

On some spectral problems of mathematical physics

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ABSTRACT. The article contains a brief survey of some spectral problems of mathematical physics that have been arising recently in optics, mesoscopic systems, quantum chaos, and other areas. In particular, problems of photonic crystal theory, waveguides, and quantum graphs are addressed. This text is a modified version of the lectures delivered at the Pan-American Advanced Studies Institute (PASI) on Partial Differential Equations, Inverse Problems and Non-Linear Analysis, January 6-18, 2003, Universidad de Chile, Santiago, Chile.

1. Introduction

This article is a brief survey of some spectral problems of mathematical physics that have been arising recently in optics, mesoscopic systems, quantum chaos, and other areas. Going into details and providing comprehensive references would make such a survey a monograph. So I chose instead to provide pointers to more extended surveys, where the interested reader could find detailed exposition and bibliography.

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2. Photonic crystals

Photonic crystals or photonic band-gap (PBG) media are artificially created optical materials that are in some sense optical analogs of semiconductors. The reader can look into recent books and surveys [80, 84, 98, 145, 153] for physics and mathematics details of photonic crystal theory, engineering, and applications. One can imagine a photonic crystal as a chunk of dielectric (insulator) with cavities (“bubbles”) carved out in a periodic manner and filled with a different dielectric (e.g., air). The name photonic crystal comes from analogies with natural crystals that are also periodic media, and also from the idea that photonic crystals behave with respect to photon propagation similarly to the behavior of semi-conductors with respect to the electron propagation. In order to make this more explicit, let us start with recalling some notions from the solid state theory (e.g., [5]).

2.1. A solid state prelude. Pure semiconductors are crystals periodic with respect to a discrete co-compact subgroup $\Gamma \subset \mathbb{R}^3$ acting on \mathbb{R}^3 by shifts. Such a group is called a *lattice*. Co-compactness means that the orbit space \mathbb{R}^3/Γ is compact, or in other words the action of Γ has a compact fundamental domain W , i.e. a domain such that its translations by elements of Γ are pairwise disjoint and tile the whole space. The choice of a fundamental domain W is not unique; one can for instance include into W all points that are closer in terms of Euclidean distance to the origin than to any other point of Γ . In physics W is sometimes called the **Wigner-Seitz cell**.

The **dual lattice** Γ^* consists of all vectors k in the dual space \mathbb{R}^{3*} such that $\langle k, \gamma \rangle$ is an integer multiple of 2π for any $\gamma \in \Gamma$. If \mathbb{R}^3 is equipped with an Euclidean structure, then its dual \mathbb{R}^{3*} can be identified with \mathbb{R}^3 , and then $\langle k, \gamma \rangle$ is just the inner product of two vectors. E.g., $(\mathbb{Z}^n)^* = 2\pi\mathbb{Z}^n$.

In the discussions that follow almost nothing will depend significantly on the choice of the group (difficulties arising sometimes, e.g. in establishing finiteness of the number of spectral gaps, will be swept under the rug in this text). So, it is safe for the reader to assume that Γ is just the integer lattice \mathbb{Z}^3 (or \mathbb{Z}^n when other dimensions are considered).

Neglecting electron-electron interaction, the wave function ψ of an electron in a semi-conductor satisfies the Schrödinger equation

$$(1) \quad -\Delta\psi + V(x)\psi = E\psi,$$

where E is the energy of the electron and $V(x)$ is a Γ -periodic real-valued function (electric potential) determined by the crystal. A significant part of the solid state theory is devoted to studying the spectrum in $L^2(\mathbb{R}^3)$ of the (appropriately defined) Hamiltonian

$$(2) \quad H = -\Delta + V(x).$$

We would like to emphasize once more that this model neglects electron-electron interaction, an approximation, which is not always acceptable. Taking this interaction into the account leads to a significantly more complex analysis of multi-particle Hamiltonians. We will not touch upon these topics, but will notice a difference with the case of photonic crystals later.

Our goal now is to sketch some important spectral features of periodic Schrödinger operators (2), referring the reader to the literature (e.g., [34, 47, 86, 96, 97, 98, 124, 135, 151, 152, 158] and references therein) for the details. However, before doing so we would like to mention the main tool for studying periodic operators, the so called Floquet theory [47, 86, 96, 97, 98, 135, 151, 152], an analog of Fourier transform suitable for work with periodic operators. In physics this theory is usually associated with the name of F. Bloch [31] rather than G. Floquet [65] (Floquet theory was developed much earlier than Bloch theory, but mostly for ODEs).

2.2. A sketch of Floquet theory. In order to explain the main idea of Floquet theory, let us start with some standard Fourier analysis. Let us consider a linear constant coefficient partial differential operator $L(D)$, where as usual $D = \frac{1}{i} \frac{\partial}{\partial x}$. This 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, after which 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 . The spectrum of such an operator coincides with the range 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 (Fig. 1). One can also understand how the point spectrum can arise. If there were a non-zero L^2 -function $f(x)$ and an eigenvalue λ such that $L(D)f(x) = \lambda f(x)$ a.e., then after the Fourier transform one obtains that $L(\xi)\widehat{f}(\xi) = \lambda\widehat{f}(\xi)$, and hence

$L(\xi) = \lambda$ on a set of positive measure. Since $L(\xi)$ is analytic (even polynomial), this would imply that $L(\xi)$ is constant.

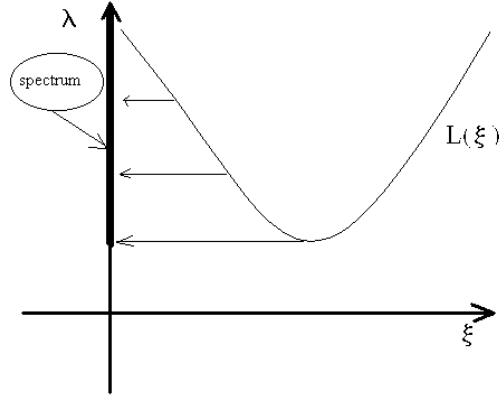


FIGURE 1. The spectrum of the operator of multiplication by $L(\xi)$.

To move closer to the situation of periodic operators, consider a constant coefficient system $L(D)$ with the symbol $L(\xi)$ that is a self-adjoint matrix function. Then the same Fourier approach shows that the spectrum can be found as follows: find the (continuous) eigenvalue branches $\lambda_j(\xi)$ (**dispersion relation** branches 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 (see Fig. 2).

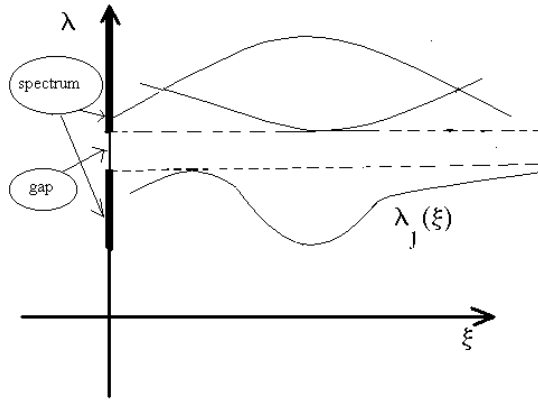


FIGURE 2. The dispersion curves and the band-gap structure of the spectrum of the operator of multiplication by the matrix $L(\xi)$.

