



The Application of Group Representation Theory in the Study of Photonic Crystals

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Abstract

In this work, we apply the theory of group representations to the study of degeneracies of modes in photonic crystals. After a rigorous mathematical description of the problem, we proceed to study induced representations, leading to a way of determining their irreducibility. We then apply this theory to symmetry groups of photonic crystals, allowing predictions on the degeneracies of photonic modes. The theory is exemplified in a number of numerical simulations of two-dimensional crystals with various wallpaper groups as their symmetry group. We find degeneracies of modes in highly symmetric structures that can be removed by breaking the symmetry. Removing these symmetries generally leads to the formation of gaps and photonic bands with low group velocity, or ‘slow light’. The use of representation theory thus comprises a novel design principle for photonic crystals. In several cases we find so called ‘accidental degeneracies’ that are not easily predicted by our mathematical framework. Further research on this issue needs to be conducted in order to achieve a robust design principle.

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Chapter 1

Introduction

The past 150 years or so have witnessed the phenomenal rise in mankind's control over (and its ultimate dependence on) electricity, magnetism and radiation. It is unlikely that early electrical engineers like Edison and Tesla could have foreseen their research paving the way for the likes of telephones, computers and outer space exploration, to name but a few consequences of basal inventions such as the telegraph and induction motor.

For most of this time, however, our mastery of light and of the optical properties of matter have lagged behind. Though technologies like laser and fiber-optic communication exemplify the existence of developments in this field, more advanced means of manipulating the flow of light would be invaluable to technological and scientific progress alike. True mastery over light demands control of matter at wavelength and sub-wavelength scales, for which the required nanofabrication technology has become available with the dawn of modern computers. Thus, we find ourselves at the onset of a new era in optical physics. Ushering in this age are photonic crystals, structures with a periodic variation in refractive index at wavelength scale that exhibit fascinating interactions with light, displaying phenomena such as confinement of light and control over its propagation speed. Applications of photonic crystals range from high reflectivity coatings, which could increase the efficiency of solar panels [1], to optical transistors, which could pave the way for the construction of optical computers. To boot, it is important to keep in mind that we, similar to Edison and Tesla in their day, are still blind to potential applications further down the road.

In this work, we aim to strengthen and possibly extend earlier established links between the study of photonic crystals and group theory. Much of the underlying theory is decades old, but it seems that the absence of a text

accessible to both mathematicians and physicists has inhibited collaboration between the fields. The main goal of this text, then, is to create the bedrock for future exchange of knowledge by providing a mathematically rigorous treatment of the subject, while staying rooted in the physical context.

Recently, much emphasis in research has been placed on the topology of bands in the fields of graphene, topological insulators and topological photonics [2]. A key role in those areas is played by degeneracies and defect modes that are protected by symmetry. Understanding these phenomena and the limitations of what is achievable seems impossible without a firm group theoretical description. Further development of the application of group theory in this field could lead to new ways of designing photonic crystals based on considerations of symmetry, potentially opening the door to yet unseen properties and phenomena.

Chapter 2

Theory

2.1 Preliminaries

Photonic crystals are the objects of interest in this work and are defined as follows.

Definition 1. For $1 \leq n \leq 3$, a *n-dimensional photonic crystal* is a smooth function $\varepsilon : \mathbb{R}^n \rightarrow \mathbb{C}$ with the periodicity of a lattice $\Lambda \subset \mathbb{R}^n$, where $\varepsilon(r)$ represents the so-called permittivity of the material at position $r \in \mathbb{R}^n$.

Several remarks concerning this definition should be made. Primarily, since ε (sometimes called the dielectric function) represents the permittivity of a material, it is subject to some physical constraints. For lossless materials, to which we shall restrict ourselves, we have $\text{Im}(\varepsilon(r)) = 0$ and $\text{Re}(\varepsilon(r)) > 0$ for all $r \in \mathbb{R}^n$. Realistically, ε also depends on the frequency of light to which the material is being exposed. However, here we are interested in transparent materials for which this frequency dependency is weak. Thus, for the sake of simplicity, we shall exclude this dependency.

In definition 1, we used the term *lattice* to mean a free abelian group of rank n , i.e. a subgroup of \mathbb{R}^n that is isomorphic to \mathbb{Z}^n (as an additive group) and which generates \mathbb{R}^n as a vector space. Note that by “periodicity of a lattice Λ ”, we mean that Λ is the finest lattice on which ε is periodic. This agreement ensures that Λ is uniquely determined by ε , as well as excluding trivial cases like a constant ε from our definition.

A one dimensional photonic crystal still exists in three dimensional space, but here the term ‘one-dimensional’ signifies its periodicity in one dimension,

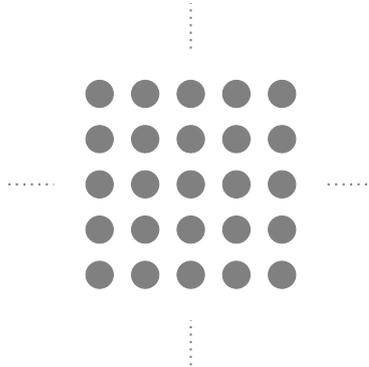


Figure 2.1: *Graphic depiction of a two-dimensional photonic crystal consisting of circular sections of a certain permittivity, surrounded by a medium with a different permittivity, as indicated by the coloring. The dotted lines indicate the crystal's periodicity in all directions.*

and its uniformity in the remaining two dimensions. Something analogous holds for a two dimensional photonic crystal.

Throughout this text, we shall use the symbol n to indicate an integer in $\{1, 2, 3\}$. Furthermore, we will consider photonic crystals where ε approximately varies in step-wise fashion (though we will assume it to be analytic, as required by definition 1). This means that we can color code values of ε , as is done in figure 2.1. For $n = 2$, we thus obtain a wallpaper pattern, thanks to the periodicity of ε on the underlying lattice. Of course, this is exactly what a photonic crystal in the real world will look like, given that different colors represent different materials.

The above clarifies the designating term ‘crystal’ in definition 1. The following sections will delve deeper into why the interaction of light with these objects is so significant as to also attach the brand ‘photonic’ to the name. This interaction becomes particularly notable when the wavelength of light is comparable to the periodicity of the crystal, i.e. the length of the shortest vector in the lattice.

2.2 Electric and magnetic fields

We are interested in how light propagates through a given photonic crystal. To analyze this, we must first consider Maxwell’s equations, prescribing the physical properties of electric and magnetic fields. After all, light is an electromagnetic wave, meaning it consists of an electric and magnetic field which both oscillate in time and travel through vacuum space at speed $c \approx 3 \times 10^8$

m/s. Mathematically, these fields can be described by analytical functions

$$\begin{aligned}\mathbf{E} &: \mathbb{R}^3 \times \mathbb{R} \rightarrow \mathbb{C}^3 & \text{and} \\ \mathbf{H} &: \mathbb{R}^3 \times \mathbb{R} \rightarrow \mathbb{C}^3\end{aligned}$$

which are elements of $L^2(\mathbb{R}^3 \times \mathbb{R}, \mathbb{C}^3)$, meaning they are square-integrable, and which obey Maxwell's equations (see below). The first argument in these functions can be seen as a spatial position r in three dimensions, where the second argument is the one-dimensional time component t . The function \mathbf{E} is formally called the macroscopic electric field, but usually just referred to as the electric field. Similarly, \mathbf{H} is formally called the macroscopic magnetic field, which is generally shortened to 'magnetic field'.

The set of Maxwell's equations, which these fields obey, is as follows.

$$\begin{aligned}\nabla \cdot \mathbf{B} &= 0, & \nabla \times \mathbf{E} &= -\frac{1}{c} \frac{\partial \mathbf{B}}{\partial t}, \\ \nabla \cdot \mathbf{D} &= 4\pi\rho, & \nabla \times \mathbf{H} &= \frac{1}{c} \left(\frac{\partial \mathbf{D}}{\partial t} + 4\pi\mathbf{J} \right).\end{aligned}\tag{2.1}$$

Here, $\nabla = (\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z})$ is the del operator with respect to the three spatial components in \mathbb{R}^3 . Furthermore, we have introduced several new functions, among which \mathbf{D} , the electric displacement field and \mathbf{B} , the magnetic induction field. Like \mathbf{E} and \mathbf{H} , these fields are analytical functions in $L^2(\mathbb{R}^3 \times \mathbb{R}, \mathbb{C}^3)$. As for the other functions in (2.1), $\rho : \mathbb{R}^3 \rightarrow \mathbb{R}$ represents the free charge density and $\mathbf{J} : \mathbb{R}^3 \times \mathbb{R} \rightarrow \mathbb{R}^3$ the free current density. In the photonic crystals we will consider, $\rho \equiv 0$ and $\mathbf{J} \equiv \mathbf{0}$, meaning there are no free charges or free currents.

The fields from (2.1) are related to one another in an additional way. For non-magnetic materials (which we will restrict ourselves to), the magnetic induction field \mathbf{B} and the macroscopic magnetic field \mathbf{H} are related by

$$\mathbf{B}(r, t) = \mathbf{H}(r, t).\tag{2.2}$$

Moreover, we will restrict ourselves to so-called mixed dielectric media, for which the electric displacement field \mathbf{D} and the macroscopic electric field \mathbf{E} are related by

$$\mathbf{D}(r, t) = \varepsilon(r)\mathbf{E}(r, t).\tag{2.3}$$

From (2.2) and (2.3), we see that, in order to find a solution to the differential equations from (2.1), we only need to determine \mathbf{E} and \mathbf{H} . After all, ε is a given function defining the photonic crystal.

The fourth equation from (2.1), together with (2.3), renders

$$\frac{1}{\varepsilon} \nabla \times \mathbf{H} = \frac{1}{c} \frac{\partial \mathbf{E}}{\partial t},$$

since ε doesn't vary with time (our structure is fixed) and, as mentioned before, we assume that $\mathbf{J} \equiv 0$. Taking the curl of both sides of this equation, we get

$$\begin{aligned} \nabla \times \left(\frac{1}{\varepsilon} \nabla \times \mathbf{H} \right) &= \frac{1}{c} \nabla \times \frac{\partial \mathbf{E}}{\partial t} \\ &= \frac{1}{c} \frac{\partial}{\partial t} (\nabla \times \mathbf{E}) \\ &= -\frac{1}{c^2} \frac{\partial^2}{\partial t^2} \mathbf{H}, \end{aligned} \tag{2.4}$$

where we have invoked Schwarz's theorem to interchange derivatives. We will denote the vector space of magnetic field functions in $L^2(\mathbb{R}^3 \times \mathbb{R}, \mathbb{C}^3)$ which obey Maxwell's equations and form a solution to (2.4) as Ω_ε .

In this work, we will often restrict ourselves to the study of so-called photonic modes, which are defined as follows.

Definition 2. A *photonic mode*, or simply *mode*, is a tuple (\mathbf{E}, \mathbf{H}) of an electric and a magnetic field, respectively, which obey Maxwell's equations and take the particular form

$$\begin{aligned} \mathbf{H}(r, t) &= \mathbf{H}(r, 0) e^{i\omega t}, \\ \mathbf{E}(r, t) &= \mathbf{E}(r, 0) e^{i\omega t}, \end{aligned} \tag{2.5}$$

where ω is some real-valued, positive constant.

Often, we will simply refer to a mode by its magnetic field \mathbf{H} . The constant ω obviously represents the frequency of the temporal oscillation of such a mode.

When dealing with photonic modes, (2.4) becomes

$$\nabla \times \left(\frac{1}{\varepsilon} \nabla \times \mathbf{H} \right) = \left(\frac{\omega}{c} \right)^2 \mathbf{H}, \tag{2.6}$$

where we have used the second equation from (2.1). Together with the first equation from (2.1), which can be rewritten as

$$\nabla \cdot \mathbf{H} = 0, \tag{2.7}$$

this determines \mathbf{H} (by Helmholtz's theorem). Note that equations (2.6) and (2.7) also hold for the spatial part $\mathbf{H}(r, 0)$, since we can take out the time-dependent factor $e^{i\omega t}$ on either side.

In order to determine how photonic modes propagate through a photonic crystal, we need to solve equation (2.6) for each frequency ω . We can then find \mathbf{E} by invoking

$$\mathbf{E} = -\frac{ic}{\omega\varepsilon}\nabla \times \mathbf{H},$$

which can easily be derived from Maxwell's equations and the restriction to photonic modes, similar to the derivation of equation (2.6). This is done in more detail in [3].

The analysis of modes in a photonic crystal thus reduces to solving equation (2.6) for each ω , which we can use to plot a diagram. We will return to such *band diagrams* in section 2.5.

Notation. For ease of notation, we define the operator

$$\begin{aligned} \Theta : \Omega_\varepsilon &\rightarrow \Omega_\varepsilon \\ \mathbf{H} &\mapsto \nabla \times \left(\frac{1}{\varepsilon} \nabla \times \mathbf{H} \right) \end{aligned} \tag{2.8}$$

So that, for photonic modes, \mathbf{H} becomes an eigenfunction of Θ with eigenvalue $(\omega/c)^2$.

The above provides a description of the problem at hand. Several strategies can be used to determine which modes may propagate through our crystal, one of which involves explicitly solving equation (2.6) numerically, which we will do in chapter 3. However, such calculations can be laborious and do not always provide much insight into the origin of certain characteristics of solutions. In the following, we shall investigate the role of the symmetry of our crystal in the underlying mechanisms to several important properties of the sought after solutions.

2.3 Symmetry groups

Given a photonic crystal ε , we can look at the group

$$\text{Sym}(\varepsilon) = \{f \in \text{ISO}(n) : \varepsilon \circ f = \varepsilon\},$$

consisting of all isometries on n -dimensional Euclidean space that leave the structure invariant. We can decompose $\text{ISO}(n)$ as the semidirect product

$\text{ISO}(n) = T(n) \rtimes O(n)$ of the translation group $T(n)$ and the orthogonal group $O(n)$. Doing so, we may write elements of $\text{ISO}(n)$ as (λ, A) , with $\lambda \in T(n)$ and $A \in O(n)$. The group multiplication rule becomes

$$(\lambda_1, A_1)(\lambda_2, A_2) = (A_1\lambda_2 + \lambda_1, A_1A_2) \quad (2.9)$$

and elements act on $r \in \mathbb{R}^n$ according to

$$(\lambda, A)r = Ar + \lambda. \quad (2.10)$$

We will occasionally uphold this notation, but will generally denote elements of $\text{ISO}(n)$ by a single letter. Note that it is not necessarily the case that $\text{Sym}(\varepsilon)$ can be written as a semidirect product. This will be investigated further in section 2.8.

By definition 1, the group of translations Λ is a subgroup of $\text{Sym}(\varepsilon)$ and equals the restriction of $T(n)$ to $\text{Sym}(\varepsilon)$. The action of $\text{Sym}(\varepsilon)$ on \mathbb{R}^n can naturally be extended to an action \star on the magnetic field functions \mathbf{H} belonging to any mode. We do this by defining, for any $g \in \text{Sym}(\varepsilon)$ and any $\mathbf{H} \in \Omega_\varepsilon$,

$$g \star \mathbf{H}(r, t) := (\det g) \cdot g\mathbf{H}(g^{-1}r, t), \quad (2.11)$$

where $\det g$ is the determinant of the non-translational part of the operator g . In (2.11), we have extended the action of g from \mathbb{R}^n to \mathbb{C}^3 by first letting g act trivially on the remaining $3 - n$ basis vectors of \mathbb{R}^3 and then extending this to an action on \mathbb{C}^3 . It is important to note that the factor $\det g$ arises from the fact that \mathbf{H} transforms as a *pseudovector* under isometries [4]. This means that it should maintain its orientation under reflections, as opposed to the electric field \mathbf{E} , which changes direction if reflected in a plane to which it is normal. The reason for this requirement is that \mathbf{H} can be defined as the curl $\mathbf{H} = \nabla \times \mathbf{A}$ of a vector potential \mathbf{A} , which is a vector that changes sign under reflection in a plane to which it is normal. Therefore, its curl does not, making \mathbf{H} a pseudovector. In later sections, this will prove to be an important property. We may also define an action of $\text{Sym}(\varepsilon)$ on the electric fields \mathbf{E} similar to the action above, only dropping the factor $\det g$.

In the preceding, we have defined a photonic crystal to be periodic over a lattice which by definition extends infinitely far throughout n -dimensional space. In reality, however, a crystal must abort at some finite boundary. A way to incorporate this fact is by thinking of the crystal as being infinite, but assuming photonic modes in the crystal to be periodic within this infinite lattice. More specifically, we shall assume that for some¹ large number $N \in$

¹This number is not as arbitrary as implied here. We will return to restrictions on N in section 2.8.

\mathbb{Z} , any mode (\mathbf{E}, \mathbf{H}) will have the periodicity of the lattice $\Lambda_N := N \cdot \Lambda$. The periodicity condition is also known as the *Born-von Kármán boundary condition*, and means that we only need to consider modes within one cell of the lattice Λ_N .

