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CRYSTAL WAVEGUIDES**

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On guided waves in photonic crystal waveguides

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Abstract

The paper addresses the issue of existence of modes guided by linear defects in photonic crystals. Such modes can be created in spectral gaps of the bulk materials and are evanescent in the bulk.

1 Introduction

A photonic crystal (or a PBG material, where PBG stands for “photonic band-gap”) is a periodic dielectric medium in which the frequency spectrum of electromagnetic waves has a gap. In other words, monochromatic electromagnetic waves of certain frequencies do not exist in this medium. Due to their high promise for applications, such materials have been intensively studied since the idea was suggested in 1987 [22, 11] (see, e.g., the recent books [10, 12, 18] and the survey of mathematical problems of this area [15]). Photonic crystalline waveguides is one of the important suggested application of PBG materials. The idea is that introducing a linear defect (a “waveguide”) into an otherwise periodic PBG material, one can create waves through it at frequencies prohibited for the bulk. Numerical

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and experimental studies have shown that such superior quality guides can be engineered very efficiently (e.g., [10, 12, 16, 18]). There also exist natural acoustic analogs of PBG materials and corresponding waveguides.

Analytic studies of such waveguides, however, are essentially absent even in the case of straight waveguide. The first questions one can ask are existence of modes at the frequencies in the band gap of the bulk material, their essential confinement to the guide (i.e., their exponential decay into the bulk), and structure of the arising spectrum in the gap (e.g., absence of bound states, absolute continuity of the spectrum). In this article we address some of these basic issues and derive simple initial results for the case of a straight linear defect. These results in fact do not use the periodicity of the bulk PBG material. Although one can obtain analogous statements for the case of full Maxwell equation, we only address the scalar model in this paper, which covers in particular the cases of TE and TM polarized electromagnetic waves in 2D photonic and waves in 2D and 3D acoustic waveguides.

We now describe the mathematical model studied in this text. Let $\varepsilon_0(x)$ and $\rho_0(x)$ be bounded positive measurable functions in \mathbb{R}^d separated from zero, i.e. $0 < c_0 \leq \varepsilon_0(x), \rho_0(x) \leq c_1 < \infty$. It is usually assumed in the photonic crystal theory that both functions are periodic with respect to a lattice $\Gamma \subset \mathbb{R}^d$, but this is not required for the basic results we obtain in this text.

One can think that the whole space \mathbb{R}^d 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, but this will be of no importance for our study). 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

$$\int \varepsilon_0^{-1} |\nabla u|^2 dx \tag{1}$$

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

We will also consider a “defect” strip

$$S_l = \{x = (x_1, x') \in \mathbb{R}^d \mid x \in \mathbb{R}, x' \in l\Omega\},$$

where Ω is the unit ball centered at the origin in \mathbb{R}^{d-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

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

Physically, a linear homogeneous defect S_l is introduced into the original medium.

We define the perturbed operator A that corresponds to the modified medium analogously to the background operator A_0 . This operator is self-adjoint in the weighted L_2 -space $L_2(\mathbb{R}^n, \rho(x) dx)$, which will from now on be denoted $L_{2,\rho}$.

Our goal is to show that for any gap (α, β) in the spectrum $\sigma(A_0)$ of the unperturbed medium and under appropriate conditions on the parameters l, ρ , and ε of the line defect, spectrum of the perturbed medium arises in the gap. One naturally wants to interpret this as existence of guided waves in the “photonic waveguide” S_l , while this would require proving some additional properties. These are first of all confinement of the wave to the guide (i.e., evanescence into the bulk), which is also proven below, and non-existence of bound states (i.e., the fact that the wave is actually propagating along the waveguide), which we have not been able to establish yet.

Our results complement the discussions of the preprint [1] by H. Ammari and F. Santosa, where spectral properties of the TM mode in a 2D PBG waveguides were studied in a situation of a linear defect aligned with a periodicity axis of an otherwise periodic medium (and hence Floquet theory [14, 17] was applicable). In particular, exponential confinement of the guided modes for this particular case was proven there. Some of the constructions presented here are similar to the ones used in [6] for localized defects.

2 Formulation of the results

Our main results are the following theorems.

