandomMatrix(6,6): feve:=RandomMatrix(6,2):
zvec:=Vector([0,0,0,0,0,0]):
devalues:=Vector([E2,E3,E4]):
evecs[1..6,1]:=ev2: evecs[1..6,2]:=zvec:
evecs[1..6,3]:=ev3a: evecs[1..6,4]:=ev3b:
evecs[1..6,5]:=ev4a: evecs[1..6,6]:=ev4b:
feva:=E1:
chiii:=ev1:
> #-----
termn:=0:
for n from 1 to 3 do
#-----
termp:=0:
for p from 0 to 1 do
uterm:=DotProduct(chiii,Mper.evecs[1..6,2*n-
1+p])*DotProduct(evecs[1..6,2*n-1+p],Mper.chiii):
lterm:=feva-devalues[n]:
term:=uterm/lterm:
termp:=termp+term:
end do:
#-----
termn:=termn+termp:
end do:
#-----
w:=simplify(termn) assuming k>0, theta::real;
> omega[i]:=Moru[1,1]+elc+w;

```

$$\begin{aligned}
w_i := & \frac{4}{3} k_0 + \frac{4}{3} k_1 - \frac{4}{3} k_2 - \frac{4}{3} k_3 + k^2 (k_0 + 2 k_1 + 2 k_2 + k_3) \\
& + \frac{k^2 (4 k_0^2 + 9 k_1^2 + 12 k_1 k_0 + 6 k_1 k_2 + 4 k_0 k_2 + k_2^2)}{k_1 - 3 k_2 - 4 k_3}
\end{aligned}$$