Now, for any eigenvalue $(\omega/c)^2$ of the aforementioned operator Θ , or rather any value of ω (which is equivalent since c is a known constant and ω positive), we can consider the eigenspace

$$E(\omega) := \ker \left(\Theta - \frac{\omega^2}{c^2} \right).$$

Note that $\text{Sym}(\varepsilon)$ commutes with Θ , since Θ only depends on ε , which by definition is invariant under the action of $\text{Sym}(\varepsilon)$. Hence, applying the action of $\text{Sym}(\varepsilon)$ to both sides of equation (2.6), we see that an eigenspace $E(\omega)$ is stable under $\text{Sym}(\varepsilon)$. As a consequence, $E(\omega)^{\Lambda_N} := \{x \in E(\omega) : \forall \lambda \in \Lambda_N : \lambda x = x\}$ is stable under the *symmetry group* $G := \text{Sym}(\varepsilon)/\Lambda_N$. Due to the Born-von Kármán boundary condition, however, the subspace $E(\omega)^{\Lambda_N}$ is equal to $E(\omega)$, meaning that eigenspaces of Θ are stable under G . This important property leads us to study the result of the action of G on modes in our crystal, which can be described with the help of group representation theory. The next section will elaborate on this idea. Those unfamiliar with group representation theory are referred to [5].

2.4 Bloch functions

The Born-von Kármán boundary condition implies that it is sufficient to only consider the group $G = \text{Sym}(\varepsilon)/\Lambda_N$ as the effective symmetries of our photonic crystal. The translation subgroup of G is Λ/Λ_N , an abelian group of order N^n which thus has only one-dimensional irreducible group representations. The group consisting of all one-dimensional representations $\rho : \Lambda/\Lambda_N \rightarrow \text{GL}(\mathbb{C}) = \mathbb{C}^*$ is often denoted by $X(\Lambda/\Lambda_N)$, the character group of Λ/Λ_N . Writing $\Lambda/\Lambda_N = \sum_{j=1}^n a_j \mathbb{Z}$, we see that for any $\lambda = \sum_{j=1}^n n_j a_j \in \Lambda/\Lambda_N$ (with n_j integers), we have

$$1 = \rho(0) = \rho(\lambda^N) = \rho(\lambda)^N,$$

so that for each j ,

$$\rho(a_j) = \exp \left(\frac{2\pi i}{N} m_j \right)$$

for some $m_j \in \mathbb{Z}/N\mathbb{Z}$ and

$$\rho(\lambda) = \prod_{j=1}^n \rho(a_j)^{n_j} = \exp \left(\sum_{j=1}^n \frac{2\pi i}{N} m_j n_j \right). \quad (2.12)$$

Hence, we can label the irreducible representations of Λ/Λ_N by their values of m_j or, equivalently, by their values of $\frac{2\pi}{N}m_j$.

To simplify these statements, we introduce the following definition.

Definition 3. Let $\Lambda \subset \mathbb{R}^n$ be a lattice. Its *reciprocal lattice* Λ^* is defined as

$$\Lambda^* := \{x \in \mathbb{R}^n : x \cdot \Lambda \subset 2\pi\mathbb{Z}\},$$

where \cdot denotes the standard inner product on \mathbb{R}^n .

Note that we have the ‘reversed’ inclusion $\Lambda^* \subset \Lambda_N^*$, and that the homomorphism

$$\begin{aligned} \Lambda_N^* &\rightarrow \text{Hom}(\Lambda/\Lambda_N, \mathbb{C}^*) \\ \lambda^* &\mapsto (\lambda \mapsto \exp(i\lambda^* \cdot \lambda)) \end{aligned}$$

has kernel Λ^* . Thus, we obtain an isomorphism

$$\Lambda_N^*/\Lambda^* \xrightarrow{\sim} \text{Hom}(\Lambda/\Lambda_N, \mathbb{C}^*) = X(\Lambda/\Lambda_N). \quad (2.13)$$

In the homomorphism above, we take an inner product of elements in Λ/Λ_N .

To define this inner product, it is necessary to choose representatives of the residue classes $\lambda \in \Lambda/\Lambda_N$. The general convention is to choose representatives as being the elements of Λ lying in the Voronoi cell of the lattice Λ_N around the origin. For those unfamiliar, a Voronoi cell of a point p in a discrete set (in this case, a lattice) within a metric space is the area around p consisting of those elements of the underlying space that are closer to p than to any other point of the discrete set in question. After choosing these elements of Λ within the Voronoi cell of Λ_N around zero as our representatives, we let the inner product $\lambda^* \cdot \lambda$ equal the standard inner product of the chosen representatives in \mathbb{R}^n .

Elements $k \in \Lambda_N^*/\Lambda^*$ are usually called *wave vectors*, due to the physical role they play, which we will get to later. From the isomorphism above, it is clear that we can label irreducible representations of Λ/Λ_N by a wave vector k . We will do this by writing such an irreducible representation as ρ^k . Indeed, for the aforementioned $\lambda \in \Lambda/\Lambda_N$ in equation (2.12), there now exists an element $k \in \Lambda_N^*/\Lambda^*$ such that

$$k \cdot \lambda = -\frac{2\pi}{N} \sum_{j=1}^n m_j n_j,$$

so that $\rho^k(\lambda) = \exp(-ik \cdot \lambda)$, where the negative sign is a matter of convention.

We may write the vector space Ω_ε of solutions mentioned in section 2.2 as a direct sum

$$\Omega_\varepsilon = \bigoplus_{k \in \Lambda_N^*/\Lambda^*} V_k$$

of ‘ k -vector spaces’

$$V_k = \{\phi \in \Omega_\varepsilon : \forall \lambda \in \Lambda/\Lambda_N : \lambda\phi = \rho^k(\lambda)\phi\},$$

effectively splitting Ω_ε into subspaces according to the way they transform under translations. Now, let ρ^k be an irreducible representation of Λ/Λ_N and let $\mathbf{H}_k \in V_k$. For any $\lambda \in \Lambda/\Lambda_N$, we have

$$\mathbf{H}_k(r - \lambda, t) = \lambda \star \mathbf{H}_k(r, t) = \rho^k(\lambda)\mathbf{H}_k(r, t) = e^{-ik \cdot \lambda} \mathbf{H}_k(r, t),$$

from which we see that

$$e^{-ik \cdot r} \mathbf{H}_k(r, t) = e^{-ik \cdot r} e^{ik \cdot \lambda} \mathbf{H}_k(r - \lambda, t) = e^{-ik \cdot (r - \lambda)} \mathbf{H}_k(r - \lambda, t),$$

implying that $e^{-ik \cdot r} \mathbf{H}_k(r, t)$ is periodic over Λ/Λ_N , and thus that \mathbf{H}_k takes the form

$$\mathbf{H}_k(r, t) = e^{ik \cdot r} \cdot \mathbf{u}_k(r, t), \quad (2.14)$$

where $\mathbf{u}_k \in L^2(\mathbb{R}^3 \times \mathbb{R}, \mathbb{C}^n)$ is an analytic function which is periodic over Λ/Λ_N . Functions of the form of \mathbf{H}_k in (2.14) are called *Bloch functions*, and we have seen that there exists a basis for Ω_ε consisting of Bloch functions.

If we are dealing with a Bloch function that is also a photonic mode, it follows from definition 2 that $\mathbf{u}_k(r, t) = \mathbf{u}_k(r, 0)e^{i\omega t}$. Hence, we can determine the magnetic field – up to a periodic amplitude modulation from $\mathbf{u}_k(r, 0)$ – by specifying k and ω . The next section will explore the relationship between these parameters.

2.5 Band diagrams

We have seen that the modes in our photonic crystal can be written as a linear combination of Bloch functions. Each of these constituent Bloch functions will also be a photonic mode, as can be seen by decomposing a mode \mathbf{H} as

$$\begin{aligned} \mathbf{H}(r, t) &= a_1 \mathbf{H}^1(r, t) + \dots + a_m \mathbf{H}^m(r, t) \\ &= \mathbf{H}(r, 0)e^{i\omega t} = (a_1 \mathbf{H}^1(r, 0) + \dots + a_m \mathbf{H}^m(r, 0))e^{i\omega t}, \end{aligned}$$

where $\mathbf{H}^1, \dots, \mathbf{H}^m \in \Omega_\varepsilon$ are Bloch functions and $a_1, \dots, a_m \in \mathbb{C}$ complex constants. By the linear independence of the \mathbf{H}^j , it follows that

$$\mathbf{H}^j(r, t) = \mathbf{H}^j(r, 0)e^{i\omega t}, \quad 1 \leq j \leq m,$$

so that these Bloch functions in the decomposition of the mode \mathbf{H} are themselves also modes. Without loss of generality, we can thus restrict ourselves to modes that are Bloch functions. For such functions $\mathbf{H}_k(r, t) = \mathbf{u}_k(r, 0)e^{ik \cdot r}e^{i\omega t}$ (note that the subscript k here indicates the wave vector), we can invoke equation (2.6) once more to obtain

$$\Theta \mathbf{H}_k = \nabla \times \left(\frac{1}{\varepsilon} \nabla \times \mathbf{u}_k(r, 0)e^{ik \cdot r}e^{i\omega t} \right) = \left(\frac{\omega}{c} \right)^2 \mathbf{H}_k = \left(\frac{\omega}{c} \right)^2 \mathbf{u}_k(r, 0)e^{ik \cdot r}e^{i\omega t},$$

where we may take out the factors $e^{i\omega t}$ on either side and rewrite this as

$$(ik + \nabla) \times \left(\frac{1}{\varepsilon} (ik + \nabla) \times \mathbf{u}_k(r, 0) \right) = \left(\frac{\omega}{c} \right)^2 \mathbf{u}_k(r, 0). \quad (2.15)$$

For any $k \in \Lambda_N^*/\Lambda^*$, the functions \mathbf{u}_k belonging to modes in our crystal correspond to the functions in $L^2(\mathbb{R}^3 \times \mathbb{R}, \mathbb{C}^n)$ that form solutions to (2.15), are periodic on Λ/Λ_N and satisfy $(ik + \nabla) \cdot \mathbf{u}_k = 0$, which can be derived from (2.7). We will denote the vector space of these functions by O_k . We can shorten equation (2.15) by defining the operator

$$\begin{aligned} \Theta_k : O_k &\rightarrow O_k \\ \mathbf{u}_k &\mapsto (ik + \nabla) \times \left(\frac{1}{\varepsilon} (ik + \nabla) \times \mathbf{u}_k \right) \end{aligned} \quad (2.16)$$

so that the functions \mathbf{u}_k become eigenfunctions of Θ_k with eigenvalue $(\omega/c)^2$.

As we saw in the previous section, we can characterize the solutions to equation (2.6) by a wave vector k and a corresponding set of possibly distinct values of ω , which together form Bloch functions. Each pair (k, ω) may have several linearly independent solutions, since a photonic mode has some degree of freedom left in the function $\mathbf{u}_k(r, 0)$. Thus, we may identify solutions with a pair (k, ω) and a corresponding *degeneracy*, which is defined as the dimension of the eigenspace

$$E_k(\omega) := \ker \left(\Theta_k - \frac{\omega^2}{c^2} \right).$$

Since the functions $\mathbf{u}_k \in O_k$ are periodic on Λ/Λ_N , we may consider equation (2.15) to be restricted to a single unit cell of the lattice Λ . As is known from the literature [3], restricting an eigenvalue problem (of a Hermitian operator) to a finite volume yields a discrete spectrum of solutions. Thus, for every $k \in \Lambda_N^*/\Lambda^*$, there will be a discrete set of frequencies ω that, together with k , constitute a set of solutions. Therefore, we may arrange the solutions (k, ω)

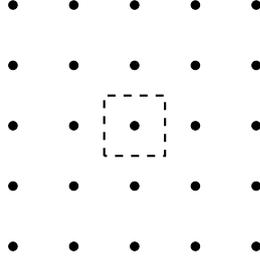


Figure 2.2: Illustration of part of the reciprocal lattice Λ^* of a photonic crystal with its Brillouin zone outlined.

belonging to a particular k in order of increasing ω and label them as (k, m) , with $m \in \mathbb{Z}_{>0}$. Here, m is the solution's position in this ordering. In this convention, m is called the *band number* of the solution (k, m) , for reasons that will become clear later in this section.

When performing calculations, it is necessary to choose representatives of the residue classes $k \in \Lambda_N^*/\Lambda^*$. Similar to before, the convention is to choose these representatives as being the elements of Λ_N^* lying in the Voronoi cell of the lattice Λ^* around the origin, as illustrated in figure 2.2. This cell is often called the *Brillouin zone* within this context.

In theory, one would have to compute solutions for every wave vector in the Brillouin zone. However, the symmetry of the crystal ensures that only a small part of the wave vectors renders unique solutions. To see why this is the case, consider a mode \mathbf{H}_k with wave vector k and corresponding frequency ω . We wish to show that, for an element $g \in \text{Sym}(\varepsilon) \cap O(n)$, the mode $g \star \mathbf{H}_k$ will have wave vector gk and the same frequency ω . Indeed, recalling the notation and definition from equations (2.9) and (2.10), we see that

$$(\lambda, 1)(0, g) = (\lambda, g) = (0, g)(g^{-1}\lambda, 1),$$

where 1 denotes the identity element of $O(n)$ and 0 that of $T(n)$. Thus, we have

$$\begin{aligned} (\lambda, 1)(0, g) \star \mathbf{H}_k &= (0, g)(g^{-1}\lambda, 1) \star \mathbf{H}_k = (0, g) \star e^{ik \cdot (g^{-1}\lambda)} \mathbf{H}_k \\ &= (0, g) \star e^{i(gk) \cdot \lambda} \mathbf{H}_k = e^{i(gk) \cdot \lambda} (0, g) \star \mathbf{H}_k, \end{aligned}$$

from which we see that $(0, g) \star \mathbf{H}_k$ is a mode with wave vector gk . Since $\text{Sym}(\varepsilon)$ commutes with Θ , this mode with wave vector gk will have the same frequency as the one with wave vector k . We may formulate this by stating that, for $g \in \text{Sym}(\varepsilon) \cap O(n)$, we have

$$\omega(k) = \omega(gk).$$

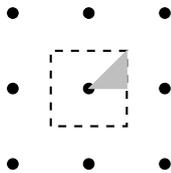


Figure 2.3: Illustration of the irreducible zone (the gray area) inside the Brillouin zone (outlined).

In fact, there is even further symmetry in the frequency. Denoting complex conjugation by a superscript $*$, it follows from the fact that Θ_k is Hermitian that

$$(\Theta_k \mathbf{H}_k)^* = \left(\left(\frac{\omega}{c} \right)^2 \mathbf{H}_k \right)^* = \left(\frac{\omega}{c} \right)^2 \mathbf{H}_k^*.$$

Furthermore, $\mathbf{H}_k^* = (e^{ik \cdot r} \mathbf{u}_k)^* = e^{i(-k) \cdot r} \mathbf{u}_k^*$ is a mode with wave vector $-k$, and the above shows that it has the same eigenvalue as the mode with wave vector k . Thus, we also have the equality $\omega(k) = \omega(-k)$, even when such an inversion is not an element of our symmetry group.

These properties permit us to further restrict the wave vectors which we need to analyze to representatives of the orbits of $\text{Sym}(\varepsilon) \cap O(n)$ and the inversion operator $k \mapsto -k$ in Λ_N^*/Λ^* . It is customary to choose these representatives to cover a certain area of the Brillouin zone, as depicted in figure 2.3. This area is called the *irreducible zone*. An alternative description may be found in [3].

It is important to realize the significance of these results, as they justify considering only this small area within the lattice Λ_N^*/Λ^* , instead of all possible wave vectors, to obtain a full picture of the solutions to (2.6).

As noted earlier in this section, we may arrange² the eigenvalues of (2.15) for a certain k as $(\omega_1(k), \omega_2(k), \dots)$, where $\omega_m(k) \leq \omega_{m+1}(k)$. For a given m we call the set of eigenvalues $\{\omega_m(k), k \in \Lambda_N^*/\Lambda^*\}$ the *m-th (energy) band* of our photonic crystal. The energy bands together form the *band structure*. We can visualize the band structure by plotting the frequency ω against the wave vectors, drawing a point wherever a mode exists for the photonic crystal we are considering. This is what we call a *band diagram* or *dispersion diagram*.

Although there is no obvious further redundancy in the considered wave vectors, it is common to analyze only a one-dimensional path within the irreducible zone, namely its contour, instead of the whole area. The reason

²Note that this ordering includes degeneracy, so that the amount of times an eigenvalue appears in this sequence equals its degeneracy.

for this is twofold: it allows us to make simple two-dimensional band diagrams, and the extrema of bands are usually assumed on the border of the irreducible zone. This approach is not always entirely justifiable, however, since it is not forbidden for band extrema to occur on the interior of the irreducible zone. A study on such occurrences in two-dimensional phononic crystals (the acoustic equivalent of photonic crystals) found that the likelihood of an extremum appearing on the interior of the irreducible zone is relatively high for crystals with low symmetry (e.g. only rotational symmetry), and decreases as reflection axes are added [6]. Although this caveat is important to bear in mind, we will henceforth follow the convention of analyzing dispersion along the irreducible zone contour.

