

EXISTENCE OF GUIDED MODES ON PERIODIC SLABS

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Abstract. We prove the existence of bound guided modes for the Helmholtz equation on lossless penetrable periodic slabs. We handle both robust modes, for which no Bragg harmonics propagate away from slab, as well as nonrobust standing modes, which exist in the presence of propagating Bragg harmonics. The latter are made possible by symmetries of the slab structure, which prevent coupling of energy to the propagating harmonics. These modes are isolated in wavevector-frequency space, as they disappear under a perturbation of the wavevector. The main tool is a volumetric integral equation of Lippmann-Schwinger type that has a self-adjoint kernel.

1. Introduction. In this work, we prove the existence of bound guided acoustic and electromagnetic modes in periodic slab structures. These are material slabs that are infinitely periodic in two spatial directions and finite in the other. Such a structure can be thought of as an acoustic or photonic crystal slab if it arises from an infinite periodic structure that is truncated to a finite width in one direction.

A bound guided mode is a traveling or standing wave that is supported by the slab in the absence of any source, such as a plane wave incident upon it from the side. The intensity of the field decays exponentially away from the slab and therefore loses no energy through the sides. In this communication, we restrict attention to the Helmholtz equation of linear acoustics. For structures that are constant in one of the directions of periodicity, our results also describe polarized electromagnetic guided modes.

It is well known that objects that are bound in space (finite in all directions) cannot support bound Helmholtz states [1]. In other words, there are no nonzero solutions of the Helmholtz equation, with different constants inside and outside a bounded domain Ω in \mathbb{R}^3 , that satisfy physical matching conditions on the boundary of Ω and an outgoing condition. However, if the structure is extended infinitely in one or two directions (as a periodic pillar or slab), it may support guided modes, which can be viewed as true bound states when one restricts analysis to a single period.

As a simple illustrative example, consider a uniform slab without any periodic structure, whose material coefficient is greater than that of the surrounding

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medium. It is a simple calculation to show that such a structure supports guided modes. More precisely, one seeks solutions $u(x, y, z)$ to the problem

$$\begin{aligned} \nabla^2 u + \epsilon \omega^2 u &= 0, \quad |z| \neq L \\ \epsilon &= \begin{cases} \epsilon_0, & |z| > L \\ \epsilon_1, & |z| < L \end{cases}, \quad \epsilon_0 < \epsilon_1 \\ u \text{ and } \frac{\partial u}{\partial z} &\text{ continuous.} \end{aligned}$$

Here, ϵ may refer to an acoustic or dielectric constant, and ω is the nondimensionalized frequency. Separation of variables leads to the form

$$u = v(z)e^{i(\kappa_1 x + \kappa_2 y)},$$

where v satisfies

$$v'' + (\epsilon \omega^2 - \kappa_1^2 - \kappa_2^2)v = 0,$$

and one arrives at extended states for $\kappa_1^2 + \kappa_2^2 < \epsilon_0 \omega^2$ ($(\kappa_1, \kappa_2, \omega)$ inside the light cone for the exterior medium) and dispersion relations $\omega = W(\kappa_1, \kappa_2)$ that describe guided modes for $\epsilon_0 \omega^2 < \kappa_1^2 + \kappa_2^2 < \epsilon_1 \omega^2$ ($(\kappa_1, \kappa_2, \omega)$ outside the exterior light cone but inside that of the interior medium). At high frequencies, these modes correspond to total internal reflection of rays by geometric optics.

Under a periodic perturbation of the slab, those guided modes that can be represented by points outside the light cone for the exterior medium ϵ_0 with wave vector inside the first Brillouin zone are robust, whereas those outside are not. This is reflected in the fact that the Green function for the exterior medium in the former case decays away from the slab (it has no propagating Fourier harmonics, also called Bragg harmonics), whereas in the latter it has a finite number of radiating Fourier harmonics. See [2] for a lucid description of extended and bound states and their relation to the light cones for photonic crystals.