One can think that in some cases the bands might have a gap between them.

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 due to analyticity implies existence of a constant branch. We would like to look at this from a different angle: if we can prove absence of constant band functions, this would imply absence of pure point spectrum. In fact, a small additional effort yields that the whole spectrum is then absolutely continuous. We will return to this discussion later.

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}^n (for instance, $\Gamma = \mathbb{Z}^n$)¹. Due to invariance of the operator with respect to this group, it is natural to apply the Fourier transform on Γ , which on $\Gamma = \mathbb{Z}^n$ amounts to the assigning to a sufficiently fast decaying function $h(l)$ on \mathbb{Z}^n the Fourier series

$$(3) \quad \hat{h}(k) = \sum_{l \in \mathbb{Z}^n} h(l) e^{ik \cdot l},$$

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

$$(4) \quad \mathcal{U}f(x, k) = \sum_{l \in \mathbb{Z}^n} f(x - l) e^{ik \cdot l}.$$

This transform is an analog of the Fourier transform for the periodic case. The parameter k is called **quasimomentum** (for physics reasons [5]) and it is an analog of the dual variable in the Fourier transform. Notice that the action of the group Γ on \mathbb{R}^n is not transitive, in contrast to the action of \mathbb{R}^n on itself. Hence, the space of orbits of this action contains more than one point, and as a result, the transformed function still depends on the old variable x . Let us notice two important relations:

$$(5) \quad (\mathcal{U}f)(x + l, k) = e^{ik \cdot l} (\mathcal{U}f)(x, k), \text{ for all } l \in \mathbb{Z}^n$$

and

$$(6) \quad \mathcal{U}f(x, k + \gamma) = \mathcal{U}f(x, k), \gamma \in 2\pi\mathbb{Z}^n.$$

The first of them (5) is the so called **Floquet condition** (or cyclic condition). It shows that it is sufficient to know the function $\mathcal{U}f(x, k)$

¹The reader can refer to [5, 80] for a brief introduction into general lattices, Brillouin zones, etc.

only at one point x of each orbit $x + \mathbb{Z}^n$ in order to recover it completely. For instance, it is sufficient to know it only for $x \in W$, where W is any fundamental domain for the action of \mathbb{Z}^n on \mathbb{R}^n .

The second identity (6) means that the function $\mathcal{U}f(x, k)$ is periodic with respect to the quasimomentum k . Notice that the lattice of the periods with respect to k is **dual (or reciprocal)** to the lattice the operator was periodic with respect to. We conclude that k can be considered as an element of the torus $\mathbb{T}^* = \mathbb{R}^n / 2\pi\mathbb{Z}^n$. 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 $\Gamma^* = 2\pi\mathbb{Z}^n$. 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 the solid state physics this domain is called the (first) **Brillouin zone**.

So, 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 . Compactness of the new domain W plays the crucial role in the whole Floquet theory.

It is sometimes useful to employ an alternative version of the transform \mathcal{U} :

$$(7) \quad \Phi f(x, k) = \sum_{l \in \mathbb{Z}^n} f(x - l) e^{-ik \cdot (x - l)} = e^{-ik \cdot x} \mathcal{U}f(x, k).$$

While the function $\mathcal{U}f(x, k)$ was periodic in k and satisfied the Floquet (cyclic) 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 :

$$(8) \quad \begin{cases} \Phi f(x + l, k) = \Phi f(x, k), & l \in \Gamma = \mathbb{Z}^n \\ \Phi f(x, k + \gamma) = e^{-i\gamma \cdot x} \Phi f(x, k), & \gamma \in \Gamma^* = 2\pi\mathbb{Z}^n \end{cases}.$$

When k changes, the values of $\Phi f(\cdot, k)$ belong to the same space of functions of x on the torus $\mathbb{T} = \mathbb{R}^n / \mathbb{Z}^n$. It is still sufficient 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.

As for the regular Fourier transforms, one can prove analogs of Plancherel and Paley-Wiener theorems that describe the ranges of the $L^2(\mathbb{R}^n)$ and of some spaces of smooth decaying functions under the Floquet transform [97]. Such theorems are very significant for many issues of spectral theory of periodic operators, same way as in the regular Fourier analysis. Let us formulate an analog of the Plancherel theorem. Below we assume that the natural measures dk on the Brillouin zone B and the dual torus \mathbb{T}^* are normalized.

THEOREM 1. *The transforms*

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

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 as 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 (5).*

This theorem, used constantly in solid state physics since Bloch [31], was introduced into mathematics for spectral analysis of periodic differential operators by I. Gelfand [71] (see XIII.16 in [135] and Chapters 2, 4 of [97] for discussion and further references). It can also be understood as expanding the space $L^2(\mathbb{R}^n)$ into a direct integral [135]. The proof of the theorem is straightforward, since (4) is just a Fourier series with coefficients in the Hilbert space $L^2(W)$ and the standard Plancherel's theorem applies to such series. It is easy to prove an analog of such a theorem for the Sobolev space $H^s(\mathbb{R}^n)$ instead of $L^2(\mathbb{R}^n)$, albeit it requires using Banach vector bundles [97].

Let us look at how a periodic differential operator $L(x, D)$ would react to the Floquet transform. A straightforward calculation shows that

$$(9) \quad \mathcal{U}(Lf)(x, k) = L(x, D_x)\mathcal{U}f(x, k)$$

and

$$(10) \quad \Phi(Lf)(x, k) = L(x, D_x + k)\Phi f(x, k) = L(k)\Phi f(\cdot, k),$$

where we indicate with the subscript x in D_x that D differentiates with respect to x rather than k .

Looking at (9), one observes that for each k the operator $L(x, D_x)$ now acts on functions satisfying the corresponding Floquet condition (5). 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

$L^2(\mathbb{R}^n)$ into the “direct integral” of operators

$$(11) \quad \int_{\mathbb{T}^*}^{\oplus} L(k) dk$$

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}^n . 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 Fig. 2 with the difference that the number of branches is now infinite. We see that the spectrum is expected to have a band-gap structure, and there is a hope of opening spectral gaps.

The transform Φ does not commute with periodic differential operators anymore. So, using it instead of \mathcal{U} we gain a fixed function space, while the differential expression for the operator $L(k)$ changes with k . The periodic operator $L(x, D)$ in \mathbb{R}^n 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} , 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 (e.g., [162], Chapter 1 of [97], discussion and further references therein). This technique is a crucial part of the study of periodic elliptic operators.

2.3. Some spectral properties of periodic elliptic operators.

We will briefly survey in this section several spectral properties of periodic Schrödinger operators that are relevant for solid state physics and whose analogs are of importance for PBG materials as well. We will touch upon the known results and open problems for such operators, as well as for more general scalar elliptic periodic operators. In the next section we will return to discussion of similar problems in the photonic crystal setting.