Up to this point, we have regarded wave vectors as being the finite set of elements of Λ_N^*/Λ^* . This arose from the assumption that solutions are periodic on Λ_N , which turned our translation subgroup into the finite abelian group Λ/Λ_N , which implied the existence of Bloch functions. It is important to recall that we required N to be very large and that it may indeed be arbitrarily large. For the purpose of constructing dispersion diagrams, we essentially let it approach infinity, so that wave vectors become elements of \mathbb{R}^n/Λ^* . If it seems dubious that we let N be finite or approach infinity at will, it is good to point out that even in calculations a discrete set of wave vectors is analyzed, so that they still belong to Λ_N^*/Λ^* for some finite N . The limit to infinity is rather an extension to be able to speak of continuity and differentiability of bands in a dispersion diagram. For instance, since k appears only as a parameter in (2.15), we expect the frequency along a certain band to vary continuously with k (in the limit where we regard k to vary continuously).

Figure 2.4 below is an example of a dispersion diagram. The horizontal axis traverses a range of wave vectors and the vertical axis a range of frequencies. We have intentionally not included specific values of frequencies of wave vectors, since this figure is just meant to illustrate the general form a band diagram might take.

In the diagram, the frequency can be seen to vary continuously along the bands. Also present in this diagram is a range of frequencies that no band enters for any wave vector. This range is called a *band gap*, and means that, regardless of its wave vector, no mode with a frequency within this gap is allowed to propagate within our crystal (since it does not offer a solution to (2.6)). Such band gaps are immensely important for practical applications of photonic crystals. For example, a band gap in a suitable range of frequencies can make a photonic crystal an effective mirror of light with precisely these

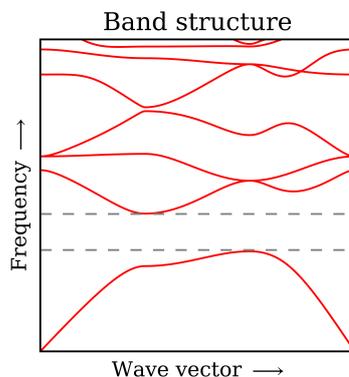


Figure 2.4: A generic band diagram. We have intentionally left the specific values of the frequencies and the wave vectors ambiguous. The dashed horizontal lines mark off a band gap: a range of frequencies for which no mode exists.

frequencies, while not reflecting light of frequencies outside the gap. This can be utilized in the construction of wave guides and reflective coatings and in a more efficient harnessing of solar energy [1], to name but a few applications. This clarifies why we are interested in the extrema of bands, since these extrema limit the size and presence of band gaps.

An important aspect in predicting the presence of band gaps is the degeneracy of modes. After all, a degeneracy may mean a touching point between two bands of non-degenerate solutions (such points occur in figure 2.4, for example), and thereby the absence of a band gap in the frequency range of the corresponding bands.

In the following, we will therefore investigate the degeneracy of modes. The next section will discuss how such degeneracies may be determined from representations of the symmetry group of our crystal.

2.6 Degeneracies and representations

The purpose of this section is to predict the degeneracy of the modes belonging to a pair (k, ω) , i.e. the dimension of $E_k(\omega)$. In the same way that G stabilizes the eigenspaces $E(\omega)$ of Θ , as mentioned in section 2.3, the eigenspace

$$E_k(\omega) = \ker \left(\Theta_k - \frac{\omega^2}{c^2} \right), \quad \omega \in \mathbb{R}_{>0}, \quad k \in \Lambda_N^* / \Lambda^*$$

is stable under the action of the group

$$G(k) := \langle \{g \in G : gk \equiv k\}, \Lambda/\Lambda_N \rangle.$$

This is because elements $g \in G$ such that $gk \equiv k$ commute with Θ_k , and functions in O_k are by definition invariant under translations in Λ/Λ_N , so that $E_k(\omega)$ is stable under these translations as well. Note that O_k is a complex vector space on which $G(k)$ acts in the same way as defined in (2.11). Therefore, O_k forms the representation space for a group representation of $G(k)$. As such, every eigenspace $E_k(\omega)$ will be a direct sum of representation spaces of irreducible representations of $G(k)$.

If we have $n = 2$ for the dimension of the photonic crystal, every eigenspace $E_k(\omega)$ consists of modes (\mathbf{E}, \mathbf{H}) with one of two possible polarizations (i.e. orientations of the electric and magnetic fields): one where \mathbf{E} is pointed in the direction along which ε is constant³, and one where \mathbf{H} is directed such. Below, we will show that these are indeed the only polarizations, and we call them *transverse-electric* (TE) and *transverse-magnetic* (TM) modes, respectively.

To prove the statement above, consider a reflection in a plane perpendicular to the axis along which ε is constant. It is such a plane that we display when depicting a two-dimensional photonic crystal. A reflection σ in this plane acts on a magnetic field $\mathbf{H}(r, t)$ – where r lies in the plane – as

$$\sigma \star \mathbf{H}_k(r, t) = (\det \sigma) \cdot \sigma \mathbf{H}_k(\sigma r, t) = -\sigma \mathbf{H}_k(r, t),$$

where we have used that $\sigma r = r$. Moreover, we know that $\sigma \star \mathbf{H}_k(r, t)$ is a mode with wave vector σk , as we saw in the previous section. Since k lies in the plane, we have $\sigma k = k$. If $\mathbf{H}_k(r, t)$ lies in the plane, we must have $\sigma \mathbf{H}_k(r, t) = \mathbf{H}_k(r, t)$, so that $\sigma \star \mathbf{H}_k(r, t) = -\mathbf{H}_k(r, t)$. If, on the other hand, $\mathbf{H}_k(r, t)$ is perpendicular to the plane of reflection, we must have $\sigma \mathbf{H}_k(r, t) = -\mathbf{H}_k(r, t)$, so that $\sigma \star \mathbf{H}_k(r, t) = \mathbf{H}_k(r, t)$. Similarly, since our definition in section 2.3 states that an electric field $\mathbf{E}_k(r, t)$ transforms as $\sigma \star \mathbf{E}_k(r, t) = \sigma \mathbf{E}_k(\sigma r, t)$, it follows that $\sigma \star \mathbf{E}_k(r, t) = \mathbf{E}_k(r, t)$ if the electric field lies in the plane and $\sigma \star \mathbf{E}_k(r, t) = -\mathbf{E}_k(r, t)$ if it is perpendicular to it. Thus, the only modes that are even under σ are those where the electric field lies in the plane of reflection and the magnetic field is perpendicular to it. We call these transverse-electric (TE) modes. Conversely, the only odd modes under σ are those where the magnetic field is parallel to the plane of reflection

³Recall from one of the remarks below definition 1 that a photonic crystal always exists in three-dimensional space. Therefore, for $n = 2$, there is one dimension along which ε does not vary.

and the electric field is perpendicular to it. We call these transverse-magnetic (TM) modes. Since σ has order two, its entire image consists of modes that transform either oddly or evenly. Thus, we find that the only modes that can exist inside a two-dimensional photonic crystal are TE and TM modes.

In the literature ([7] – [12]), the link between the irreducible representations of $G(k)$ and the eigenspaces $E_k(\omega)$ – or the modules of TE and TM modes therein – is usually formulated along the following (paraphrased) lines:

An irreducible representation of $G(k)$ will correspond to a module of eigenfunctions with wave vector k and a certain eigenvalue ω (or rather, $(\omega/c)^2$). As the possible range of eigenvalues is, a priori, continuous, it is unlikely that two irreducible representations will correspond to such modules for precisely the same eigenvalue. Hence, an irreducible representation of $G(k)$ will generally correspond not just to a submodule of (TE or TM modes within) an eigenspace, but rather the entire (module of such modes within an) eigenspace. This motivates us to determine the degeneracies of modes by examining the irreducible representations of $G(k)$. Of course, it is not forbidden for an eigenspace to be the direct sum of distinct modules within the mode eigenspace, but in this case the resulting degeneracy is called accidental, as it cannot be predicted from the study of irreducible representations of $G(k)$.

It is quite astonishing that this reasoning has been accepted as correct and unambiguous and has been used seemingly without further scrutiny throughout the past century. It is not at all evident why it would be ‘coincidental’ for irreducible submodules to correspond to the same eigenvalue. Nor is it clear why the foregoing ‘accidental degeneracies’ should be rare or of little importance. However, the principle as outlined above has been used consistently in solid state physics and seems to stand firm, despite a lack of mathematical rigour within the theory. This is likely because counterexamples are rare in most situations of interest. In this light, we shall take it as a postulate that submodules of TE and TM modes within eigenspaces $E_k(\omega)$ form irreducible representations of $G(k)$. However, we once more stress the importance of a more developed theory here.

The above provides incentive to study irreducible representations of finite groups, which shall be the focus of the next section. We work towards results that apply to the type of groups akin to symmetry groups of photonic crystals.

2.7 Group representation theory

For an introduction to representation theory of finite groups, we refer to [5]. Those unfamiliar with the topic should find the first two or three chapters provide sufficient groundwork for this section. In the following, we will always take groups to be finite. The aim of this section is to provide conditions for the irreducibility of induced representations of finite groups.

We begin by recalling some properties of induced representations. Let G be a finite group and $H \subset G$ a subgroup. A $\mathbb{C}[G]$ -module V is said to be induced by a $\mathbb{C}[H]$ -module W if

$$V \cong \mathbb{C}[G] \otimes_{\mathbb{C}[H]} W.$$

This is equivalent to stating that

$$V \cong \bigoplus_{r \in R} rW,$$

where $R \subset G$ is a set of representatives of G/H . Here, the action of G on a coordinate rw of an element in this direct sum is defined as $grw = r_g hw$, where $r_g \in R$ is such that $gr = r_g h$ for some $h \in H$. Note that hw is an element of W , since this is a $\mathbb{C}[H]$ -module. The isomorphism above now follows by realizing that the elements $r \in R$ form a basis of $\mathbb{C}[G]$ as a right module over $\mathbb{C}[H]$. We shall denote the induced representation of W in G as $\text{Ind}_H^G(W)$.

We can extend this notion of induction to class functions. A function $f : H \rightarrow \mathbb{C}$ is called a class function of H if $f(xyx^{-1}) = f(y)$ for all $x, y \in H$, i.e. if it is constant on the conjugacy classes of H . We can define the function $\text{Ind}_H^G(f)$ on $G \supset H$ by

$$\text{Ind}_H^G(f)(g) = \frac{1}{\#H} \sum_{x \in G, x^{-1}gx \in H} f(x^{-1}gx)$$

Note that characters of representations are also class functions of the group they represent. The following proposition shows that the induction of characters is compatible with the induction of the corresponding representation.

Proposition 1. *If χ is the character of a representation W of H , then $\text{Ind}_H^G(\chi)$ is the character of the induced representation $\text{Ind}_H^G(W)$ of $G \supset H$.*

Proof. Write $\rho : G \rightarrow \text{GL}(V)$ for the representation induced by $\sigma : H \rightarrow \text{GL}(W)$, so that

$$V \cong \bigoplus_{r \in R} rW$$

with R a set of representatives of G/H inside G . Let $g \in G$. The map $\rho(g)$ sends a space rW to r_gW , where $r_g \in R$ is such that $gr = r_g h$ for some $h \in H$. Choosing a union of bases of the spaces rW as a basis for V , we see that the matrix form of $\rho(g)$ will have zero diagonal entries wherever $r_g \neq r$. The trace $\text{tr}_V(\rho(g))$ will therefore consist of the sums of the traces of $\rho(g)$ on rW wherever $r = r_g$. Since the equality $r = r_g$ holds if and only if $gr = rh$, i.e. $r^{-1}gr \in H$, we obtain

$$\text{tr}_V(\rho(g)) = \sum_{r \in R, r^{-1}gr \in H} \text{tr}_{rW}(\rho(g)),$$

where we understand that $\rho(g)$ in the last term is restricted to rW . Furthermore, since ρ and σ coincide on H , it follows that

$$\rho(r) \circ \sigma(r^{-1}gr) = \rho(r) \circ \rho(r^{-1}gr) = \rho(g) \circ \rho(r),$$

from which we see that $\text{tr}_W(\sigma(r^{-1}gr)) = \text{tr}_{rW}(\rho(g))$, since $\rho(r)$ gives an isomorphism from W to rW . Now writing χ_ρ for the character of ρ and χ_σ for that of σ , we obtain

$$\chi_\rho(g) = \text{tr}_V(\rho(g)) = \sum_{r \in R, r^{-1}gr \in H} \text{tr}_W(\sigma(r^{-1}gr)) = \sum_{r \in R, r^{-1}gr \in H} \chi_\sigma(r^{-1}gr).$$

Since $\chi_\sigma(r^{-1}gr) = \chi_\sigma(x^{-1}gx)$ for all elements $x \in G$ in the coset rH , we indeed see that

$$\chi_\rho(g) = \frac{1}{\#H} \sum_{x \in G, x^{-1}gx \in H} \chi_\sigma(x^{-1}gx) = \text{Ind}_H^G(\chi_\sigma)(g).$$

□

In addition to the notion of induction, we may denote by $\text{Res}_H(f)$ the restriction of a class function f on G to a subgroup $H \subset G$. For a representation $\rho : G \rightarrow \text{GL}(V)$, we may denote such a restriction as $\text{Res}_H(V)$. We will show that induction and restriction are Hermitian adjoint operators, a fact that is known as Frobenius reciprocity. To prove this, we first define an inner product $\langle \cdot, \cdot \rangle_G$ on the space of class functions of G as

$$\langle f_1, f_2 \rangle_G = \frac{1}{\#G} \sum_{g \in G} f_1(g^{-1})f_2(g).$$

Similarly, we define a bi-additive function for $\mathbb{C}[G]$ -modules as

$$\langle V_1, V_2 \rangle_G = \dim(\text{Hom}^G(V_1, V_2)),$$

where $\text{Hom}^G(V_1, V_2)$ denotes the vector space of $\mathbb{C}[G]$ -homomorphisms from V_1 to V_2 . These two functions are compatible in the following sense.

Lemma 1. *Let χ_1 and χ_2 be the characters of $\mathbb{C}[G]$ -modules V_1 and V_2 , respectively. Then*

$$\langle \chi_1, \chi_2 \rangle_G = \langle V_1, V_2 \rangle_G.$$

To prove this statement, we need the following results.

Lemma 2 (Schur's lemma). *Let $\rho : G \rightarrow \text{GL}(V_1)$ and $\sigma : G \rightarrow \text{GL}(V_2)$ be two irreducible representations of a finite group G , and let $f \in \text{Hom}^G(V_1, V_2)$, so that*

$$\sigma(g) \circ f = f \circ \rho(g)$$

for all $g \in G$. If V_1 and V_2 are non-isomorphic, we have $f = 0$. If, on the other hand, we have $V_1 = V_2$ and $\rho = \sigma$, then f is a scalar multiple of the identity.

Proof. Suppose that $f \neq 0$. For $x \in \ker(f)$, we have $f(\rho(g)x) = \sigma(g)(f(x)) = 0$, so that $\rho(g)x \in \ker(f)$. Hence, $\ker(f)$ is stable under G . From the irreducibility of ρ , it follows that either $\ker(f) = 0$ or $\ker(f) = V_1$, but the latter is excluded from our assumption that $f \neq 0$. In a similar manner, we find that $\text{im}(f) = V_2$, so that f must be an isomorphism from V_1 to V_2 . Consequently, if V_1 and V_2 are non-isomorphic, we have $f = 0$.

Now suppose that $V_1 = V_2$ and $\rho = \sigma$. Since \mathbb{C} is algebraically closed, f has an eigenvalue $\lambda \in \mathbb{C}$ (we only consider complex representations, so that V_1 and V_2 are complex vector spaces). The function $f' = f - \lambda \cdot \text{id}_{V_1}$ has a non-trivial kernel, and we have $\sigma(g) \circ f' = f' \circ \rho(g)$ since $\rho = \sigma$. The same reasoning as before now shows that either $\ker(f') = 0$ or $\ker(f') = V_1$. Since we know that the kernel is non-trivial, we find $\ker(f') = V_1$, so that $f' = 0$ and $f = \lambda \cdot \text{id}_{V_1}$. \square

Theorem 1. *If χ and ψ are the characters of two irreducible representations of a finite group G , we have $\langle \chi, \psi \rangle_G = 0$ if the representations corresponding to respectively χ and ψ are non-isomorphic, and $\langle \chi, \psi \rangle_G = 1$ if they are isomorphic.*

Proof. Let $\rho : G \rightarrow \text{GL}(V_1)$ and $\sigma : G \rightarrow \text{GL}(V_2)$ be the representations corresponding to the characters χ and ψ , respectively. Let $f : V_1 \rightarrow V_2$ be a linear mapping between the representations and define the function

$$f' = \frac{1}{\#G} \sum_{g \in G} \sigma(g)^{-1} f \rho(g),$$

which is also a linear map from V_1 to V_2 . Note that, for any $h \in G$, we have

$$\begin{aligned}\sigma(h)^{-1}f'\rho(h) &= \frac{1}{\#G} \sum_{g \in G} \sigma(h)^{-1}\sigma(g)^{-1}f\rho(g)\rho(h) \\ &= \frac{1}{\#G} \sum_{g \in G} \sigma(hg)^{-1}f\rho(hg) = f',\end{aligned}$$

so that $\sigma(h)f' = f'\rho(h)$. From Schur's Lemma, it follows that $f' = 0$ if ρ and σ are not isomorphic. We choose bases of V_1 and V_2 and write ρ and σ in matrix form over these bases as $\rho(g) = (r_{i_1 j_1}(g))$ and $\sigma(g) = (s_{i_2 j_2}(g))$. Similarly, we write $f = (x_{i_2 i_1})$ and $f' = (x'_{i_2 i_1})$. We have

$$x'_{i_2 i_1} = \frac{1}{\#G} \sum_{g \in G} \sum_{j_1, j_2} s_{i_2 j_2}(g^{-1}) x_{j_2 j_1} r_{j_1 i_1}(g).$$

As said, if ρ and σ are not isomorphic, then this equation equals zero, regardless of the form of f . In particular, we can choose f such that all entries $x_{i_2 i_1}$ except one $x_{j_2 j_1}$ equal zero. it follows that we must have

$$\langle s_{i_2 j_2}, r_{j_1 i_1} \rangle_G = \frac{1}{\#G} \sum_{g \in G} s_{i_2 j_2}(g^{-1}) r_{j_1 i_1}(g) = 0$$

for every i_1, i_2, j_1, j_2 . Since $\chi(g) = \sum_i r_{ii}(g)$ and $\psi(g) = \sum_j s_{jj}(g)$, we indeed see that $\langle \chi, \psi \rangle_G = 0$.

