Chapter 7

The Mathematics of Photonic Crystals

Peter Kuchment

7.1 Introduction

A photonic crystal, or photonic band gap (PBG) optical material, is an artificially created periodic low-loss dielectric medium in which electromagnetic waves of certain frequencies cannot propagate. The range of the prohibited frequencies is called the complete band gap. A simple example of such a medium is a dielectric background material with a periodic array of air bubbles. The reason why the band gap arises (if it does) is the coherent multiple scattering of waves and destructive interference. To put it simply, if a wave of a prohibited frequency somehow managed to propagate in the medium, it would reflect and self-interfere in such a way that it would cancel itself completely. It is expected that industrial manufacturing of photonic crystals will bring about a new technological revolution in optics, computing, information transmission, and other areas. The idea of photonic crystals was coined in [107, 192], though simpler versions of such materials like layered media and optical gratings have been known for a long time. We will not dwell much on the physics aspects of this field of research, since the reader can refer to the surveys and proceedings [33, 101, 108, 134, 154, 156, 167, 168, 182, 189] devoted to this topic, and especially to the lovely book [106]. The bibliography [153] and the collection of photonic crystal links [190] are also very useful.

The area of photonic crystal research presents a bonanza of beautiful, important, and hard problems for a mathematician, most of which are still unexplored or explored only tangentially. The number of mathematics publications dealing with PBG materials is growing (see [3, 7, 8, 21, 41, 42, 44, 45, 50, 51], [61]–[81], [86, 87, 100, 126, 127, 155, 188]) but is probably still not sufficient. We hope that this survey will play some role in publicizing the topic. One of the big attractions and advantages of the PBG research is that the mathematical model one studies is considered to be practically precise in most circumstances (see, for instance, [106]), a luxury not very often enjoyed by applied mathematicians.

In this article the author tries to expose some basic analytic ideas and techniques, to collect the recent mathematical results on PBG materials and their acoustic analogs, to present some basic problems that still await their resolution, and to indicate analogies with research in other areas (mostly related to solid-state physics) that could provide some leads for the PBG studies. Due to the limited space, the reader is referred to the corresponding literature for the details, complete formulations of the results, precise conditions on the coefficients, or exact definitions of some operators. Since the surveys [101, 152, 189] and collections cited before do a good job describing the numerical techniques that are commonly used, this paper addresses only a few recent, less standard numerical approaches that are not covered by these surveys.

There are many areas of the photonic crystal research that deserve and have not yet enjoyed close mathematical attention, but which we were not able to include in this survey. Among these are effects of losses, finiteness of samples, surface waves, nonlinear effects, magnetic effects, effects of metallic inclusions, gap solitons, and many others. The reader can find discussion of all of these and many other exciting topics in the surveys and bibliography quoted above and also in the papers [3, 41, 63, 66, 67, 86, 87, 188]. Regretfully, the important topic of Anderson localization of classical waves, where crucial results have recently been achieved, is just briefly mentioned due to the space limitations. We provide references to the relevant publications on this subject in section 7.6.6.

The theory of PBG materials as an area of mathematics is still in its childhood. As a result, there is no common choice of topics, approaches, etc. This article, therefore, reflects the author's views and interests and would probably be written in a totally different (maybe even orthogonal) manner by other researchers.

7.2 The Maxwell Operator

The reader has probably already seen the Maxwell equations many times in this book. We need, however, to briefly address them again. Our goal is to summarize the information we need and to mention some specific mathematical questions relevant to the theory of photonic crystals and to optics in general. Good general references concerning the Maxwell equations are [103, 135]. A mathematician can also be interested in the discussion of these equations presented in [53].

The macroscopic Maxwell equations that govern the light propagation in a photonic crystal in absence of free charges and currents look as follows:

$$\begin{cases} \nabla \times \mathbf{E} = -\frac{1}{c}\frac{\partial \mathbf{B}}{\partial t}, & \nabla \cdot \mathbf{B} = 0, \\ \nabla \times \mathbf{H} = \frac{1}{c}\frac{\partial \mathbf{D}}{\partial t}, & \nabla \cdot \mathbf{D} = 0. \end{cases} \tag{7.1}$$

Here c is the speed of light, $\mathbf{E}$ and $\mathbf{H}$ are the macroscopic electric and magnetic fields, and $\mathbf{D}$ and $\mathbf{B}$ are the displacement and magnetic induction fields, respectively.

All these fields are vector-valued functions from $\mathbb{R}^3$ (or a subset of $\mathbb{R}^3$) into $\mathbb{R}^3$. We denote such fields with boldface letters. The standard vector notations $\nabla\times$ (or $\nabla^\times$), $\nabla\cdot$, and ∇ are used for the curl, divergence, and gradient, although we will also use curl, div, and grad. The system (7.1) is incomplete until we add the so-called constitutive relations that describe how the fields $\mathbf{D}$ and $\mathbf{H}$ depend on $\mathbf{E}$ and $\mathbf{B}$. Although in general these relations are nonlinear and even nonlocal, in materials other than ferroelectrics and ferromagnets and when the fields are weak enough, the following linear approximations to the constitutive relations work:

$$\mathbf{D} = \varepsilon\mathbf{E}, \qquad \mathbf{B} = \mu\mathbf{H}. \tag{7.2}$$

Here ε and μ are the so-called material tensors. We will mostly address the case of isotropic media, where ε and μ can be considered as scalar time-independent functions called electric permittivity (or dielectric constant) and magnetic permeability, correspondingly. In most photonic crystals considerations it is assumed that the material is nonmagnetic, and hence $\mu = 1$.

After introducing the above assumptions, the Maxwell system reduces to the form

$$\begin{cases} \nabla\times\mathbf{E} = -\frac{1}{c}\mu(x)\frac{\partial\mathbf{H}}{\partial t}, & \nabla\cdot\mu\mathbf{H} = 0, \\ \nabla\times\mathbf{H} = \frac{1}{c}\varepsilon(x)\frac{\partial\mathbf{E}}{\partial t}, & \nabla\cdot\varepsilon\mathbf{E} = 0, \end{cases} \tag{7.3}$$

or, in the nonmagnetic case,

$$\begin{cases} \nabla\times\mathbf{E} = -\frac{1}{c}\frac{\partial\mathbf{H}}{\partial t}, & \nabla\cdot\mathbf{H} = 0, \\ \nabla\times\mathbf{H} = \frac{1}{c}\varepsilon(x)\frac{\partial\mathbf{E}}{\partial t}, & \nabla\cdot\varepsilon\mathbf{E} = 0. \end{cases} \tag{7.4}$$

These linear partial differential equations have time-independent coefficients, so the Fourier transform in the time domain reduces considerations to the case of monochromatic waves $\mathbf{E}(x,t) = e^{i\omega t}\mathbf{E}(x)$, $\mathbf{H}(x,t) = e^{i\omega t}\mathbf{H}(x)$. This leads from (7.3) to

$$\begin{cases} \nabla\times\mathbf{E} = -\frac{i\omega}{c}\mu(x)\mathbf{H}, & \nabla\cdot\mu\mathbf{H} = 0, \\ \nabla\times\mathbf{H} = \frac{i\omega}{c}\varepsilon(x)\mathbf{E}, & \nabla\cdot\varepsilon\mathbf{E} = 0, \end{cases} \tag{7.5}$$

which can be rewritten in the matrix form as

$$\begin{pmatrix} 0 & -\frac{i}{\varepsilon}\nabla^\times \\ \frac{i}{\mu}\nabla^\times & 0 \end{pmatrix} \begin{pmatrix} \mathbf{E} \\ \mathbf{H} \end{pmatrix} = \frac{\omega}{c} \begin{pmatrix} \mathbf{E} \\ \mathbf{H} \end{pmatrix} \tag{7.6}$$

on the subspace of vectors $\binom{\mathbf{E}}{\mathbf{H}}$ satisfying

$$\nabla\cdot\varepsilon\mathbf{E} = 0, \qquad \nabla\cdot\mu\mathbf{H} = 0. \tag{7.7}$$

We use in (7.6) and in the rest of the text the notation $\nabla^\times$ for the curl operator.

We are now facing the spectral problem for the Maxwell operator

$$M = \begin{pmatrix} 0 & -\frac{i}{\varepsilon}\nabla^\times \\ \frac{i}{\mu}\nabla^\times & 0 \end{pmatrix} \tag{7.8}$$

on the subspace (7.7). One of the principal tasks of the photonic crystals theory is to choose periodic functions $\varepsilon(x) \geq 1$ and μ (although μ is usually assumed to be equal to 1) such that the corresponding spectrum has a gap. Existence of such a gap would mean that electromagnetic waves with a frequency ω in the gap cannot propagate in the material.

7.2.1 Defining a Self-Adjoint Maxwell Operator

Before studying the spectrum of the problem (7.8), one needs to define the corresponding self-adjoint operator. It is not hard to define the operator in the case when the material tensors are smooth and the operator is considered either in the whole space or in a smooth domain with conducting boundaries. In fact, smoothness of the material tensors is also not a big issue when one deals with the whole space (or with a torus, as one often does in the photonic crystal theory). However, if the domain has nonsmooth conducting boundaries, the solutions can develop singularities. Although we will constrain ourselves to the case when no metallic inclusions are present, PBG materials with nonsmooth metallic inclusions and/or boundaries are actually considered. In such cases one should consult with a comprehensive study of the Maxwell operator done by Birman and Solomyak in [22, 23].

Let us assume that $\mu(x)$ and $\varepsilon(x)$ are positive measurable functions uniformly bounded by positive constants from below and from above. In most of our discussion μ is equal to 1 and $\varepsilon(x) \geq 1$ is periodic and piecewise constant. We want to define the Maxwell operator as a self-adjoint operator in appropriate spaces. We will use notation $L^2(\mathbb{R}^3, w(x)dx)$ for the weighted L^2-space with the norm

$$||f||^2 = \int |f(x)|^2 \, w(x)dx$$

and $L^2(\mathbb{R}^3, w(x)dx; \mathbb{C}^3)$ for the corresponding space of vector fields.

Consider now the subspace J of the space

$$L^2(\mathbb{R}^3, \varepsilon(x)dx; \mathbb{C}^3) \oplus L^2(\mathbb{R}^3, \mu(x)dx; \mathbb{C}^3)$$

that consists of all pairs of vector fields (u_1, u_2) such that

$$\nabla \cdot \varepsilon u_1 = \nabla \cdot \mu u_2 = 0. \tag{7.9}$$

On the space J we can define the Maxwell operator M with the matrix (7.8) and the domain consisting of pairs (u_1, u_2) such that

$$\nabla \times u_j \in L^2(\mathbb{R}^3), \qquad j = 1, 2.$$

The derivatives here are understood in the distributional sense.

THEOREM 7.1 (Lemma 2.2 in [22]). *The Maxwell operator M defined this way is self-adjoint.*

7.2.2 Ellipticity

The trouble with the Maxwell operator is that it is neither elliptic nor semi-bounded (so its spectrum extends to both positive and negative infinity). There are ways to cope with both of these problems. Squaring the operator produces a new operator

$$M^2 = \begin{pmatrix} \frac{1}{\varepsilon}\nabla\times\frac{1}{\mu}\nabla\times & 0 \\ 0 & \frac{1}{\mu}\nabla\times\frac{1}{\varepsilon}\nabla\times \end{pmatrix},$$

which is already positive definite. Thus, as is customarily done in photonic crystals theory, we can consider either one of the following positive definite spectral problems:

$$\begin{cases} \frac{1}{\varepsilon}\nabla\times\frac{1}{\mu}\nabla\times E = \lambda E, \\ \nabla\cdot\varepsilon E = 0 \end{cases} \tag{7.10}$$

or

$$\begin{cases} \frac{1}{\mu}\nabla\times\frac{1}{\varepsilon}\nabla\times H = \lambda H, \\ \nabla\cdot\mu H = 0, \end{cases} \tag{7.11}$$

each of which contains only one of the electric and magnetic fields. Here we denote $\lambda = (\omega/c)^2$. This notation will be used from now on. The spectrum of either of these two problems determines the spectrum of M.

We will be mostly concerned with the case when $\mu = 1$, so (7.10) and (7.11) reduce to

$$\begin{cases} \frac{1}{\varepsilon}\nabla\times\nabla\times E = \lambda E, \\ \nabla\cdot\varepsilon E = 0 \end{cases} \tag{7.12}$$

and

$$\begin{cases} \nabla\times\frac{1}{\varepsilon}\nabla\times H = \lambda H, \\ \nabla\cdot H = 0. \end{cases} \tag{7.13}$$

The problem (7.12) can also be rewritten after introducing a new vector field $F = \varepsilon^{1/2}E$ as follows:

$$\begin{cases} -\varepsilon^{-1/2}\Delta\Pi\varepsilon^{-1/2}F = \lambda F, \\ \nabla\cdot\varepsilon^{1/2}F = 0, \end{cases}$$

where Δ is the Laplace operator and Π is the orthogonal projector onto the space of transverse vector fields. This restatement of the problem has proven to be useful, for instance, in localization problems (see [42]). In most cases when we refer to the Maxwell equations, we will mean (7.13).

Note that for $\lambda \neq 0$ the second equation in either of the systems (7.10) or (7.11) is a consequence of the first one. One is thus tempted to eliminate the zero divergency conditions altogether and to study only the "Schrödinger-type" first equations in (7.12) or (7.13), which can be called the eigenvalue problem for the unrestricted Maxwell operator. This introduces a large kernel consisting of longitudal waves (gradients of scalar functions), without changing the spectrum otherwise. Sometimes this trick works well, but in many cases the huge kernels that arise in this approach make analytic and numerical studies harder. This is related to the nonellipticity of the Maxwell operator. In fact, the truth is that the Maxwell operator *is* elliptic, if ellipticity is understood in an appropriate sense. Namely, this operator should not be considered alone, but rather as a part of what is usually called an elliptic complex of operators. Rather than going into the details of the general notion of an elliptic complex (which does not seem to bring any insights about photonic crystals), we will provide a simple explanation of some of the corresponding notions. Let us consider for simplicity the curl operator $\nabla^\times$ instead of the full Maxwell operator M. What are the indications that the curl is not an elliptic operator? If it were, then on a compact manifold its kernel (considered in appropriate spaces) would be finite dimensional, while its range would have finite codimension. Consider the case of the torus $\mathbb{T} = \mathbb{R}^3/\mathbb{Z}^3$, where $\mathbb{Z}^3$ is the integer lattice in $\mathbb{R}^3$. Then the gradient of any function on $\mathbb{T}$ belongs to the kernel of $\nabla^\times$, which shows that the kernel is infinite dimensional. There is a similar situation with the range: every function in the range of $\nabla^\times$ has zero divergence, which means that the range is of infinite codimension. The nonellipticity of curl is also clear from its Fourier domain representation as multiplication (up to a scalar factor) by the matrix

$$\begin{pmatrix} 0 & -\xi_3 & \xi_2 \\ \xi_3 & 0 & -\xi_1 \\ -\xi_2 & \xi_1 & 0 \end{pmatrix}$$

with the determinant identically equal to zero.

The correct point of view at the operator $\nabla^\times$ is to include it into the sequence of operators

$$0 \to C^\infty(\mathbb{T}) \xrightarrow{\nabla} [C^\infty(\mathbb{T})]^3 \xrightarrow{\nabla^\times} [C^\infty(\mathbb{T})]^3 \xrightarrow{\nabla\cdot} C^\infty(\mathbb{T}) \to 0$$

(where the C^∞ spaces can be replaced by appropriate spaces of Sobolev type). This is an example of an elliptic complex. This means that, first, composition of any two consecutive operators is zero. Second, the cohomologies of this complex (i.e., the quotient spaces of the kernel of each next operator modulo the range of the previous one) are finite dimensional. The whole Maxwell operator M can be included into an elliptic complex in a similar way. There is a trick commonly used in geometry that naturally reduces the study of such a complex to a single elliptic matrix operator. A similar technique is known in the study of overdetermined systems of partial differential equations, where it is sometimes called the method of orthogonal extension (see [93]). Let us show how it works in the particular cases of the curl and Maxwell operators. Consider the operator $\nabla^\times$ acting on vector fields E, add one more scalar function f so the operator now acts on pairs (E, f), and define the extended operator as

$$\begin{pmatrix} \nabla^\times & \nabla \\ -\nabla\cdot & 0 \end{pmatrix}.$$

One can easily check ellipticity of this extended operator (for instance, by taking the Fourier transform). The subspace of vectors of the form $(\mathbf{E}, 0)$, where $\mathbf{E}$ is divergence free, reduces the extended operator, and on this subspace it coincides with the curl. Analogously, one can include the Maxwell operator M into the larger elliptic operator

$$\mathfrak{M} = \begin{pmatrix} 0 & 0 & -\frac{i}{\varepsilon}\nabla\times & -i\nabla \\ 0 & 0 & i\nabla\cdot\mu & 0 \\ \frac{i}{\mu}\nabla\times & i\nabla & 0 & 0 \\ -i\nabla\cdot\varepsilon & 0 & 0 & 0 \end{pmatrix}$$

acting in the space

$$L^2(\mathbb{R}^3, \varepsilon(x)dx; \mathbb{C}^3) \oplus L^2(\mathbb{R}^3, dx) \oplus L^2(\mathbb{R}^3, \mu(x)dx; \mathbb{C}^3) \oplus L^2(\mathbb{R}^3, dx).$$

Here we denoted by $\nabla \cdot \varepsilon$ the operator acting on a vector field u as $\nabla \cdot \varepsilon u$. One can easily define $\mathfrak{M}$ as a self-adjoint operator. This extension to a larger elliptic problem is often useful in obtaining estimates and in other situations (see, for instance, [22, 93]).