In this paper, we prove the existence of bound guided modes on periodic slabs outside the light cone for the exterior medium. These are robust, for there are no propagating Bragg harmonics that can carry energy away from the slab. We also prove that, even in the wavevector and frequency regimes for which there are propagating Bragg harmonics (this is the region inside the light cone for the exterior medium), certain symmetry conditions allow for bound standing modes on the slab—the energy is confined to the nonpropagating harmonics. In Corollary 2.2, we show that this confinement of the energy of the mode to the slab is described by the vanishing of certain integrals, which depend on the frequency and wavenumber, over a period of the structure. They are hence nonrobust—they disappear under a perturbation of the wavevector and are thus isolated states within the light cone. Nonrobust states correspond to eigenvalues embedded in the continuous spectrum of the Helmholtz operator in \mathbb{R}^3 in the presence of the slab; it is known that they exist in hard acoustic waveguides in the presence of certain obstacles [3].

Our main tool is the volumetric integral with a self-adjoint Green function as the convolution kernel. The material coefficient of the slab, with the exterior material coefficient fixed, essentially becomes the eigenvalue of an integral operator with frequency and wave number as parameters. The approach is applicable to a wider class of problems than that which we present in this Proceedings communication. In future communication, we will present similar results for guided electromagnetic modes (satisfying the full Maxwell equations), Helmholtz modes with more general boundary conditions, and bound states in waveguides with obstacles.

2. Pseudo-periodic fields and guided modes. The structure for which we investigate guided modes is described by a domain Ω in \mathbb{R}^3 that is doubly periodic, with period 2π in x and y , and bounded in z . Ω has a C^2 boundary $\partial\Omega$ with outward-pointing normal vector field n . The structure is penetrable, with real positive material constants ϵ_0 exterior to the structure and ϵ_1 interior to it. We consider harmonic solutions $u(x, y, z)e^{-i\omega t}$ of the linear wave equation, with nonzero real frequency ω , that are continuous and have continuous gradients across $\partial\Omega$. The spatial factor u satisfies the Helmholtz equation:

$$\begin{aligned} \nabla^2 u + \epsilon_0 \omega^2 u &= 0 \quad \text{in } \mathbb{R}^3 \setminus \overline{\Omega}, \\ \nabla^2 u + \epsilon_1 \omega^2 u &= 0 \quad \text{in } \Omega, \\ u \text{ and } \frac{\partial u}{\partial n} &\text{ are continuous on } \partial\Omega. \end{aligned}$$

Because of the periodicity of the structure, we let u have the Bloch pseudo-periodic form

$$u(x, y, z) = v(x, y, z)e^{i(\kappa_1 x + \kappa_2 y)},$$

where v is 2π -periodic in x and y . The periodic factor v satisfies

$$\begin{aligned} (\nabla + i\boldsymbol{\kappa})^2 v + \epsilon_0 \omega^2 v &= 0 \quad \text{in } \mathbb{R}^2 \setminus \overline{\Omega}, \\ (\nabla + i\boldsymbol{\kappa})^2 v + \epsilon_1 \omega^2 v &= 0 \quad \text{in } \Omega, \\ v \text{ and } \frac{\partial v}{\partial n} &\text{ are continuous on } \partial\Omega, \end{aligned}$$

in which $\boldsymbol{\kappa} = \langle \kappa_1, \kappa_2, 0 \rangle$ and $i = \sqrt{-1}$. We seek solutions of this problem that decay to zero as $|z| \rightarrow \infty$.

The radiating periodic Green function for the operator $(\nabla + i\boldsymbol{\kappa})^2 + \epsilon_0 \omega^2$ is $G(r - r')$, where $r = (x, y, z)$, $r' = (x', y', z')$, and G satisfies

$$(\nabla + i\boldsymbol{\kappa})^2 G + \epsilon_0 \omega^2 G = \sum_{k, \ell = -\infty}^{\infty} \delta(x + 2\pi k, y + 2\pi \ell, z).$$

δ is the Dirac δ -distribution with unit strength at the origin. The expansion of G in its Fourier harmonics is

$$G(x, y, z) = -\frac{1}{8\pi^2} \sum_{n, m = -\infty}^{\infty} \frac{1}{\gamma_{mn}} e^{\gamma_{mn}|z|} e^{i(mx + ny)},$$

in which $\gamma_{mn}^2 = -\epsilon_0 \omega^2 + (m + \kappa_1)^2 + (n + \kappa_2)^2$. It is assumed that $\gamma_{mn} \neq 0$ for all pairs (m, n) . We take $i\gamma_{mn} < 0$ for the finite number of propagating Fourier harmonics, so that they are outgoing as $|z| \rightarrow \infty$, and $\gamma_{mn} < 0$ so that the rest of the harmonics decay as $|z| \rightarrow \infty$.