Suppose, on the other hand, that $V_1 = V_2$ and $\rho = \sigma$. It then follows from Schur's Lemma that $f' = \lambda \cdot \text{id}_{V_1}$, with $\lambda \in \mathbb{C}$ some constant, so that $x'_{i_2 i_1} = \lambda \delta_{i_2 i_1}$ (with δ the Kronecker delta symbol). Writing $n = \dim(V_1)$, note that we have

$$n\lambda = \text{tr}(f') = \frac{1}{\#G} \sum_{g \in G} \text{tr}(\rho(g^{-1})f\rho(g)) = \text{tr}(f),$$

so that

$$\lambda = \frac{1}{n} \text{tr}(f) = \frac{1}{n} \sum_{j_1, j_2} \delta_{j_2 j_1} x_{j_2 j_1}.$$

Putting these equalities together, we see that

$$\frac{1}{\#G} \sum_{g \in G} \sum_{j_1, j_2} s_{i_2 j_2}(g^{-1}) x_{j_2 j_1} r_{j_1 i_1}(g) = x'_{i_2 i_1} = \lambda \delta_{i_2 i_1} = \frac{1}{n} \sum_{j_1, j_2} \delta_{j_2 j_1} x_{j_2 j_1} \delta_{i_2 i_1}.$$

Again, the form of f is arbitrary, so we must have

$$\langle s_{i_2 j_2}, r_{j_1 i_1} \rangle_G = \frac{1}{\#G} \sum_{g \in G} s_{i_2 j_2}(g^{-1}) r_{j_1 i_1}(g) = \frac{1}{n} \delta_{i_2 i_1} \delta_{j_2 j_1}.$$

Indeed, we see that $\langle \chi, \psi \rangle_G = 1$. □

Proof of lemma 1. If V_1 and V_2 are reducible, we may decompose them uniquely into irreducible subspaces, turning the function $\langle V_1, V_2 \rangle_G$ into a sum of terms containing these irreducible subspaces (since this function is bi-additive). Thus, we may assume that V_1 and V_2 are irreducible. If $V_1 = V_2$, it follows from Schur's Lemma that any $\mathbb{C}[G]$ -homomorphism from V_1 to V_2 is a multiple of the identity, so that $\langle V_1, V_2 \rangle_G = 1$. If, on the other hand, V_1 and V_2 are not isomorphic, it follows from the same lemma that $\langle V_1, V_2 \rangle_G = 0$. Finally, theorem 1 gives us the desired statement. \square

With the results above, we are ready to prove the previously announced Frobenius reciprocity.

Theorem 2 (Frobenius reciprocity). *Let χ_1 be the character of a representation $\rho : H \rightarrow \text{GL}(W)$ of a finite group H and χ_2 the character of a representation $\sigma : G \rightarrow \text{GL}(V)$ of a finite group $G \supset H$. Then*

$$\langle \chi_1, \text{Res}_H(\chi_2) \rangle_H = \langle \text{Ind}_H^G(\chi_1), \chi_2 \rangle_G.$$

Proof. From lemma 1, it suffices to show that

$$\langle W, \text{Res}_H(V) \rangle_H = \langle \text{Ind}_H^G(W), V \rangle_G.$$

This fact follows from a known property of tensor product, namely

$$\text{Hom}^G(\mathbb{C}[G] \otimes_{\mathbb{C}[H]} W, V) \cong \text{Hom}^H(W, V).$$

To see why this holds true, consider a homomorphism $\varphi \in \text{Hom}^G(\mathbb{C}[G] \otimes_{\mathbb{C}[H]} W, V)$. By composing it with the map

$$\begin{aligned} W &\rightarrow \mathbb{C}[G] \otimes_{\mathbb{C}[H]} W \\ w &\mapsto 1 \otimes w, \end{aligned}$$

we obtain a $\mathbb{C}[H]$ -linear homomorphism from W to V . Conversely, a homomorphism $\psi \in \text{Hom}^H(W, V)$ can be extended to $\mathbb{C}[G] \otimes_{\mathbb{C}[H]} W$ by mapping

$$\sum_{g \in G} g \otimes w_g \mapsto \sum_{g \in G} g\psi(w_g) \in V.$$

Indeed, this forms a $\mathbb{C}[G]$ -homomorphism. It is clear that these two mappings between the spaces of homomorphisms are each others inverse, so we obtain the required isomorphy. \square

Regarding the inner products, the following theorem is of significant value.

Theorem 3. *Let $\rho : G \rightarrow \text{GL}(V)$ be a representation of a finite group G with corresponding character ψ . We may decompose V into irreducible subspaces as*

$$V = W_1 \oplus W_2 \oplus \cdots \oplus W_m.$$

For an irreducible representation W of G with character χ , the number of W_i isomorphic to W equals $\langle \psi, \chi \rangle_G$. This number is what is meant by the ‘number of times’ that W appears in V .

Proof. Writing ψ_i for the character of W_i , we see that $\psi = \psi_1 + \psi_2 + \cdots + \psi_m$, so that

$$\langle \psi, \chi \rangle_G = \langle \psi_1, \chi \rangle_G + \cdots + \langle \psi_m, \chi \rangle_G.$$

As follows from theorem 1, the inner product $\langle \psi_i, \chi \rangle_G$ equals 1 if W_i and W are isomorphic, and 0 otherwise. Summing these terms gives us the wanted result. \square

Corollary 1. *Let G be a finite group and $H \subset G$ a subgroup. Given an irreducible representation V of G and an irreducible representation W of H , the number of times that W occurs in $\text{Res}_H(V)$ is equal to the number of times that V occurs in $\text{Ind}_H^G(W)$.*

Proof. The result follows immediately from the theorem above and Frobenius reciprocity. \square

As expressed in the beginning of this section, we wish to determine when an induced representation is irreducible. To this end, let G be a finite group, $A, B \subset G$ two subgroups and $\rho : A \rightarrow \text{GL}(W)$ a representation of A , with $V = \text{Ind}_A^G(W)$ the corresponding induced representation of G . It will be useful to know how to determine $\text{Res}_B(V)$. To this end, let R be a set of representatives of the (double) cosets BrA of G . For r in R , we define $A_r = rAr^{-1} \cap B$ and for each $x \in A_r$, we set

$$\rho_r(x) = \rho(r^{-1}xr).$$

In this way, $\rho_r : A_r \rightarrow \text{GL}(W)$ becomes a homomorphism and thus we obtain a representation of A_r . To distinguish it from ρ when writing only the vector space to denote the representation as a whole, we denote it as $\rho_r : A_r \rightarrow \text{GL}(W_r)$. It induces a representation $\text{Ind}_{A_r}^B(W_r)$ of B .

Proposition 2. *For the groups as in the preceding, we have the following isomorphism:*

$$\text{Res}_B(\text{Ind}_A^G(W)) \cong \bigoplus_{r \in R} \text{Ind}_{A_r}^B(W_r).$$

Proof. Let $S \subset G$ be a set of representatives for the cosets in G/A , so that $V = \bigoplus_{s \in S} sW$. For $r \in R$, we define $V(r) = \bigoplus_{x \in BrA} xW$. We have the following equalities:

$$V = \bigoplus_{s \in S} sW \cong \bigoplus_{r \in R} \left(\bigoplus_{b \in B} brW \right) \cong \bigoplus_{r \in R} \left(\bigoplus_{x \in Br} xW \right) \cong \bigoplus_{r \in R} \left(\bigoplus_{x \in BrA} xW \right),$$

where the last identity follows from the fact that W is a $\mathbb{C}[A]$ -module. It follows that $V \cong \bigoplus_{r \in R} V(r)$. Each $V(r)$ is stable under B , so we obtain

$$\text{Res}_B(\text{Ind}_A^G(W)) \cong \bigoplus_{r \in R} V(r).$$

What remains is to show that $V(r)$ is isomorphic to $\text{Ind}_{A_r}^B(W_r)$ as a $\mathbb{C}[B]$ -module. Indeed, we have

$$V(r) \cong \bigoplus_{x \in BrA} xW \cong \bigoplus_{x \in B} xrW,$$

and since $xrW = rW$ holds only for $x \in A_r$, we see that $V(r)$ may be written as the direct sum of the spaces xrW for $x \in B/A_r$. Hence, $V(r) \cong \text{Ind}_{A_r}^B(rW)$, and the isomorphism $rW \mapsto W_r$ gives us the wanted result. \square

We can apply the above to the case where $A = B = H$ for some subgroup $H \subset G$. Again, we denote by H_r the group $rHr^{-1} \cap H$.

Proposition 3 (Mackey's criterion). *Let $\rho : H \rightarrow W$ be a representation of H . The induced representation $V = \text{Ind}_H^G(W)$ is irreducible if and only if the following conditions are met:*

- (a) W is irreducible.
- (b) For each $r \in G \setminus H$, the representations ρ_r and $\text{Res}_{H_r}(\rho)$ of H_r are disjoint in the sense that $\langle \rho_r, \text{Res}_{H_r}(\rho) \rangle_{H_r} = 0$.

Proof. It follows from lemma 2 that V is irreducible if and only if $\langle V, V \rangle_G = 1$, as we already saw in the proof of lemma 1. Due to Frobenius reciprocity (combined with lemma 1) and proposition 2, we have

$$\begin{aligned} \langle V, V \rangle_G &= \langle W, \text{Res}_H(V) \rangle_H = \langle W, \bigoplus_{r \in R} \text{Ind}_{H_r}^H(W) \rangle_H \\ &= \sum_{r \in R} \langle W, \text{Ind}_{H_r}^H(W_r) \rangle_H = \sum_{r \in R} \langle \text{Res}_{H_r}(W), W_r \rangle_{H_r} \\ &= \sum_{r \in R} \langle \text{Res}_{H_r}(\rho), \rho_r \rangle_{H_r} \end{aligned}$$

where R is a set of representatives of the double cosets of $H \backslash G / H$ in G . Note that $\langle \text{Res}_{H_1}(\rho), \rho_1 \rangle_{H_1} = \langle \rho, \rho_1 \rangle_H = \langle \rho, \rho \rangle_H \geq 1$, with equality if and only if W is irreducible. Under this condition, we see that $\langle V, V \rangle_G = 1$ if and only if $\langle \text{Res}_{H_r}(\rho), \rho_r \rangle_{H_r} = 0$ for all $1 \neq r \in R$ (i.e. for all $r \in G \setminus H$). \square

In the case where G decomposes as the semidirect product $G = A \rtimes H$ of an abelian normal subgroup A and a subgroup H , Mackey's criterion provides us with an explicit way to construct the irreducible representations of G , which we will now investigate. Being an abelian group, A only has one-dimensional irreducible representations, which form the group $X := X(A) = \text{Hom}(A, \mathbb{C}^*)$. We can let G act on X by defining

$$(g\chi)(a) = \chi(g * a) = \chi(g^{-1}ag) \quad (2.17)$$

for $g \in G$, $\chi \in X$, and $a \in A$. Here, $g * a = g^{-1}ag$ is the standard action of G on A . Under the action above, let $(\chi_i)_{i \in X/H}$ be a system of representatives for the orbits of H in X . Define the stabilizer $H_i := \{h \in H : h\chi_i = \chi_i\}$ and let $G_i = A \rtimes H_i$. By setting $\chi_i(ah) = \chi_i(a)$, we may extend χ_i to a character of G_i of degree 1. Note that it is indeed a character of G_i , as we have $h\chi_i = \chi_i$ for $h \in H_i$. Similarly, we can extend any irreducible representation ρ of H_i to G_i by composing it with the canonical projection from G_i to H_i . This gives an irreducible representation $\tilde{\rho}$ of G_i , since any $\mathbb{C}[G_i]$ -submodule is also a $\mathbb{C}[H_i]$ -submodule, the latter of which can only be the zero space or the whole representation space. With this, we construct an irreducible representation $\chi_i \otimes \tilde{\rho}$ of G_i (where the tensor product is taken over \mathbb{C}). The following proposition states how this can be used to construct the irreducible representations of G .

Proposition 4. *Following the notation of the preceding paragraph, we have that*

$$\text{Ind}_{G_i}^G(\chi_i \otimes \tilde{\rho})$$

is an irreducible representation of $G = A \rtimes H$. Moreover, up to isomorphism, such a representation is uniquely determined by i and ρ and every irreducible representation of G is isomorphic to such a representation.

Proof. To prove the first part of the statement, we use Mackey's criterion. As stated above, $\chi_i \otimes \tilde{\rho}$ is irreducible, so it remains to prove the second part of the criterion. To this end, let $r \in G \setminus G_i$ and define $K_r = rG_i r^{-1} \cap G_i$. We obtain representations of K_r by composing $\chi_i \otimes \tilde{\rho}$ with either the canonical imbedding $K_r \rightarrow G_i$ or the injection $x \mapsto r^{-1}xr$. To show that these two representations are disjoint, it is enough to show that they are disjoint when restricted to A . Indeed, these restrictions result in a multiple of χ_i and a

multiple of $r\chi_i$, respectively (due to the defined action of G on X), which are unequal since $r \notin G_i$. Therefore, the restrictions are disjoint (by theorem 1), implying that the corresponding representations of K_r are disjoint, too.

To show that $\text{Ind}_{G_i}^G(\chi_i \otimes \tilde{\rho})$ is uniquely determined by i and ρ , it suffices to show that such a given representation pins down i and ρ . Indeed, restricting $\text{Ind}_{G_i}^G(\chi_i \otimes \tilde{\rho})$ to A returns characters in the same orbit of H as χ_i , hence the same representative χ_i (and the same index i). Now, denote by W the representation space of $\text{Ind}_{G_i}^G(\chi_i \otimes \tilde{\rho})$ and define

$$W_i = \{w \in W : \text{Ind}_{G_i}^G(\chi_i \otimes \tilde{\rho})(a)w = \chi_i(a)w \quad \forall a \in A\}$$

as the subspace of W that transforms according to χ_i under A . Since W_i is stable under H_i , we obtain a representation $H_i \rightarrow \text{GL}(W_i)$ which is naturally isomorphic to ρ .

Lastly, let $\sigma : G \rightarrow \text{GL}(V)$ be an irreducible representation of G . The restriction $\text{Res}_A(V)$ may be decomposed as $\bigoplus_{\chi \in X} V_\chi$, where

$$V_\chi = \{v \in V : \sigma(a)(v) = \chi(a)v \quad \forall a \in A\}.$$

Some of these subspaces may equal the zero space, but at least one V_χ is nonzero. For v in this V_χ , we have

$$\begin{aligned} \sigma(a)\sigma(g)(v) &= \sigma(ag)(v) = \sigma(g)\sigma(g^{-1}ag)(v) = \sigma(g)(\chi(g^{-1}ag)v) \\ &= \sigma(g)((g\chi)(a)v) = (g\chi)(a)\sigma(g)(v). \end{aligned}$$

It follows that V_χ is mapped under $\sigma(g)$ to the space $V_{g\chi}$. Consequently, V_{χ_i} is stable under H_i , thus producing a representation $H_i \rightarrow \text{GL}(V_{\chi_i})$. For any irreducible $\mathbb{C}[H_i]$ -submodule V_i of V_{χ_i} , we obtain an irreducible representation $\tau : H_i \rightarrow \text{GL}(V_i)$. It induces a representation of $G_i = A \rtimes H_i$ as before, by composing τ with the canonical projection $G_i \rightarrow H_i$ to obtain an irreducible representation $\tilde{\tau}$ of G_i , and taking the tensor product with χ_i to obtain an irreducible representation $\chi_i \otimes \tilde{\tau}$ of G_i . Hence, this representation will occur at least once in $\text{Res}_{G_i}(\sigma)$. According to corollary 1, the representation σ will thus appear at least once in $\text{Ind}_{G_i}^G(\chi_i \otimes \tilde{\tau})$, and it follows from its irreducibility that $\sigma = \text{Ind}_{G_i}^G(\chi_i \otimes \tilde{\tau})$, proving the last part of the proposition. \square

Example 1. Let m be an even integer. We have $D_m = C_m \rtimes C_2$, where D_m is the dihedral group of order $2m$ and C_m is the cyclic group of order m . Using the proposition above, we will determine the irreducible representations of D_m using those of the two subgroups. Firstly, note that the character group $X = X(C_m)$ is isomorphic to C_m , since C_m is abelian. Identifying C_m with $\mathbb{Z}/m\mathbb{Z}$, we see that the group C_2 acts on X by inversion, sending $i \in X$ to

$-i$, hence leaving only 0 and $m/2$ fixed. In this way, we obtain $m/2 + 1$ distinct orbits of C_2 in C_m . For each representative of an orbit, we have the stabilizers $(C_2)_0 = (C_2)_{m/2} = C_2$ and $(C_2)_i = \{1\}$ for $i \in \{1, 2, \dots, m/2 - 1\}$ (to clarify, these stabilizers are denoted by H_i in the proposition above). The corresponding subgroups of D_m (corresponding to G_i in the proposition) are

$$(D_m)_0 = (D_m)_{m/2} = C_m \rtimes C_2$$

and

$$(D_m)_i = C_m \rtimes \{1\} \cong C_m$$

for $i \neq 0, m/2$. There are two irreducible representations of C_2 , which have degree one since C_2 is abelian. Therefore, for both $(D_m)_0$ and $(D_m)_{m/2}$ we get two irreducible representations of degree 1 (since the representation of C_m is fixed), which each induces an irreducible representation of degree $[C_2 : C_2] = 1$ of D_m . To each of the remaining $(D_m)_i$ belongs one irreducible representation (since, again, the representation of C_m is fixed by i), which each induces an irreducible representation of D_m of degree $[C_2 : \{1\}] = 2$. Thus, for D_m we obtain a total of 4 irreducible representations of degree 1 and $(m - 2)/2$ of degree 2.