7.2.3 Variational Formulation and Energy

The energy density of the field (E, H) in (7.1) can be defined as

$$\mathcal{E}(x,t) = \frac{1}{2}\left\{\varepsilon(x)\left|E(x,t)\right|^2 + \mu(x)\left|H(x,t)\right|^2\right\}$$

with the corresponding physical energy

$$E = \int \mathcal{E}(x,t)dx.$$

Each of the problems (7.12) and (7.13) allows a variational formulation of finding stationary points of the ratios

$$\frac{\int \left|\nabla \times E(x)\right|^2 dx}{\int \left|E(x)\right|^2 \varepsilon(x)dx}$$

and

$$\frac{\int \left|\nabla \times H(x)\right|^2 \varepsilon^{-1}(x)dx}{\int \left|H(x)\right|^2 dx},$$

respectively (subject to the natural zero divergence restrictions). This formulation is used, for instance, in the numerical treatment of these problems by finite element methods.

7.2.4 Scaling Properties

The problems (7.12) and (7.13) look similar to the spectral problem for a Schrödinger operator (with $\varepsilon(x)$ playing the role of a "potential," or rather of a metric). Although this analogy is useful, it can be misleading, since the Maxwell operator enjoys many properties different from those of Schrödinger operators. The scaling property is one of them. Consider, for instance, the problem (7.12):

$$\begin{cases} \nabla \times \nabla \times E = \lambda \varepsilon(x) E, \\ \nabla \cdot \varepsilon E = 0. \end{cases}$$

It is straightforward to compute that change of variables $x' = sx$ and simultaneous change of the spectral parameter $\lambda' = \lambda/s^2$ reduces the problem (7.12) to the similar one with the rescaled dielectric function $\varepsilon'(x) = \varepsilon(x/s)$. This means that in rescaling the dielectric function of a medium, we do not need to recompute the spectrum, since its simple rescaling would do. This observation has significant implications. It shows that the Maxwell equations do not have any fundamental length scale besides the requirement that they be macroscopic. For instance, if one finds some spectral phenomenon on the microwave scale, then the similar (rescaled) effect holds in the visible light region of frequencies. This is a significant departure from the Schrödinger case, where the Bohr radius provides a fundamental length scale for potentials. However, one should realize that manufacturing the materials for one length scale (for instance, for the visual light wave length) could be much harder than for another (microwaves).

Another important scaling property deals with the values of the electric permittivity function $\varepsilon(x)$. Assume that it is multiplied by a constant scaling factor s: $\varepsilon'(x) = s\varepsilon(x)$. It is obvious that the spectral problem for the new dielectric function ε' is reduced to the old one by rescaling the eigenvalues according to the formula $\lambda = s\lambda'$. This means that there is no fundamental value of the dielectric constant. In particular, in any homogeneous medium the spectrum always starts at zero, the property that is in striking contrast with the Schrödinger case. Among the important implications are different mechanisms of opening spectral gaps and of creating impurity spectra.

7.2.5 Two-Dimensional Case. TM and TE Polarizations

If a medium has material tensors independent of one of the coordinates, we will call it a "two-dimensional medium." Let us assume that $\mu = 1$ and $\varepsilon(x) = \varepsilon(x_1, x_2)$ is independent on the third coordinate x_3. We will consider the waves propagating in the (x_1, x_2)-plane only. In other words, the electromagnetic field $(\mathbf{E}, \mathbf{H})$ is x_3-independent. It is straightforward to check that on the space of such fields the Maxwell operator

$$M = \begin{pmatrix} 0 & -\frac{i}{\varepsilon}\nabla\times \\ i\nabla\times & 0 \end{pmatrix}$$

is reduced by the direct decomposition $S_1 \oplus S_2$, where S_1 consists of the fields $(E_1, E_2, 0, 0, 0, H)$ and S_2 consists of the fields $(0, 0, E, H_1, H_2, 0)$. In other words,

S_1 consists of the transverse electric (TE) polarized fields (or H-fields), in which the magnetic field is directed along the x_3 axis and the electric field is normal to this axis. Analogously, S_2 consists of transverse magnetic (TM) polarized fields (E-fields) with the electric field parallel and magnetic field normal to the x_3 axis. One can come to the conclusion that this reduction of the operator is due to the fact that in this case the Maxwell equations are mirror symmetric with respect to any mirror orthogonal to the axis x_3 (see [106]).

On the space S_2 the spectral problem for the Maxwell operator reduces to the scalar problem of Helmholtz type

$$-\Delta E = \lambda \varepsilon E, \tag{7.14}$$

while on S_1 it reduces to the divergence-type problem

$$-\nabla \cdot \frac{1}{\varepsilon} \nabla H = \lambda H. \tag{7.15}$$

These two spectral problems also arise when one considers acoustic waves in media with periodically varying parameters. Thus, many results obtained for photonic crystals can be transferred to the case of such waves. The acoustic interpretation also makes the consideration of the three-dimensional analogs of the scalar spectral problems (7.14) and (7.15) meaningful, although they do not reduce the Maxwell operator anymore. We will not, however, concentrate on the acoustic situation.

We would like to mention a rather standard transformation that can be applied to the problem (7.15) in $\mathbb{R}^d$ with smoothly varying $\varepsilon(x)$ to transfer it to a problem resembling (7.14). Here we will assume that the medium is isotropic, and hence the material tensor ε is just a sufficiently smooth periodic function $\varepsilon \geq 1$. We are interested in invertibility of the (suitably defined by quadratic forms) operator

$$L_\lambda u = -\nabla \cdot \frac{1}{\varepsilon} \nabla u - \lambda u$$

in $L^2(\mathbb{R}^d)$. The transformation works as follows:

$$L_\lambda \to H_\lambda = \sqrt{\varepsilon} L_\lambda \sqrt{\varepsilon}. \tag{7.16}$$

The multiplication by $\sqrt{\varepsilon}$ is an invertible operator in $L^2(\mathbb{R}^d)$ and, if ε is smooth enough, it preserves the domain of the operator L_λ. Thus, the operators L_λ and H_λ are invertible simultaneously. A straightforward calculation shows that

$$H_\lambda = -\Delta + V - \lambda \varepsilon,$$

where

$$V = \frac{3(\nabla \varepsilon)^2}{4\varepsilon^2} - \frac{\Delta \varepsilon}{2\varepsilon}.$$

We conclude that λ is in the spectrum of the operator $-\nabla \cdot \frac{1}{\varepsilon} \nabla$ if and only if the operator H_λ is not invertible, i.e., when λ is in the spectrum of the Schrödinger operator pencil $-\Delta + V - \lambda \varepsilon$.

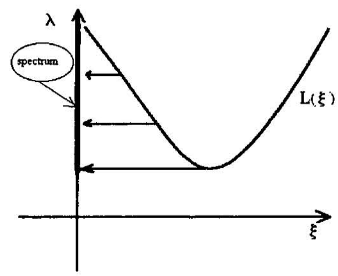

Figure 7.1: The spectrum of the operator of multiplication by $L(\xi)$.

The transform described above is sometimes called Liouville–Green transform and is frequently used in problems of spectral theory (see, for instance, [16, 25, 26, 49, 117]). In particular, nonexistence of bound states for the Schrödinger operator H_λ implies their absence for the operator L_λ. Unfortunately, this transform does not work in the case when the material tensors are piecewise constant, which is the standard situation for photonic crystals.

7.3 Periodic Media and Floquet–Bloch Theory

So far our considerations do not involve any periodicity requirement for the medium. However, as has already been mentioned, the main feature of a (pure) photonic crystal is periodicity of its structure. Let us discuss in very general terms why periodicity is a favorable environment for spectral gaps. In order to do this we need to provide some information about periodic (elliptic) differential operators and Floquet theory, which in the periodic case plays the role of the Fourier transform. Many aspects of this theory are discussed in detail in books and surveys [54, 116, 123, 124, 145, 157, 173, 174, 179, 185]. Some additional references on this subject will be provided later in the text. Many physics books also address this topic, for instance, [5, 36].

Let us start considering a constant coefficient partial differential operator[1] $L(D)$ in $L^2(\mathbb{R}^n)$, where $D = -i\nabla$. In fact, what we will discuss is also applicable to more general convolution operators, where $L(\xi)$ does not have to be a polynomial. The operator is invariant with respect to the (transitive) action of the additive group $\mathbb{R}^n$ on itself via translations. This leads to the natural idea of applying the Fourier transform on this group, which is the standard Fourier transform. After applying the Fourier transform, L becomes the operator of multiplication by the function $L(\xi)$ in $L^2(\mathbb{R}^n)$, where ξ denotes the variable dual to x. It is clear that the spectrum of such an operator coincides with the (closure of the) set of all values of $L(\xi)$. In other words, if we draw the graph of the function $\lambda = L(\xi)$, its projection on the λ-axis produces the spectrum (Figure 7.1).

It is also important to understand when the point spectrum can arise. If there is a nonzero L^2-function $f(\xi)$ and an eigenvalue λ such that $L(\xi)f(\xi) = \lambda f(\xi)$ a.e., one immediately concludes that $L(\xi) = \lambda$ on a set of positive measure. The converse

[1] We intentionally avoid here any discussion of exact definition of the operator, its domain, etc.

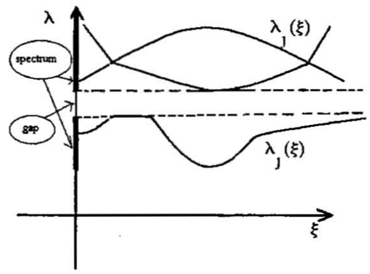

Figure 7.2: The band gap structure of the spectrum in the matrix case.

statement is also correct: positivity of the measure of the set where $L(\xi) = \lambda$ implies existence of an eigenfunction. In the important particular case when $L(\xi)$ is analytic, this would imply that $L(\xi)$ is constant.

Another step toward periodic operators is to consider a system $L(D)$ (i.e., the symbol $L(\xi)$ is a self-adjoint matrix function). It is rather clear then that the spectrum can be found as follows: find the (continuous) eigenvalue branches $\lambda_j(\xi)$ ("dispersion relations" or "band functions") of the matrix function $L(\xi)$ and take their ranges (i.e., project their graphs onto the λ-axis). Each of the branches then provides a band (i.e., a segment) in the spectrum. One can expect that in some cases the bands might have a gap between them (Figure 7.2).

As in the scalar case, existence of the point spectrum is equivalent to existence of flat pieces on the graphs of the band functions, which in the analytic situation implies existence of a constant branch.

Let us now tackle periodic operators. Consider a linear partial differential operator $L(x, D)$, whose coefficients are periodic with respect to a discrete group of translations Γ acting on $\mathbb{R}^d$. Assume, for instance, that Γ is the integer lattice $\mathbb{Z}^d$; this assumption is made for simplicity only and does not restrict generality of our consideration.[2] In analogy with the constant coefficient case, due to invariance of the operator with respect to this group, it is natural to apply the Fourier transform on Γ. "Fourier transform" on $\Gamma = \mathbb{Z}^d$ is in fact the Fourier series, which assigns to a sufficiently fast decaying function $h(n)$ on $\mathbb{Z}^d$ the Fourier series

$$\widehat{h}(k) = \sum_{n \in \mathbb{Z}^d} h(n) e^{ik \cdot n},$$

where $k \in \mathbb{R}^d$ (or $\mathbb{C}^d$). We have to somehow apply this transform to functions defined on $\mathbb{R}^d$. Let $f(x)$ be a function decaying sufficiently fast. We can define its *Floquet transform* (sometimes called *Gelfand transform*) as follows:

$$\mathcal{U}f(x, k) = \sum_{n \in \mathbb{Z}^d} f(x - n) e^{ik \cdot n}. \tag{7.17}$$

This transform is an analog of the Fourier transform for the periodic case. The parameter k is called *quasi momentum*, and it is an analogue of the dual variable

[2]The reader can refer to [5, 106] for a brief introduction into general lattices, Brillouin zones, etc.

in the Fourier transform. Notice that in contrast to the Fourier transform the transformed function still depends on the old variable x. The reason is that the action of the group Γ on $\mathbb{R}^d$ is not transitive, and hence the space of orbits of this action contains more than one point, while in the constant coefficient case we deal with a transitive action of $\mathbb{R}^d$ on itself. One should notice the two following important relations. If we shift x by a period $m \in \mathbb{Z}^d$, then we get the relation

$$(\mathcal{U}f)(x+m,k) = e^{ik\cdot m}(\mathcal{U}f)(x,k). \tag{7.18}$$

This is the *Floquet condition.* It shows that it is sufficient to know the function $\mathcal{U}f(x,k)$ only at one point x on each orbit $x+\mathbb{Z}^d$ in order to recover it completely. For instance, it is sufficient to know it only for $x \in F$, where F is a fundamental domain for the action of $\mathbb{Z}^d$ on $\mathbb{R}^d$. A domain F in $\mathbb{R}^d$ is called a fundamental domain for the action of $\mathbb{Z}^d$ if each orbit has a representative in the closure $\overline{F}$ of F and every point of F is a unique representative in F of its orbit. In other words,

$$\cup_{m\in\mathbb{Z}^d}(\overline{F}+m) = \mathbb{R}^d$$

and $\overline{F}+m$ and $\overline{F}$ can intersect only along their boundaries. One way to find a fundamental domain is to consider all points x that are closer to the origin $0 \in \Gamma$ than to any other point of Γ. An example of a fundamental domain for the action of $\mathbb{Z}^d$ on $\mathbb{R}^d$ by translation is the unit cube

$$W = \left\{x \in \mathbb{R}^d \,|\, 0 \le x_j \le 1,\ j=1,\dots,d\right\}.$$

In physics the fundamental domains are often called *Wigner–Seitz cells.*

The second simple observation is that the function $\mathcal{U}f(x,k)$ is periodic with respect to the quasi momentum k. Indeed,

$$\mathcal{U}f(x,k+2\pi m) = \mathcal{U}f(x,k), \qquad m \in \mathbb{Z}^d.$$

Notice that the lattice of the periods with respect to k is different from the lattice with respect to which the operator was periodic. Now it is $\Gamma^* = 2\pi\mathbb{Z}^d$, which is the *dual (or reciprocal) lattice* to $\Gamma = \mathbb{Z}^d$. We conclude that k can be considered as an element of the torus $\mathbb{T}^* = \mathbb{R}^d/2\pi\mathbb{Z}^d$. Another way of saying this is that all information about the function $\mathcal{U}f(x,k)$ is contained in its values for k in the fundamental domain of the dual lattice $\Gamma^* = 2\pi\mathbb{Z}^d$. We can define such a domain B as the set of all vectors k that are closer to the origin than to any other point of Γ^*. In solid-state physics this domain is called the (first) *Brillouin zone.*

As the result, after the Floquet transform one ends up with a function $\mathcal{U}f(x,k)$, which can be considered as a function of k on the torus $\mathbb{T}^*$ (or on the Brillouin zone B) with values in a space of functions of x on the compact Wigner–Seitz cell W. As we will soon see, compactness of the new domain plays the crucial role in the whole Floquet theory.

Now consider the effect of the Floquet transform on a periodic differential operator $L(x,D)$. Due to periodicity, the operator commutes with the transform

$$\mathcal{U}(Lf)(x,k) = L(x,D_x)\mathcal{U}f(x,k),$$

where by the subscript x in D_x we indicate that D differentiates with respect to x rather than k. For each k the operator $L(x, D_x)$ now acts on functions satisfying the corresponding Floquet condition (7.18). In other words, although the differential expression of the operator stays the same, its domain changes with k. If we denote this operator by $L(k)$, we see that the Floquet transform expands the operator L in $L^2(\mathbb{R}^d)$ into the "direct integral" of operators

$$\int_{\mathbb{T}^*}^{\oplus} L(k)dk$$

(see, for instance, discussion of this notion in [157]). This is analogous to the situation of the constant coefficient systems of equations, only instead of matrices $L(\xi)$ we have to deal with operators $L(k)$ in infinite-dimensional spaces. The crucial circumstance is that these operators act on functions defined on a compact manifold (a torus), while the original operator L acted in $\mathbb{R}^d$. Thus, under appropriate ellipticity conditions, these operators have compact resolvents, and hence discrete spectra. Then we can define again the *band functions (dispersion relations)* $\lambda_j(k)$ and obtain a picture analogous to Figure 7.2 with the difference that the number of branches is now infinite. We see that the spectrum is expected to have a band structure, and there is hope of opening spectral gaps.

We will now provide a slightly more detailed discussion of the Floquet transform $\mathcal{U}$ and of its effects on function spaces and differential operators. We will still assume that $\Gamma = \mathbb{Z}^d$, since the case of a general lattice of translations does not at this stage introduce any actual difficulties besides complicating the notations.

Let us introduce an alternative version of the transform $\mathcal{U}$. This version is often useful. We define the transform Φ as follows:

$$\Phi f(x,k) = \sum_{n \in \mathbb{Z}^d} f(x-n)e^{-ik\cdot(x-n)} = e^{-ik\cdot x}\mathcal{U}f(x,k).$$

While the function $\mathcal{U}f(x,k)$ was periodic in k and satisfied the Floquet condition with respect to x, the function $\Phi f(x,k)$ is periodic with respect to x and satisfies a cyclic condition with respect to k:

$$\begin{cases} \Phi f(x+n,k) = \Phi f(x,k), & n \in \Gamma = \mathbb{Z}^d, \\ \Phi f(x,k+\gamma) = e^{-i\gamma\cdot x}\Phi f(x,k), & \gamma \in \Gamma^* = 2\pi\mathbb{Z}^d. \end{cases} \tag{7.19}$$

Now when k changes, the values of $\Phi f(\cdot,k)$ belong to the same space of functions of x on the torus $\mathbb{T} = \mathbb{R}^d/\mathbb{Z}^d$. It is still sufficient, however, to know the values of $\Phi f(x,k)$ for x in the Wigner–Seitz cell W and k in the Brillouin zone B in order to recover the whole function. The transform Φ does not commute with periodic differential operators anymore. A straightforward calculation shows that

$$\Phi(Lf)(x,k) = L(x, D_x + k)\Phi f(x,k) = L(k)\Phi f(\cdot,k). \tag{7.20}$$

So, while we gained a fixed function space, now the differential expression for the operator changes with k.