2.3.1. Band-gap structure of the spectrum. We have already concluded that the spectra of periodic elliptic differential operators exhibit band-gap structure (see [97, 98, 135, 152] for details and references). If we have a self-adjoint periodic operator $L = L(x, D)$ in $L^2(\mathbb{R}^n)$, the Floquet transform expands it into the direct integral of operators

$L(k) = L(x, D + k)$ on the torus \mathbb{T} . The main spectral statement is:

$$(12) \quad \sigma(L) = \bigcup_{k \in B} \sigma(L(k))$$

(see [47, 97, 98, 135, 152]). Ellipticity of the operator and compactness of W imply that 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 and one can choose continuous eigenvalue branches $\lambda_j(k)$ (the j th eigenvalue of $L(k)$ counted in the increasing order with the multiplicity) called **band functions** or branches of the **dispersion relation**. We conclude that the spectrum $\sigma(L)$ consists of the closed intervals (spectral bands) S_j

$$(13) \quad S_j = [\min_k \lambda_j(k), \max_k \lambda_j(k)],$$

where $\min_k \lambda_j(k) \rightarrow \infty$ when $j \rightarrow \infty$.

Existence of spectral gaps, i.e. intervals of the spectral axis not covered by any spectral bands is what makes a crystal a semi-conductor and brings about most marvels of electronics [5]. We talk here about finite gaps only, rather than the infinite gap below the spectrum.

It is well known that for ordinary differential operators of the second order the bands cannot overlap (although they can touch) [47, 135, 158], which explains why it is a generic situation in $1D$ that all spectral gaps are open between adjacent bands (see [135]). In dimensions two and higher the bands can and normally do overlap, which makes opening gaps much harder [47, 97, 135, 152]. It is still conceivable that at some selected locations the bands might not overlap and hence open a gap in the spectrum.

In the next subsection we will deal with the questions of existence and number of spectral gaps.

2.3.2. Existence and the number of gaps. Unlike the one-dimensional case, when generically infinitely many spectral gaps exist, it is believed that in dimensions two and higher only finitely many gaps can exist in the spectrum of a self-adjoint periodic elliptic operator. This is the so called Bethe-Sommerfeld conjecture [19, 152]. It has been proven for Schrödinger operators with periodic electric potentials [44, 85, 86, 152], [159]–[161] and recently in dimension two also for such operators in presence of periodic magnetic potentials as well [118, 87]. Although the proofs in the papers cited are different, most of them are of a perturbative nature. Namely, one considers first the “free” operator, where all potentials are equal to zero. In this case one shows that spectral bands are overlapping, with the size and multiplicity of

the overlap growing at large energies. This often requires some number theory results. Then it is shown that the band overlap is so strong that turning on the potentials cannot eliminate it (and hence open gaps) at high energies.

Since in the multiple dimensions the number of gaps is finite, one can ask whether the gaps must exist at all. The answer is: they do not have to. For instance, it is easy to show that the Schrödinger operator with a sufficiently small periodic electric potential does not possess any spectral gaps at all [86, 97, 152]. So, not every crystal is a semi-conductor. This is in a stark contrast with the 1D case, where the celebrated Borg's uniqueness theorem [33] says that absence of gaps implies that the electric potential is constant. Luckily for our technology, many natural crystals with such gaps exist. As we will see, we do not have such a luck with photonic crystals, which practically do not exist in nature and need to be manufactured.

It is interesting to figure out what regimes favor opening the spectral gaps. For Schrödinger and for more general periodic elliptic operators

$$(14) \quad - \sum_{i,j=1}^n \frac{\partial}{\partial x_i} a_{i,j}(x) \frac{\partial}{\partial x_j} + \sum_{i=1}^n b_i(x) \frac{\partial}{\partial x_i} + c(x),$$

there are three types of such regimes well known.

The most common one works for the Schrödinger operator (2) as follows (the hand-waving below can easily be made precise). Let us start for simplicity with the (negative) Laplace operator $-\Delta$ (i.e., $V(x) = 0$), which has the non-negative half-axis \mathbb{R}^+ as its spectrum. Let us now introduce a negative localized potential $V_0(x)$ (a potential well). This is known to possibly (and in 1D necessarily) produce a negative eigenvalue λ_0 that corresponds to an eigenfunction $\phi_0(x) \in L^2(\mathbb{R}^n)$ (the electron with the energy λ_0 is trapped by the potential well $V_0(x)$ in the bound state $\phi_0(x)$). Let us now create a new (periodic) potential $V(x) = \sum_{\gamma \in M\Gamma} V_0(x - \gamma)$, where Γ is a lattice in \mathbb{R}^n and M is a large parameter. In other words, the periodic potential is constructed by a periodic repetition of copies of $V_0(x)$ far apart from each other. If the eigenfunction $\phi_0(x)$ had compact support, then for large M we would have its Γ -shifted copies as eigenfunctions as well. This would add infinite multiplicity to the eigenvalue λ_0 without moving it. However, due to standard uniqueness theorem, compactness of support would imply that the eigenfunction were identically equal to zero. Hence, the eigenfunction has a long tail and senses the presence of other wells. Thus, the electron has a chance to tunnel to them. So, periodizing

the potential changes this portion of the spectrum. However, if M is large, and so the copies of $V_0(x)$ are far apart, the tunnelling is weak (an electron in one potential well feels only slightly presence of other wells). Hence, the spectrum shifts just a little bit, and one obtains a very narrow band of spectrum near λ_0 . This means that there will remain a gap between this band and the rest of the spectrum above it. This is how spectral gaps can be created using the tunnelling effect. Let us notice that the crucial ingredient in this construction was our ability to shift the bottom of the spectrum to a new position λ_0 below the initial 0. We will see that this possibility is missing in the case of photonic crystals.

The second way to open a gap is to employ high contrasts in the properties of the medium. This technique is normally not used for Schrödinger operators. It is important, though, for more general operators, e.g. Laplace-Beltrami operator, where high contrast in the metric a_{ij} in (14) can be used successfully for opening spectral gaps. One can find discussion of the results in this direction in [74, 98, 134]. We will also see later on in this text that this is a favorite approach in the optics case.

The third possibility for gap opening that has been discussed in the literature is to use identical scatterers distributed throughout the medium [130, 131]. This approach (which in fact does not necessarily require periodicity of the medium) will be addressed more in the section devoted to quantum graphs (see also [9, 104, 147]).

2.3.3. Absolute continuity of the spectrum. Another physically important property is the structure of the spectrum. Namely, understanding presence or absence of the pure point, absolute continuous, or singular continuous parts in the expansion

$$(15) \quad \sigma(L) = \sigma_{pp} \cup \sigma_{ac} \cup \sigma_{sc}.$$

Physically, the eigenfunctions of the pure point spectrum correspond to the bound (or trapped) states, while the ones of the absolutely continuous spectrum are interpreted as propagating modes. It has been known for a long time that the singular continuous part is missing from the spectra of periodic Schrödinger operators (e.g., [97, 135, 151, 157]). Close inspection of the proof (e.g., the one given in [97, 151]) shows that it works for any periodic elliptic operator. This was explicitly stated in [72], where it was proved for general “analytically fibered” operators $\int L(k)$, where each $L(k)$ has compact resolvent. The task of proving absolute continuity of the spectrum boils down now to showing absence of eigenvalues. Although it has been unanimously believed by physicists for a long time (since beginnings of the quantum solid state

theory), proving this statement happens to be a hard problem (it is false, by the way, for periodic elliptic operators of higher order [97]). For the Schrödinger case in 3D it was proven in the celebrated paper [157] by L. Thomas and then extended to more general potentials in [135]. A significant advance was started by the paper [26], where absolute continuity was proven in 2D for the Schrödinger operator with both magnetic and electric periodic potentials. This result was extended in [154] to any dimension (see also [107] for a simplification). One can find more references and a nice survey of most known results in [28]. The deficiency of all these result was that they addressed only operators with constant coefficients in the leading terms, or those that could be reduced to this case (for instance, by using isothermal coordinates). A breakthrough was made in [69], where absolute continuity was proven for essentially arbitrary periodic elliptic operator (14) of second order (under some smoothness conditions on the coefficients). The only caveat is that it is required in [69] that (if \mathbb{Z}^n is the lattice of the periods) the operator commutes with the change of sign of one of the coordinates. This symmetry condition does not seem necessary, but no one has succeeded in removing it yet.