The adjoint of G as an integral kernel is the ‘‘antiradiating’’ analog of G , obtained by taking $i\gamma_{mn} > 0$ for the propagating modes, so that they are incoming. We shall make use of the self-adjoint pseudo-periodic Green function, which is the mean of the radiating and antiradiating functions:

$$\begin{aligned} H(x, y, z) &= -\frac{1}{8\pi^2} \sum_{\text{prop}} \frac{1}{\mu_{mn}} \sin \mu_{mn}|z| e^{i(mx + ny)} + \\ &\quad + \frac{1}{8\pi^2} \sum_{\text{decay}} \frac{1}{\nu_{mn}} e^{-\nu_{mn}|z|} e^{i(mx + ny)}, \end{aligned} \tag{2.1}$$

in which $\mu_{mn} = \sqrt{\epsilon_0\omega^2 - (m + \kappa_1)^2 - (n + \kappa_2)^2}$, $\nu_{mn} = \sqrt{(m + \kappa_1)^2 + (n + \kappa_2)^2 - \epsilon_0\omega^2}$, and \sum_{prop} and \sum_{decay} indicate sums over the finitely many Fourier harmonics that are propagating in z and the rest of the harmonics, which are decaying in z .

We now establish an integral representation theorem that is a form of the Lippmann-Schwinger equation [4]. Let \mathcal{S} denote the three-dimensional strip

$$\mathcal{S} = \{(x, y, z) : -\pi \leq x \leq \pi, -\pi \leq y \leq \pi, -\infty < z < \infty\}.$$

Theorem 2.1. *Let $\epsilon = \epsilon_0$ in the exterior to Ω and $\epsilon = \epsilon_1$ in the interior.*

1. *Let $v : \mathbb{R}^3 \rightarrow \mathbb{C}$ be a continuously differentiable function that satisfies*
 - (a) $(\nabla + i\boldsymbol{\kappa})^2 v + \epsilon\omega^2 v = 0$ in \mathbb{R}^3 ,
 - (b) $v(x, y, z)$ is 2π -periodic in x and y ,
 - (c) $v(x, y, z) \sim \sum_{\text{prop}} (A_{mn} e^{i\mu_{mn}z} + B_{mn} e^{-i\mu_{mn}z}) e^{i(mx+ny)} \quad (z \rightarrow \infty)$,
 $v(x, y, z) \sim - \sum_{\text{prop}} (A_{mn} e^{i\mu_{mn}z} + B_{mn} e^{-i\mu_{mn}z}) e^{i(mx+ny)} \quad (z \rightarrow -\infty)$.

Then v satisfies the integral equation

$$v(x, y, z) = \omega^2(\epsilon_1 - \epsilon_0) \int_{\Omega \cap \mathcal{S}} H(x - x', y - y', z - z') v(x', y', z') dV(x', y', z'), \quad (2.2)$$

for all $(x, y, z) \in \mathbb{R}^3 \setminus \partial\Omega$ and the coefficients A_{mn} and B_{mn} are given by

$$\begin{aligned} -16\pi^2 i \mu_{mn} A_{mn} = \\ \omega^2(\epsilon_1 - \epsilon_0) \int_{\Omega \cap \mathcal{S}} e^{-i\mu_{mn}z'} e^{-i(mx'+ny')} v(x', y', z') dV(x', y', z'), \end{aligned} \quad (2.3)$$

$$\begin{aligned} 16\pi^2 i \mu_{mn} B_{mn} = \\ \omega^2(\epsilon_1 - \epsilon_0) \int_{\Omega \cap \mathcal{S}} e^{i\mu_{mn}z'} e^{-i(mx'+ny')} v(x', y', z') dV(x', y', z'), \end{aligned} \quad (2.4)$$

2. *A solution of (2.2) for $(x, y, z) \in \Omega$ extends to a solution of (a), (b), and (c). The extension is the natural one, in which the same formula is applied for $(x, y, z) \in \mathbb{R}^3 \setminus \bar{\Omega}$.*