The main tools needed when one uses Fourier transform are the Plancherel and Paley–Wiener theorems. In the periodic case we need similar statements for the Floquet transforms $\mathcal{U}$ and Φ, since they become crucial in all aspects of spectral theory of periodic operators. Let us first formulate an analogue of the Plancherel theorem. In the theorem below we assume that the natural measures dk on the Brillouin zone B and the dual torus $\mathbb{T}^*$ are normalized.

THEOREM 7.2. *The transforms*

$$\mathcal{U}: L^2(\mathbb{R}^d) \to L^2(\mathbb{T}^*, L^2(W)), \qquad \Phi : L^2(\mathbb{R}^d) \to L^2(B, L^2(\mathbb{T}))$$

are isometric. Their inverse transforms are

$$\Phi^{-1}v(x) = \int_B e^{ix\cdot k} v(x,k)dk$$

and

$$\mathcal{U}^{-1}w(x) = \int_{\mathbb{T}^*} w(x,k)dk,$$

where the function $v(x,k) \in L^2(B, L^2(\mathbb{T}))$ is considered a periodic function with respect to $x \in \mathbb{R}^n$ and $w(x,k) \in L^2(\mathbb{T}^*, L^2(W))$ is extended from W to all $x \in \mathbb{R}^n$ according to the Floquet condition (7.18).

This theorem, used constantly in solid-state physics since Bloch [28], was introduced into mathematics for spectral analysis of periodic differential operators by Gelfand [85] and further investigated in [149, 191] (see section XIII.16 of [157] and Chapters 2 and 4 of [123] for discussion and further references). The proof is straightforward if one notices that (7.17) is just a Fourier series with coefficients in the Hilbert space $L^2(W)$ and uses the standard Plancherel's theorem for such series. It is easy to prove an analogue of such a theorem for the Sobolev space $H^s(\mathbb{R}^d)$ instead of $L^2(\mathbb{R}^d)$. Namely, it is transformed by Φ isomorphically onto the space $L^2(B, H^s(\mathbb{T}))$. In terms of the transform $\mathcal{U}$ the situation becomes more technical. Let us define for each $k \in \mathbb{T}^*$ the closed subspace H^s_k of the space $H^s(W)$ consisting of restrictions to W of all functions from $H^s_{loc}(\mathbb{R}^d)$ which satisfy the Floquet condition (7.18). It is easy to conclude (see Theorem 2.2.1 in [124]) that

$$\mathcal{E}^s = \bigcup_{k\in\mathbb{T}^*} H^s_k$$

is a Hilbert vector bundle over $\mathbb{T}^*$. Then one can show that the transform $\mathcal{U}$ maps isomorphically the space $H^s(\mathbb{R}^d)$ onto the Hilbert space $L^2(\mathbb{T}^*, \mathcal{E}^s)$ of L^2-sections over $\mathbb{T}^*$ of the bundle $\mathcal{E}^s$.

Let us now move to the Paley–Wiener-type theorems. By this we mean the theorems that describe the images under the Floquet transform of spaces of sufficiently fast decaying functions on $\mathbb{R}^n$. One can notice that while the classical Paley–Wiener theorem deals with spaces of compactly supported functions, such a theorem, although easily provable, has not been useful so far for the Floquet transform.

It is a commonplace that Paley–Wiener theorems require extension into the complex domain of the dual variable. The same is true for the Floquet transform. One can see that both transforms $\mathcal{U}$ and Φ can be defined on compactly supported or sufficiently fast decaying functions also for complex quasi momenta k. The bundles $\mathcal{E}^s$ also extend into the complex domain to analytic infinite-dimensional bundles (see Theorem 2.2.1 in [124]). The reader unfamiliar with the technique of infinite-dimensional bundles can think of a closed subspace of a fixed Hilbert space, where the subspace depends analytically upon the parameter k (for instance, there is a projector onto the subspace, which depends analytically on k). One can now obtain analogues of the Paley–Wiener theorem for several spaces of decaying functions. This is done in the Theorem 2.2.2 of [124]. In order to avoid technicalities, we will loosely describe the corresponding results, referring the reader to [124] for details. For instance, the space of functions that belong to $H^s_{loc}(\mathbb{R}^n)$ and decay exponentially in the H^s sense

$$||f||_{H^s(W+n)} \leq Ce^{-a|n|} \tag{7.21}$$

goes over to the space of sections of the bundle $\mathcal{E}^s$ that are analytic over a specific neighborhood of the real space $\mathbb{R}^d$ in $\mathbb{C}^d$. Availability of the estimate (7.21) for arbitrary $a > 0$ is equivalent to the fact that the function $\mathcal{U}f$ is entire with respect to k. If the estimate (7.21) is strengthened to require decay of order higher than 1,

$$||f||_{H^s(W+n)} \leq Ce^{-a|n|^p}, \qquad p > 1,$$

this is reflected in growth estimates on the corresponding entire function. All these theorems are important for periodic partial differential equations and for the spectral theory in particular, as will be mentioned later (one can also refer to Chapter 4 of [124] and to papers [9, 10, 78, 120, 131, 132] for examples of such applications).

Let us now reflect a little bit on the effect that the Floquet transform has on the operators. As we have mentioned already, the periodic operator $L(x, D)$ in $\mathbb{R}^d$ after the Floquet transform becomes a family (in fact, a polynomial with respect to k) of operators $L(k) = L(x, D+k)$. Here each of the operators $L(k)$ acts on the torus $\mathbb{T}$, which is a compact closed manifold. In particular, if L is elliptic, we are dealing with an analytic (polynomial) operator function $L(k)$ whose values are Fredholm operators in appropriate spaces. This enables one to invoke the rich theory of such operator functions (see, for instance, [193] and Chapter 1 of [124] for its discussion and further references).

Ellipticity (or at least hypoellipticity, for instance, parabolicity) of the operator is crucial. It influences not only the technique, but also the results one might expect (see [124]). Here one can see what kind of difficulties can be expected with the Maxwell operator. As we have already discussed before, the Maxwell operator taken alone is not elliptic. The correct idea is to include it into an elliptic complex (or to extend to a larger elliptic operator, which is essentially the same). Consider the example of the homogeneous Maxwell operator $M = (\nabla^{\times})^2$ acting from the cokernel of the gradient into the kernel of divergence. Here arises the problem: after the Floquet transform the operator $M(k)$ will act between the cokernel of grad$(k) = (\nabla + ik)$ and the kernel of div$(k) = (\nabla + ik)\cdot$, where all operators are acting now on periodic functions. It is easy to check by the Fourier series expansion, however, that these spaces (i.e., cokernel and kernel, respectively) do not depend analytically on k. If

$$F(x) = \sum F_\gamma e^{i\gamma\cdot x}$$

is the Fourier series of a periodic vector field F, then

$$(\nabla - ik)\cdot F = \sum i(\gamma + k)\cdot F_\gamma e^{i\gamma\cdot x}.$$

One can see a degeneration of the kernel at the point $k = 0$. Namely, for $k \neq 0$ the condition $(\nabla + ik)\cdot F = 0$ implies that the vectors $(\gamma + k)$ and F_γ are orthogonal, and so F_γ belongs to the two-dimensional orthogonal complement of $(\gamma + k)$. On the other hand, for $k = 0$ the coefficient F_0 can be arbitrary. This means a non-analytic behavior of Ker(div(k)) at $k = 0$. The same thing is true for the cokernel of grad(k). In technical terms this requires one to work with sections of analytic sheaves instead of sections of analytic vector bundles. Although this is possible (see, for instance, [150], where the main result of [123, 124] was extended to the case of elliptic complexes), the technical complications can sometimes be severe.

7.4 Spectra in Periodic Media

In this section we will focus on the spectral properties of periodic (elliptic) differential operators, including the Maxwell operator.

7.4.1 Band Gap Structure

As we have already explained, the spectra of periodic elliptic differential operators exhibit band gap structure. Let us discuss this a little bit more (see [157, 179, 124] for details and references). If we have a self-adjoint periodic operator $L = L(x, D)$ in $L^2(\mathbb{R}^d)$, the Floquet transform expands it into the direct integral of operators $L(k) = L(x, D + k)$ on the torus $\mathbb{T}$.

One can prove the main spectral statement:

$$\sigma(L) = \bigcup_{k\in B} \sigma(L(k)) \tag{7.22}$$

(see [91, 54, 149, 157, 179, 124]). Due to ellipticity, the spectrum of each $L(k)$ is discrete. If L is bounded from below, the spectrum of $L(k)$ accumulates only at the positive infinity. Let us denote by $\lambda_n(k)$ the nth eigenvalue of $L(k)$ (counted in increasing order with their multiplicity). This continuous function of $k \in B$ is called a *band function* (or one branch of the *dispersion relations*). We conclude that the spectrum $\sigma(L)$ consists of the closed intervals (called the spectral bands)

$$S_n = [\min_k \lambda_n(k), \max_k \lambda_n(k)],$$

where $\min_k \lambda_n(k) \to \infty$ when $n \to \infty$. It is well known that for ordinary differential operators of the second order the bands cannot overlap (although they can touch), which explains why it is a generic situation in one dimension that gaps open in the spectrum between adjacent bands (see [157]). In dimensions 2 and higher the bands can and normally do overlap, which makes opening gaps much harder. It is still conceivable that at some selected locations the bands might not overlap and hence open a gap in the spectrum. What we have just described is called the band gap structure of the spectrum for elliptic (or hypoelliptic) periodic differential operators. This is what triggered hopes for creating photonic crystals as dielectric materials of periodic structure.

It is not difficult to derive the band gap structure of the spectrum of the periodic Maxwell operator. This can be done either by including it into an elliptic complex (and following the line of [150]) or by using an orthogonal extension to an elliptic operator, as was discussed above. It looks like this standard derivation of the band gap structure of the spectrum for the periodic Maxwell operator has never been written down, except the two-dimensional version described in [78]. One usually refers to this as "according to the Floquet theory" (with no references provided).

One can make a simple useful remark about the representation (7.22). Namely, not all quasi momenta k are needed in the right-hand side of (7.22). It is sufficient to use any dense subset S of the Brillouin zone B and then take closure of the union of the corresponding spectra:

$$\sigma(L) = \overline{\bigcup_{k \in S} \sigma(L(k))}. \tag{7.23}$$

There are at least two important choices for the subset S. First, as we mentioned in section 7.3, there are values of the quasi momentum that are "bad" for the Maxwell operator (i.e., at which the cokernel of the gradient and the kernel of the divergence lose analyticity). One can just skip these values and then take the closure of the union of the remaining spectra instead. In some cases (like, for instance, in [78]) this works just fine, while it does not eliminate the problem completely in other situations. This trick can also be used in numerics, when some values of quasi momenta cause trouble. Second, it is often useful and commonly used in solid-state physics to represent the spectrum $\sigma(L)$ as the limit of spectra on finite domains. Consider a cube K in $\mathbb{R}^d$ and stretch it: $K_m = mK, m = 1, 2, \ldots$. We can naturally define operators L_m in $L^2(K_m)$ using the differential expression $L(x, D)$ with periodic boundary conditions on K_m. If L is elliptic with sufficiently decent coefficients, there is no ambiguity in such a definition. Then one can show that the spectrum $\sigma(L)$ coincides with the closure

$$\overline{\bigcup_m \sigma(L_m)} = \lim_{m \to \infty} \sigma(L_m). \tag{7.24}$$

This is clearly just a particular case of (7.23) when we use the subset of all quasi momenta with components commensurable with a given number. The important relation (7.24) is often proven for specific operators, although it holds for periodic elliptic operators in general and follows from (7.23).

7.4.2 Fermi and Bloch Varieties

We are now going to define two objects of paramount importance for the theory of periodic elliptic (and hypoelliptic) operators. Although they are often used in solid-state physics, their roles are not always completely appreciated. They are analogues of the set of zeros of the symbol of a constant coefficient operator, which is known to determine many properties of such an operator.

Let $L(x, D)$ be a periodic elliptic operator in $\mathbb{R}^d$. We define its *complex Bloch variety* as follows:

$B(L)$ consists of all points $(k, \lambda) \in \mathbb{C}^{d+1}$ such that the equation $L(k)u = \lambda u$ has a nonzero solution $u(x)$ satisfying (7.18).

The *real Bloch variety* $B_R(L)$ is the intersection of $B(L)$ with the real space $\mathbb{R}^{d+1}$. It is clear that the real Bloch variety of the operator L is just the union of graphs of all band functions $\lambda_j(k)$. In other words, the Bloch variety is the graph of the multivalued dispersion relations for the operator L. In particular, the spectrum of the self-adjoint operator L is equal to the projection of $B_R(L)$ onto the λ-axis.

The level sets of the dispersion relations are also of interest. For a given $\lambda \in \mathbb{C}$ we call the *Fermi surface* of the operator L on the level λ the set $F_\lambda(L)$ consisting of all points $k \in \mathbb{C}^d$ such that the equation $L(k)u = \lambda u$ has a nonzero solution $u(x)$ satisfying (7.18). Analogously to the real Bloch variety, we define

$$F_{R,\lambda}(L) = F_\lambda(L) \cap \mathbb{R}^d.$$

It is immediately clear that for a self-adjoint operator L

$$\lambda \in \sigma(L) \Longleftrightarrow F_{R,\lambda}(L) \neq \emptyset.$$

One can imagine that when λ changes, the (complex) Fermi surface moves, and the values of λ for which the surface touches the real space constitute the spectrum of the operator.

The following theorem establishes an important property of the Bloch and Fermi varieties.

THEOREM 7.3 ([124]; see also [120, 123]). *The set $B(L)$ coincides with the set of all zeros of an entire function $f(k, \lambda)$ of a finite order in $\mathbb{C}^{d+1}$. (Here an entire function $f(z)$ in C^n is said to be of the finite order p if it satisfies an estimate $|f(z)| \leq C \exp a\, |z|^p$.) A similar statement holds for the Fermi surface at any level λ.*

One can refer to Theorem 4.4.2, Corollary 3.1.6, and Theorem 3.1.7 of [124] for exact formulations, including the precise order of the entire function (see also further discussion and references in sections 3.5 and 4.7 of [124]). In particular, one concludes that $B(L)$ is an analytic subset of $\mathbb{C}^{d+1}$ in the sense of several complex variables [94], i.e., that it can be locally (and even globally) described by analytic equations (this particular corollary was probably first proven in [191]).

As is explained in [124], a similar statement holds for matrix operators. One can also show that it holds for the Maxwell operator as well (analyticity of $B(L)$ for this case, although without estimates, can be also extracted from [150]).

There is a natural action of the dual lattice Γ^* on the Bloch and Fermi varieties by shifts: $(k, \lambda) \to (k + \gamma, \lambda)$ and $k \to k + \gamma$ correspondingly, where $\gamma \in \Gamma^*$. Considering the case of a constant coefficient operator $L(D)$ one easily finds that

$$B(L) = \{(k, \lambda) |\, L(k + \gamma) - \lambda = 0 \,\text{for some}\, \gamma \in \Gamma^*\}$$

and

$$F_\lambda(L) = \{k |\, L(k + \gamma) - \lambda = 0 \,\text{for some}\, \gamma \in \Gamma^*\}\,.$$

In other words, one needs to find the set of zeros of the symbol $L(k) - \lambda$ and then take its orbit with respect to Γ^*.

An analytic set X is said to be *reducible* if it can be represented as the union of two smaller analytic subsets: $X = X_1 \cup X_2$. We remind the reader not familiar with this concept that if the function $f(z)$ whose set of zeros is X allows a nontrivial factorization $f = f_1 f_2$, then the sets of zeros of factors reduce X. An analytic set that is not reducible is called *irreducible* [94]. The example of a constant coefficient operator in the previous paragraph shows that one should discuss irreducibility of the Bloch and Fermi varieties only modulo the dual lattice. Irreducibility plays an important role in many problems of the spectral theory of periodic operators: in inverse spectral problems [90, 120], behavior with respect to impurities [131, 132], and others. The irreducibility of $B(L)/\Gamma^*$ was proven for the one-dimensional periodic Schrödinger operator by Kohn [121] and conjectured for the general periodic Schrödinger operator in [6, 120, 145]. It was proven in [120] in two dimensions using an intricate algebrogeometric approach. It is conjectured that $F_\lambda(L)/\Gamma^*$ is also irreducible in this case.

CONJECTURE 7.4. *The varieties $B(L)/\Gamma^*$ and $F_\lambda(L)/\Gamma^*$ are irreducible for any periodic second-order elliptic operator L, including the Maxwell operator.*

This problem looks even harder for the Fermi surface than for the Bloch variety. It was studied in detail for the discrete Schrödinger operator in the book [90] and for the discrete Maxwell operator in [9]. In both cases results on irreducibility of the Fermi surface $F_\lambda(L)/\Gamma^*$ were obtained by methods of algebraic geometry. It was shown in [10] that $F_\lambda(L)/\Gamma^*$ is irreducible for the Schrödinger operator in two dimensions with a separable periodic potential $v_1(x_1) + v_2(x_2)$ and in three dimensions for a separable periodic potential $v_1(x_1) + v_2(x_2, x_3)$.

Another consideration of interest is the following. When λ approaches the spectrum, the Fermi surface approaches the real space, and when λ enters the spectrum, $F_{R,\lambda}$ is not empty. It is natural to expect that when λ goes into the interior of a spectral band, the Fermi surface becomes sufficiently "massive." In fact, one can show that if λ belongs to the interior of a spectral band, then the Fermi surface $F_{R,\lambda}$ as a real analytic set has dimension at least $d - 1$.