Theorem 1 *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:*

$$l^4 \delta^2 \rho^2 \varepsilon^2 > \nu_{d-1}, \tag{2}$$

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 theorem guarantees that when (2) is satisfied, defect modes in the spectral gaps of the background medium exist, and the corresponding spectrum forms a δ -net in the gap. One is tempted to associate these modes with the guided waves. In order to do so one needs first to establish their confinement to the waveguide (i.e., their evanescent nature in the bulk of the material) and secondly, that they do not correspond to discrete spectrum (bound states). The first of these tasks is achieved in the next simple result, while the second is much harder and still awaits its solution. Before formulating the theorem, we remind the reader about existence of the so called generalized eigenfunction expansions. In the case of the operators we consider, for almost all points $z \in \mathbb{R}$ with respect to the spectral measure, such a generalized eigenfunction $u \in H_{loc}^1$ of the operator A has the properties $(1 + |x|)^{-N}u(x) \in L_2(\mathbb{R}^d)$ and $(1 + |x|)^{-N}\nabla u(x) \in L_2(\mathbb{R}^d)$ for some $N > 0$. The eigenvalue problem $Au = zu$ is satisfied in the distributional sense. This is a well known fact for elliptic operators with smooth coefficients [3], while for operators of the type we study one can find the corresponding results in [13]. We will use the polynomial boundedness condition in the following form:

$$\|u\|_{L_2(K+x)} + \|\nabla u\|_{L_2(K+x)} \leq C_K(1 + |x|)^N \quad (3)$$

for any compact K and $x \in \mathbb{R}^d$. We summarize (3) as polynomial growth of order N .

Theorem 2 *Let u be a polynomially bounded generalized eigenfunction of A that corresponds to a value z in a gap G of $\sigma(A_0)$, then it decays exponentially away from the defect strip S_l .*

The exact meaning of the exponential decay will be provided in the reformulation of this theorem given in Theorem 3 of the next section.

3 Proofs of the results

We adopt the following notations: the norm and inner product in $L_2(\mathbb{R}^n)$ will be denoted by $\|\cdot\|$ and $\langle \cdot, \cdot \rangle$ respectively, while those in the weighted space $L_2(\mathbb{R}^n; \rho(x)dx)$

will be denoted with the subscript ρ : $\|\cdot\|_\rho, \langle \cdot, \cdot \rangle_\rho$. Notice that the norms $\|\cdot\|, \|\cdot\|_\rho$, and $\|\cdot\|_{\rho_0}$ are equivalent.

3.1 Proof of Theorem 1

Let $(\mu - \delta, \mu + \delta)$ be a sub-interval of the gap G . The idea of the proof is that under the conditions of the theorem one is able to provide an approximate eigenfunction $u(x)$ for the operator A , such that $\|u\|_\rho = 1$ and

$$\|Au - \mu u\|_\rho^2 < \delta^2. \quad (4)$$

Finding such an approximate eigenfunction would imply immediately the statement of the theorem. For functions u supported in the defect strip, where $\rho(x) = \rho$, this is equivalent to finding a function u such that $\|u\| = 1$ and

$$\|Au - \mu u\|^2 < \delta^2. \quad (5)$$

So, let us construct such a function.

Let a real valued function $\phi(x') \in C_0^\infty(\Omega)$ have unit L_2 -norm and $\phi_l(x') = l^{(1-d)/2} \phi(x'/l)$. We will also need real valued functions $\psi(x_1) \in C_0^\infty(\mathbb{R})$ with a unit L_2 -norm and $\psi_n(x_1) = n^{-1/2} \psi(x_1/n)$ for $n > 0$. It is clear that the functions ϕ_l, ψ_n still have unit norms in the corresponding spaces. Introducing $k = \sqrt{\mu\rho\varepsilon}$, we consider the function

$$u_{l,n}(x) = \phi_l(x') \psi_n(x_1) e^{ikx_1}, \quad (6)$$

which will be our try for an approximate eigenfunction.

Instead of estimating the left hand side of (5), we will estimate $\|\varepsilon\rho(Au - \mu u)\|^2$. Taking into account that the function u is supported inside the defect, the needed inequality (5) can be also rewritten as

$$\|\Delta u + \mu\varepsilon\rho u\|^2 < \delta^2 \rho^2 \varepsilon^2. \quad (7)$$

Let us calculate directly the left hand side of (7) for the function u introduced above, understanding all norms as the norms in L_2 :

$$\|\Delta u + \mu\varepsilon\rho u\|^2 = \|(\Delta_{x'} \phi_l) \psi_n + \phi_l \psi_n'' + 2ik\phi_l \psi_n'\|^2 = \|(\Delta_{x'} \phi_l) \psi_n + \phi_l \psi_n''\|^2 + 4\mu\rho\varepsilon \|\phi_l \psi_n'\|^2.$$