We will now indicate the main thrust of the Thomas' proof and of all its extensions. The major step is to use analytic continuation into the domain of complex quasimomenta k . The following basic theorem first proven in [157] for Schrödinger operators holds:

THEOREM 2. *Let L be a periodic elliptic operator. Then the following statements are equivalent:*

- a) The point λ is an eigenvalue of L in $L^2(\mathbb{R}^n)$, i.e., there is a non-zero L^2 -solution of the equation $Lu = \lambda u$ in \mathbb{R}^n ;*
- b) For any $k \in \mathbb{C}^n$ there exists a non-zero solution of the equation $L(k)v = \lambda v$ on the torus.*

The proof is not hard [97] and follows the idea stated previously: having an eigenvalue λ of L , after Floquet transform one concludes that it is an eigenvalue of $L(k)$ for a positive measure set of (real) quasimomenta k . Then analytic continuation shows that this must also be true for all complex k . The converse statement is also simple.

Let us interpret this result in a different way. One obtains the following key corollary:

COROLLARY 3. *If for any λ there exists a quasimomentum $k \in \mathbb{C}^n$ such that the equation $L(k)v = \lambda u$ has no non-trivial solutions on the torus \mathbb{T} , then the spectrum of the operator L is absolutely continuous.*

All the known proofs of absolute continuity (including [69]) follow the following pattern: using the freedom of going into the domain of complex quasimomenta, one finds a vector $k \in \mathbb{C}^n$ such that the equation $L(k)v = \lambda u$ has no non-trivial solutions. Except in [69], this is done by the method that can be easily explained for the case considered first in [157]: Schrödinger operator $-\Delta + v(x)$ with a periodic potential v . If one can show the absence of periodic solutions of the equation $(D + k)^2 u + vu = \lambda u$ for an appropriately chosen (depending on λ) complex quasimomentum k , the job is done. It is not hard to choose a quasimomentum with a large imaginary part in such a way that the L^2 -norm of $(D + k)^2 u$ term dominates the norm of zero order terms $vu - \lambda u$, and hence no non-trivial solutions can exist (see for instance [157, 135, 97] for details). Although the idea stays the same, treatment of more general operators involving non-constant first order terms becomes much more complex. This method of dominating the lower order terms by the leading ones had essentially precluded proving absolute continuity for the case when variable coefficients are present in the leading terms of the operator (the two-dimensional case is an exception, due to the availability of isothermal coordinates). The situation changed with the appearance of [69], where the “domination” approach described above was not used, while the rest of the general Thomas’ scheme was still preserved.

2.3.4. Impurity spectra. Both in the solid state physics and in the photonic crystal studies it is important to understand what happens to the spectrum of a periodic operator when the operator is perturbed in some specific ways. In the case of a Schrödinger operator, the case of interest is adding either a localized, or randomly distributed perturbation to the potential. This corresponds to adding impurities to the periodic medium (crystal). The reason for studying these questions is not just that often the media are not purely periodic and one wants to know what is the effect of having such impurities. Indeed, it is often (e.g, in laser physics) desirable to have such impurities, and so studying impurity spectra becomes an important task.

In the case of a compactly supported perturbation of the potential, usually a version of the Weyl’s theorem [135] is applicable that guarantees that the essential spectrum is not perturbed. This means that only additional eigenvalues of finite multiplicity can arise. In principle, one can expect two distinct types of those: impurity eigenvalues arising in the gaps of the spectrum, and the ones arising on the original essential spectrum (so called embedded eigenvalues). It is generally expected that embedded eigenvalues should be absent if the perturbation is decaying fast enough (otherwise there are counterexamples). There

is a rather large body of work devoted to proving the absence of embedded eigenvalues in the case when the background potential is zero (e.g., [43, 48] and references therein). Although the case of a periodic background potential is completely resolved in $1D$ [136, 137], for dimensions two and higher there appears to be only one rather limited result of [111] known. It was also shown in [111] that the problem of absence of embedded eigenvalues appears to be linked to the extremely hard problem of analytic irreducibility of the so called Fermi surface.

Most of the attention has been paid to the impurity eigenvalues inside the gaps, which are responsible for many useful properties of doped semi-conductors. We will not dwell on this, referring the reader to available surveys (e.g., [20]-[22]).

An important case is of a random perturbation of the potential, the subject of studies of the so called Anderson localization. We will skip this issue and direct the reader to [38, 129, 156] and references therein.

2.3.5. Spectral behavior near the gap edges. Suppose that $[a, b]$ is a gap in the spectrum of one of the periodic problems we have been discussing. 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, non-degenerate, etc.? There is a conjecture that the band edges generically are non-degenerate single extrema of dispersion relations. Unfortunately, there is almost no information about this. The only exception is the recent result of [89], which states that generically each gap end-point is an extremal value of a single band function λ_j (nothing is still known about it being isolated and non-degenerate). The problem still remains a challenge.

The bottom of the spectrum (which is the upper end of the infinite gap $(-\infty, a]$) is the only gap end at which the behavior of the dispersion curves is well understood. The result of [88] concerns a periodic Schrödinger operator $H = -\Delta + V(x)$ in \mathbb{R}^n and establishes that the bottom of the spectrum truly is a single non-degenerate minimum. Let us denote as before

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

Let the band functions $\lambda_j(k)$ provide the eigenvalues of $H(k)$, with $\lambda_1(k)$ being the lowest one.

THEOREM 4. (*Theorem 2.1 in [88]*) *Let ψ_0 be the positive periodic solution of $H\psi_0 = \lambda_1(0)\psi_0$. Then*

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

This theorem implies that the bottom of the spectrum is attained only at the zero quasimomentum $k = 0$, and that 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 .

A thorough study of the behavior at the bottom of the spectrum of dispersion curves of periodic elliptic operators (including matrix operators, in particular Pauli and Maxwell operators) has been done recently in a series of papers by M. Birman and T. Suslina [27, 29] (see also [133]).

Any results of this kind for the higher gaps that we described for the bottom of the spectrum would be of great importance, since the band edge behavior is closely related to many issues. One can list among them homogenization theory [18, 29, 78], Liouville type theorems about the structure and dimension of the spaces of polynomially growing solutions [110], Anderson localization (already mentioned above), and behavior of the impurity spectra in the gaps [20, 22]. The notion of the effective masses, common in solid state physics [5] also assumes non-degeneracy of the band edge. One should mention the recent advance in [23], where a version of homogenization theory was developed for internal gap edges for periodic ODEs (the standard homogenization is related to the bottom of the spectrum only). A PDE analog is considered in [30].