It is also natural to assume that one should be able to estimate the distance from the point λ to the spectrum by the distance between the Fermi surface F_λ and the real space. Here is how this argument can go. First, if the Fermi surface is at a certain distance from the real space, this means that the equation $Lu = \lambda u$ has a Floquet–Bloch solution $u = e^{ik\cdot x}v(x)$ with a periodic $v(x)$ and with an estimate on $|\text{Im}k|$. In other words, we have an exponential estimate on $u(x)$. Then an argument of the type provided in the section 54 of [91] for the Schrödinger operator should lead to an estimate on the distance $d(\lambda, \sigma(L))$. It would be very interesting to extend this type of an argument to more general operators than Schrödinger (in particular, to the Maxwell operator) and to improve the estimates of [91] to the extent that one can deduce exponential localization estimates obtained in [42] (see section 7.6.3).

Concluding this section, I want to emphasize that analytic properties of the Bloch and Fermi varieties are very important for understanding spectra of corresponding operators: analyticity of these sets imply absolute continuity of the spectrum (section 7.4.3), irreducibility is crucial for inverse spectral problems [120] and for the absence of embedded impurity eigenvalues (section 7.6.4), and the way the Fermi surface approaches the real space is related to embedded eigenvalues (section 7.6.4) and to the exponential localization of impurity modes (section 7.6.3).

7.4.3 Absolute Continuity

As we have already discussed, the spectrum of any periodic elliptic or hypoelliptic operator L has a band gap structure. The natural question is about the type of spectrum that can arise (e.g., absolutely continuous, singular continuous, point). The general expectation is that in principle the spectrum must be absolutely continuous; i.e., no eigenvalues or singular continuous spectrum can arise. In fact, this is not true in general, since one can show existence of periodic elliptic operators of the fourth order that do have point spectrum (see [124, pp. 135–136]). However, there is very little doubt that absolute continuity holds for any second-order periodic elliptic operator, including Maxwell. There is one simple thing one can prove for a periodic elliptic operator of any order: the singular continuous spectrum is empty. The reason is that (as was understood since [28, 85]) the Floquet–Bloch transform represents the operator L as the infinite sum of operators of multiplication by the band functions $\lambda_n(k)$. Another important ingredient is that the band functions are piecewise analytic. Then it is not hard to conclude that each of these multiplication operators either is absolutely continuous or has an eigenvalue. In the latter case, the corresponding band function must be constant on a positive measure set of quasi momenta k and hence constant. This kind of consideration goes back to [184] and is presented in several places, for instance, in [157, 174, 124].

The task of proving absolute continuity of the spectrum now reduces to showing absence of eigenvalues. Although it has been unanimously believed by physicists for a long time, proving this statement happens to be a hard problem. For the Schrödinger case in three dimensions it was proven in the celebrated paper [184] by Thomas and then extended to more general potentials in [157] (see also [14]). Attempts to extend this theorem to more general periodic elliptic operators had failed for about 20 years, except the results of [50] for the Dirac operator and [98] for the magnetic Schrödinger operator with small magnetic potential. Then an avalanche of papers was triggered in 1997 by the paper [24], where absolute continuity was proven in two dimensions for the Schrödinger operator with both magnetic and electric potentials. The same year this result was extended in [180] to any dimension, which required a new technique. The proof of [180] was simplified in [128, 129]. The recent paper [142] contained the absolute continuity result for the two-dimensional Schrödinger operator with periodic metric. The paper [170] contains improved conditions on the potential. One can find more references and a nice survey of known results in [26].

We will now indicate the main thrust of Thomas's proof [184] and of all its extensions. The major step is to use analytic continuation into the domain of complex quasi momenta. The following theorem holds.

THEOREM 7.5 (Theorems 4.1.5 and 4.1.6 in [124]). *Let L be a periodic elliptic operator. Then the following statements are equivalent:*

(a) *The point λ is an eigenvalue of L in $L^2(\mathbb{R}^d)$, i.e., there is a nonzero L^2-solution of the equation $Lu = \lambda u$ in $\mathbb{R}^d$;*

(b) *The Fermi surface F_λ coincides with the whole space $\mathbb{C}^d$;*

(c) *There exists a nonzero solution of the equation $Lu = \lambda u$ in $\mathbb{R}^d$ that decays faster than any exponent:*

$$|u(x)| \leq C \exp(-a\,|x|) \quad \textit{for all } a > 0;$$

(d) *There exists a nonzero solution of the equation $Lu = \lambda u$ in $\mathbb{R}^d$ that decays superexponentially:*

$$|u(x)| \leq C \exp(-\,|x|^{1+\alpha}) \quad \textit{for some } \alpha > 0.$$

In fact, statements (c) and (d) are not needed for the standard proof of absolute continuity, but they are interesting on their own. The exact technical conditions on the operator can be found in [124]. Let us concentrate on the equivalence of (a) and (b), which can be easily explained. As we have already discussed, the operator of multiplication by $\lambda_n(k)$ has an eigenvalue λ if and only if the level set $\lambda_n(k) = \lambda$ has a positive measure. In terms of the Fermi surface $F_{R,\lambda}(L)$ this means that $F_{R,\lambda}(L)$ has a positive measure in $\mathbb{R}^d$. However, as we know already, it is an analytic set. The uniqueness theorems for analytic functions immediately imply that this can happen only when $F_\lambda(L) = \mathbb{C}^d$, and thus the equivalence of (a) and (b) is proven.

Let us interpret this result in a different way. If for each λ we can prove that $F_\lambda \neq \mathbb{C}^d$, then we conclude that there are no eigenvalues and hence that the spectrum is absolutely continuous. Recalling the definition of the Fermi surface, one obtains the following key corollary.

COROLLARY 7.6. *If for any λ there exists a quasi momentum $k \in \mathbb{C}^d$ such that the equation $L(k)u = \lambda u$ has no nontrivial solutions on the torus $\mathbb{T}$, then the spectrum of the operator L is absolutely continuous.*

Now one proves absolute continuity of the spectrum of the Schrödinger operator $-\Delta + v(x)$ with a periodic potential v if one can show the absence of periodic solutions of the equation $(D+k)^2u+vu = \lambda u$ for an appropriately chosen (depending on λ) quasi momentum k. It is not hard to choose a quasi momentum with a large imaginary part in such a way that the $(D+k)^2$ term dominates the zero-order terms, and hence no nontrivial solutions are allowed (see, for instance, [184, 157, 124] for details). Although the idea stays the same, treatment of more general operators becomes much more complex when one wants to show that $F_\lambda \neq \mathbb{C}^d$.

At this moment we want to address the case of the Maxwell operator, which is of main interest here. Unfortunately, absolute continuity of its spectrum has not been proven yet even for the case of smooth material tensors and for the isotropic medium.[3] Considerations of [128, 129] show that the technology developed in [180] leads for the Maxwell operator with smoothly varying parameters to a model problem that involves a simple covariant Cauchy–Riemann derivative operator on the torus.

For the case of a two-dimensional medium and for the waves propagating in the periodicity plane the result on absolute continuity can be extracted from the known results about operators of the Schrödinger type. Let us recall that, as was discussed in section 7.2.5, in this case the spectral problem for the Maxwell operator splits into the direct sum of two scalar problems:

$$-\Delta u = \lambda\varepsilon(x)u$$

and

$$-\nabla \cdot \frac{1}{\varepsilon}\nabla u = \lambda u.$$

Now the following theorem resolves the problem of absolute continuity in two dimensions (although its first statement holds in any dimension).

THEOREM 7.7. (a) *Under the conditions*[4] *on the periodic dielectric function* $\varepsilon(x)$ *that imply the absolute continuity of the spectrum of the Schrödinger operator* $(-\Delta - \varepsilon)$, *the spectrum of the problem*

$$-\Delta u = \lambda\varepsilon(x)u$$

is absolutely continuous in $\mathbb{R}^d$.

(b) *Let the dielectric tensor* $\varepsilon(x)$ *be smooth and periodic (not necessarily scalar); then the spectrum of the operator* $-\nabla \cdot \varepsilon^{-1}\nabla$ *in* $L^2(\mathbb{R}^2)$ *is absolutely continuous.*

Proof. (a) If $-\Delta u = \lambda\varepsilon(x)u$ has a nonzero L^2-solution, then the Schrödinger operator $(-\Delta - \lambda\varepsilon)$ has a zero eigenvalue, which is impossible according to the known results. (b) This is essentially the result of [142], modulo an application of the transform (7.16).

The equivalence of (a) and (b) in the Theorem 7.5 for Schrödinger operators is essentially due to Thomas [184]. We now want to call the reader's attention to the statements (c) and (d) of this theorem. The proof requires a technique from the several complex variables theory [124]. In principle, these statements suggest a different way of proving absolute continuity of spectra of periodic elliptic operators of the second order. Namely, for such operators existence of a superexponentially

[3]When the author was finishing the last revision of this text, the preprint [143] appeared, where the absolute continuity result for the isotropic periodic Maxwell operator was proven.

[4]The best currently known conditions were established in [26, 170]. In dimension $d = 2$ it is that $\varepsilon \in L^r_{loc}(\mathbb{R}^2)$ for some $r > 1$ (or equivalently $\varepsilon \in L^r(W)$, where W is the Wigner–Seitz cell). For $d = 3$ and 4 one requires $\varepsilon \in L^0_{d/2,\infty}(W)$. This means that the function $\rho_\varepsilon(t) = mes\{x \in W \,|\, |\varepsilon(x)| \geq t\}$ satisfies $\rho_\varepsilon(t) = o(t^{-d/2})$. In dimensions $d \geq 5$ the (nonoptimal) condition is $\varepsilon \in L^{d/2}(W)$. Shen has recently announced the optimal condition for any dimension [171].

decaying solution like in (d) should be an impossible pathology that would violate uniqueness of continuation at infinity (see, for instance, [84, 136, 137, 140], and references therein). If one could prove nonexistence of such solutions, the immediate consequence would be absolute continuity of the spectrum. However, partial differential equation results that guarantee absence of such solutions are probably not currently available for periodic operators.

7.4.4 Spectral Gaps

In this section we will consider the nature, existence, and number of gaps in the spectrum of a periodic operator. This is probably the central issue of the whole photonic crystals theory. Existence of gaps is a prerequisite to most applications of photonic crystals.

Let us discuss briefly one mechanism of opening gaps that exists in the case of a periodic Schrödinger operator $-\Delta + v(x)$. Imagine that we start with a constant potential. Then the spectrum of the operator is continuous and covers a semiaxis $[\alpha, \infty)$. Let us add a localized potential well. This will create a few eigenvalues below the continuous spectrum. The corresponding eigenfunctions (bound states) are localized in a vicinity of the well. Let us now repeat the well periodically with a sufficiently large period. The former bound states can now tunnel to the other wells and hence will not be localized anymore. This will lead to spreading the eigenvalues into narrow bands, which correspondingly will be separated from the rest of the spectrum by gaps. So, the major factor in opening gaps is that by adding a potential one can change the bottom of the spectrum. In the case of photonic crystals, however, this is exactly what is missing. The operators involved in both two- and three-dimensional photonic cases are multiplicative rather than additive perturbations of the corresponding free operators:

$$\frac{1}{\sqrt{\varepsilon}} \left(\nabla^{\times}\right)^2 \frac{1}{\sqrt{\varepsilon}}$$

in three dimensions and

$$-\frac{1}{\sqrt{\varepsilon}} \Delta \frac{1}{\sqrt{\varepsilon}}$$

and

$$-\nabla \cdot \frac{1}{\varepsilon} \nabla$$

in two dimensions (TM and TE polarizations). The outcome is that in all these cases the spectrum starts at zero. Indeed, consider, for instance, the TM case. If ϕ_n is an approximate eigenfunction for $L = -\Delta$ at zero, i.e., if $||\phi_n||_{L^2} > c > 0$ and $||L\phi_n|| \to 0$, then the functions $\psi_n = \sqrt{\varepsilon}\phi_n$ are approximate eigenfunctions for $\left(-\varepsilon^{-1/2}\Delta\varepsilon^{-1/2}\right)$. This shows that the mechanism of opening gaps in the PBG case is different. In particular, while the gaps for the Schrödinger operator can be opened at the bottom of the spectrum, in the photonic case they normally open in the medium-frequency range (see, for instance, [106]).

It is well known that in one dimension (i.e., for the Hill operator) the generic situation is that infinitely many gaps are open (see, for instance, [157]). On the other hand, it is commonly believed that the number of gaps one can open in a periodic medium in dimension higher than 1 is finite. In the case of a periodic Schrödinger operator, this constitutes the Bethe–Sommerfeld conjecture [15], first proven by M. Skriganov (see [52, 96], [110]–[116], [124, 141], [175]–[179], [181, 187] for the discussion of this problem and several different approaches to its proof). The proofs are by no means simple and often employ results from number theory. The following analogue of the Bethe–Sommerfeld conjecture almost certainly holds true.

CONJECTURE 7.8. *In dimensions* 2 *and higher the spectrum of any photonic crystal (or of its acoustic analogue) has at most a finite number of gaps.*

The main idea of the proof in the case of Schrödinger operators is that the overlap of spectral bands of the free Hamiltonian for sufficiently high energies is so strong that addition of a periodic potential cannot open gaps at these energies. However, in the photonic case one deals with a multiplicative rather than additive perturbation of the free Hamiltonian, which will probably lead to the necessity of involving a different approach to the proof. On the other hand, it looks like it is harder to open gaps in the photonic case, which raises a hope that the proof of finiteness of number of gaps could be simpler than in the solid-state situation.

Let us now address the problem of existence of spectral gaps for the periodic Maxwell operator. While there is a lot of numerical and experimental evidence of it (see the surveys [33, 101, 106, 108, 134, 156, 182, 189]), analytic results on existence of gaps are scarce. We are not aware of any such theorems for the full-vector three-dimensional case, which is the main interest in the PBG theory (the result announced in [75] is erroneous). There are, however, a few cases when existence of gaps was proven for the scalar problems analogous to (7.14) and (7.15) in two and higher dimensions. The authors of [49] studied the Laplace–Beltrami operator

$$L_g f = -\frac{1}{\sqrt{|g|}} \sum_{i,j} \partial_i (g^{ij} \sqrt{|g|} \partial_j f)$$

in $\mathbb{R}^d$ with a conformally flat periodic metric $g_{ij} = a(x)\delta_{ij}$. In the one-dimensional case it reduces to

$$-\left(\frac{1}{\sqrt{a}}\frac{d}{dx}\right)^2,$$

which in turn can be reduced by a simple change of variables to $-d^2/dy^2$. This shows that when $d = 1$ the spectrum of L_g coincides with the positive half-axis and hence has no gaps. This is in contrast with the case of periodic Schrödinger operators, since such an operator in one dimension (the Hill operator) generically possesses infinitely many spectral gaps. Experience with Schrödinger operators also shows that when dimension increases, it becomes increasingly difficult to create spectral gaps. Surprisingly enough, the situation with the periodic Laplace–Beltrami operators is different: while there are no gaps in the spectrum of such an operator in one dimension, it was shown in [49] that in any higher dimension there exist periodic metrics such that the corresponding Laplace–Beltrami operators have gaps in the spectrum. The idea of the proof is that using a procedure similar to the one described in section 7.2.5, one can reduce the operator to a Schrödinger form. If one succeeds in reducing to a Schrödinger operator with a separable potential, then one can use the well-developed theory of spectra of the Hill operators to check existence of gaps. This study was continued in the paper [92], where it was shown that in two dimensions one can achieve any finite number of gaps in the spectrum of a periodic Laplace–Beltrami operator. It is not known whether the number of gaps must always be finite and whether it is not limited in dimensions higher than 2. It is interesting to note that the method used in [92] to show that the number of gaps is not limited in two dimensions is essentially the same one that was applied in [76]–[78] for showing existence of gaps in spectra of some two-dimensional photonic crystals (see description of these results below).

There is not much hope for analytic (rather than purely numerical) prediction of spectral gaps in a general situation. However, when some parameters of the problem approach extremal values (for instance, the dielectric contrast becomes very high, the dielectric regions become very narrow, etc.), one can try to understand the asymptotic situation and therefore to predict the behavior of the spectrum. This is the idea that was employed in [76]–[81] and [8, 100, 126, 127, 172] for studying spectra of the problems (7.14) and (7.15). Due to their specific flavor, we will address these results in the next section.

Suppose that $[a, b]$ is a gap in the spectrum of one of the periodic problems we discuss. This means that a is the maximal value of a band function $\lambda_j(k)$. Analogously, b is the minimal value of another band function. In many cases (some of which will be mentioned later) it is important to know in which way these extrema are attained: are they isolated, nondegenerate, etc.? Unfortunately, there is almost no information about this, except the recent result of [119] on generic simplicity of the endpoints of bands. Probably the only thing known for some periodic operators is the behavior of the band functions at the bottom of the spectrum (which is the upper end of the infinite gap $(-\infty, a]$). The result obtained in [117] concerns a periodic Schrödinger operator $H = -\Delta + V(x)$ in $\mathbb{R}^d$. Let us denote as before

$$H(k) = (D + k)^2 + V(x).$$

Then the band functions $\lambda_j(k)$ provide the eigenvalues of $H(k)$, where $\lambda_1(k)$ is the lowest one.

THEOREM 7.9 (Theorem 2.1 in [117]). *Let ψ_0 be the positive periodic solution of $H\psi_0 = \lambda_1(0)\psi_0$. Then*

$$(\min \psi_0 / \max \psi_0)^2 k^2 \le \lambda_1(k) - \lambda_1(0) \le k^2.$$

This theorem implies that the bottom of the spectrum is attained only at the zero quasi momentum $k = 0$, and around that point the lowest band function behaves as

$$\lambda_1(k) = \lambda_1(0) + \gamma(k) + O(k^4),$$

where $\gamma(k)$ is a positive definite quadratic form of k.

The analogous result was recently obtained in [25] for periodic Pauli operators

$$P_{\pm} = (D - A)^2 \pm B$$

in two dimensions, where $A = (A_1, A_2)$ is a periodic magnetic potential and $B = \partial_1 A_2 - \partial_2 A_1$ is the corresponding magnetic field. Besides, it was shown that the quadratic form $\gamma(k)$ has the form αk^2 with an explicit formula for the coefficient α.