We used the definition of k and the condition that functions ϕ and ψ are real valued.
Let $\gamma > 0$. Using the inequality

$$(a + b)^2 \leq (1 + \gamma) a^2 + \left(1 + \frac{1}{\gamma}\right) b^2$$

and normalization of the functions, we can estimate the last expression from above to get the following upper bound for the expression in question:

$$\|\Delta u + \mu \varepsilon \rho u\|^2 \leq \frac{1 + \gamma}{l^{d+3}} \|\Delta \phi \left(\frac{x'}{l}\right)\|_{L_2(\Omega)}^2 + \frac{1 + \frac{1}{\gamma}}{n^5} \|\psi'' \left(\frac{x_1}{n}\right)\|_{L_2(\mathbb{R})}^2 + \frac{4\mu \rho \varepsilon}{n^3} \|\psi' \left(\frac{x_1}{n}\right)\|_{L_2(\mathbb{R})}^2. \quad (8)$$

By changing variables to $(x_1/n, x'/l)$, this expression reduces to

$$\frac{1 + \gamma}{l^4} \|\Delta \phi(x')\|_{L_2(\Omega)}^2 + \frac{1 + \frac{1}{\gamma}}{n^4} \|\psi''(x_1)\|_{L_2(\mathbb{R})}^2 + \frac{4\mu \rho \varepsilon}{n^2} \|\psi'(x_1)\|_{L_2(\mathbb{R})}^2. \quad (9)$$

Since n can be chosen arbitrarily large (without changing the defect strip), the last two terms can be made arbitrarily small (uniformly with respect to k on any finite interval). Hence, one needs to control only the first term by an appropriate choice of a test function ϕ . In other words, one is interested in

$$v_{d-1} = \inf \|\Delta \phi(x')\|_{L_2(\Omega)}^2,$$

where the *infimum* is taken over real functions in $C_0^\infty(\Omega)$ of unit L_2 -norm. This is then the lowest eigenvalue of the bi-harmonic operator Δ^2 with Dirichlet boundary conditions in Ω . In particular, $v_{d-1} > 0$. Now, due to arbitrariness of $\gamma > 0$ our condition boils down to

$$\frac{v_{d-1}}{l^4} < \delta^2 \rho^2 \varepsilon^2 \quad (10)$$

or

$$l^4 \delta^2 \rho^2 \varepsilon^2 > v_{d-1}, \quad (11)$$

which proves the statement of the theorem.

3.2 Proof of Theorem 2

Let G be a spectral gap of A_0 and $z \in \sigma(A) \cap G$. Let also $u(y)$ be a polynomially growing generalized eigenfunction for the operator A that corresponds to z (in the meaning explained in the introduction). Let $x = (x_1, x') \in \mathbb{R}^d$ and $\chi_x(y)$ be the characteristic function of the cube $\{y \mid |y_j - x_j| \leq 1\}$ centered at x .

We now give a more precise formulation of Theorem 2:

Theorem 3 *There exist positive constants C_1 and $C(z)$ such that*

$$\|\chi_x u\| \leq C_1 (1 + |x_1|)^N e^{-C(z)\text{dist}(x, S_l)}, \quad (12)$$

where N is the order of polynomial growth of u .

Remark 4 *One might be concerned with the fact that albeit the eigenfunction decays exponentially away from the defect strip, the factor in front of the expression grows polynomially along the strip. However, for a generalized eigenfunction that grows polynomially one cannot expect anything better. In the periodic situation, using Floquet-Bloch theory, one can guarantee absence of this growth (see the comments at the end of the paper).*

Proof. Define the sesqui-linear form

$$Q[\varphi, w] := \langle \nabla \varphi, \frac{1}{\varepsilon_0} \nabla w \rangle - z \langle \varphi, w \rangle_{\rho_0}$$

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

Let $R(z) = (A_0 - z)^{-1}$ and $\varphi := R(z)\chi_x u$. We use here that z is not in the spectrum of A_0 . Note that $\varphi \in D(A_0)$.

Let $p = \max(2\text{dist}(x, S_l), 1)$ and $\xi_x(y)$ be a nonnegative smooth cutoff function that depends on y_1 only, is supported in $(x_1 - (p+1), x_1 + (p+1))$ and such that it is equal to 1 on $[x_1 - p, x_1 + p]$. We assume further that $\xi_x(y) \leq 1$ and $|\nabla \xi_x(y)| = |\xi'_x(y_1)| \leq C$ for some constant C and all $x, y \in \mathbb{R}^d$. For simplicity of notation, we drop the subscript x in $\xi = \xi_x$. Note that $\xi u \in H^1(\mathbb{R}^d)$. Using $w = \xi u$, one gets

$$Q[\varphi, \xi u] = \langle A_0 \varphi, \xi u \rangle_{\rho_0} - \langle z \varphi, \xi u \rangle_{\rho_0} = \langle \chi_x u, \xi u \rangle_{\rho_0} = \|\chi_x u\|_{\rho_0}^2.$$