Example 2. The alternating group of order 4 can be decomposed as $A_4 = V_4 \rtimes A_3$, where V_4 is the Klein four-group. The character group $X = X(V_4)$ is isomorphic to V_4 , and A_3 acts on the nontrivial characters χ_1, χ_2, χ_3 by permuting the indices. We obtain two distinct orbits, which we label as 0 and 1. Here, 0 corresponds to the trivial character in X and 1 to the (orbit of the) remaining three characters in X . The stabilizer of the trivial character is A_3 , whereas the stabilizer of the χ_i is the identity. We thus have $(A_4)_0 = V_4 \rtimes A_3$ and $(A_4)_1 = V_4 \rtimes \{1\} \cong V_4$. The abelian group A_3 has three one-dimensional irreducible representations. Hence, we acquire three irreducible representations of $(A_4)_0$ of degree 1, which each induces an irreducible representations of A_4 of degree $[A_3 : A_3] = 1$. Similarly, from $(A_4)_1$ we get one irreducible representations of degree 1, which induces a representation of A_4 of degree $[A_3 : \{1\}] = 3$. Thus, for A_4 we obtain a total of 3 irreducible representations of degree 1 and one of degree 3.

2.8 Categorization

Throughout this section, we let N be a fixed, even integer (the reason for its parity will be discussed).

We can categorize photonic crystals based on their symmetry group $G = \text{Sym}(\varepsilon)/\Lambda_N$. As part of this categorization, we distinguish between *symmorphic* and *non-symmorphic* symmetry groups.

Definition 4. Let ε be a photonic crystal, $G = \text{Sym}(\varepsilon)/\Lambda_N$ its symmetry group and $T := \Lambda/\Lambda_N$ its translation subgroup. We call G *symmorphic* if the short exact sequence

$$0 \rightarrow T \rightarrow G \rightarrow G/T \rightarrow 0 \quad (2.18)$$

splits. Otherwise, G is called *non-symmorphic*.

Proposition 5. *The symmetry group G of a photonic crystal is symmorphic if and only if it can be written as the semidirect product*

$$G = T \rtimes H,$$

where $H \subset G$ is a subgroup isomorphic to G/T .

Proof. If $G = T \rtimes H$, then the section $s : G/T \rightarrow G$ mapping \bar{g} to $(0, g)$ splits the short exact sequence (2.18), making G symmorphic. If, on the other hand, we know that G is symmorphic, the section $s : G/T \rightarrow G$ that splits (2.18) gives rise to an isomorphism $T \rtimes H \xrightarrow{\sim} G$ given by $(\lambda, g) \mapsto \lambda s(\iota(g))$, where $\iota : H \rightarrow G/T$ is an isomorphism. \square

In the case of two-dimensional photonic crystals, we can classify their symmetry by identifying $\text{Sym}(\varepsilon)$ with the corresponding wallpaper group. A wallpaper group is simply a discrete group of isometries of two-dimensional Euclidean space which contains two linearly independent translations. Indeed, these translations make a wallpaper group the symmetry group of a two-dimensional periodic pattern. There are only 17 types of wallpaper groups, with which the symmetry of all such periodic structures can be described. We will uphold the so-called Hermann-Mauguin notation [13] to denote these groups.

Example 3. The photonic crystal illustrated in figure 2.5 has wallpaper group $\text{Sym}(\varepsilon) = pm$. It is generated by two independent translations and a reflection. The canonical embedding $G/T \hookrightarrow G$ (which maps an element in G/T to a representative in G with no translation part) splits the short exact sequence

$$0 \rightarrow T \rightarrow G \rightarrow G/T \rightarrow 0,$$

so that G is symmorphic and, using proposition 5, we have $G = T \rtimes D_1$, where $T \cong C_N \times C_N$. We can now use proposition 4 to determine the irreducible representations of G . According to our discussion in section 2.6, this will provide insight into the possible degeneracies of modes. This is

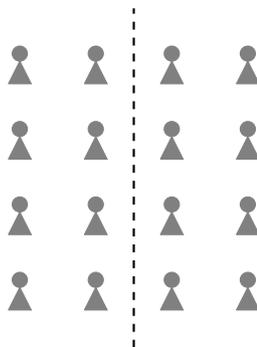


Figure 2.5: Part of a two-dimensional photonic crystal with wallpaper group pm . The colors in this figure correspond to different values of $\varepsilon(r)$. A reflection axis is indicated with a dashed line.

because any $\mathbb{C}[G]$ -submodule is in particular a $\mathbb{C}[G(k)]$ -submodule, so that any irreducible representation of $G(k)$ which is also a representation of G must be an irreducible representation of G .

To be able to use proposition 4, we need to know how $G/T \cong D_1$ acts on the characters of T , i.e. on $\Lambda_N^*/\Lambda^* = \Lambda^*/N\Lambda^*$. Since Λ is a square lattice, Λ^* will be too, and they are isomorphic as G/T -modules. Instead of studying the action of G/T on the characters of T , we may therefore instead study its action on $T = \Lambda/N\Lambda$ itself. From figure 2.5, we see that there are $N - 1$ translations that are stable under reflection. There is the trivial translation that is also stable under the whole group G/T , and the remaining $N^2 - N$ elements have trivial stabilizer. Further note that $G/T \cong D_1$ only has two irreducible representations, and these have degree 1. Following the method of proposition 4, we see that the N translations stabilized by G/T each induce two irreducible representations of degree $[D_1 : D_1] = 1$, and the remaining $N(N - 1)$ elements each induce one irreducible representation of degree $[D_1 : \{1\}] = 2$. We thus expect to find only one- and twofold degeneracies in the band diagram of this photonic crystal.

Example 4. The photonic crystal depicted in figure 2.6 has a symmorphic symmetry group. We can show this as follows. The wallpaper group of the crystal is $p4m$, which is generated by two independent translations, a rotation of order 4 and a reflection. It contains glide reflections, which are the composition of a reflection and a translation (which is not in T) along the line of reflection. Let G_0 be the subgroup of G consisting of elements that fix the origin. Any element $g \in G$ transforms the origin to a point which is removed from it by some translation vector $\lambda \in T$, i.e. $\lambda^{-1}g \in G_0$. It follows that we have $G = T \rtimes G_0$, and since there exist a natural injections between

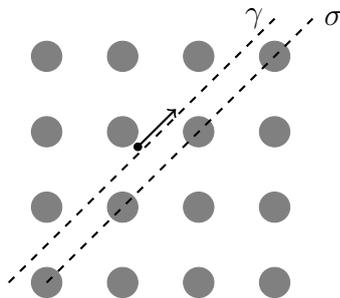


Figure 2.6: Part of a two-dimensional photonic crystal with wallpaper group $p4m$. Two symmetry elements - a reflection σ and a glide γ - are indicated by their reflection axes with a dashed line, and an arrow for the subsequent translation for γ .

G_0 and G/T , we must have $G/T \cong G_0 \cong D_4$. We may again use proposition 4 to determine the irreducible representations of G , where we can study the action of G on T instead of on the characters of T because, as in the previous example, we are dealing with a square lattice. Looking at figure 2.5, we see that there are $N - 1$ elements of T that are fixed under a reflection in a horizontal axis, and the same amounts are fixed for a vertical and two diagonal axes, corresponding to a stabilizer $\langle \sigma \rangle$, with $\sigma \in G$ such a reflection. These subgroups $\langle \sigma \rangle$ have index 4 in D_4 , and since they are abelian, we obtain $4N - 4$ irreducible representations of G of degree 4 by using proposition 4. Of course, there is a trivial element in T that is fixed by D_4 . From example 1, we know the irreducible representations of D_4 , which now give rise to one irreducible representation of G of degree 2 and four of degree 1. Lastly, the remaining $N^2 - 4N + 4 - 1$ elements of T have trivial stabilizer with index 8 in D_4 , corresponding to a single irreducible representation of degree 8. In total, then, G has four irreducible representations of degree 1, one of degree 2, $4N - 4$ of degree 4 and $N^2 - 4N + 3$ of degree 8. We thus expect to see one-, two-, four- and eightfold degeneracies in the band diagram for this photonic crystal (although not all are required to appear).

Example 5. The photonic crystal shown in figure 2.7 has wallpaper group pmg (and hence a non-symmorphic symmetry group G , as we shall prove), which is generated by two independent translations, a rotation of order 2 and a reflection. It also contains glide reflections. A major difference between this structure and the one from the previous example is that a glide here does not transform the origin (or any point, for that matter) to a point which is removed from it by a lattice vector. This is precisely what will cause G to be non-symmorphic. Indeed, the group G/T is generated by representatives of

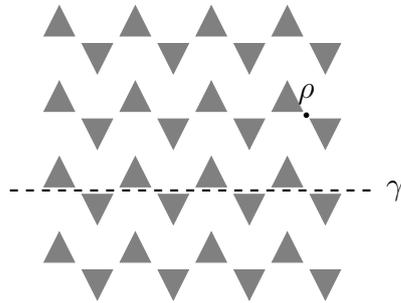


Figure 2.7: Part of a two-dimensional photonic crystal with wall-paper group pmg . A glide γ is indicated by its reflection axis and a rotation ρ by its center of rotation.

a reflection σ with vertical reflection axis and a rotation ρ , which is indicated in figure 2.7 by its center of rotation. The representative of a glide γ also lies in this group (as it should), since we have the equality $\bar{\gamma} = \bar{\sigma}\bar{\rho}$ as elements of G/T . Thus, we have $G/T = \langle \bar{\rho}, \bar{\sigma} \rangle \cong V_4$. A lift $x \in G$ of $\bar{\gamma}$ has order 2. Therefore, x must be a reflection, rotation, a translation of order 2 inside G or any combination of these. The composition of a reflection and a rotation equals a glide reflection, since the centers of rotation do not lie on reflection axes. The glide reflections in G translate over an element which does not lie in T . Note that a translation of order 2 must be an element of T , since N is even (recall that T has order N^2). It follows that the translational part of a glide in G cannot have order 2, hence the glide cannot have order 2. The only possible lifts of $\bar{\gamma}$ are therefore reflections and rotations (possibly composed with translations from T). However, these are sent under a mapping $G \rightarrow G/T$ to $\bar{\sigma}$ and $\bar{\rho}$, respectively. It follows that we cannot lift $\bar{\gamma}$ to G in such a way that a mapping $G \rightarrow G/T$ sends this lift back to $\bar{\gamma}$. In other words, there is no section of the sequence $0 \rightarrow T \rightarrow G \rightarrow G/T \rightarrow 0$. Thus, this sequence does not split, proving that G is non-symmorphic.

From the preceding examples, it is clear that the only way a symmetry group can be non-symmorphic is if G/T contains elements outside of the orthogonal group $O(n)$, i.e., elements that carry with them some translation. This is because such an element will have a different order in G/T than in G , so it is not always possible to lift it to G . As an example, the glide in figure 2.7 squares to a translation, so that it has order 2 in G/T but order $2N$ in G , and indeed we saw in example 5 that it was not possible to lift the glide from G/T to G . The elements composed of a transformation from $O(n)$ and a subsequent translation that may appear in G/T are glide reflections and screw rotations, the latter of which is a rotation followed by a translation along the rotation axis (which does not appear for $n < 3$). Thus, the only

elements that can make G non-symmorphic if $n = 2$ are glides, which square to a translation.

Before we proceed, we will take some time to elaborate on the chosen restriction of N to be even.

Consider a photonic crystal ε which is invariant under the isometries in the group $\text{Sym}(\varepsilon)$. Recall that its symmetry group equals $G = \text{Sym}(\varepsilon)/\Lambda_N$. The Born-von Kármán boundary condition permitted us to work with finite groups by modding out Λ_N , but one needs to remain vigilant as not to alter certain properties of the groups involved. In particular, if the sequence

$$0 \rightarrow \Lambda \rightarrow \text{Sym}(\varepsilon) \rightarrow \text{Sym}(\varepsilon)/\Lambda \rightarrow 0 \quad (2.19)$$

does not split, we also want the sequence

$$0 \rightarrow T \rightarrow G \rightarrow G/T \rightarrow 0 \quad (2.20)$$

not to split, in order to reflect reality accurately. For this to be the case, we must choose a suitable value of N . If $n = 2$, we will show that we need N to be even.

Proposition 6. *Let ε be a two-dimensional photonic crystal with symmetry group $G = \text{Sym}(\varepsilon)/\Lambda_N$ and translation subgroup $T = \Lambda/\Lambda_N$, for a certain choice of N . If N is even, then the sequence (2.20) splits if and only if (2.19) splits. If N is odd, (2.20) always splits.*

Proof. Let N be even. Suppose that (2.19) splits, so that there are homomorphisms $\varphi : \text{Sym}(\varepsilon) \rightarrow \text{Sym}(\varepsilon)/\Lambda$ and $\psi : \text{Sym}(\varepsilon)/\Lambda \rightarrow \text{Sym}(\varepsilon)$ such that $\varphi \circ \psi = \text{id}_{\text{Sym}(\varepsilon)/\Lambda}$. Precomposing ψ with the canonical isomorphism $G/T \xrightarrow{\sim} \text{Sym}(\varepsilon)/\Lambda$ and composing the resulting map with the standard quotient map $\text{Sym}(\varepsilon) \rightarrow G$, we obtain a section $G/T \rightarrow G$ that splits (2.20).

Conversely, suppose that N is even and (2.19) does not split. Since orthogonal maps (reflections and rotations) have the same order in $\text{Sym}(\varepsilon)$ and $\text{Sym}(\varepsilon)/\Lambda$, this is only possible if $\text{Sym}(\varepsilon)$ contains a glide that translates over a vector not in Λ . By modding out Λ , this glide is sent to an element $x \in \text{Sym}(\varepsilon)/\Lambda \cong G/T$. A lift $\tilde{x} \in G$ of x must have order 2 since x squares to 1 inside G/T . Hence, \tilde{x} must be a reflection or rotation composed with a translation which squares to the trivial element of G . Since T has even order N^2 , such a translation must be an element of T . Hence, \tilde{x} is either a rotation or a reflection composed with such a translation in T . A mapping $G \rightarrow G/T$ now sends \tilde{x} to this rotation or reflection. This image cannot equal x , since (2.19) does not split. It follows that (2.18) also does not split.

Now let N be odd and let $x \in G/T$ be the equivalence class of a glide. As expressed before, only glides can inhibit the splitting of (2.20), so it suffices to only consider such elements. To split (2.20), we lift x to an element $\tilde{x} \in G$. We see that \tilde{x} must square to a translation, since x has order 2 in G/T . Since N is odd, T has odd order. It follows that there is an odd integer m such that $(\tilde{x}^2)^m = 1 \in G$, and $\tilde{x}^m \in G$ gets mapped to $x^m = x \in G/T$ (where the equality follows from the fact that m is odd). Hence, the element \tilde{x}^m is a lift of x that squares to 1 inside G , and therefore splits the sequence. \square

More generally, when $n = 3$, the elements that may cause G to be non-symmorphic also include screw rotations (as remarked above), which can have arbitrary order. However, since G/T is finite, it contains only a finite number of glides and screw rotations. Let M be the product of their orders in G/T (if $n = 2$, this will be a power of 2). These orders do not depend on N since we have $G/T \cong \text{Sym}(\varepsilon)/\Lambda$. If N is coprime to M , then it follows analogously to the proof above that the sequence $0 \rightarrow T \rightarrow G \rightarrow G/T \rightarrow 0$ always splits. However, choosing N to be a multiple of M will ensure that the sequence does not automatically split. These restrictions on N are not paramount to our understanding of the theory, since N never takes on explicit values in this work, but it is important to realize that such constraints do exist. Since the examples in this work cover only two-dimensional cases ($n = 2$), we have fixed N to be even.