It is interesting to mention that such band edge behavior is closely related to Liouville-type theorems on the structure and dimension of the spaces of polynomially growing solutions of periodic elliptic equations [130].

A similar result about the way the bottom of the spectrum is attained has been obtained recently by Birman and Suslina [21] for the full-vector Maxwell operator in three dimensions (in which case the statement applies to the two first band functions). This, in particular, provides a rigorous justification of the known linear behavior of the band functions $\omega(k)$ at zero frequency (recall that the eigenvalues are related to the frequencies as $\lambda = (\omega/c)^2$). From the physical point of view the situation is rather clear: long waves do not notice the periodic structure of the medium and see it as a homogeneous one. Clearly, some kind of homogenization technique (see [13, 104]) is required in order to find the slope of the dispersion relation close to zero frequency. This was done for several cases in physics papers (see, for instance, [48, 95, 122]) although it looks like a rigorous mathematical analysis is still due.

Any results for the higher gaps of the kind that we described for the bottom of the spectrum would be of great importance. It is very common to see in papers devoted to impurity spectra and localization (see section 7.6.2 below) conditions of the following kind. Let $[a, b]$ be a gap in the spectrum. Then a is the maximum of a band function $\lambda_j(k)$. It is assumed that this function attains its maximum at a single point (or a finite set of points) in the Brillouin zone and that this maximum is nondegenerate (i.e.,

$$\lambda_j(k) = \lambda_j(k_0) + \gamma(k - k_0) + O(|k - k_0|^3),$$

where γ is a positive definite quadratic form). However, it is apparently not known how to verify such a condition, or even how common it is. It is believed that this condition holds generically. The only result in this direction known to the author is that of [119], where the simplicity of the band edge was shown in the generic situation.

7.5 Asymptotic Analysis of High-Contrast PBG Materials

It has been recognized (see [106, 189]) that high dielectric contrast of a photonic crystal favors spectral gaps. Under some circumstances it was also noticed that gaps could benefit from narrowness of optically dense dielectric "walls" separating the air bubbles. It is natural to try to understand what happens in the asymptotic limits when the contrast goes to infinity and the filling fraction of the dielectric (or the air)

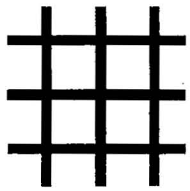

Figure 7.3: Two-dimensional square PBG structure. The dark strips of width δ represent dielectric with $\varepsilon > 1$. The white areas are filled with air ($\varepsilon = 1$).

portion of the medium goes to zero. In this section we will address spectral results known for the PBG materials in such asymptotic situations. One should notice, however, that neither very high contrasts nor very low dielectric filling fractions are currently achievable technologically (for instance, 12 is considered to be a high value for the dielectric contrast). The asymptotic study still makes sense for several reasons. First, it might reveal spectral effects which are hard to recognize otherwise. Second, since often the asymptotic problems are much simpler to study numerically and analytically, they might provide quick ways to estimate the situation. Third, information obtained for the asymptotic models can suggest better algorithms for numerics for the full problem. In particular, one can try to use the spectra and eigenmodes computed for the asymptotic models as seeds for iterative methods for the full problem and/or for creating suitable preconditioners for such methods. One also discovers that asymptotic results can sometimes provide unexpectedly good approximation in the cases when neither the contrast is very high, nor the structure is very thin [8]. One can hope that with further advances in technology the values of parameters closer to the asymptotic limits might become one day technologically feasible. Finally, in the acoustic situation, which is also of interest, one can already achieve such high contrasts. This section is devoted to discussion of the known asymptotic results about PBG materials.

7.5.1 Square Geometry

Probably the first successful asymptotic study of the PBG materials was undertaken in [76]–[78] and in a less detailed form in [172].[5] These papers addressed the square geometry of a two-dimensional PBG medium (Figure 7.3).

The medium has period 1 in both x- and y-directions. The dark areas have thickness $\delta < 1$ and are filled with a dielectric with the dielectric constant $\varepsilon > 1$, while the light areas are filled with air ($\varepsilon = 1$). The dielectric function $\varepsilon(x)$ then takes values ε and 1 in the dielectric and air regions correspondingly. The scaling properties of the Maxwell equations (see section 7.2.4) guarantee that our choice of the period and of the dielectric constant of the "air" regions does not restrict generality of the consideration. The square structure was chosen for its simplicity with the hope that one could understand it and then move on to more complex geometries.

[5]We use the word "successful" here since the three-dimensional result announced in [75] was erroneous.

We remind the reader that for the in-plane harmonic waves the Maxwell system reduces to the following two scalar spectral problems (7.15) and (7.14):

$$-\nabla \cdot \frac{1}{\varepsilon(x)}\nabla u = \lambda u$$

(TE polarization) and

$$-\Delta u = \lambda\varepsilon(x)u$$

(TM polarization), where $\lambda = (\omega/c)^2$. The papers [76]–[78] are devoted to the study of these two spectral problems for the square two-dimensional geometry described above in the asymptotic limit when $\varepsilon\delta \to \infty$ and $\varepsilon\delta^2 \to 0$. The TE polarization happens to be the simplest one, and its asymptotic spectral behavior is described by the following result.

THEOREM 7.10 (see [76]). *Let N be an arbitrary positive number and*

$$S_1 = \left\{\pi^2(n_1^2 + n_2^2) \mid \mathbf{n} = (n_1, n_2) \in \mathbb{Z}^2\right\}.$$

Denote by σ_{TE} the spectrum of the problem (7.15) for the square geometry described above. Then the Hausdorff distance between $S_1 \cap [0, N]$ and $\sigma_{TE} \cap [0, N]$ tends to zero when $\varepsilon\delta \to \infty$ and $\varepsilon\delta^2 \to 0$. Moreover,

$$d\left(S_1 \cap [0, N], \sigma_{TE} \cap [0, N]\right) \leq C_N \max\left\{(\varepsilon\delta)^{-1}, \varepsilon\delta^2\right\},$$

where d denotes the Hausdorff distance.

This theorem says that the spectrum of the TE modes for small values of $(\varepsilon\delta)^{-1}$ and $\varepsilon\delta^2$ concentrates in a small vicinity of the discrete set S_1, and hence large gaps at exactly known locations open up. The reader has probably noticed that the set S_1 to which the spectrum σ_{TE} converges is just the spectrum of the Neumann Laplacian on the unit square (which is the Wigner–Seitz cell of the considered geometry). A more precise description of this result can be found in [76]. An additional observation made in [76] was that the Floquet–Bloch eigenmodes have most of their energy concentrated in the air region.

We would also like to mention that the same result holds for the problem (7.15) for the cubic geometry in three dimensions [76], where one can think of (7.15) as describing acoustic rather than electromagnetic waves.

This study was finished in [78], where the asymptotic behavior of the TM modes (7.14) was investigated. We will present here the main result of [78], omitting some details.

Consider the spectral problem (7.14) for the square structure in two dimensions. Denote by S_2 the following set:

$$S_2 = \left\{\pi^2(n_1^2 + n_2^2) \mid \mathbf{n} = (n_1, n_2) \in \mathbb{Z}^2 \backslash \{(0,0)\}\right\}.$$

It is clear that S_2 is the spectrum of the Dirichlet Laplacian on the unit square.

THEOREM 7.11 (see [78]). *The spectrum σ_{TM} of the problem (7.14) for the square geometry described above splits into two parts: $\sigma_{TM} = \sigma_1 \cup \sigma_2$.*

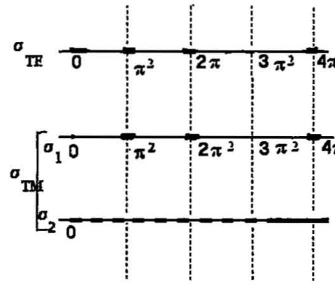

Figure 7.4: The three asymptotic spectra arising in the high-contrast square PBG structure.

If $w = (\varepsilon\delta)^{-1} \to 0$ *and* $\varepsilon\delta^{4/3} \to 0$, *then the following spectral asymptotics hold: Let* N *be an arbitrary positive number.*

(a) *The Hausdorff distance between* $S_2 \cap [0, N]$ *and* $\sigma_1 \cap [0, N]$ *tends to zero. Moreover,*

$$d\left(S_2 \cap [0, N], \sigma_1 \cap [0, N]\right) \leq C_N \left(\varepsilon\delta\right)^{-1}.$$

(b) *There exists a set of disjoint segments*

$$\mathcal{D} = \bigcup_{n \geq 0} [D_n^-, D_n^+]$$

not depending on ε *and* δ *such that*

$$D_0^- = 0, \quad D_0^+ = 4, \quad D_{n+1}^- > D_n^+, \quad D_n^- \sim 2\pi n, \quad D_n^- \sim 2\pi n + \pi$$

when $n \to \infty$. *The spectrum* σ_2 *allows the representation*

$$\sigma_2 \cap [0, N] = \left\{ \bigcup_{n \geq 0} [w_n^- D_n^-, w_n^+ D_n^+] \right\} \cap [0, N],$$

where $w_n^\pm \sim w = (\varepsilon\delta)^{-1}$.

One can find a more precise formulation in [78]. This theorem shows that the two subspectra σ_1 and σ_2 behave differently in our asymptotic limit. The subspectrum σ_1 behaves essentially like σ_{TE}, except for the absence of the band at zero. The bands shrink to the spectrum of the Dirichlet Laplacian on the unit square, therefore becoming almost discrete and opening large gaps at exactly described locations. Another similarity with σ_{TE} is that the eigenmodes are also the air modes, which have most of the energy concentrated in the air bubbles. A completely different behavior is observed in the second subspectrum σ_2. Namely, it splits into narrow bands separated by narrow gaps, both of the asymptotic size $w = (\varepsilon\delta)^{-1}$. Besides, the Floquet–Bloch eigenmodes behave differently: they concentrate in the dielectric regions, quickly dying out in the air. One can attribute this effect to the total internal reflection [103]; i.e., the narrow dielectric regions behave as a waveguide. Figure 7.4 represents these three spectra schematically.

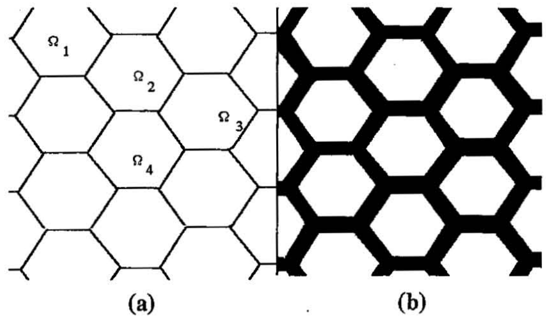

Figure 7.5: (a) The graph Σ and its faces Ω_j. (b) The dielectric PBG material corresponding to the graph Σ. The dark areas of width δ represent dielectric with dielectric constant $\varepsilon > 1$. The white areas are the air bubbles with $\varepsilon = 1$.

One of the by-products of this study is the following statement.

THEOREM 7.12 (see [78]). *For the square geometry of the two-dimensional material, for any given integers N and M the number of gaps in* $(\sigma_{TE} \cup \sigma_{TM}) \cap [0, N]$ *is at least M for sufficiently small values of* $\varepsilon\delta^{4/3}$ *and* $(\varepsilon\delta)^{-1}$. *The spectral bands in* $[0, N]$ *are of asymptotic size* $(\varepsilon\delta)^{-1}$ *and are separated by gaps of the same asymptotic size.*

This theorem proves in particular that it is possible to open spectral gaps in PBG materials. It also shows that the TM modes responsible for the subspectrum σ_2 present the main obstacle for the gaps opening, since all other TM and TE waves tend to create an almost discrete spectrum with large gaps.

The proofs of the quoted theorems are rather technical and rely on availability of an exactly solvable model with separable variables in a vicinity of the spectral problem of interest. This approach restricts the consideration to the square case. On the other hand, both the result about splitting the spectrum into subspectra with different asymptotics and the understanding of behavior of the corresponding eigenmodes are of general importance. They will be exploited in our further considerations.

7.5.2 General Two-Dimensional Geometry

The results of the previous section raise several natural questions. The main ones are about the possibility of carrying over a similar analysis for nonsquare geometries, which do not allow separation of variables, and the explanation of the origin of the spectrum σ_2. To some extent, these questions were answered in [79, 80]. The proofs presented in [80] are much simpler than the ones in [76]–[78]. A wide range of PBG geometries is covered. On the other hand, the price paid was a somewhat weaker nature of the results.

Consider a periodic graph Σ on the plane that divides it into compact faces Ω_j. Imagine that all its edges are fattened to the width δ (the dark areas in Figure 7.5) and filled with a dielectric with the dielectric constant $\varepsilon > 1$. The rest of the plane (the white faces Ω_j) is filled with air (Figure 7.5).

We will consider now the asymptotic behavior of the spectrum of TM modes when $\delta \to 0$ and $(\varepsilon\delta)^{-1} \to W < \infty$. We address the TM modes since in the asymptotic limit they are the "worst" modes as far as gaps are concerned (see the previous section). The case of the TE modes will be discussed in [81]. One can notice that in the previous theorems we assumed that $W = 0$. We now allow nonzero (albeit finite) limits of $(\varepsilon\delta)^{-1}$. This is a much more realistic assumption, at least at the current level of technology, since the technologically feasible values of $(\varepsilon\delta)^{-1}$ are of order 1.

Theorem 7.11 shows that the sizes of bands and gaps of the "worst" spectrum σ_2 are of order $(\varepsilon\delta)^{-1}$. It is natural, then, before trying to understand this spectrum, to zoom in on it by introducing a rescaled spectral parameter $D = (\varepsilon\delta)\lambda$. Then the spectral problem (7.14) becomes

$$-\Delta u = (\varepsilon\delta)^{-1} D\varepsilon(x)u. \tag{7.25}$$

THEOREM 7.13 ([80]; see also [79]). *For any positive N the part of the spectrum σ (in terms of the parameter D) of the problem* (7.25) *that belongs to* $[0, N]$ *converges to the corresponding part of the spectrum of the following problem:*

$$-\Delta u = D(\delta_\Sigma + W)u. \tag{7.26}$$

Here δ_Σ is the delta function supported by the graph Σ; i.e., for any compactly supported smooth function $\phi(x)$

$$\langle \delta_\Sigma, \phi \rangle = \int_\Sigma \phi(x)dx.$$

There are several comments on this theorem:

(1) All the details, exact definitions of the operators, etc., can be found in [80].

(2) The constant $W = \lim(\varepsilon\delta)^{-1}$ plays the role of a coupling constant. We saw that when $W = 0$ (i.e., in the situation considered in the previous section) the air and dielectric modes decouple.

(3) This theorem allows nonzero values of W, which is much more realistic under the current technological conditions.

(4) Although the statement of the theorem looks similar in spirit to the ones of the previous section, it is in fact weaker for $W = 0$. Indeed, if in the previous section we stated results of convergence of any finite part of the spectrum in terms of the spectral parameter λ, this is now done in terms of the rescaled parameter $D = (\varepsilon\delta)\lambda$. If $D \in [0, N]$, then $\lambda \in [0, (\varepsilon\delta)^{-1}N]$. This shows that when $(\varepsilon\delta) \to \infty$ (i.e., when $W = 0$), we are zooming in on an ever smaller segment of the λ-axis. It is desirable to extend this result to any finite part of the spectrum, in the spirit of Theorem 7.11.

When $W = 0$, the problem (7.26) reduces to

$$-\Delta u = D\delta_\Sigma u. \tag{7.27}$$

In this case the natural domain for consideration of this spectral problem is the graph Σ itself. In order to understand this we need to introduce the notion of the *Dirichlet-to-Neumann (D–N) operator* on the graph Σ. Take a function $\phi(x)$ defined along the edges of the graph Σ. We will further assume that $\phi \in L^2(\Sigma)$, but so far one can think of a sufficiently smooth compactly supported function on the plane restricted to the graph Σ. Take any of the compact faces Ω_j and solve the following Dirichlet problem:

$$\begin{cases} -\Delta u_j(x) = 0, & x \in \Omega_j, \\ u_j|_{\partial\Omega_j} = \phi. \end{cases}$$

Then on each face Ω_j we obtain a harmonic function u_j. Due to the construction, these functions agree across the graph's edges, while their normal derivatives disagree. Let us now define a function ψ on the graph as the sum of all exterior normal derivatives of all the functions u_j:

$$\psi = \sum_j \frac{\partial u_j}{\partial \mathbf{n}_j},$$

where $\mathbf{n}_j$ are the exterior normal vectors to $\partial\Omega_j \subset \Sigma$.

The D–N operator on the graph Σ is the operator

$$\Lambda_\Sigma : \phi \to \psi.$$

It is not hard to define Λ_Σ as a self-adjoint operator on $L^2(\Sigma)$ (see, for instance, [80, 126]).

THEOREM 7.14 (see [80]). *The spectrum of the operator* Λ_Σ *coincides with the spectrum of the problem* (7.27).

This theorem explains the origin of the "bad" spectrum σ_2 in the previous section: it asymptotically behaves as the spectrum of the D–N operator Λ_Σ rescaled with the small parameter $(\varepsilon\delta)^{-1}$.

The operator Λ_Σ can be thought of as a "pseudodifferential" operator on the graph Σ. Although this is probably possible, we will not try to define the notion of a pseudodifferential operator on graphs. It is known that if the graph is smooth (and in particular has no vertices or loose ends) the operator Λ_Σ is in fact a pseudodifferential operator. D–N operators have been intensively studied recently, in particular due to the needs of inverse problems (see, for instance, [186] and references therein). The only thing different in the photonic situation is that the operator Λ_Σ is a "two-sided" one. This means that in order to define it, we solve Dirichlet problems on both sides of an edge and then take the jump of normal derivatives from both sides, while in standard considerations the Dirichlet problem is solved on only one side, and then the exterior normal derivative at the boundary is taken. For a standard D–N operator it is known that it is pseudodifferential and that its symbol is the square root of the symbol of the Laplace–Beltrami operator on the boundary (see, for instance, [183]). It is easy to conclude then that if the graph Σ is smooth, the operator Λ_Σ is pseudodifferential with the symbol $2|\xi|$ (i.e., the symbol of the operator $2\sqrt{-d^2/ds^2}$, where s is the arc length). This understanding is important for what follows.