2.4. PBG materials and the spectral structure of periodic Maxwell operators. We are finally moving now to the optics case. As it was explained before, a photonic crystal, or a PBG (photonic band-gap) medium is a dielectric (i.e., insulator) material with a spatially periodic structure. One is interested in propagation of electromagnetic waves in such a material (and in fact tailoring the material to obtain desired properties). While in solid state physics the governing equation is Schrödinger equation, in optics it is the Maxwell system [77, 115]. A thorough study of spectral theory of Maxwell operators in bounded domains can be found in [24, 25].

2.4.1. The governing equations. The macroscopic Maxwell equations that govern the light propagation in absence of free charges and

currents look as follows:

$$(16) \quad \begin{cases} \nabla \times \mathbf{E} = -\frac{1}{c} \frac{\partial \mathbf{B}}{\partial t}, & \nabla \cdot \mathbf{B} = 0 \\ \nabla \times \mathbf{H} = \frac{1}{c} \frac{\partial \mathbf{D}}{\partial t}, & \nabla \cdot \mathbf{D} = 0 \end{cases}$$

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 [77, 115]. 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 ∇^\times), $\nabla \cdot$, and ∇ are used for the curl, divergence, and gradient, although we will use *curl*, *div*, and *grad* as well. The system (16) is incomplete until we add the so-called constitutive relations that describe how the fields \mathbf{D} and \mathbf{B} depend on \mathbf{E} and \mathbf{H} . Although in general these relations are non-linear and even non-local, in materials other than ferroelectrics and ferromagnets and when the fields are weak enough, the following linear approximations to the constitutive relations work:

$$(17) \quad \mathbf{D} = \varepsilon \mathbf{E}, \mathbf{B} = \mu \mathbf{H}.$$

Here ε and μ are the so called material tensors. We will only 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 crystal considerations it is assumed that the material is non-magnetic and so we can take $\mu = 1$. The electric permittivity function $\varepsilon(x)$ will be assumed periodic with respect to a lattice in \mathbb{R}^3 .

The linear PDE system (16) has time-independent coefficients, so the Fourier transform in the time domain reduces considerations to the case of monochromatic waves $\mathbf{E}(x, t) = e^{i\omega t} \mathbf{E}(x)$, $\mathbf{H}(x, t) = e^{i\omega t} \mathbf{H}(x)$, where ω is the time frequency. From now on we will consider such waves only. This leads from (16) to

$$(18) \quad \begin{cases} \nabla \times \mathbf{E} = -\frac{i\omega}{c} \mathbf{H}, & \nabla \cdot \mathbf{H} = 0 \\ \nabla \times \mathbf{H} = \frac{i\omega}{c} \varepsilon(x) \mathbf{E}, & \nabla \cdot \varepsilon \mathbf{E} = 0 \end{cases} ,$$

or after eliminating the electric field \mathbf{E} , to

$$(19) \quad \nabla \times \frac{1}{\varepsilon(x)} \nabla \times \mathbf{H} = \lambda \mathbf{H}, \nabla \cdot \mathbf{H} = 0.$$

Here $\lambda = (\omega/c)^2$ plays the role of the spectral parameter. Now (19) will be our replacement for the Schrödinger spectral problem that we discussed in the solid state case.

We would like to mention that in applications of interest photon-photon interaction is negligible, and the Maxwell system is considered to be an extremely good model. This is in contrast with the solid

state case, where the one-particle Schrödinger operator often cannot be considered as a very precise model. On the other hand, the constitutive relations might become more complex (nonlinear and non-local). Then one arrives to the nonlinear optics, where the Maxwell equations must be modified to some nonlinear versions [116]. We will not address the nonlinear problems here and refer the reader to [12]-[15], [153] for further reading and references on nonlinear photonic crystals.

One of the principal tasks of the photonic crystals theory is to choose a periodic function $\varepsilon(x) \geq 1$ such that the spectrum of the corresponding problem (19) 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. This in turn would make many wonderful applications to light sources, lasing, optical waveguides, optical computing, mirrors, etc. possible [80, 84, 145].

The vector nature of the Maxwell operator and presence of zero-divergence conditions in (19) sometimes complicate the study a lot in comparison with the Schrödinger case. There is one important exception, though, where this complication disappears. This is the case of a $2D$ medium, i.e. a medium where the electric permittivity $\varepsilon(x)$ does not depend on one of the variables (say, z) and is periodic with respect to the other two $x \in \mathbb{R}^2$. One can think of such a medium as $2D$ -periodic in the x -variables and homogeneous with respect to the “vertical” variable z . One can check then that the Maxwell system is reduced by the complementary subspaces, / one consisting of the fields where the electric field \mathbf{E} is normal to the periodicity plane (and hence has the form $\mathbf{E} = (0, 0, E(x))$, where $E(x)$ is a scalar periodic function), while the other has magnetic field $\mathbf{H} = (0, 0, H(x))$ normal to the periodicity plane. In these two subspaces the spectral problem (19) reduces respectively to the following scalar ones:

$$(20) \quad -\Delta E = \lambda \varepsilon(x) E$$

and

$$(21) \quad -\nabla \cdot \frac{1}{\varepsilon(x)} \nabla H = \lambda H,$$

where as before λ is related to the time frequency ω as $\lambda = (\omega/c)^2$.

2.4.2. Floquet theory for periodic Maxwell operators. Let us denote by M the operator $M = \nabla^\times \frac{1}{\varepsilon(x)} \nabla^\times$ on the subspace of fields \mathbf{F} satisfying $\nabla \cdot \mathbf{F} = 0$ (the precise definition of the operator requires some technicalities that we skip, the reader can refer for instance to

[24, 29, 56, 59, 61]). Our task is to study the spectrum of this operator and to design periodic dielectric permittivity functions $\varepsilon(x)$ such that the spectrum has desired properties (for instance, gaps).

The first question to ask is whether the Floquet theory described above applies to the Maxwell operator. The answer is essentially a “yes,” but some additional difficulties do arise. The main results of Floquet theory as indicated above and as described in more detail in [97] work for elliptic (or at least hypoelliptic) operators. Ellipticity influences not only the technique, but also the results one might expect (see, e.g. [97, 98]). What one needs, is that the operators $L(k)$ (acting on a torus) in the Floquet decomposition (11) have compact resolvents. Ellipticity guarantees this. However, the Maxwell operator M taken alone is not elliptic. The correct idea is to include it into an elliptic complex (or to extend to a larger elliptic operator [75, 24, 25], 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, it is a part of an elliptic complex formed by the operators $grad$, M , and div . In other words, M is the middle part of an elliptic complex of operators containing besides M also the gradient and divergence, but not an elliptic operator standing alone.