In this section, we have predicted degeneracies in band diagrams by considering irreducible representations of G . These results don't tell us, however, where (i.e. for which $k \in \Lambda_N^*/\Lambda^*$) to expect such a degeneracy to take place. To give such 'local' predictions, we need to look at the irreducible representations of $G(k)$, as already discussed in section 2.6. Recall the definition

$$G(k) := \langle \{g \in G : gk \equiv k\}, T \rangle$$

for the stabilizer of a wave vector $k \in \Lambda_N^*/\Lambda^*$. If G is symmorphic, we now have a splitting short exact sequence

$$0 \rightarrow T \rightarrow G(k) \rightarrow G(k)/T \rightarrow 0$$

for every $k \in \Lambda_N^*/\Lambda^*$, as follows simply from restricting the homomorphism $G/T \rightarrow G$ that splits (2.18) to $G(k)/T$. Hence, for symmorphic symmetry groups, we have the equality $G(k) = T \rtimes H'$, where $H' \cong G(k)/T$, for all $k \in \Lambda_N^*/\Lambda^*$. This makes it possible to use proposition 4 to determine the irreducible representations of $G(k)$, which we can use to acquire information about the degeneracies at k . For example, at $k = 0$, we

have $G(k) = G$, so that every irreducible representations of G may form an eigenspace $E_k(\omega)$ here. On the contrary, there are many points of low symmetry where $G(k) = T$, so that there should not be any degeneracies here (except for possible accidental ones).

For non-symmorphic symmetry groups, there does not exist such a neat theorem as proposition 4 to determine its irreducible representations, which is what generally makes them harder to study. Some non-symmorphic groups are solvable groups, for which theorems on determining irreducible representations do exist. However, this treatment is beyond the scope of this text.

In the next chapter, we shall explore several examples of two-dimensional photonic crystals and use numerical computations to analyze their band diagrams. We will then compare the degeneracies that show up to the theoretical predictions as outlined in the preceding section.

Examples and numerical simulations

In the examples in this chapter, we calculate the photonic band structures of crystals with symmetry groups corresponding to various wallpaper groups. In general, degeneracies of modes are expected in more symmetric structures and at points of high symmetry. Removing or lowering symmetry thus provides an opportunity to create a band gap, i.e. a range of frequencies for which no propagating modes exist. Such gaps play a pivotal role in the functionality and design of photonic crystals. Of particular interest for our understanding are structures where the symmetry can be changed continuously, without affecting other properties of the crystal. We will illustrate that this can be achieved by either moving a scatterer in a complex unit cell with two scatterers, or by rotating a single scatterer.

Although we cannot always solve equation (2.15) by hand, it is possible to solve it numerically with the help of a computer. For the numerical simulations in this chapter, we used the software package MPB (*MIT Photonic Bands*) to calculate band structures, employing the language Scheme to program the crystals. The code for this can be found in the Appendix. In Scheme, one can define a periodic structure by specifying the values of ε within the unit cell, with the help of certain standard geometric shapes (circles, triangles, et cetera). One can further specify the wave vectors at which equation (2.15) should be solved and the resolution with which this is to be carried out. MPB then outputs several files, one of which contains a visualization of ε . Another contains the frequencies of modes, i.e. the eigenvalues of (2.15), at every k . These frequencies can be divided into those of TE and those of TM modes. For each of these modes, the frequencies can then be plotted against the corresponding wave vectors (using, for example, a Python script), thus giving us the TE and TM band diagrams. In these diagrams, wave vectors are often indicated by certain symbols. These symbols

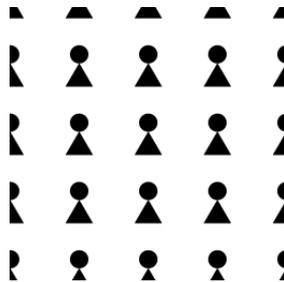


Figure 3.1: A symmorphic crystal with wallpaper group pm , as recreated in MPB. The scatterers (black) have permittivity $\varepsilon = 12$ (e.g. Si or GaAs at wavelength $\lambda = 1.5\mu\text{m}$) and the surrounding medium (white) has $\varepsilon = 1$ (air or vacuum). By ‘scatterer’, we mean a shape of constant permittivity ε .

are conventional within solid state physics [14], but other than that quite arbitrary.

For the sake of completeness, we will mention the conventions regarding physical units that Scheme and MPB employ. Vectors and lengths are defined in multiples of the fundamental lattice constants, i.e. the lengths of the smallest translations that span the lattice. Similarly, vectors and lengths in the reciprocal lattice are defined in multiples of 2π divided by these lattice constants – that is, in multiples of the fundamental reciprocal lattice constants. The output frequencies are given in units of the speed of light c divided by the smallest fundamental lattice constant, which we will denote by a throughout this section.

3.1 Wallpaper group pm

We begin with the structure previously treated in example 3. Figure 3.1 displays the structure as recreated in MPB using the Scheme code from appendix A.1. The first part of the code in appendix A.1 defines the structure of the crystal, whereas the latter part instructs MPB on the wave vectors we want to consider. MPB then finds solutions to equation (2.6) at these wave vectors. Using a Python script, we extract the frequencies of these solutions and plot the TE and TM modes separately, giving us the band diagrams in figure 3.3. Note that we have purposefully traced a path larger than the outline of the irreducible zone in order to directly compare the bands to that of a less symmetric structure, where the irreducible zone will be larger. The path in reciprocal space is depicted in figure 3.2.

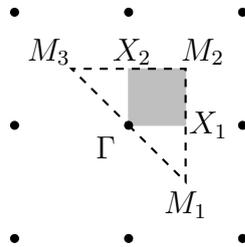


Figure 3.2: Illustration of the irreducible zone (gray area) inside the reciprocal lattice of the structure depicted in figure 3.1. The path traced to obtain the band diagrams is indicated by the dashed line. Special points (corners and midpoint of edges) and the zero point Γ are indicated by symbols which we will continue using for square lattices.

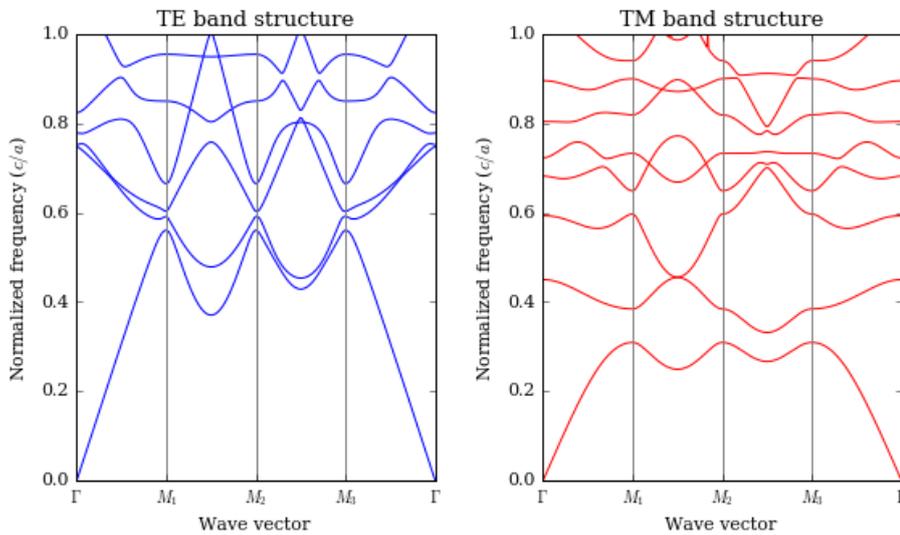


Figure 3.3: Band diagrams of TE and TM modes for the structure from figure 3.1

The band diagrams in figure 3.3 show several points where bands cross. From our analysis in example 3 in section 2.8, we expected only one- and twofold degeneracies to occur. More specifically, the wave vectors k between M_1 and M_2 have stabilizer $G(k) = G$, since the reflection from G transform these elements into equivalent wave vectors, in the sense that they are displaced by an element of Λ^* . Thus, for these wave vectors k , the group $G(k) = G$ has one- and two-dimensional irreducible representations (as we saw in example 3) and we expect one- and twofold degeneracies to occur in this range. The band diagrams in figure 3.3 indeed display such degeneracies. The same holds for the point X_2 , as it lies on the reflection axis, so that $G(X_2) = G$.

There are points in the band diagram where bands cross despite the lack of higher dimensional irreducible representations of the corresponding group $G(k)$. For example, at wave vectors in the range between (but not including) Γ and M_1 , the group $G(k)$ simply equals T , as there are no other symmetries that stabilize these elements. Since T only has one-dimensional irreducible representations, we do not expect degeneracies to occur here. Nonetheless, a crossing of bands does take place in this range in the TE diagram. Indeed, this crossing is an example of the aforementioned phenomenon of an accidental degeneracy, which is not protected by symmetry and may disappear for slightly different parameters.

3.2 Wallpaper group $p1$

We now simulate a less symmetric crystal with wallpaper group $p1$ consisting only of translations, so that $G = T$. This structure is obtained from figure 3.1 by a translation of the circular scatterer. Since the symmetry group is now abelian and only has one-dimensional irreducible representations, we expect no degeneracies to take place, and therefore no bands to cross. The structure, for which the code can be found in appendix A.2, is depicted in figure 3.4.

Due to the lack of symmetry, the irreducible zone in the crystal's reciprocal lattice equals half of the Brillouin zone (the structure has inversion symmetry, but no other point symmetries). Thus, the contour of the irreducible zone equals the path we traversed in the previous example (see figure 3.2) and allows a direct comparison with this example. The band diagrams are depicted in figure 3.5. The bands from figure 3.3 are included as gray dotted lines to facilitate the comparison.

Note that the derivative $\frac{\partial\omega}{\partial k}$ for small ω is the same for both structures. This is expected, because this slope at small ω represents the ‘effective index’

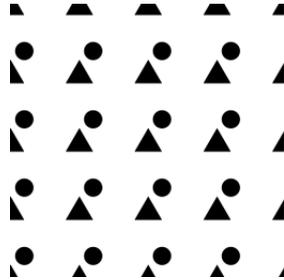


Figure 3.4: A symmorphic crystal with wallpaper group $p1$, as recreated in MPB. The scatterers (black) have permittivity $\varepsilon = 12$ and the surrounding medium (white) has $\varepsilon = 1$.

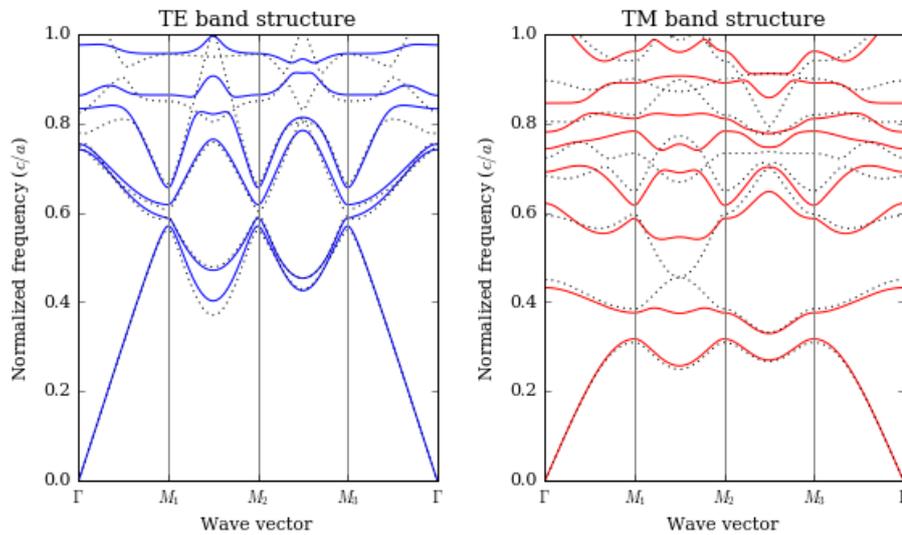


Figure 3.5: Band diagrams for the structure from figure 3.4, with the bands from figure 3.3 in gray dotted lines for comparison.

of the structure, which relates to the average value of ε in the unit cell. Since we have not changed this value by translating the circular scatterer, the slopes of both band diagrams near zero are equal. The fact that the effective index remains constant implies that the average interaction is identical, so that changes in the band structure are primarily due to a change in symmetry.

As expected, we see from figure 3.5 that we have ‘lifted’ all degeneracies from the previous example by lowering the symmetry, and there are no band crossings. In this particular example, this lack of band crossings has opened up quite a large band gap (a concept which we discussed in section 2.5) between the second and third band in the TM diagram. Since moving the circle in figure 3.4 can be done continuously, this band gap could be maximized by fine-tuning the position of the circle. We will not do so here, in order not to digress too far from our path of studying symmetry, but this example provides a promising route for further study.

The fact that we can continuously move from figure 3.1 to a structure of lower symmetry has another interesting implication. Since certain bands of the former structure cross and those of the latter do not, a crystal that is only slightly different from figure 3.1 (for example, by a minuscule translation of the circle) will have bands that come very close together, though they will not cross. Conversely, moving a structure ‘further away’ from symmetry can thus have the effect of distancing its bands further from one another. Since a band diagram is periodic with respect to wave vectors, bands must start and terminate at the same frequency. From this it follows that every band has an extremum, where $\frac{\partial\omega}{\partial k} = 0$. If bands were allowed to cross, this would not have been necessarily true, since band crossings would form points where this derivative cannot be unambiguously defined. A lack of symmetry ensures that such crossings do not happen and the slope $\frac{\partial\omega}{\partial k}$ must therefore equal zero at least at two points. Being ‘far away’ from a symmetric structure (meaning it would take relatively large translations or rotations of scatterers to obtain a structure with higher symmetry), bands will likely bound each other to small frequency ranges, which implies that these bands will remain quite flat throughout the irreducible zone. Since the derivative $\frac{\partial\omega}{\partial k}$ represents the group velocity of a wave, the above suggests the prevalence of ‘slow light’ in photonic crystals with low symmetry. To support this statement, we study another crystal with the same symmetry group, but which is not as ‘close’ to a symmetric structure as the one we just studied. The crystal is depicted in figure 3.6 and its band diagrams in figure 3.7.

It is clear that the wallpaper group of this pattern is indeed $p1$, and no isometry can transform it into a structure with which it almost coincides. More quantitatively: a non-translational element of a wallpaper group applied to this pattern would render a structure with little overlap with respect

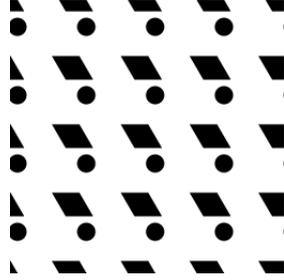


Figure 3.6: A symmorphic crystal with wallpaper group $p1$, as recreated in MPB. The scatterers (black) have permittivity $\varepsilon = 12$ and the surrounding medium (white) has $\varepsilon = 1$.

to the total black area in figure 3.6 (as opposed to figure 3.4, where a reflection would leave the triangles overlapping). Therefore, we expect the bands in the dispersion diagram of this crystal to repel one another more strongly, likely leading to even flatter bands. The calculated band structure is shown in figure 3.7 and is in line with these predictions, particularly for the TM polarization.

Again, the circle in figure 3.6 could be continuously moved to optimize the flatness of bands, but we shall refrain from doing so, for the reason of not digressing too far from the study of symmetry. Nonetheless, the procedure outlined above gives a ‘recipe’ for designing photonic crystals which display slow light dispersion that has seemingly not been described before [15].

3.3 Wallpaper group $p6m$

The structure shown in figure 3.8 (for which the code can be found in appendix A.3) can be easily shown to have wallpaper group $\text{Sym}(\varepsilon) = p6m$. The only glides that this group possesses translate over a whole lattice vector, so from our discussion in section 2.8 it is clear that G is symmorphic. It can therefore be written as the semidirect product $G = T \rtimes D_6$. To identify the stabilizers of the characters of T , it is important to realize that some wave vectors $k \in \Lambda_N^*/\Lambda^*$, hence some characters of T , are transformed by elements of G to equivalent wave vectors within Λ_N^*/Λ^* that are separated from one another by an element of Λ^* . This can only happen if k lies on the boundary of the Brillouin zone, as is illustrated in figure 3.10. Here, we see the reciprocal lattice Λ^* of the structure from figure 3.8. Since this structure has the periodicity of a triangular lattice Λ (as can be easily verified), it follows that Λ^* is also triangular. The Brillouin zone is outlined in figure 3.10 and can be seen to form a hexagon. The encircled points on the corners are examples

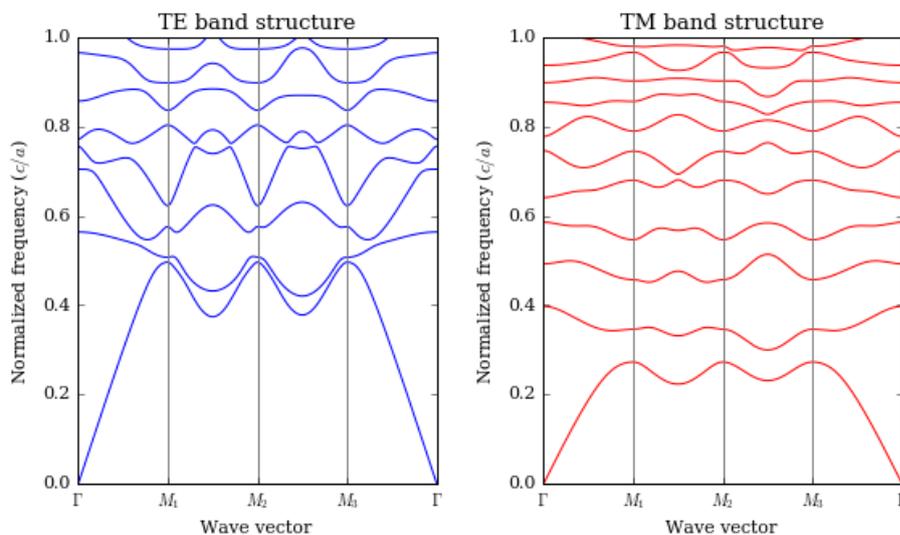


Figure 3.7: Band diagrams for the structure from figure 3.6, demonstrating flat bands in a structure of low symmetry.

of equivalent wave vectors (hence corresponding to the same character of T), since they are separated by a lattice vector of Λ^* . They are permuted among one another by symmetries of G/T . Thus, the stabilizer of such a point is not merely a reflection that runs through it, but also contains a rotation of degree three and combinations of the two, making it isomorphic to the symmetric group S_3 . This group has one- and two-dimensional irreducible representations and has index 2 in D_6 , so it follows from proposition 4 that this stabilizer induces two- and four-dimensional irreducible representations of G .