The study of [80] was devoted to the case of TM modes in two dimensions only. It is continued in the paper under preparation [81], where the TE modes in two dimensions are treated in a similar asymptotic limit. It is shown, in particular, that the spectrum of the TE modes converges to the spectrum of the following problem:

$$\begin{cases} -\Delta u = \lambda u, & x \in \mathbb{R}^2 - \Sigma, \\ \left[\frac{\partial u}{\partial n}\right] = 0, & x \in \Sigma, \\ \frac{\partial u}{\partial n} = W[u], & x \in \Sigma, \end{cases} \tag{7.28}$$

where $\left[\frac{\partial u}{\partial n}\right]$ and $[u]$ stand for the jumps of $\partial u/\partial n$ and of u, respectively, across Σ and $\partial/\partial n$ is the normal derivative at smooth points of Σ. Some three-dimensional cases were also considered in [81].

7.5.3 Study of the Graph Models

As we saw in the previous section, study of thin high-contrast dielectric structures leads to spectral problems on graphs. In three dimensions, analogous study also leads to similar problems on surface structures. It is interesting to mention that in recent years, due to progress in nanotechnology and microelectronics, problems in thin domains ("fattened" points, graphs, or surfaces) were considered in mesoscopic physics. These are in particular studies of circuits of thin semiconductor strips ("quantum wires"; see a mathematical discussion in [59]), thin superconducting structures [160]–[162]), and others. In all these cases a natural asymptotic consideration was applied, which led to differential problems on graphs. One can also mention related considerations in different branches of mathematics ([30]–[32], [37]–[39], [57, 58, 165, 82, 83, 89, 133], [146]–[148], [163, 166]), chemistry [164], and other areas. The eigenvalue problems that arise in these studies usually look as follows: along each edge of the graph one has the problem

$$-\frac{d^2u}{ds^2} = \lambda^2 u$$

with "appropriate" boundary conditions at each vertex. These boundary conditions at the vertices are still problematic, since it looks like convergence of spectra on thin domains to spectra on graphs are harder to prove in mesoscopic physics than in the photonic case. The only known results of this kind are probably the ones obtained in [82, 83, 133, 166, 163]. The theorems proved there and some handwaving in other cases show that normally these conditions are probably the following: the function u must be continuous through each vertex, and at each vertex the sum of the outgoing derivatives along each edge must be equal to zero. A further study of this problem is required.

Let us now discuss some spectral properties of the operator Λ_Σ on a periodic graph Σ in the plane. We remind the reader that this is the asymptotic model for the TM waves propagating mostly in the thin dielectric regions along the edges of the graph and that waves of this kind are responsible for the main difficulties in opening spectral gaps in the high-contrast case.

A thorough numerical and analytic study of this operator was done in [8, 126, 127]. We refer the reader to [126] for a description of the numerical algorithm used

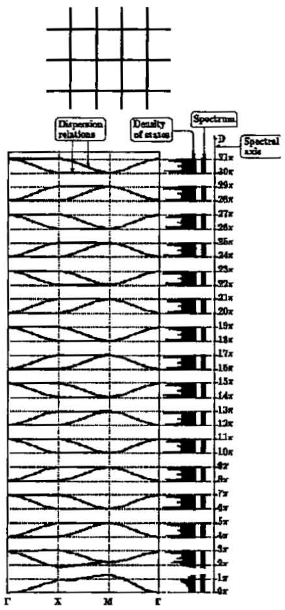

Figure 7.6: Square structure and its spectrum.

for finding spectra of operators Λ_Σ and present here only some of the obtained results.

Figure 7.6 presents the spectrum computed for the square lattice graph formed by the lines $x = n$ and $y = m$ $(n, m \in \mathbb{Z})$ and also explains our graphing system. In this picture the spectral axis is vertical. The first column represents the graphs of several branches of the dispersion relations $D_j(\mathbf{k})$ (we remind the reader that we have a rescaled spectral parameter D instead of the former λ). In order to avoid graphing surfaces, the dispersion relation is commonly graphed only for the values of the quasi momentum $\mathbf{k}$ on the boundary of the irreducible Brillouin zone, which in this case is the triangle with the vertices $\Gamma(0,0)$, $X(\pi, 0)$, and $M(\pi, \pi)$. The second column contains the graph of the density of states over the spectral axis. The third column shows the band gap structure of the spectrum.

Consider now disconnected graphs Σ. For instance, take a circle of a radius less than 0.5 and repeat it periodically with the period group $\mathbb{Z}^2$. One can view the resulting disconnected graph as a model of the structure of thin optically dense dielectric pipes in the air. A similar procedure can be applied to a segment, cross, square, etc., each time yielding a disconnected graph Σ. The numerical study of all of these and of some other disconnected structures produced dispersion relations with band functions that flatten very fast with the growing band number, leading to spectra that consist of very narrow spectral bands and thus are almost discrete for high frequencies. Besides, the spectra appear to be asymptotically periodic. Figure 7.7 represents the results of the calculation for the disconnected structure composed of disjoint circles of radii 0.2.

We present now an analytic result that explains this spectral behavior. It holds in any dimension, not necessarily in two dimensions. Let S be a smooth closed

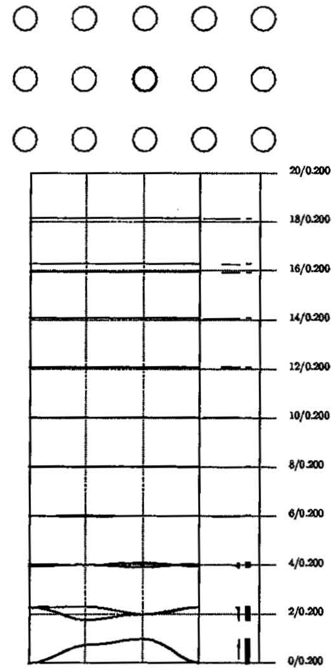

Figure 7.7: The disconnected structure of period 1 consisting of circles of radius 0.2 (top) and its spectrum (bottom).

hypersurface in $\mathbb{R}^d$ and $\Sigma = \cup_{\mathbf{n}\in\mathbb{Z}^d}(S+\mathbf{n})$ be the disjoint union of the integer shifts of S. One can define the D–N operator Λ_Σ on Σ, as was done above for $d = 2$.

THEOREM 7.15 (see [126]). *Let $\{D_n\} \subset \mathbb{R}$ be the (discrete) spectrum of the (positive) Laplace–Beltrami operator Δ_S on the surface S. Then there exists a sequence of positive numbers $\rho_n \to 0$ such that the spectrum of operator Λ_Σ on Σ belongs to the union of intervals*

$$\sigma(N) \subset \bigcup_n \left[2\sqrt{D_n} - \rho_n, 2\sqrt{D_n} + \rho_n\right],$$

and each of these intervals contains a nonempty portion of $\sigma(N)$.

Remark. In fact, if S is smooth, one can guarantee that

$$\rho_n \le c_p D_n^{-p}$$

for any p. The case when S is a circle can be solved explicitly using Fourier series. It shows that analyticity of S probably implies exponential decay of ρ_n.

Theorem 7.15 explains the "almost discrete" nature of the spectrum and provides its asymptotic location for disconnected smooth structures. For instance, in the two-dimensional case we conclude that the spectrum at higher frequencies must concentrate around values $4\pi n L^{-1}$, where L is the length of S. In particular, for a circle of radius R this leads to $2nR^{-1}$. These numbers are indicated along the spectral axis in Figure 7.7, and one can see perfect agreement with the numerical results. This also provides an explanation of the asymptotic periodicity of the spectrum in two dimensions that was observed in numerics.

A few words are due about the method of proof. First, one can show that for high frequencies the eigenmodes decay very fast in the air regions, so the distinct copies of S essentially decouple. Then one is almost in the situation when the wave is zero on a surface surrounding a copy of S. Now the standard technique shows that we are dealing with a first-order pseudodifferential operator on S which is equal to $2\sqrt{\Delta_S} + R$, where Δ_S is the (positive) Laplace–Beltrami operator on S and R is a smoothing pseudodifferential operator. This in turn leads to the properties of the spectrum claimed in the theorem.

We would like to mention that numerics show a very fast convergence of the asymptotics claimed in the last theorem. So, one can make rather accurate predictions about the spectra using this theorem.

A very restrictive assumption is smoothness of S, since graphs that represent thin dielectric structures will normally have vertices and/or corners. One might expect that if instead of circles we use squares of the same length, the asymptotic nature of the spectrum will stay the same. However, numerical tests show that this is not the case. One could suspect that maybe just the rate of the asymptotic convergence is much slower in the nonsmooth case, but in fact the spectra look systematically shifted from the values predicted according to the formula $4\pi nL^{-1}$. Our current understanding is that this effect is due to the vertices (corners), which require some special boundary conditions. These conditions will be discussed later. So, the treatment of nonsmooth graphs (which are most common) requires additional study.

Connected structures are certainly the most interesting. The paper [126] contained results of computations for different geometries that show how the spectrum reacts to geometry. We will not present all these numerical results here, but rather address an interesting resonance phenomenon observed in [126]. Consider, for instance, the same disconnected circle structure and add dielectric edges connecting the circles along the symmetry axes of the structure. Figure 7.8 represents the computed dispersion relations and spectrum for this model.

One can notice resonance-type behavior: some branches of the dispersion relation become practically flat, and the density of states shows high delta-type peaks at the corresponding locations. As the following result (which at the moment of initial submission of this article was stated as a conjecture) shows, this does not indicate presence of actual eigenvalues, but rather of resonances.

THEOREM 7.16 (see [27]). *For any periodic graph Σ, the spectrum of Λ_Σ is absolutely continuous.*

It is interesting to look at the Floquet–Bloch eigenmodes that correspond to these observed resonances. Figure 7.9 represents the density plot of two such eigenmodes.

What one can see is that the wave is strongly localized at one circle (it is stuck in the loop), in spite of availability of the dielectric edges connecting different circles that allow the wave to propagate. One can also observe that the frequencies at which these resonances occur coincide with a subset of the spectrum computed for the disconnected circle structure. This is not a coincidence. One can show (the corresponding theorem is proven in [126]) that the eigenmodes of the disconnected

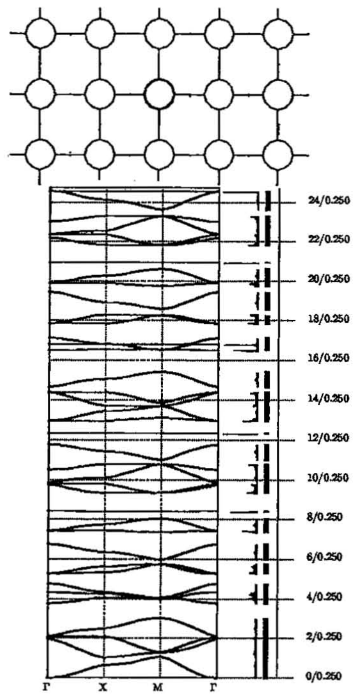

Figure 7.8: The structure of connected circles of radius 0.25 (top) and its spectrum (bottom).

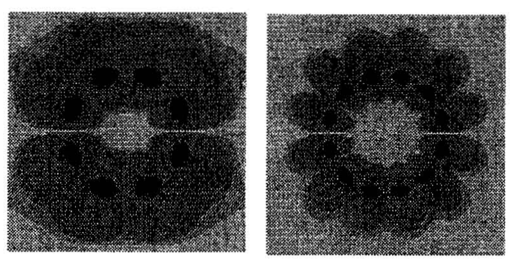

Figure 7.9: Density plots of the first two "localized" eigenmodes for the connected circle structure. Notice that the modes apparently do not propagate along the dielectric edges connecting the circles.

circle structure that are antisymmetric with respect to both symmetry axes of the structure, lead to resonances in the connected structure.

Similar resonant behavior was also observed in [126] for several other geometries, including, for instance, the honeycomb one. There is, however, no complete understanding of this effect. For instance, one can show both analytically and numerically that these resonances do not occur in the square geometry. It is not clear yet what differentiates this geometry from those with resonances. The study of these resonances suggests that it is in principle conceivable to "almost localize" electromagnetic waves in a purely periodic PBG material with no impurities, just by using an appropriate geometry. It is interesting to note that existence of significantly flattened band functions is of practical importance and has recently been used successfully for enhancement of spontaneous emission [29] and lasing [102].

The results of [126] show that there are often infinitely many gaps in the spectrum of the D–N operator Λ_Σ on a periodic graph Σ in the plane. Is the same true for higher dimensions? The following theorem shows that the answer is probably negative.

THEOREM 7.17 (see [126]). *Let the space $\mathbb{R}^3$ be tiled with unit cubes and Σ be the union of their surfaces. The spectrum of the corresponding D–N operator Λ_Σ has only a finite number of gaps. Moreover, there are no gaps in the spectrum for the values of the spectral parameter $D \geq 40\pi$.*

This theorem was proved by separating variables and consequently studying the resulting system of transcendental inequalities. It is interesting to note that the threshold between infinite and finite numbers of gaps lies for the periodic D–N operators between dimensions 2 and 3, while for the periodic Schrödinger operators it is between 1 and 2. The reason is probably that the D–N operator on a graph Σ is to a large extent a one-dimensional, rather than a purely two-dimensional, operator. Similarly, such an operator in three dimensions acts on a surface and hence is to some extent a two-dimensional operator. One should remember, however, that the operator Λ_Σ on a graph Σ still has two-dimensional features; for instance, its spectral bands can overlap.

CONJECTURE 7.18. *For any periodic hypersurface structure $\Sigma \subset R^d, d \geq 3$, the number of gaps in the spectrum of Λ_Σ is finite.*

Let us now address the most interesting case of nonsmooth graphs Σ. The main feature of Theorem 7.15 is that it reduces a complex pseudodifferential problem to a much simpler (especially in two dimensions) differential one. The question is whether such reduction is possible in the nonsmooth case. It is not clear whether the answer is affirmative in general. However, there are situations when this is possible. First, since the D–N operator is "almost" twice the square root of the negative second derivative with respect to the arc length, it is clear that it is reasonable to consider the eigenvalue problem

$$-\frac{d^2u}{ds^2} = \left(\frac{D}{2}\right)^2 u \tag{7.29}$$

along each edge (or maybe

$$(-1)^m \frac{d^{2m}u}{ds^{2m}} = \left(\frac{D}{2}\right)^{2m} u$$

for some integer m). The difficult question arises, however, of what boundary conditions at the vertices and corners one should use. Although the general answer is not known, some special geometries can be treated. The analysis developed in [127], although not completely rigorous, provides an interesting heuristic technique. Due to space limitations, we cannot discuss the details of this method. In order to understand the boundary behavior at a vertex or corner (junction of several edges), one blows it up by applying the Mellin transform in the radial directions from the vertex. Then one needs to study the singularities of analytic continuation of the resulting function. The spectral problem for the D–N operator becomes a functional equation that can be used to study these singularities. We will just present one of the results that can be obtained this way. If one has a symmetric junction of three edges at a vertex and u_j is the restriction of the function to the jth edge, then our analysis leads to the following conditions at the vertex:

$$\begin{cases} u_1(0) = u_2(0) = u_3(0), \\ \sum\limits_{j=1,2,3} \frac{du_j}{ds}(0) = -(\frac{3D}{2}) \cot \frac{\pi}{3} u(0). \end{cases} \tag{7.30}$$

An interesting feature here (besides a funny trigonometric factor) is that the spectral parameter D also enters the boundary conditions. The problem (7.29) with conditions similar to (7.30) leads to simple algebraic equations and hence in many cases can be analyzed analytically. For instance, the dispersion relations for the case of the honeycomb structure with the edge size L can be found explicitly. Namely, one can derive existence of a series of eigenvalues $D = 2n\pi/L$ and of a series of nonflat bands given by

$$D_n(\mathbf{k}) = \frac{2}{L}\left(\pi n + \frac{\pi}{3} \pm \arcsin\sqrt{\frac{1}{4} + \frac{1}{6}\cos k_2 \pm \frac{1}{6}\sqrt{(1+\cos k_1)(1+\cos k_2)}}\right). \tag{7.31}$$

Tests on the disconnected union of three-edge stars, honeycomb structures, and some other geometries lead to an amazing agreement between the differential and pseudodifferential results. Figure 7.10 presents the results of computing the spectrum using the differential model (7.29)–(7.30) and the pseudodifferential operator Λ_Σ for the honeycomb lattice in the plane.

One can see that the pictures differ a little bit for the lowest band functions, but otherwise are practically identical. No rigorous justification of this effect is known. One should note, though, an important difference between the pseudodifferential and differential models. Namely, the almost flat band functions for the pseudodifferential model (left graph) are not exactly flat and do not correspond to actual eigenvalues [27], while one can show that the corresponding bands for the differential model (right) are flat and lead to infinitely degenerate eigenvalues (bound states).