Now one can apply the Floquet transform to the whole elliptic complex. And here the problem arises: after the 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 . Indeed, let us expand the field F into the Fourier series $\sum_{\gamma \in \Gamma} e^{i\gamma \cdot x} F_\gamma$. Then 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 situation forces one to work with sections of analytic sheaves instead of sections of analytic vector bundles. Although this is possible (see for instance [128], where the main result of [96]-[97] was extended to the case of elliptic complexes), the technical complications can sometimes be severe.

In any case, one can extend to the Maxwell system the basics of the Floquet theory, including Floquet transforms, band-gap structure of the spectrum, and analyticity of dispersion curves (see, for instance

[29, 56, 59, 61]). Now one can attempt a detailed spectral analysis similar to the one done for periodic Schrödinger operators.

2.4.3. *Problems of spectral theory of PBG materials.* We want now to address the spectral problems for (19) analogous to the ones discussed above for periodic Schrödinger operators.

- **The band-gap structure** of $\sigma(M)$ still holds, as it was mentioned above. This means that the piecewise analytic band functions (branches of the dispersion curve) $\lambda_j(k)$ can be defined, and the spectrum consists of the union of their ranges S_j (**bands**) such that each S_j is a finite closed interval $S_j = [a_j, b_j]$ and $\lim_{j \rightarrow \infty} a_j = \infty$.

- **Absence of the singular continuous spectrum** still holds, with no change in the proof for analytically fibered operators [72].

- **Absolute continuity of the spectrum** (or absence of bound states) has been established in the case of sufficiently smooth dielectric function $\varepsilon(x)$. This was done in [120], where it was shown that this problem can be reduced to a similar one for a non-self-adjoint matrix Schrödinger operator, for which the standard Thomas' approach works (see also [107]). In practical applications, though, the photonic crystals are created by mixing two different dielectrics (e.g., cutting air holes in a dielectric slab). This means that $\varepsilon(x)$ is piecewise constant, and hence not even continuous. The problem of extending this result to such dielectric functions remains open (as well as for other spectral results to be discussed).

The case of a $2D$ photonic crystal is simpler, at least for the E -polarized waves (20), where the absolute continuity of the spectrum for a piecewise-constant electric permittivity follows from the Thomas' result for the Schrödinger operator. The H -polarized case (21) is still waiting for the treatment of the piecewise-constant $\varepsilon(x)$.

- **Gaps opening** is the main goal to be achieved when creating a photonic crystal. After initial failures, photonic crystals have been created for which both numerics and experiments confirm existence of spectral gaps (see [80, 84, 145]). One has to be careful with such evidence, though, since numerics needs to be done carefully to avoid miscalculations of the spectra (which had occurred initially). Secondly, both numerics and experiments have a hard time distinguishing between true gaps and so called pseudo-gaps, where the spectrum is very "thin" (i.e., the density of states is very low). So, analytic studies are fully warranted.

It is much harder to guarantee analytically existence of gaps in the photonic rather than the solid state case. Here is the reason. We have

described before the idea of using periodically repeated local perturbations to the potential in a Schrödinger operator for gap opening. As we indicated there, the main effect used was the possibility of lowering the bottom of the spectrum by perturbing the potential. This mechanism is absent in the Maxwell case. Indeed, the operator is non-negative, and so its spectrum is contained in the positive half-axis. On the other hand, constants satisfy the equation (19) with $\lambda = 0$ and thus provide generalized eigenfunctions guaranteeing that zero is in the spectrum. So, the spectrum of the Maxwell operator M **always** starts from zero. We see, in particular, that gaps do not open at the bottom of the spectrum. On the other hand, analogously to the Bethe-Sommerfeld statement, one expects that there are no gaps at high frequencies. Therefore, gaps could possibly open in some middle range of frequencies only, which makes this effect harder to achieve.

Here, however, the second technique comes to rescue: using high contrast materials (i.e. the ones with high variations in the electric permittivity function). The first truly analytic confirmation of the possibility of opening spectral gaps for some photonic crystals, as well as analysis of those gaps, was obtained for $2D$ crystals [60]-[62]. In $2D$, the spectral problems (20)-(21) are scalar and much easier to study. Existence of gaps was shown for PBG materials that consist of very narrow graph-like strips of an optically dense dielectric (i.e., $\varepsilon \gg 1$) separating large “air bubbles” with $\varepsilon = 1$. Similar analysis for the full $3D$ model remains a challenge. The only exception is the paper [63], where the magnetic properties were also involved and high contrasts in both ε and μ were required. It is not clear yet whether there exist regimes (i.e. specific geometries of the material and choices of the electric permittivity) where one can show analytically (rather than numerically) existence of gaps for a truly $3D$ periodic dielectric (i.e., non-magnetic) medium.

An interesting activity was started in [41, 42] of optimizing gaps in a PBG medium (see also [46] on optimization of impurities). Here one starts with a medium with a gap and then uses non-smooth optimization methods to change the geometry and dielectric function in order to maximize the gap. There is also a version of the method, in which gaps are forced to open at locations where they did not exist before.

- **The number of gaps** is believed to be finite, like in the Bethe-Sommerfeld conjecture for the Schrödinger case, however no results are known.

- **Localized impurities** added to a periodic ε are known not to change the essential spectrum [55]-[59] and hence introduce only eigenvalues of finite multiplicity. In the same papers sufficient conditions are

provided for the “strength” (i.e., size and dielectric constant) of a homogeneous impurity that would guarantee that an impurity eigenvalue does arise at a prescribed location in the gap. The corresponding eigenfunctions decay exponentially with the rate dependent on the proximity of the essential spectrum.

We will not address the popular activity in physics literature concerning random perturbations to a photonic crystals and the corresponding classical analog of Anderson localization, which in fact was one of the initial reasons for pursuing photonic crystals (e.g., [81]–[83]). There are also some initial analytic results in this direction [17, 39, 55, 58].

The effects of introducing linear defects into a photonic crystal will be addressed in the next section.

3. Waveguides

In this section we will survey very briefly some spectral problems concerning waveguides that are of the nature similar to the ones discussed above. We will consider two types of waveguides, which we will call “hard wall” and “soft” waveguides, meaning that in the first case one has boundary conditions imposed that confine the wave to the guide (e.g., electric field in a waveguide with metallic walls), while in the second one the waves can leak into the exterior, where they are forced to decay exponentially.

3.1. Periodic hard wall waveguides. In this section, by a waveguide we will mean an elliptic problem in a cylindrical domain (possibly with a multi-dimensional axis and with a variable cross-section). A common example is a Helmholtz operator in cylindrical tube with either Dirichlet, or Neumann conditions [117]. We call such waveguides “hard wall,” since the wave is confined to the tube to start with.

Let $Q \subset \mathbb{R}^n$ be a smooth domain in

$$(22) \quad \mathbb{R}^n = \mathbb{R}^{n_1} \oplus \mathbb{R}^{n_2}$$

The points of Q are denoted by (t, x) corresponding to the decomposition (22). It is assumed that for each t the cross-section $Q_t = \{x \mid (t, x) \in Q\}$ is bounded and periodic with respect to t . We consider a regularly elliptic spectral boundary value problem in Q :

$$(23) \quad \begin{cases} L(t, x, D_t, D_x)u(t, x) = \lambda u(t, x) & \text{in } Q \\ B_j(t, x, D_t, D_x)u|_{\partial Q} = 0, & j = 1, \dots, m \end{cases}$$

where $2m$ is the order of the elliptic operator L , the boundary operators B_j are of orders $m_j \leq 2m - 1$, and the coefficients of L and B_j , as well

as the domain Q , are periodic in t . Such problems arise as models of periodic electromagnetic and optical waveguides.