This means that our goal should be to estimate $Q[\varphi, \xi u]$ from above. On the other hand, using the equality $Au = zu$, one gets

$$\begin{aligned} Q[\varphi, \xi u] &= \langle \nabla \varphi, \frac{1}{\varepsilon_0} \nabla(\xi u) \rangle - \langle \varphi, \xi zu \rangle_{\rho_0} \\ &= \langle \nabla \varphi, \frac{1}{\varepsilon_0} \nabla(\xi u) \rangle - \langle \varphi, \xi Au \rangle_{\rho_0} + \langle \varphi, \frac{\rho}{\rho_0} \xi Au \rangle_{\rho_0} - \langle \varphi, \frac{\rho}{\rho_0} \xi Au \rangle_{\rho_0} \end{aligned}$$

Simple algebraic transformations and easily justifiable integration by parts allow one to rewrite the last sum as

$$\langle \nabla \varphi, \xi \tilde{\varepsilon} \nabla u \rangle + \langle \varphi, \xi \rho \tilde{\rho} Au \rangle_{\rho_0} + \langle \nabla \xi, \frac{u}{\varepsilon_0} \nabla \varphi - \frac{\varphi}{\varepsilon} \nabla u \rangle_{\rho_0}. \quad (13)$$

In these calculations we used the notations

$$\tilde{\varepsilon}(x) = \frac{1}{\varepsilon_0(x)} - \frac{1}{\varepsilon(x)}, \quad \tilde{\rho}(x) = \frac{1}{\rho_0(x)} - \frac{1}{\rho(x)}.$$

Notice that both these functions are supported inside the strip S_l .

Our last task in proving the theorem is to estimate from above the terms in (13). In order to do so, we need an auxiliary statement concerning the exponential decay of the resolvent, which is a result of [2, 6]:

Lemma 5 [2, 6] *There exist a positive number m_z that depends only on the distance of the point z from the gap edges, such that for a positive constant C the following estimates hold for the local $L_2(\mathbb{R}^d)$ -norm of the resolvent $R(z)$:*

$$\begin{aligned} \|\chi_u R(z) \chi_v\| &\leq C e^{-m_z |u-v|} \\ \|\chi_u \nabla R(z) \chi_v\| &\leq C e^{-m_z |u-v|} \end{aligned} \quad (14)$$

for any $u, v \in \mathbb{R}^d$. Here the norms in the left hand side are the operator norms in $L_2(\mathbb{R}^d)$.

We can now get the needed estimates. Let $V = [x_1 - p - 1, x_1 + p + 1] \times I\Omega$. This is a compact domain that can be covered by the union of p fixed size domains $V_j = [a_j, a_j + 2] \times I\Omega$ and which contains the supports of $(\xi \tilde{\varepsilon})$ and $(\xi \tilde{\rho})$. Also note that $\text{dist}(x, V_j) \geq \text{dist}(x, S_l)$. Now using the lemma above and (3) we get

$$\begin{aligned} |\langle \nabla \varphi, \xi \tilde{\varepsilon} \nabla u \rangle| &\leq \|\chi_V \nabla \varphi\| \|\xi \tilde{\varepsilon} \nabla u\| \leq C \left\| \sum_j \chi_{V_j} \nabla R(z) \chi_{x^u} \right\| \left\| \sum_j \chi_{V_j} \nabla u \right\| \\ &\leq C p^2 (|x_1| + p + 1)^{2N} e^{-m_z \text{dist}(x, S_l)} \leq C (|x_1| + 1)^{2N} e^{-(m_z - \eta) \text{dist}(x, S_l)} \end{aligned} \quad (15)$$

We used here that $p = \max(2\text{dist}(x, S_l), 1)$. We also denoted by C different constants.

Analogously,

$$|\langle \varphi, \xi \rho \tilde{\rho} A u \rangle_{\rho_0}| \leq C |z| \sum_j \|\chi_{V_j} \varphi\| \|\xi \tilde{\rho} u\| \leq C (1 + |x_1|)^{2N} e^{-(m_z - \eta) \text{dist}(x, S_l)} \quad (16)$$

Let us move now to estimating the last term in (13). Denote by $a > 0$ a number such that shifts of $l\Omega$ by vectors aj with $j \in \mathbb{Z}^{d-1}$ cover the whole space \mathbb{R}^{d-1} . We denote

$$W_j := ([x_1 - p - 1, x_1 - p] \cup [x_1 + p, x_1 + p + 1]) \times (l\Omega + aj).$$

Then $W_j = W_0 + (0, aj)$. Notice that $W = \cup_j W_j$ covers $\text{supp } \nabla \xi$ and $\text{dist}(x, W_j) \geq C_1(p + |j|) - C_2$.