Let us now address the asymptotic problem with $W \neq 0$:

$$-\Delta u = D(\delta_\Sigma + W)u.$$

In this case there is the dielectric-air coupling, and the problem cannot be conveniently reduced to the graph Σ. One of the ways one can handle this is to consider the auxiliary problem with two spectral parameters (c, D):

$$-\Delta u - cu = D\delta_\Sigma u \tag{7.32}$$

and then to intersect its spectrum in the (c, D)-plane with the line $c = WD$. Figure 7.11 represents the results of such calculation for the square structure (i.e.,

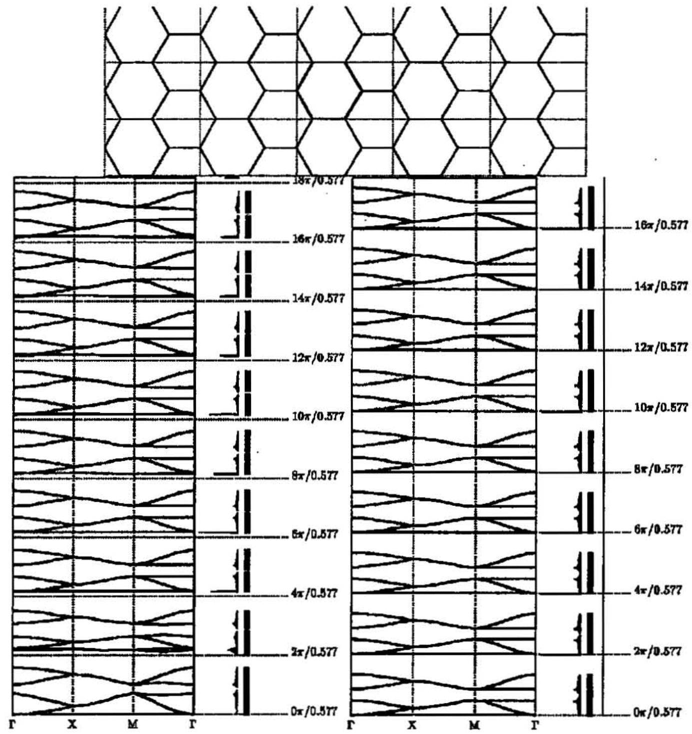

Figure 7.10: The honeycomb structure (top), the spectrum of the corresponding D–N operator (bottom left), and the spectrum of the differential model (bottom right).

formed by the lines $x = n$ and $y = m$, $m, n \in \mathbb{Z}$). The case of the square structure is exactly solvable. Analogous graphs for other geometries can be obtained numerically. The computation of the spectrum is done by fixing c, using the Green's function to rewrite the problem on Σ, and finally numerically finding the spectrum with respect to D. Doing so for many values of c, one can recover the two-dimensional spectrum of the problem.

The D-axis is horizontal and the c-axis is vertical. The shaded areas show the two-dimensional spectrum and the inclined line is $c = D$. One can see that the (c, D)-spectrum shows two distinct patterns. First, almost vertical strips originate at $c = 0$ from the bands of the spectrum of the D–N operator. Another set of narrowing strips goes in the horizontal direction. The horizontal lower edges of these strips indicate that at the corresponding values of c the D-spectrum of the problem (7.32) degenerates and covers the whole real line (and hence, due to an analyticity statement, the whole complex plane). The two different patterns intersect the line $c = D$ over two different subspectra, which correspond to the subspectra σ_1 (horizontal strips) and σ_2 (vertical strips), respectively (these spectra were discussed in section 7.5.1). The next result explains when the spectral degeneration observed at the straight edges of the horizontal strips can occur. This can provide guidance for creating geometry in a way that eliminates or lifts the horizontal pattern higher.

THEOREM 7.19 (see [127]). *The degeneration observed on the picture occurs at a level c if and only if*

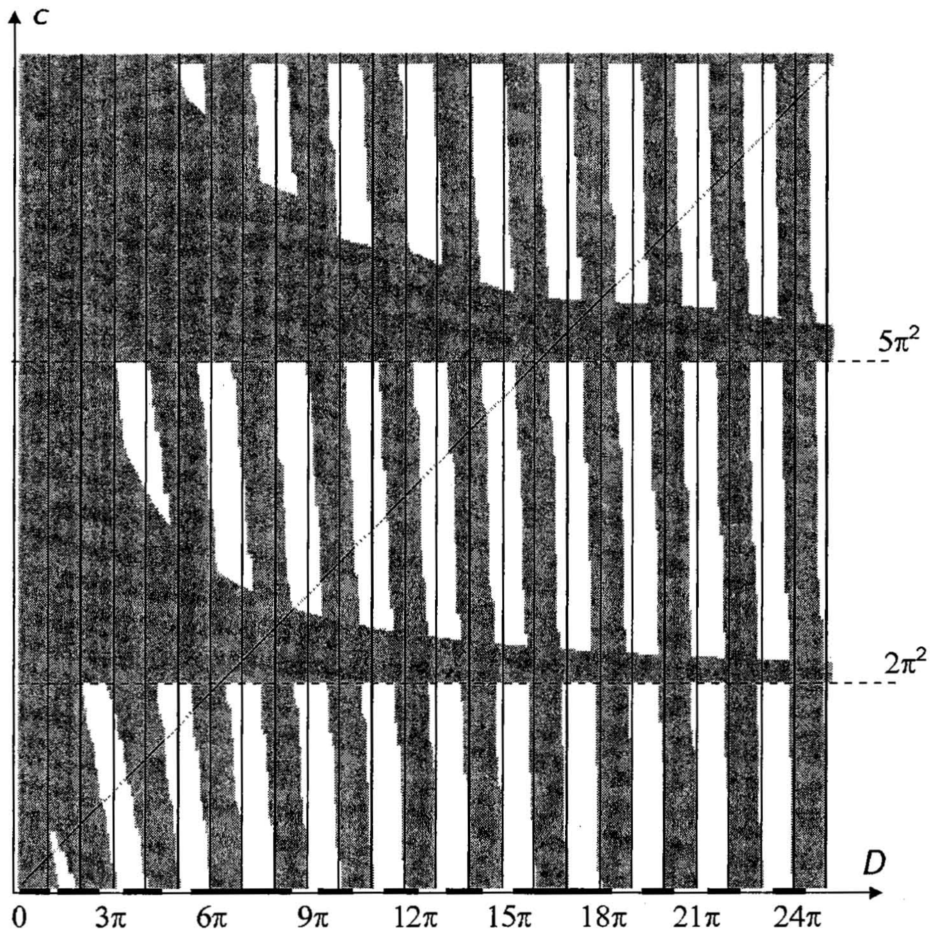

Figure 7.11: Calculation of the spectrum of the problem $-\Delta u - cu = D\delta_\Sigma u$ for the square structure.

(a) *c is in the spectrum of the Floquet Laplacian* $-\Delta_k = (-i\nabla + k)^2$ *on the torus for some real value of the quasi momentum* k*;*

(b) Σ *is in the nodal set of an eigenfunction* ϕ *of* $-\Delta_k$ *corresponding to the eigenvalue* c.

7.5.4 High-Contrast Materials with Dielectric Inclusions

In this section we present the results obtained in [100].

Let $\Omega \subset \mathbb{R}^d$ be an open connected set, which is periodic with respect to $\mathbb{Z}^d$. The complement $M = \Omega^c$ is assumed to have a positive distance from the boundary of the Wigner–Seitz cell $W = [0,1]^d$. Denoting by M_0 the part of M that resides inside W, we see that $M = \bigcup_{\mathbf{n}\in Z^d}(M_0 + \mathbf{n})$. Let χ_Ω be the characteristic function of the domain Ω. Now consider the spectral problem for the following operator:

$$T_\nu = -\nabla \cdot (1 + \nu\chi_\Omega)\nabla, \qquad \nu >> 1$$

(the operator must be defined in a standard way through the quadratic form).

In two dimensions this represents the case of TE modes in a high-contrast PBG material formed by an array of optically dense dielectric columns with sections $M_0 + \mathbf{n}, \mathbf{n} \in Z^d$. In three dimensions we may think of this as a model of acoustic waves in a high-contrast periodic medium. We are interested in the asymptotic behavior of the spectrum when the coupling constant ν (and hence the dielectric contrast) tends to infinity. In particular, do the gaps open in the case of high contrast? The positive answer is given by the following theorem.

THEOREM 7.20 (see [100]). (a) *Let $\sigma_{n,\nu}$ and $\beta_{n,\nu}$ denote the lower and upper band edges of T_ν, listed in increasing order, so that $\sigma(T_\nu) = \bigcup_n [\sigma_{n,\nu}, \beta_{n,\nu}]$.*

Then there exists a sequence of numbers μ_n satisfying $0 = \mu_1 < \mu_2 \leq \cdots$ that interlaces with the eigenvalues δ_n of the Dirichlet Laplacian $(-\Delta_{M_0})$ on M_0,

$$\mu_n \leq \delta_n \leq \mu_{n+1}$$

such that the spectrum of T_ν converges to $\bigcup_n [\mu_n, \delta_n]$ in the sense that for all n

$$\lim_{\nu \to \infty} \sigma_{n,\nu} = \mu_n, \qquad \lim_{\nu \to \infty} \beta_{n,\nu} = \delta_n.$$

(b) *If $\delta_{k-1} < \delta_k = \cdots = \delta_m < \delta_{m+1}$ for some $k \leq m$, and additionally there exists an eigenfunction u of $-\Delta_{M_0} u = \delta_k u$ that satisfies*

$$\int u dx \neq 0,$$

then $\mu_k < \delta_k$ and $\delta_m < \mu_{m+1}$. In particular, a gap opens above δ_m and a band extends below δ_k when $\nu \to \infty$.

Under some mild conditions on regularity on M_0, one can conclude from this theorem that the gap between the first two bands necessarily opens when $\nu \to \infty$. As a by-product one can also extract a statement about absolute continuity of the bottom part of the spectrum.

It was also established in [100] that although the bands in the asymptotic limit are extended and do not shrink into points, the density of states concentrates mostly at the Dirichlet eigenvalues δ_n, so the rest of each band becomes what is often called a pseudogap.

7.6 Defects in a Photonic Crystal

We have dealt so far with purely periodic media only. However, it is well known that practically important modifications of properties of materials can be made by doping them, i.e., by introducing localized or random defects into a purely periodic structure (see, for instance, [5, 106]). In this section we address the mathematics of impurities in PBG materials. The analogous problem for perturbations of periodic Schrödinger operators has been studied intensively in recent decades. We will not describe the corresponding results, referring the reader to the surveys [18]–[20].

7.6.1 Stability of the Essential Spectrum

Consider the dielectric medium described by a periodic electric permittivity $\varepsilon_0(x) \geq 1$, which is assumed to be a bounded measurable function. Then, as we have already discussed, the frequency spectrum of waves propagating in this medium is determined by the spectrum of the Maxwell operator $M_0 = \nabla^{\times}\frac{1}{\varepsilon_0}\nabla^{\times}$ appropriately defined on the subspace of transversal fields.[6] Inserting a localized defect into this periodic structure means adding a compactly supported perturbation $\varepsilon_1(x)$ to $\varepsilon_0(x)$: $\varepsilon = \varepsilon_0 + \varepsilon_1 \geq 1$. Then the operator itself is perturbed: $M = M_0 + M_1$. The first question we want to address is what kind of change of the spectrum this perturbation can bring. A similar question can be posed for the acoustic operator $-\nabla \cdot \frac{1}{\varepsilon}\nabla$. The answer is given by the following result.

THEOREM 7.21. *In both the electromagnetic and acoustic cases introduction of a localized defect does not change the essential spectrum of the operator.*

This theorem was established in the stated form in [72] by using Corollary 4 to Weyl's Theorem XIII.14 in [157]. This required showing that the perturbation is relatively compact in the sense of quadratic forms with respect to a power M_0^n of the unperturbed operator. A similar statement for the acoustic case was also proved in [1]. A general approach that implies this theorem is presented in [16].

Assume now that the unperturbed (acoustic or Maxwell) operator has a gap in the spectrum. Then the last theorem shows that the spectrum that might arise in the gap due to the added defect must consist of isolated eigenvalues of finite multiplicity. The physical meaning of this is rather simple. In the purely periodic medium these values of frequencies are prohibited. If, due to a localized impurity, a wave of a prohibited frequency does arise around the defect, it must decay fast as soon as it enters the unperturbed periodic part of the medium. Thus a bound state (eigenvector) is created. As we will see soon, these impurity modes must decay exponentially (another term used for such waves is "evanescent"). The question is, however, whether these impurity levels actually arise and, if so, in what number. This problem is addressed in the next section, along with a study of the corresponding impurity modes.

7.6.2 Impurity Levels in Spectral Gaps

Probably the first paper where the problem of defect modes was considered in a setting relevant for photonic crystals was [1]. In that paper a divergence-type operator in $\mathbb{R}^d$ was studied:

$$A = -\sum \partial_i a_{ij}(x)\partial_j$$

with a positive definite, Lipschitz continuous, bounded away from zero, and infinity matrix function $a_{ij}(x)$. This operator is perturbed by

$$B = -\sum \partial_i b_{ij}(x)\partial_j$$

with a nonnegative definite matrix b decaying to zero at infinity. Assume that the spectrum of A has a gap and that E belongs to this gap. The perturbed operator

[6] We use here the letter M to denote the operator $\nabla^{\times}\frac{1}{\varepsilon}\nabla^{\times}$, while in section 7.1 M was used for a different version of the Maxwell operator.

$A + \kappa B$ is considered for $\kappa > 0$. As is noted in the preceding section, the essential spectra of the operators A and $A + \kappa B$ are the same. Hence, if E belongs to the spectrum of the perturbed operator $A + \kappa B$, it must be an eigenvalue of finite multiplicity. One can introduce the counting function

$$N(\kappa, b, E) = \#\{0 < \mu < \kappa |\ E \in \sigma(A + \mu B)\}.$$

The following theorem establishes the possibility of creating an impurity eigenvalue at E if the support of the perturbation is sufficiently large.

THEOREM 7.22 (see [1]). *There exists $R > 0$ such that if $b(x)$ is positive definite for any x in the ball of radius R, then $E \in \sigma(A + \kappa B)$ for some $\kappa > 0$.*

The next statement deals with perturbations of small support. In particular, it shows the impossibility of creating an eigenvalue at E if the support of the perturbation is too small.

THEOREM 7.23 (see [1]). *Let $d \geq 2$. There exists a constant $c_0 > 0$ such that*

$$N(\kappa, b, E) < c_0 R^d$$

for all $R > 0$, $\kappa > 0$, and all $b(x)$ with support in the ball of radius R. In particular

$$N(\kappa, b, E) = 0$$

if the support of $b(x)$ is too small.

The paper [1] also contained a study of the asymptotic behavior of $N(\kappa, b, E)$ for large values of κ under additional conditions on the behavior of $b(x)$ at infinity. One can find some further extensions of these results in [17, 34]. One should also note a difference between dimension $d > 2$, where no impurity spectrum in the gap arises below a threshold value of κ, and $d = 2$, where no such threshold exists.

A series of papers, [72]–[74], attacks the problem of defect modes in a setting coming from the photonic crystal theory. Namely, acoustic

$$A_0 = -\nabla \cdot \frac{1}{\varepsilon_0} \nabla$$

and Maxwell

$$M_0 = \nabla^\times \frac{1}{\varepsilon_0} \nabla^\times$$

operators are considered (the latter one on the subspace of transverse fields). The dielectric function $\varepsilon_0(x)$ is assumed to be a periodic measurable function bounded from above and below by positive constants. Suppose that the spectrum of the operator has a gap. Let us now create a localized defect as follows. Choose a cube with the side l and fill it with a dielectric material with a constant electric permittivity ε. The considerations of the previous section show that only isolated eigenvalues of finite multiplicity can be created inside the gap. The questions are whether such eigenvalues do arise and, if so, then in what quantity. The next theorem guarantees existence of defect eigenvalues if the defect is "strong enough."

THEOREM 7.24 (see [72, 73]). *Let* (λ_a, λ_b) *be a gap in the spectrum of* M_0. *Also let* $\tau \in (\lambda_a, \lambda_b)$ *be such that* $[\tau(1-\gamma), \tau(1+\gamma)] \subset (\lambda_a, \lambda_b)$ *for some* $\gamma \in (0,1)$. *If we change the value of* $\varepsilon(x)$ *to* ε *in a cube of side* l *such that*

$$l^2\varepsilon > \frac{79}{\tau\gamma^2},$$

then the corresponding Maxwell operator has at least one defect eigenvalue inside the segment $[\tau(1-\gamma), \tau(1+\gamma)]$.

The papers [73, 74] also contain important theorems that provide estimates from above of the total number of defect eigenvalues that can arise in the gap. They require, however, some conditions of regularity of the ends of the gaps (see the discussion of this topic in the section 7.4.4). In particular, the following statement on the absence of defect eigenvalues in the case of "weak" defects holds.

THEOREM 7.25 (see [73, 74]). *Let* $\varepsilon_0(x)$ *be a measurable periodic function such that*

$$0 < \varepsilon_- \le \varepsilon_0(x) \le \varepsilon_+ < \infty$$

and (λ_a, λ_b) *be a gap in the spectrum of the corresponding Maxwell operator* M_0. *Let us insert a defect by changing the dielectric function as follows:*

$$\varepsilon(x) = \frac{\varepsilon_0(x)}{1+\theta(x)},$$

where $\theta(x)$ *is a measurable function supported inside of a cube of side* l *and such that*

$$-1 < \theta_- \le \theta(x) \le \theta_+ < \infty.$$

Then

(a) *if the left end* λ_a *of the gap is regular (in an appropriate sense) and* $\theta_- = 0$, *then there exists a constant* $c > 0$ *depending only on* λ_a, $\varepsilon_\pm$, *and* l *such that if* $\theta_+ < c$, *then there are no defect eigenvalues in* (λ_a, λ_b);

(b) *if the right end* λ_a *of the gap is regular and* $\theta_+ = 0$, *then there exists a constant* $c > 0$ *depending only on* λ_b, $\varepsilon_\pm$, *and* l *such that if* $|\theta_-| < c$, *then there are no defect eigenvalues in* (λ_a, λ_b).

The papers [73, 74] also contain an approach to the problem of the mid-gap defect modes based on a version of the Birman–Schwinger method. A Birman–Schwinger-type compact operator depending upon the mid-gap frequency $\lambda \in (\lambda_a, \lambda_b)$ is defined such that its eigenvalues considered as functions of λ completely determine behavior of the defect eigenvalues. This method is probably also suitable for numerical implementation. We refer the reader to the papers [73, 74] for further details.