A simple example is of a Schrödinger operator $L = -\Delta_{t,x} + g(t, x)$ in a cylinder along the t -axis, with Dirichlet or Neumann conditions, where the potential g is t -periodic.

The general Floquet theory is applicable to such elliptic (as well as parabolic) problems (see Section 5.4 in [97]). One can ask questions similar to the ones discussed before for such waveguides. For instance, one is interested in the absolute continuity of the spectrum. Until recently, there had been barely any progress in this direction, besides a couple of simple old results ([45] and Theorem 5.4.9 in [97]). However, the recent advances in general studies of the absolute continuity problem (see the discussion above in this text) have led to the significant progress in this area as well. Namely, various results on absolute continuity for hard wall waveguides were obtained in [149, 150, 155] based on Thomas' method, as well as a waveguide analog [70] of the breakthrough paper [69].

3.2. Soft PBG waveguides. One of the main suggested applications of PBG materials (photonic crystals) is to guiding light. Here is the idea. Assume that we would like to guide the light of certain frequency ω . We also assume that we have a PBG material such that this particular frequency falls into its spectral gap. Let us create a linear (straight or bent) defect in this bulk medium (for instance, putting a different dielectric, or altering the material design in any other way along the defect). One can now try to send a wave of the “prohibited” frequency ω through the defect, where it might be able to propagate. On the other hand, when leaking into the bulk, the wave would have to decay exponentially fast (be evanescent), since there this frequency is not allowed. This is an intensively discussed topic in photonics area (e.g., [35, 54, 80, 84, 145]), due to suggested applications to optical circuits. There are quite a few questions to answer here, though. First of all, one wonders whether waves of prohibited frequencies do exist inside the line defect. The second is to show that the wave is evanescent into the bulk (i.e., it is essentially confined to the defect “guide”), which is probably the simplest among the problems that arise. The next question is whether the wave (if it does exist) might “stuck” in the guide rather than propagating through, or be reflected back from bends or junctions without sufficient transmission. There are also other issues that we will not address, e.g. in what way one could trigger such waves in the defect by coupling to an external source.

Let us notice that one deals here with a “soft” waveguide, since the waves are allowed to penetrate the bulk and gladly do so, although they will be forced to decay fast there. Analysis of such waveguides poses additional difficulties in comparison with the hard wall case.

There has been only a handful of mathematics publications devoted to these problems [4, 108, 109]. In all of them a bulk medium is described by a dielectric function $\varepsilon(x)$, which is assumed to be either periodic [4] or just bounded from below and above $1 \leq \varepsilon(x) \leq C < \infty$ [108, 109]. In [4, 108] the scalar model (20) is considered, while in [109] the full Maxwell system is treated. It is assumed that the spectrum of the bulk medium has a gap (α, β) . A linear cylindrical strip defect is considered, which is assumed to be filled with a homogeneous dielectric. In [4] it is additionally assumed that the defect is aligned with one of the periodicity axes. It was shown [4, 108, 109] that if the spectrum of the medium with the defect contains a frequency inside the bulk of the gap, then the associated generalized eigenfunctions are evanescent into the bulk (i.e., in the directions transversal to the defect). This is a rather simple result based on the known decay estimates for the Green’s function in the gap [17, 40, 59]. It was also shown in [108, 109] that if the defect strip is sufficiently wide and optically dense, then there is spectrum of the medium in the gap of the bulk, and this “guided wave” spectrum can be made to be as dense inside the gap as needed.

Let us formulate the main result of [108] more precisely. One can think that the whole space \mathbb{R}^n is filled with a dielectric or acoustic material with properties described by the functions ε_0 and ρ_0 (the physical interpretation of these functions depends on whether one deals with electromagnetic or acoustic case). In the case of periodic functions this models a photonic or acoustic crystal.

The operator A_0 is the self-adjoint realization of

$$-\frac{1}{\rho_0(x)}\nabla \cdot \frac{1}{\varepsilon_0(x)}\nabla$$

in $L_2(\mathbb{R}^n, \rho_0(x) dx)$ defined by means of its quadratic form

$$(24) \quad \int \varepsilon_0^{-1} |\nabla u|^2 dx$$

with the domain $H^1(\mathbb{R}^n)$.

We also consider a “defect” strip

$$\mathcal{S}_l = \{x = (x_1, x') \in \mathbb{R}^n \mid x \in \mathbb{R}, x' \in l\Omega\},$$

where Ω is the unit ball centered at the origin in \mathbb{R}^{n-1} (the ball can be easily replaced by other bounded domains) and $l\Omega$ is the ball of radius

$l > 0$. We can now introduce the perturbed medium, for which

$$\varepsilon(x) = \begin{cases} \varepsilon > 0 & \text{for } x \in \mathcal{S}_l \\ \varepsilon_0(x) & \text{for } x \notin \mathcal{S}_l \end{cases}, \quad \rho(x) = \begin{cases} \rho > 0 & \text{for } x \in \mathcal{S}_l \\ \rho_0(x) & \text{for } x \notin \mathcal{S}_l \end{cases}.$$

Physically, a linear homogeneous defect \mathcal{S}_l is introduced into the original medium. The perturbed operator A corresponds to the modified medium. This operator is self-adjoint in the weighted L_2 -space $L_2(\mathbb{R}^n, \rho(x) dx)$.

THEOREM 5. *Let $G = (\alpha, \beta)$ be a non-empty finite gap in the spectrum of the “background medium” operator A_0 (in particular, $\alpha > 0$). Assume that for some $\delta \in (0, \frac{\beta-\alpha}{2})$ the following inequality is satisfied:*

$$(25) \quad l^4 \delta^2 \rho^2 \varepsilon^2 > \nu_{d-1},$$

where $\nu_{d-1} > 0$ is the lowest eigenvalue of the bi-harmonic operator Δ^2 in Ω with Dirichlet boundary conditions.

Then any interval of length 2δ in the gap G contains at least one point of the spectrum $\sigma(A)$ of the perturbed operator.

This result has been extended to the full 3D Maxwell system in [109].

Not much is known otherwise about the structure of the “guided wave” spectrum in the gap (e.g., what part of the gap it fills). The next question to ask is whether this spectrum can contain any eigenvalues. If this does occur, then the corresponding waves are not propagating through the guide, but rather stuck inside of it. The last possibility is unlikely, at least in the case of a periodic bulk. The natural idea of trying to model after the Thomas’ proof of absolute continuity of the spectrum for a periodic Schrödinger operator meets with difficulties. The main obstacle here is that in the case of soft waveguides the fiber operators $L(k)$ in the direct integral Floquet expansion are defined on non-compact manifolds, and hence do not have purely discrete spectra (which does not happen for hard wall waveguides, where the Thomas’ approach works smoothly). One should also mention the recent preprint [64], where absolute continuity is shown for Schrödinger operators with potentials periodic in some directions and decaying in others. One can also apply successfully the Thomas’ method in some asymptotic cases of infinitely thin defects [68, 109]. Such defects can be modeled by δ -type potentials supported on periodic curves, which serve as another model of “soft” waveguides (e.g., [53] and references therein).