Some wave vectors, such as those indicated by a cross in figure 3.10, are transformed under a reflection to a point that lies a reciprocal lattice vector away. If the point also happens to lie on another reflection axis, its stabilizer has order 4. If not, it has order 2. Either way, the stabilizer is an abelian group with index 3 or 6 in D_6 , inducing three- and six-dimensional irreducible representations of G .

Of course, there is a trivial character which is stable under D_6 . From example 1 in section 2.7, we know that D_6 only has one- and two-dimensional irreducible representations, so we now obtain one- and two-dimensional irreducible representations of G . Lastly, there are wave vectors with trivial stabilizer, which has index 12 in D_6 , giving rise to twelve-dimensional irreducible representations of G .

We thus expect one-, two-, three-, four-, six- and twelvefold degeneracies

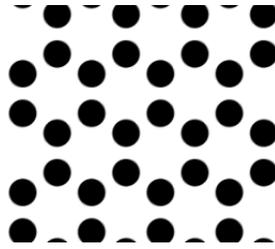


Figure 3.8: A symmorphic crystal with wallpaper group $p6m$, as recreated in MPB. This particular structure is also called a ‘honeycomb lattice’. The scatterers (black) have permittivity $\varepsilon = 12$ and the surrounding medium (white) has $\varepsilon = 1$. The radius r of the circles relative to the fundamental lattice constant a is $r/a = 0.2$.

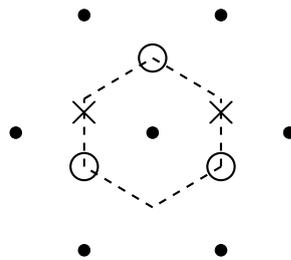


Figure 3.9: Illustration of part of the reciprocal lattice Λ^* (solid dots) of the structure from figure 3.8, with its Brillouin zone outlined. The equivalent wave vectors of two distinct points in the Brillouin zone are indicated by either a cross or a circle.

to potentially appear in our band diagram. Of course, not all need occur, since not all representations of G necessarily appear as eigenspaces, but the theory dictates that these are the only options. Note that degeneracies may occur anywhere in the band diagram: for the wave vectors k we consider here, there is always a reflection in G that leaves k invariant.

In figure 3.11, we see that the band diagrams for this structure indeed possess twofold degeneracies. Three- and fourfold degeneracies are very close to occurring, especially in the TM band structure. We see no higher degeneracies.

In figure 3.8, one can imagine drawing the inscribed circle within every ‘honeycomb’. In this way, one would obtain a pattern with the same sym-

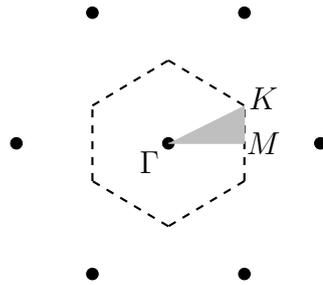


Figure 3.10: Illustration of part of the reciprocal lattice Λ^* of the structure from figure 3.8, with its irreducible zone colored gray. The corners of the irreducible zone are indicated by symbols which we will continue to use for triangular lattices.

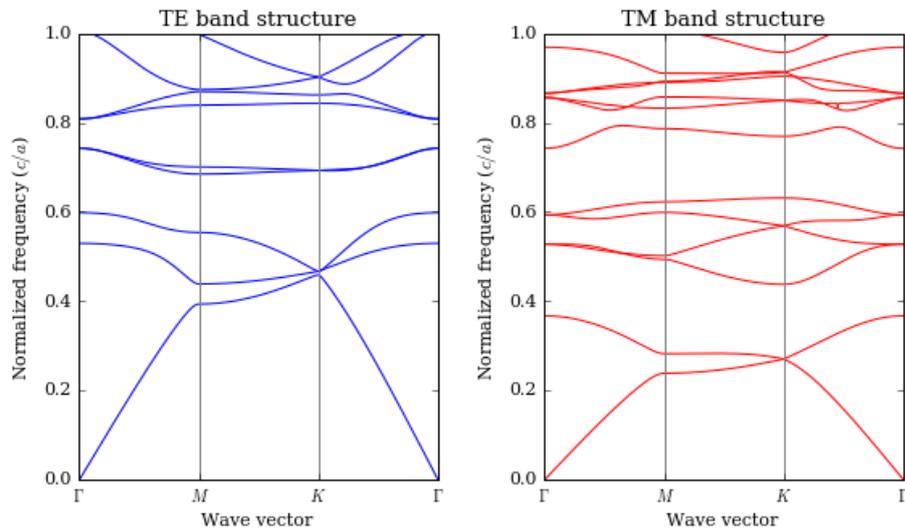


Figure 3.11: Band diagrams of the structure from figure 3.8.

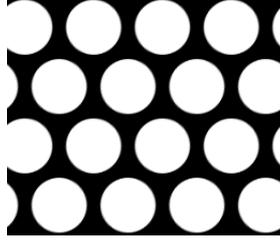


Figure 3.12: A symmorphic crystal with wallpaper group $p6m$, as recreated in MPB. The scatterers (white) have permittivity $\varepsilon = 1$ and the surrounding medium (black) has $\varepsilon = 12$. The radius r of the circles relative to the fundamental lattice constant a is $r/a = 0.4$.

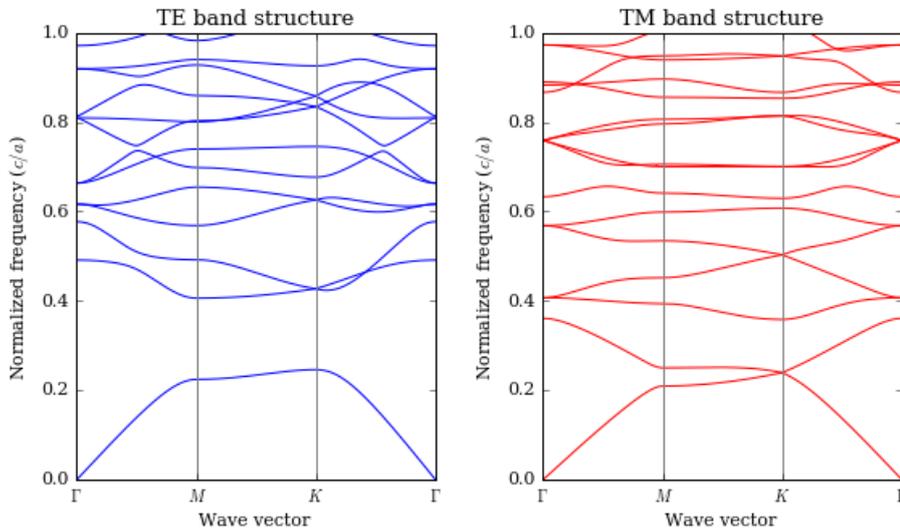


Figure 3.13: Band diagrams of the structure from figure 3.12.

metry. Moreover, if we choose these circles to have the same value of ε as the white space had in figure 3.8, and choose the remaining space to have the same value of ε as the circles had in figure 3.8, we obtain a structure that is similar not only in symmetry, but also in distribution of the values of ε . Precisely this structure is depicted in figure 3.12. We expect its band diagrams to bear much resemblance to the ones before. In particular, we again expect to see several of one-, two-, three-, four-, six- and twelfold degeneracies, though all need not appear. The band diagrams are displayed in figure 3.13.

In addition to the twofold degeneracies we saw before, we now also see that three- and fourfold degeneracies have manifested. Moreover, the TM bands for this crystal (particularly the lowest bands) have a striking level of

resemblance to those in figure 3.11. The TE diagrams, on the other hand, differ quite notably. This might have to do with the idea of ‘connectivity’, i.e. the fact that the region of high ε in this example is connected, as opposed to before. A detailed treatment of the concept of connectivity and its role in photonic band structures can be found in chapter 5 of [3].

3.4 Shifting between wallpaper groups by rotating scatterers

In the first example in section 3.2, we saw that by altering ε slightly (with respect to the crystal from the section before), we could drastically change the band diagram and remove degeneracies. However, changing ε by ‘shifting’ a scatterer might not be very practical in applications. As an alternative, we rotate scatterers in the following examples.

We begin with the structure displayed in figure 3.14. The wallpaper group belonging to this pattern is pmm , which is generated by translations and reflections in two perpendicular directions. The symmetry group of this crystal is thus symmorphic, and we can determine its irreducible representations as before. For this, we look at the action of the group $G/T \cong D_2$ on the characters of T . Since Λ is a square lattice, the Brillouin zone will have a square shape. It is easy to see that there are characters (that is to say, elements of Λ_N^*/Λ^*) on the border of the Brillouin zone that are stable under both reflections in D_2 , so that their stabilizer has index one in D_2 , giving rise to a one-dimensional irreducible representation of G (note that D_2 only has one-dimensional irreducible representations). Other elements of Λ_N^*/Λ^* that lie on a reflection axis but not on the border of the Brillouin zone have a stabilizer with index 2 in D_2 , hence inducing a two-dimensional irreducible representation of G . Lastly, there are characters with a trivial stabilizer of index 4 in D_2 , rendering four-dimensional irreducible representations of G . Thus, we expect at most two- and fourfold degeneracies to appear in the band diagrams. The irreducible zone of this crystal is the same as in figure 3.2, and we also trace the same path of wave vectors to enable a comparison. The diagrams are depicted in figure 3.15, and indeed show twofold degeneracies. In particular, the degeneracies only show up at zero and in the range between M_1 and M_2 and between M_2 and M_3 . This is expected, since these are precisely the wave vectors with non-trivial stabilizer.

As expressed above, we would like to remove or ‘lift’ these degeneracies by rotating the scatterers (the rectangles in this case). This is what is done to obtain the structure from figure 3.16. To be clear, the ‘average’ value of

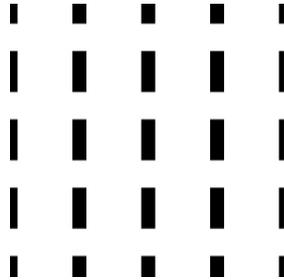


Figure 3.14: A symmorphic crystal with wallpaper group pmm , as recreated in MPB. The scatterers (black) have permittivity $\varepsilon = 12$ and the surrounding medium (white) has $\varepsilon = 1$. In term of the fundamental lattice constant a , the scatterers have length $0.65a$ and width $0.65a/3$.

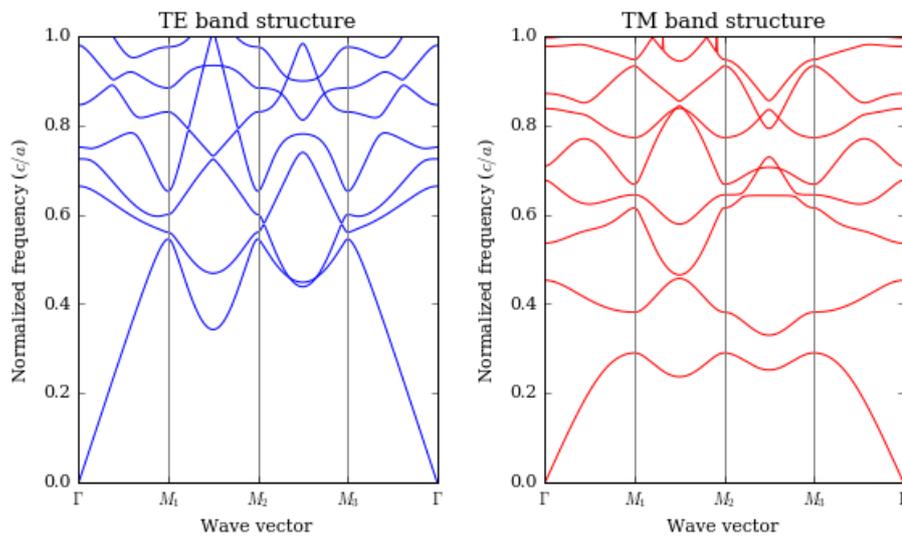


Figure 3.15: Band diagrams of the structure from figure 3.14.

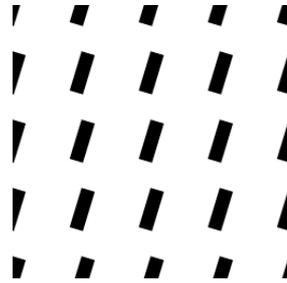


Figure 3.16: A symmorphic crystal with wallpaper group $p2$, as recreated in MPB. The scatterers (black) have permittivity $\varepsilon = 12$ and the surrounding medium (white) has $\varepsilon = 1$. In term of the fundamental lattice constant a , the scatterers have length $0.65a$ and width $0.65a/3$, and they are rotated under an angle of $\tan(0.3)$ rad $\approx 17.8^\circ$.

ε over all of space is the same as before, the shape is simply rotated. The effect of this rotation is to transform the wallpaper group to $p2$, consisting only of translations and rotations of order 2. To understand why this would have the effect of lifting degeneracies, recall from the previous chapter that, if G is symmorphic, we also have $G(k) = T \rtimes H'$ with $H' \cong G(k)/T$ and that the irreducible representations of $G(k)$ correspond to the degeneracies at that specific wave vector k . In this case, it is not hard to see that the only nonzero wave vectors k such that the group $G(k)$ contains more than just T are the elements M_1 , M_2 and M_3 , as well as the midway points between them. For these elements, we have $G(k) = G$, since a rotation of order 2 transforms them to an equivalent wave vector (i.e. the same element within Λ_N^*/Λ^*). For every other nonzero wave vector k we have $G(k) = T$. Since T is abelian and only has one-dimensional irreducible representations, there should not be any degeneracies (i.e. crossings of bands) in the band diagram, except potentially at the points M_1 , M_2 , M_3 and the points X_1 and X_2 halfway between them, as well as at Γ . Indeed, at these points, we have $G(k) = G = T \rtimes C_2$. Thus, characters with trivial stabilizer (which has index 2 in C_2) will induce a two-dimensional irreducible representation of G . The band diagrams for this structure should therefore only have twofold degeneracies at the aforementioned points, but all other degeneracies must now be lifted. This is indeed exactly what we see in figure 3.17. Although the structures in figure 3.14 and figure 3.16 are quite different from those in figures 3.1 and 3.4, the similarity between the band structures in figures 3.17 and 3.5 is striking. This clearly illustrates the important role of symmetry in the study of photonic crystals and underlines the concept of symmetry as a design principle.

We can repeat the procedure outlined above for different structures to

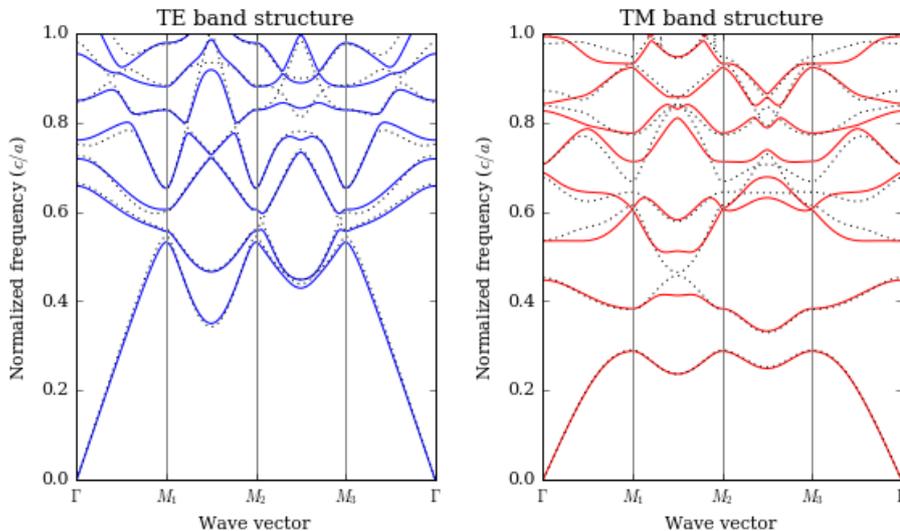


Figure 3.17: Band diagrams of the structure from figure 3.16, with the bands from figure 3.15 in gray dotted lines for comparison.