7.6.3 Exponential Localization

As we mentioned in the section 7.6.1, the impurity modes (eigenfunctions) that arise in spectral gaps due to localized defects are exponentially localized. Although the physics explanation of this effect is rather clear, its rigorous justification and especially determination of the rate of the exponential decay require some work. The main idea is that if A is either acoustic or a Maxwell operator that has a gap (λ_a, λ_b) in its spectrum, then the Green's function $G(\lambda, x, y)$ of $A - \lambda I$ for λ in this gap decays exponentially with $|x - y|$. As soon as one establishes this, the rest is simple. If we have a localized perturbation operator B and an eigenfunction f with the eigenvalue $\lambda \in (\lambda_a, \lambda_b)$, then we get the equation

$$(A - \lambda I) f = -Bf \tag{7.33}$$

or

$$f(x) = -\int G(\lambda, x, y)\,(Bf)\,(y)dy.$$

Now the exponential decay of the Green's function together with the local nature of the operator B yield the exponential decay of f. This type of argument was made precise in the papers [72]–[74], where a version of the arguments of [43] was used to get the resolvent estimates.

If an eigenfunction decays as $O(\exp(-|x|/L))$, the constant L is called the radius of localization. It is often important to have some information about this radius. The considerations of [72]–[74] and [43] yield an estimate of the exponential decay of the type $O(\exp(-C\text{dist}(\lambda, \sigma(A))\,|x|))$ for a defect eigenfunction corresponding to the eigenvalue λ in a finite gap (λ_a, λ_b) in the spectrum $\sigma(A)$ of the unperturbed operator A. In other words, it estimates the radius of localization from above by the inverse distance to the spectrum of the unperturbed operator. It is known, however, that this estimate is not optimal close to the spectrum. Section 3 of [11] contains a general operator-theoretic approach that improves on the estimates of [43] and enables one to obtain a decay estimate of the form

$$O(\exp(-C\sqrt{|\lambda - \lambda_a|\,|\lambda - \lambda_b|}\,|x|)) \tag{7.34}$$

(we remind the reader that λ belongs to the spectral gap (λ_a, λ_b) of the unperturbed operator). Although considerations of [11] were devoted to the magnetic Schrödinger operator only, the approach is rather general and works for acoustic and Maxwell operators as well, as is shown in Appendix 3 of [42]. These estimates actually do not rely on periodicity. There is, however, a different approach, which does employ periodicity of the unperturbed medium. Although it is limited to periodic media only and besides it has not led to the precise estimates (7.34) yet, it might be useful in some circumstances. Here is how it goes. Consider (7.33) and apply the Floquet transform $\mathcal{U}$ to it:

$$A(k)\mathcal{U}f(\cdot, k) = -\mathcal{U}(Bf)(\cdot, k), \tag{7.35}$$

where we denoted by $A(k)$ the operator $A - \lambda I$ restricted to the space of functions on the Wigner–Seitz cell that satisfy the Floquet condition with the quasi momentum k. Due to the local nature of the operator B and Paley–Wiener theorems for the

Floquet transform, the vector function $\mathcal{U}(Bf)(\cdot, k)$ is analytic with respect to k in a neighborhood of the real space. Taking into account that we are at some distance from the spectrum of the operator A (since λ is in a spectral gap), it is possible to show that the analytic operator function $A(k)$ is invertible in a neighborhood of the real space. This statement is equivalent to the following: distance to the spectrum of A can be estimated using the distance of the complex Fermi surface to the real space (see section 7.4.2). Then solving (7.35), $\mathcal{U}f(k) = -A(k)^{-1}\mathcal{U}(Bf)(k)$, we derive analyticity of $\mathcal{U}f(k)$ in a neighborhood of the real space, which in turn, due to a Paley–Wiener theorem for the Floquet transform, implies that f decays exponentially. Implementation of this program for the Schrödinger case using results of [91] leads to an estimate weaker than (7.34). It would be interesting to extend this to the Maxwell case and to achieve (7.34).

7.6.4 Embedded Impurity Levels

In the discussions of the previous two sections we considered a background self-adjoint operator A (an elliptic periodic differential operator) with a gap in the spectrum and then added a local perturbation operator B. Then we discussed the behavior of the impurity spectrum in the gap. However, the natural question arises of whether the impurity eigenvalues can arise inside the spectrum of the operator A rather than in its gaps. Such eigenvalues (if they exist) are called the *embedded* ones. If this does occur, then we have a peculiar situation. Consider, for instance, the Schrödinger operator with a periodic potential $A = -\Delta + v(x)$ and add to it a localized potential $w(x)$. If there is an impurity eigenvalue λ of $-\Delta + v(x) + w(x)$ that resides inside the spectrum of A, then the corresponding bound state u of the electron is very strange: the electron has sufficient energy to propagate (since $\lambda \in \sigma(A)$), but for some reason it stays attached to the defect. There is large literature devoted to discussion of embedded eigenvalues (see, for instance, the book [55]). It is known that if the impurity potential does not decay sufficiently fast, then embedded eigenvalues can occur. There are plenty of results saying that if the perturbation decays fast enough, then there are no embedded eigenvalues. However, no such results appear to cover the case of a periodic background operator (even for Schrödinger operators). The only exception is the one-dimensional result of [158, 159] that states that for sufficiently fast decaying perturbations of the Hill operator no embedded eigenvalues arise. Probably the only known multidimensional result of this kind is proved in [131, 132] (papers [88, 118] contain theorems about discreteness of the set of embedded eigenvalues). Let us introduce some notation first. We denote by $H_0 = -\Delta + q(x)$ the unperturbed Schrödinger operator with a periodic potential q, whose spectrum has the band structure

$$\sigma(H_0) = \bigcup_{i \geq 1} [a_i, b_i].$$

We now add a decaying perturbation potential $v(x)$ to get the operator $H = -\Delta + q(x) + v(x)$.

THEOREM 7.26 (see [131, 132]). *If a real periodic potential $q(x)$ belongs to $L^\infty(\mathbb{R}^d)$ $(d \leq 3)$, the operator H_0 satisfies Conjecture 7.4 about the Fermi surface, and the impurity potential $v(x)$ is measurable and satisfies the estimate*

$$|\nu(x)| \leq Ce^{-|x|^r} \text{ for some } r > 4/3 \tag{7.36}$$

almost everywhere in $\mathbb{R}^d$, then the spectrum of H contains no embedded eigenvalues. In other words,

$$\{\lambda_j\} \cap \bigcup_{i \geq 1} (a_i, b_i) = \emptyset,$$

where $\{\lambda_j\}$ is the impurity point spectrum of H.

As was mentioned in section 7.4.2, in the case when the potential $q(x)$ is separable, Conjecture 7.4 holds true. Hence, in this case the theorem claims that no embedded impurity spectra can arise.

It would be very interesting to extend this result to arbitrary periodic potentials and to other periodic elliptic operators of interest, including the ones arising in PBG studies. However, this is probably a difficult task, since the considerations of [131, 132] show that validity of Conjecture 7.4 is crucial. In fact, we believe that the following conjecture holds true.

CONJECTURE 7.27. *If for a periodic self-adjoint elliptic operator A and a point $\lambda \in \sigma(A)$ there is an irreducible component of the complex Fermi surface $F_\lambda(A)$ that does not intersect the real space, then there exists a local perturbation operator B such that λ is an eigenvalue for $A + B$.*

This conjecture is supported by the following example. For a fourth-order self-adjoint ordinary differential equation with periodic coefficients the Fermi surface F_λ is discrete and contains four points. When λ belongs to the spectrum, two of these points (irreducible components) can be complex. In this particular case we do have irreducible components "hidden" in the complex domain. One can construct an example of such an equation and of a local perturbation that leads to an embedded eigenvalue [151].

7.6.5 Linear Defects and Waveguides

Besides localized impurities linear defects are of great importance for applications. By a linear defect we mean a strip (column) of a dielectric, whose dielectric properties differ from the ones dictated by the underlying periodic structure. For instance, imagine a row of a homogeneous dielectric material inserted into a periodic structure. It is conceivable that such a row might support a propagating mode, whose frequency falls into the frequency gap of the background periodic material. In this case such a mode must be evanescent when it leaves the defect. In other words, one creates a perfect optical waveguide without standard drawbacks of the fiber-optic cables, like leakage through sharp bends. This explains attention paid to this topic in physics literature (see, for instance, [60, 106, 138, 139] and references therein). Although a rather extensive study was done numerically and experimentally, no rigorous mathematical analysis of the problem is available. Some statements are easy to prove. For instance, similarly to the case of the localized defects one can show that the propagating modes with frequencies in the gap must be evanescent in the periodic part of the crystal. This can be done either by using the estimates of the exponential decay of the Green's function or by employing the Paley–Wiener theorems for the Floquet transform (see section 7.3). It would be interesting to have a study similar to the one done in [72]–[74] that would guarantee existence or nonexistence of the propagating modes depending on the properties of the linear defect. When this is done, a study is due of transmission through a bend in a linear defect (a numerical study of this problem was done in [139]).

7.6.6 Anderson Localization

An important and extensively studied part of the photonic crystal research is Anderson localization of classical (for instance, electromagnetic or acoustic) waves in a periodic medium perturbed by random impurities. While the study of a similar phenomenon for the Schrödinger operator has attracted a lot of attention from mathematicians, the case of classical waves has been considered in only a handful of articles. We, however, cannot address this problem here due to space limitations. A large survey article could probably be written on this topic alone. The reader can consult with the physics surveys [4, 107]–[109] and with the recent publications [42], [68]–[71], and [73] that rigorously established important results on existence of Anderson localization of acoustic and electromagnetic waves.

7.7 Some Numerical Methods and Optimization

The numerical approaches commonly used in the photonic crystals theory amount to the plane wave (Fourier expansion) methods, transfer matrix methods, finite-difference time-domain methods, and some others. The surveys [101, 152, 189] describe most of these techniques rather well. Links to websites containing descriptions of algorithms and codes can be found in [153, 190]. So, in this section we will briefly discuss only a few recent developments in this area.

7.7.1 Finite Elements and Vector Elements

The finite element method has been successfully used in many applied areas, including electromagnetics. We address the reader to the book [105] for a survey of electromagnetics applications. A finite element approach to computing dispersion relations and spectra of two-dimensional PBG materials was developed independently in the papers [7, 50]. Although the algorithms developed there are not identical, they are very close. The method is applicable to both TE and TM modes described by (7.15) and (7.14), respectively. First, a mesh is generated that has the same periodicity as the problem. In [7] the mesh generator Easymesh 1.4 created by Bojan Niceno, University of Trieste, was used. This generator, which produces high-quality triangular two-dimensional meshes, adjusts the mesh to the prescribed geometry of the air-dielectric interfaces. A square mesh was utilized in [50]. Consider the TE polarization (the TM polarization is handled similarly)

$$-\nabla \cdot \frac{1}{\varepsilon(x)} \nabla \psi = \lambda \psi.$$

The algorithm handles arbitrary lattices of periods, but as before we will concentrate on the case when the structure is one-periodic with respect to each variable. For the Floquet waves with the quasi momentum k the problem reduces to

$$-(\nabla + ik) \cdot \frac{1}{\varepsilon(x)} (\nabla + ik) u = \lambda u \tag{7.37}$$

on periodic functions u. One can rewrite (7.37) as follows:

$$\int_{\mathbb{T}} \frac{1}{\varepsilon(x)} (\nabla + ik) u \cdot \overline{(\nabla + ik) v} dx = \lambda \int_T u \bar{v} dx.$$

Here $\mathbb{T}$ is the two-dimensional torus $\mathbb{T} = \mathbb{R}^2/\mathbb{Z}^2$, $\mathbb{Z}^2$ is the two-dimensional integer lattice, u is the eigenmode, and v is an arbitrary periodic function from $H^1(\mathbb{T})$. Using the mesh, a basis of functions $\phi_j(x)$ is chosen (in [7] the basis functions are linear, and in [50], bilinear on each element). Representing $u = \sum \xi_j \phi_j$ and then choosing $v = \phi_l$, we get a generalized eigenvalue problem

$$A(k)\xi = \lambda B \xi \tag{7.38}$$

on the corresponding subspace of linear combinations of the basis functions in $L_2(\mathbb{T})$. Here

$$A_{jl} = \int_T \frac{1}{\varepsilon(x)} (\nabla + ik) \phi_j \cdot \overline{(\nabla + ik) \phi_l} dx$$

and

$$B_{jl} = \int_T \phi_j \overline{\phi_l} dx.$$

Now the task is to solve numerically the generalized eigenvalue problem (7.38) to find the band functions $\lambda_j(k)$. Since the matrices A and B are very sparse, in order to cut the memory requirements and to increase the speed of calculations, one wants to use eigenvalue solvers that employ this sparsity pattern efficiently. In both papers [7, 50] versions of the subspace iteration method were used. The algorithm described in [7] uses the SICOR (simultaneous coordinate overrelaxation) method [169], while [50] is based on the (similar in spirit) subspace preconditioning method developed in [35]. The advantage of [50] is usage of clever preconditioners of two types. First, moving along a path in the Brillouin zone, the algorithm uses the results obtained for the previous value of the quasi momentum as a seed for the current one. Second, each iteration step involves solving the problem for a homogeneous medium. These preconditioners significantly speed up the convergence.

Testing of both algorithms shows good numerical convergence and good agreement with previously known numerical results and with explicitly solvable models. The algorithms are fast. Due to economical use of memory and employing sparseness, they can handle significantly larger meshes in comparison with the number of modes that one can use with the plane wave methods. The finite element method is also known to capably handle nonsmooth interfaces and singular solutions, the factors that significantly slow down convergence of Fourier series. For instance, the analysis of the high-contrast PBG structures presented in this survey shows existence of modes (the dielectric modes that led to the "bad" spectrum σ_2) would be hard to catch with the plane wave methods.

The full-vector three-dimensional case can also be handled by the finite element method, but in this case the method is known to lead to spurious spectra [105]. Using the so-called vector (or edge) elements one completely (or almost completely) eliminates this problem [105] (see [144] for mathematical theory of vector elements). This project was realized in [51].

7.7.2 Using Soluble Models

Analysis of the two-dimensional square structure done in [76]–[78] led in [64, 155] to development of an unusual method of computing spectral characteristics of PBG materials. Namely, in the case of the square structure one can find exactly solvable models in a vicinity of both problems (7.14) and (7.15). If one now finds explicit eigenfunctions and spectra for these approximate models, one hopes that they represent a good basis of functions to use for the accurate model. For instance, one can use Galerkin-type methods, or any other variation on the theme. This was done a little bit differently in the cited papers, but the general ideas are the same. The results presented in [64, 155] agree very well with each other, and also with the computations presented in [7]. The drawback of this approach is that it relies on existence of an analytically solvable model sufficiently close to the one that we want to solve, which is probably a rather exceptional situation.

7.7.3 Optimization

The question of optimizing a PBG structure comes naturally to mind. How should one change geometric and physical parameters of a medium in order to widen an existing gap or to try to open a new gap between a couple of bands? Until recently, noone had tried to consider this as an optimization problem in the technical sense. This was done for the first time for the TM modes in two dimensions in [44]. The results are rather promising. The Helmholtz equation $\Delta u + \lambda^2 \varepsilon u = 0$ in two dimensions is considered, where the electric permittivity ε is a measurable periodic function satisfying fixed bounds $0 < c_1 \leq \varepsilon(x) \leq c_2 < \infty$. The idea is to start with a dielectric function ε_0 in this class for which existence of a gap between the bands $\lambda_j(k)$ and $\lambda_{j+1}(k)$ is known, i.e., $\lambda_j(k) < \alpha < \lambda_{j+1}(k)$ for all k in the Brillouin zone B. Then one considers the goal of maximizing the function

$$G(\varepsilon) = \inf_{k \in B} (\min\{\alpha - \lambda_j(k), \lambda_{j+1}(k) - \alpha\})$$

over the set of dielectric functions satisfying

$$c_1 \le \varepsilon(x) \le c_2.$$

The problem is with nonsmoothness of the goal function. This forces us to create a clever generalized gradient ascent algorithm, where the generalized gradient is understood in the sense described in [40]. Due to the multivaluedness of the generalized gradient, choosing the directions on each step involves solving an auxiliary linear programming problem. Although convergence of the algorithm was not rigorously established, the results of the performed numerical experiments are very encouraging [44]. The TE case was recently treated in a similar manner in [45]. This direction of study definitely deserves further development. One also notices that the optimization procedure involves multiple computations of spectra of PBG materials. This explains the need to have efficient methods of computing the PBG spectra like those described in section 7.7.1.

7.8 Conclusions

I would divide the mathematical problems of the photonic crystals theory into two broad categories. The first one consists of problems whose answers are known with a high level of certainty, while justification of these answers is hard to achieve. I can mention here the problems of absence of bounded states (localized waves) in a purely periodic photonic crystal, finiteness of the number of gaps, absence of embedded impurity eigenvalues, and some others. Although neither physicists nor mathematicians doubt what the correct answers to these questions are, our inability to provide rigorous proofs shows that sufficient understanding of these phenomena has probably not been achieved yet. Another category consists of problems whose resolution could have an immediate impact on applications. Among these I would mention developing tools of analytic prediction of existence and size of gaps depending on the geometric and physical parameters of the medium, understanding the behavior of the impurity spectra, creating significantly flattened bands, and studying properties of PBG waveguides, nonlinear effects, tunable crystals, Anderson localization, and many other phenomena. Some of the outstanding problems are mentioned in the text. Many more can be easily found in the available physics literature.

I hope that the reader is persuaded by now that the field of photonic crystals research is an applied mathematician's dream: it is of high practical importance; its mathematical models are practically exact; it involves great mathematics ranging from algebraic geometry to several complex variables, to functional analysis, to numerics—you name it; most mathematical problems are largely unexplored.

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