The next important question is of creating bent guides and junctions that allow significant propagation of guided waves without much of a reflection back. Physics studies have shown [35, 54, 80, 84, 145] that special engineering of bends can lead to high transmission. This problem is still waiting for analytic results and is being currently considered.

4. Quantum graphs

In this section we would like to mention a new kind of spectral problems that have been emerging recently from a variety of sources in chemistry, physics, engineering, and mathematics. The section is necessarily very short and we do not plan to give much of specific information. The reader can refer to the surveys [99, 101, 102] and the journal issue [103] for more details and references.

4.1. What is a quantum graph? A quantum graph is a graph G equipped with two additional structures that will be mentioned later. It is assumed that all vertices have finite degrees (i.e., finite number of edges incident to a vertex). While in combinatorics and graph theory graphs are usually considered as combinatorial objects, we would like to consider G as a one-dimensional variety. We will call G a **metric graph** if its each edge e is identified with a segment of the real axis, and hence some coordinate x_e is introduced along the edge (we will disregard the subscript in x_e and call the coordinate x , which should not lead to misunderstanding). This enables one to introduce standard notions of analysis on G : metric, measure, integration, derivatives along edges, and some standard function spaces like $L^2(G)$ (notice that functions $f(x)$ here take values at all points along the edges, rather than at vertices only, as is common in graph theory). In particular, it is possible to introduce differential operators on G (as opposed to the usual difference operators customarily studied on graphs). While it is easy to write differential expressions on a graph, to define a differential operator one needs also to impose some boundary conditions at all vertices. We will see examples of such operators and conditions below. So far we can complete the definition of a **quantum graph** saying that it is a metric graph equipped additionally with a self-adjoint differential operator (Hamiltonian).

The operators of interest in the simplest cases are:
the second derivative along each edge

$$(26) \quad f(x) \rightarrow -\frac{d^2 f}{dx^2},$$

a more general Schrödinger operator

$$(27) \quad f(x) \rightarrow -\frac{d^2 f}{dx^2} + V(x)f(x),$$

or a magnetic Schrödinger operator

$$(28) \quad f(x) \rightarrow \left(\frac{1}{i} \frac{d}{dx_j} - A(x) \right)^2 + V(x)f(x).$$

In order for the definition of the operators to be complete, one needs to describe their domains. The natural conditions require that f belongs to the Sobolev space H^2 on each edge e . One also needs to impose boundary value conditions at the vertices. It is possible to describe all the vertex conditions that make these operators self-adjoint (see [52, 90, 91] and references therein and also [101]). One standard type of such “Kirchhoff” boundary conditions for operators 27 is

$$(29) \quad \begin{cases} f(x) \text{ is continuous on } \Gamma \\ \text{at each vertex } v \text{ one has } \sum_{\{e|v \in e\}} \frac{df}{dx_e}(v) = \alpha_v f(v) \end{cases},$$

where the sum is taken over all edges e containing the vertex v , and derivatives are taken in the directions away from the vertex. Here α_v are some fixed real numbers. The most common case is when $\alpha_v = 0$, i.e.

$$(30) \quad \begin{cases} f(x) \text{ is continuous on } \Gamma \\ \text{at each vertex } v \text{ one has } \sum_{\{e|v \in e\}} \frac{df}{dx_e}(v) = 0 \end{cases}.$$

There are many other plausible vertex conditions [52, 90, 91, 101].

Higher order differential operators and pseudo-differential operators on graphs arise as well [106, 127].

Historically, probably the first graph model of the type discussed above was developed in chemistry (e.g., [144]), where it was used to model π -electron orbitals in conjugated molecules.

4.2. Where do quantum graphs come from? Why is it interesting to study quantum graphs? One of the leading reasons is studying wave propagation in thin structures. Imagine that we have a medium that is a thin neighborhood of a graph and are interested in propagation of electromagnetic, acoustic, or electronic waves in this domain. This propagation is usually governed by a differential equation (Schrödinger, Helmholtz, Maxwell, etc.) with suitable boundary conditions. Examples come for instance from the **mesoscopic physics** and **nanotechnology**. **Mesoscopic systems** (e.g., [1, 6, 51, 76, 79, 121, 148]) are

physical systems whose one, two, or all three dimensions are reduced to a few nanometers. They hence look as surfaces, wires, or dots and are called correspondingly **quantum walls**, **quantum wires**, and **quantum dots**. Circuits of quantum wires, due to recent progress of microelectronics, are subjects of intensive studies. One can also consider thin graph-like acoustic or optical structures [11, 60, 61, 62, 105, 106]. Interest in such systems comes from the area of photonic crystals. There have also been studies of wave propagation through thin graph-like superconducting media [3]. One can expect that wave transport through thin graph-like media could be studied using some approximate models on graphs (when the “thin” dimensions are ignored). This is exactly what leads to quantum graphs.

There are quite a few other cases when one wants to use a graph model. One can think, for instance, of thin acoustic, electromagnetic, or quantum waveguides. Another option is to use graph models for studying the features that depend upon multiple connectedness of the material, for instance Aharonov-Bohm effect [8, 10]. One can also address quantum graph models when the full scale ones are too complex to be treated. Examples of this kind come from quantum chaos [16, 32, 93, 94, 95], Anderson localization [7], and scattering [2, 51, 73, 90, 91, 92, 114, 125, 126, 132].

Yet another source of such models is averaging in dynamical systems in the presence of a slow motion in graph directions and a fast one across the graph. Then averaging naturally leads to the models of the kind described above [66, 67].

Quantum graph models also arise in the spectral theory of differential operators in singular domains [49, 50].

4.3. Justification of quantum graph models. One wonders whether quantum graphs are justified as asymptotic models for wave transport in thin structures. Here is a brief overview of the situation.

The graph models have been justified as approximations for superconducting networks in [112, 113], [138]–[143], [146].

The quantum graph models arising in the photonic crystal theory were obtained and studied in [60]–[62], [105, 106]. One notices here appearance of pseudo-differential Hamiltonians on graphs, as well as differential operators of orders higher than 2.

Development of quantum graph models for quantum wires circuits [51] still faces problems. It is not clear whether such models can be developed. See the discussion of this issue and relevant references in [99].

4.4. Spectral properties of quantum graphs. Most of the problems leading to quantum graphs require one to study their spectra (i.e., the spectra of the corresponding Hamiltonians). The reader can refer to surveys [99, 101, 102, 103] for more details and the bibliography concerning such studies. We will just mention briefly one interesting gap opening effect that has been discovered in the graph situation and bears a potential for important applications. Imagine that each vertex of a quantum graph is equipped with an additional graph structure (same for all vertices). This can be done either by incorporation a fixed graph into each vertex (kind of adding some internal structure to the vertex), or by attaching an additional graph to each vertex “sideways”. In both cases it has been argued that this process of incorporating geometric scatterers into each vertex leads to gap opening at some specific locations [9, 147, 101, 104]. This seems to be a much more controllable gap opening mechanism than the one due to periodicity.

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