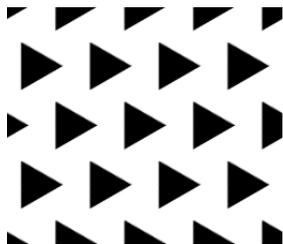


Figure 3.18: A symmorphic crystal with wallpaper group $p31m$, as recreated in MPB. The scatterers (black) have permittivity $\varepsilon = 12$ and the surrounding medium (white) has $\varepsilon = 1$.

target specific wave vectors at which we would like to lift a degeneracy. As an example, consider the structure from figure 3.18. This crystal has wallpaper group $p31m$, generated by translations, reflections in three directions, rotations of order three and glide reflections. These glides translate over a whole lattice vector, so the symmetry group G of this crystal is symmorphic. We thus have $G = T \rtimes D_3$. Since the underlying lattice Λ is triangular, the Brillouin zone will be a hexagon, and we have the same irreducible zone as depicted in figure 3.10.

Again, to determine the irreducible representations of G , we look at the stabilizers within $G/T \cong D_3$ of characters of T . Characters on a corner of the Brillouin zone are stable under all three reflections in D_3 , so that the stabilizer of such a character is equal to D_3 , which has one- and two-

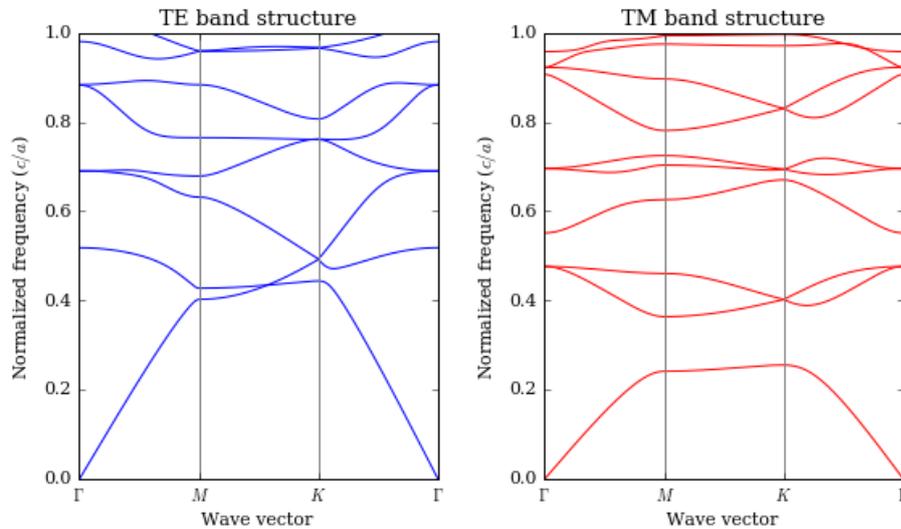


Figure 3.19: Band diagrams of the structure from figure 3.18.

dimensional irreducible representations. Other characters on the edge of the Brillouin zone (but not on a corner) are stable only under one reflection, making their stabilizer isomorphic to C_2 , which has index 3 in D_3 . This induces three-dimensional irreducible representations of G . Lastly, there are characters with trivial stabilizer with index 6 in D_3 , inducing six-dimensional irreducible representations of G . Hence, we expect any (but not necessarily all) of one-, two-, three- and sixfold degeneracies to appear. In particular, at the wave vector indicated by the letter K in figure 3.10, i.e. a corner of the Brillouin zone, we expect degeneracies to appear, since here $G(K) = T \rtimes D_3$. The band diagrams for this structure are shown in figure 3.19. Indeed, we see several twofold degeneracies, in particular at the K -point. There are also twofold degeneracies along the line between M and K , which is as expected, since these points are stable under a reflection in G (through a horizontal line), making the group $G(k)$ for these points k equal to $T \rtimes C_2$, which has one- and two-dimensional irreducible representations.

If we now rotate the scatterers, we obtain the structure from figure 3.20, which has wallpaper group $p3m1$. It differs from $p31m$ mainly in the fact that its rotation centres do not all lie on reflection axes. It is still a symmorphic group, so again we have $G = T \rtimes D_3$. Thus, we expect the same degeneracies to occur as before. However, since the K point is no longer on a reflection axis, the group $G(K)$ will equal T . Hence, there should no longer be any degeneracies at the K -point. Conversely, points on the line between Γ and M now lie on a reflection axis, so that twofold degeneracies may appear in



Figure 3.20: A symmorphic crystal with wallpaper group $p3m1$, as recreated in MPB. The scatterers (black) have permittivity $\varepsilon = 12$ and the surrounding medium (white) has $\varepsilon = 1$.

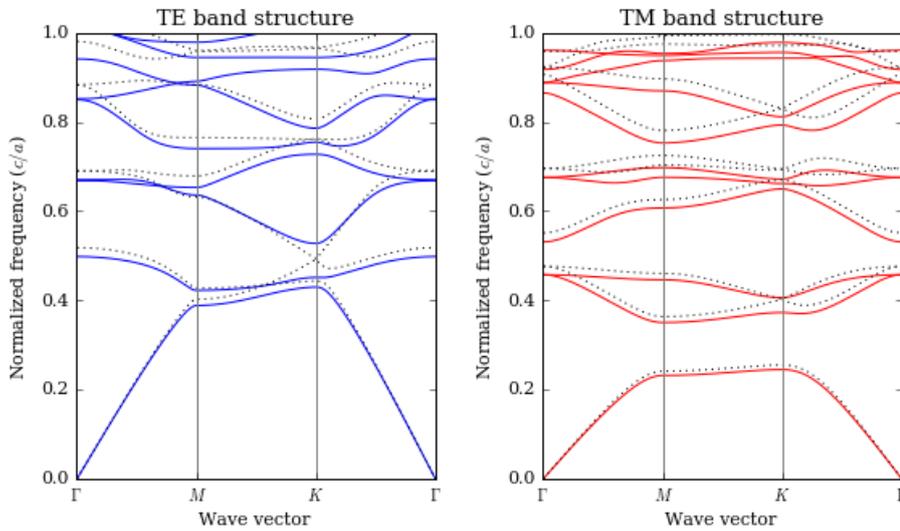


Figure 3.21: Band diagrams of the structure from figure 3.20, with the bands from figure 3.19 in gray dotted lines for comparison.

this range. The band diagrams for this crystal are depicted in figure 3.21. Indeed, we see twofold degeneracies in the range between Γ and M , and the degeneracies at K have been lifted. This result has previously been found by [16], although without a formal group theoretical basis.

Conclusion

We have presented a rigorous description of photonic crystals using the mathematical language of group representation theory. Studying the concept of irreducible representations of finite groups led us to a description of such representations for groups that can be written as a semidirect product. In the context of photonic crystals, such groups are called symmorphic, and we provided several examples of how to determine degeneracies of photonic modes in crystals with symmorphic symmetry groups. More than being just expository, these examples were carefully selected to display various interesting properties. Specifically, we described a way to design crystals with tunable dispersion by lowering symmetry. This allows for the creation of gaps by lifting degeneracies, as well as slow light modes using (the lack of) symmetry as a novel design principle. We report the removal of degeneracies at certain symmetry points in a continuously tuneable structure by either rotating scatterers, or by a continuous translation of a scatterer in a unit cell with multiple scatterers.

We urge further study on the link between eigenspaces and irreducible representations of symmetry groups. In particular, the nature and occurrence of accidental degeneracies is not yet understood and might point to some hidden symmetry in the problem. Thus far, this point has not been studied much by physicists because accidental degeneracies are rare and have little influence on the design of highly symmetric structures. Based on our work, it seems that such accidental degeneracies are important in the study of artificial structures that have low symmetry by design.

Similarly, it is still unclear why, given the same symmetry, some degeneracies will show up in one structure, but not in another. An example of this situation can be found in section 3.3, where one structure displays a four-

fold degeneracy, which the other lacks. Our characterization of degeneracies amounts to predictions of what may happen, but cannot say whether a degeneracy will occur with certainty. An understanding of this would require a deeper mathematical study.

A study of how changing parameters (such as the size of scatterers) without altering the symmetry affects the band diagrams might be a fruitful endeavour. The symmetry group G can be characterized by a continuous manifold with respect to these parameters, so applying existing mathematical theories on manifolds could give an understanding of the role of parameters that determine the structure of band diagrams.

Many interesting effects take place when introducing defects in photonic crystals [16]. An important prerequisite to creating a defect or localized mode is to have a photonic band gap inside the crystal. Lowering the symmetry of the underlying lattice removes degeneracies and we have given several examples of structures where lowering the symmetry led to the formation of gaps. A local change of the size, orientation or permittivity of a single scatterer leads to a defect mode and the study of the properties and role of symmetry on these defects is an interesting direction. However, this local change in properties does not fit into the description of a photonic crystal as being periodic over a lattice and cannot be described in terms of the representation theory used in this thesis. Understanding these defects and finding examples of defects that are protected by symmetry would require a different approach than the one taken here.

Appendix A

Scheme code

A.1 Code for 3.1

```
(define-param r 0.2)
(set-param! resolution 64)
(set! geometry (list (make cone
  (center 0 0 0) (radius r) (height (* (sqrt 3) r))
  (axis
    (rotate-lattice-vector3 (vector3 0 0 1)
      (deg->rad 90) (vector3 1 0)))
  (material (make dielectric (epsilon 12))))))
(make cylinder
  (center 0 (* 1.5 r) 0) (radius (/ r 1.5)) (height (* (sqrt 3) r))
  (material (make dielectric (epsilon 12)))
  (axis (vector3 0 0 1))))
(set! geometry-lattice (make lattice (size 1 1 no-size)
  (basis1 1 0)
  (basis2 0 1))) ;square lattice

(set! num-bands 16)
(set! k-points (list (vector3 0 0 0) ; Gamma
  (vector3 (/ 1 2) (/ -1 2) 0) ; M_1
  (vector3 (/ 1 2) (/ 1 2) 0) ; M_2
  (vector3 (/ -1 2) (/ 1 2) 0) ; M_3
  (vector3 0 0 0))) ; Gamma

(set! k-points (interpolate 64 k-points))
(run)
```

A.2 Code for 3.2

A.2.1 Code for the structure from figure 3.4

```
(define-param r 0.2)
(set-param! resolution 64)
(set! geometry (list (make cone
  (center 0 0 0) (radius r) (height (* (sqrt 3) r))
  (axis
    (rotate-lattice-vector3 (vector3 0 0 1)
      (deg->rad 90) (vector3 1 0)))
    (material (make dielectric (epsilon 12))))
  (make cylinder
    (center r (* 1.5 r) 0) (radius (/ r 1.5))
    (height (* (sqrt 3) r))
    (material (make dielectric (epsilon 12)))
    (axis (vector3 0 0 1))))))
(set! geometry-lattice (make lattice (size 1 1 no-size)
  (basis1 1 0)
  (basis2 0 1))) ;square lattice
(set! num-bands 16)
(set! k-points (list (vector3 0 0 0) ; Gamma
  (vector3 (/ 1 2) (/ -1 2) 0) ; M_1
  (vector3 (/ 1 2) (/ 1 2) 0) ; M_2
  (vector3 (/ -1 2) (/ 1 2) 0) ; M_3
  (vector3 0 0 0))) ; Gamma
(set! k-points (interpolate 64 k-points))
(run)
```

A.2.2 Code for the structure from figure 3.6

```
(define-param r 0.2)
(set-param! resolution 64)
(set! geometry (list (make cone
  (center 0 0 0) (radius r) (height (* (sqrt 3) r))
  (axis
    (rotate-lattice-vector3 (vector3 0 0 1)
      (deg->rad 90) (vector3 1 0)))
    (material (make dielectric (epsilon 12))))
  (make cone
    (center (* -1 r) 0 0) (radius r)
```

```

      (height (* (sqrt 3) r))
      (axis
        (rotate-lattice-vector3 (vector3 0 0 1)
          (deg->rad -90) (vector3 1 0)))
      (material (make dielectric (epsilon 12))))
    (make cylinder
      (center (* 0.5 r) (* -2 r) 0)
      (radius (/ r 1.5)) (height (* (sqrt 3) r))
      (material (make dielectric (epsilon 12)))
      (axis (vector3 0 0 1))))
  (set! geometry-lattice (make lattice (size 1 1 no-size)
    (basis1 1 0)
    (basis2 0 1))) ;square lattice
  (set! num-bands 16)
  (set! k-points (list (vector3 0 0 0) ; Gamma
    (vector3 (/ 1 2) (/ -1 2) 0) ; M_1
    (vector3 (/ 1 2) (/ 1 2) 0) ; M_2
    (vector3 (/ -1 2) (/ 1 2) 0) ; M_3
    (vector3 0 0 0))) ; Gamma
  (set! k-points (interpolate 64 k-points))
  (run)

```

A.3 Code for 3.3

A.3.1 Code for the structure from figure 3.8

```

  (define-param r 0.2)
  (set! geometry-lattice (make lattice (size 1 1 no-size)
    (basis1 (/ (sqrt 3) 2) 0.5)
    (basis2 (/ (sqrt 3) 2) -0.5))) ;triangular lattice
  (set! geometry (list (make cylinder
    (center (/ 6) (/ 6) 0) (radius r) (height infinity)
    (material (make dielectric (epsilon 12))))
    (make cylinder
    (center (/ -6) (/ -6) 0) (radius r) (height infinity)
    (material (make dielectric (epsilon 12))))))
  (set! k-points (list (vector3 0 0 0) ; Gamma
    (vector3 0 0.5 0) ; M
    (vector3 (/ -3) (/ 3) 0) ; K
    (vector3 0 0 0))) ; Gamma

```

```
(set! k-points (interpolate 64 k-points))
(set-param! resolution 64)
(set-param! num-bands 16)
(run)
```

A.3.2 Code for the structure from figure 3.12

```
(define-param r 0.4)
(set! geometry-lattice (make lattice (size 1 1 no-size)
    (basis1 (/ (sqrt 3) 2) 0.5)
    (basis2 (/ (sqrt 3) 2) -0.5))) ;triangular lattice
(set! default-material (make dielectric (epsilon 12)))
(set! geometry (list (make cylinder
    (center 0.5 0.5 0) (radius r) (height infinity)
    (material (make dielectric (epsilon 1))))))
(set! k-points (list (vector3 0 0 0) ; Gamma
    (vector3 0 0.5 0) ; M
    (vector3 (/ -3) (/ 3) 0) ; K
    (vector3 0 0 0))) ; Gamma
(set! k-points (interpolate 64 k-points))
(set-param! resolution 64)
(set-param! num-bands 16)
(run)
```

A.4 Code for 3.4

A.4.1 Code for the structure from figure 3.14

```
(define-param r 0.65)
(set-param! resolution 64)
(set! geometry (list (make block
    (center 0 0 0) (size (/ r 3) r 0)
    (material (make dielectric (epsilon 12))))))
(set! geometry-lattice (make lattice (size 1 1 no-size)
    (basis1 1 0)
    (basis2 0 1))) ;square lattice
(set! num-bands 16)
(set! k-points (list (vector3 0 0 0) ; Gamma
    (vector3 (/ 1 2) (/ -1 2) 0) ; M_1
    (vector3 (/ 1 2) (/ 1 2) 0) ; M_2
```

```

                (vector3 (/ -1 2) (/ 1 2) 0)      ; M_3
                (vector3 0 0 0))                ; Gamma
(set! k-points (interpolate 64 k-points))
(run)

```

A.4.2 Code for the structure from figure 3.16

```

(define-param r 0.65)
(set-param! resolution 64)
(set! geometry (list (make block
                    (center 0 0 0) (size (/ r 3) r 0)
                    (e1 1 -0.3 0)
                    (e2 0.3 1 0)
                    (material (make dielectric (epsilon 12))))))
(set! geometry-lattice (make lattice (size 1 1 no-size)
                                     (basis1 1 0)
                                     (basis2 0 1))) ;square lattice
(set! num-bands 16)
(set! k-points (list (vector3 0 0 0)           ; Gamma
                    (vector3 (/ 1 2) (/ -1 2) 0) ; M_1
                    (vector3 (/ 1 2) (/ 1 2) 0) ; M_2
                    (vector3 (/ -1 2) (/ 1 2) 0) ; M_3
                    (vector3 0 0 0)))          ; Gamma
(set! k-points (interpolate 64 k-points))
(run)

```

A.4.3 Code for the structure from figure 3.18

```

(define-param r 0.35)
(set-param! resolution 64)
(set! geometry (list (make cone
                    (center 0 0 0) (radius r) (height (* (sqrt 3) r))
                    (axis
                     (rotate-lattice-vector3 (vector3 0 0 1)
                                               (deg->rad 0) (vector3 1 0)))
                    (material (make dielectric (epsilon 11))))))
(set! geometry-lattice (make lattice (size 1 1 no-size)
                                     (basis1 1 0)
                                     (basis2 0.5 (/ (sqrt 3) 2)))) ;triangular lattice
(set! num-bands 16)
(set! k-points (list (vector3 0 0 0)           ; Gamma

```

```
(vector3 0 (/ 1 2) 0)      ; M
(vector3 (/ 3) (/ 2 3) 0) ; K
(vector3 0 0 0)))        ; Gamma
(set! k-points (interpolate 64 k-points))
(run)
```

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