We are now ready to estimate the last term of (13) from above. We proceed as before, using the lemma, the polynomial growth of u , and uniform boundedness of $\nabla \xi$.

$$\begin{aligned} |\langle \nabla \xi, \frac{u}{\varepsilon_0} \nabla \varphi \rangle_{\rho_0}| &\leq C \sum_j \|\chi_{W_j} u\| \|\chi_{W_j} \nabla R(z) \chi_x u\| \\ &\leq C \sum_j (|x_1| + p + |j| + 1)^{2N} e^{-m_z \text{dist}(x, W_j)} \\ &\leq C (|x_1| + p + 1)^{2N} e^{-m_z^1 \text{dist}(x, S_l)} \sum_j (1 + |j|)^{2N} e^{-m_z^2 |j|} \\ &\leq C (|x_1| + 1)^{2N} e^{-(m_z^1 - \eta) \text{dist}(x, S_l)} \end{aligned} \quad (17)$$

where m_z^1 and m_z^2 are positive constants.

The expression $|\langle \nabla \xi, \frac{\varphi}{\varepsilon} \nabla u \rangle_{\rho_0}|$ is estimated analogously. Combining the above estimates, we get

$$\|\chi_x u\|^2 \leq C \|\chi_x u\|_{\rho_0}^2 = \mathcal{Q}[\varphi, \xi u] \leq C_\eta (1 + |x_1|)^{2N} e^{-m_z^1 \text{dist}(x, S_l)}.$$

This finishes the proof of the theorem.

4 Remarks

In this section we present some comments concerning the results of this paper and possible further developments.

1. The sufficient conditions for existence of “guided” modes provided in Theorem 1 are certainly not necessary. It would be interesting to obtain similar results under weaker conditions on the guide.

The number v_{d-1} that enters the conditions can be estimated numerically. For instance, when $d = 2$, one can easily write a secular equation which gives an approximate value of v_1 of about 31.29.

2. Theorem 1 provides existence of a δ -net of the defect spectrum inside the gap. One wonders how much of the gap the spectrum occupies. When does it fill the whole gap? Can it have gaps on its own? There seem to be no rigorous results available concerning these questions.
3. Results of [2] on improved Combes-Thomas resolvent estimates show that the exponential decay constant m_z , which clearly depends on the distance of the point z from the spectrum, behaves as $\sqrt{(z - \alpha)(\beta - z)}$.
4. One is interested in eliminating the polynomially growing factor in the exponential decay estimate (12). Its appearance is due to polynomial growth of generalized eigenfunctions, which in general might not be possible to get rid of.

In the case when the background medium (i.e., the functions $\rho_0(x)$ and $\varepsilon_0(x)$) is periodic with respect to a lattice Γ in \mathbb{R}^d and when the linear defect is directed along one of the lattice vectors, one can apply Floquet-Bloch theory [14, 17] that shows that one has generalized (Bloch) eigenfunctions with $N = 0$. Then one obtains exponential decay estimates that do not change along the waveguide.

5. The results of the paper have their analogs for the full Maxwell system. The authors intend to present those elsewhere.
6. As it has already been mentioned, in order to have the full right to call the discovered modes “guided”, one needs to show that they do not correspond to point spectrum (i.e., to bound states). Here the most treatable case should be of a periodic medium with a linear defect aligned along one of the lattice vectors. In this situation one can apply the Floquet-Bloch theory with respect to the axial variable of the waveguide and hope to use standard techniques applied in the case of Schrödinger operators with periodic potential (e.g., [4, 8, 14, 17]). This happens to be not an easy task. Even in the case of “hard wall” periodic waveguides, when waves are contained in a periodic

waveguide by Dirichlet, Neumann, or more general boundary conditions, this problem is non-trivial. Although it has been considered for rather long time [5, 14], the first real advances are very recent [9, 19, 20, 21]. The case of photonic crystalic waveguides is more complex, due to absence of complete confinement of the waves, which exponentially decay into the bulk, but do not vanish completely.

7. The next issue is engineering bent waveguides in such a way that there is no significant reflection back at bends. Physics analysis and experiments (e.g., [12, 10, 16, 18]) show that this is possible. To the best of our knowledge, no rigorous analysis of this problem is available yet.

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