PROOF. Condition (a) implies

$$(\nabla + i\boldsymbol{\kappa})^2 v + \epsilon_0\omega^2 v = 0 \quad \text{in } \mathbb{R}^3 \setminus \bar{\Omega}, \quad (2.5)$$

$$(\nabla + i\boldsymbol{\kappa})^2 v + \epsilon_0\omega^2 v = -\omega^2(\epsilon_1 - \epsilon_0)v \quad \text{in } \Omega. \quad (2.6)$$

Define $\tilde{v} : \mathbb{R}^3 \rightarrow \mathbb{C}$ by

$$\tilde{v}(x, y, z) = \omega^2(\epsilon_1 - \epsilon_0) \int_{\Omega \cap \mathcal{S}} H(x - x', y - y', z - z') v(x', y', z') dV(x', y', z'). \quad (2.7)$$

Then \tilde{v} also satisfies (2.5) and (2.6) and is periodic, for the factor $e^{i(mx+ny)}$ can be extracted from the Green function. Furthermore, using the expression (2.1) for H ,

we obtain the asymptotics

$$\tilde{v}(x, y, z) \sim \sum_{\text{prop}} (a_{mn}e^{i\mu_{mn}z} + b_{mn}e^{-i\mu_{mn}z}) e^{i(mx+ny)} \quad (z \rightarrow \infty) \quad (2.8)$$

$$\tilde{v}(x, y, z) \sim - \sum_{\text{prop}} (a_{mn}e^{i\mu_{mn}z} + b_{mn}e^{-i\mu_{mn}z}) e^{i(mx+ny)} \quad (z \rightarrow -\infty). \quad (2.9)$$

in which

$$\begin{aligned} -16\pi^2 i\mu_{mn}a_{mn} = \\ \omega^2(\epsilon_1 - \epsilon_0) \int_{\Omega \cap \mathcal{S}} e^{-i\mu_{mn}z'} e^{-i(mx'+ny')} v(x', y', z') dV(x', y', z') \end{aligned} \quad (2.10)$$

$$\begin{aligned} 16\pi^2 i\mu_{mn}b_{mn} = \\ \omega^2(\epsilon_1 - \epsilon_0) \int_{\Omega \cap \mathcal{S}} e^{i\mu_{mn}z'} e^{-i(mx'+ny')} v(x', y', z') dV(x', y', z') \end{aligned} \quad (2.11)$$

Now define $w = v - \tilde{v}$. Then

$$(\nabla + i\boldsymbol{\kappa})^2 w + \epsilon_0 \omega^2 w = 0 \quad \text{in } \mathbb{R}^3,$$

and w has the asymptotic behavior

$$w(x, y, z) \sim \sum_{\text{prop}} (c_{mn}e^{i\mu_{mn}z} + d_{mn}e^{-i\mu_{mn}z}) e^{i(mx+ny)} \quad (z \rightarrow \infty) \quad (2.12)$$

$$w(x, y, z) \sim - \sum_{\text{prop}} (c_{mn}e^{i\mu_{mn}z} + d_{mn}e^{-i\mu_{mn}z}) e^{i(mx+ny)} \quad (z \rightarrow -\infty) \quad (2.13)$$

where $c_{mn} = A_{mn} - a_{mn}$ and $d_{mn} = B_{mn} - b_{mn}$. Since w satisfies a homogeneous Helmholtz equation throughout \mathcal{S} , the decomposition of w into Fourier harmonics as z tends to ∞ or $-\infty$ must be the same. It follows that $w \equiv 0$.

Part 2 of the Theorem is straightforward.

The following corollary give necessary and sufficient conditions for a pseudo-periodic field to be a bound state and follows directly from the Theorem.

Corollary 2.2. *Let $\epsilon = \epsilon_0$ in the exterior to Ω and $\epsilon = \epsilon_1$ in the interior.*

A function $v : \mathbb{R}^3 \rightarrow \mathbb{C}$ satisfies

- (a) $(\nabla + i\boldsymbol{\kappa})^2 v + \epsilon \omega^2 v = 0$ in \mathbb{R}^3 ,
- (b) $v(x, y, z)$ is 2π -periodic in x and y ,
- (c) $v(x, y, z) \rightarrow 0$ as $|z| \rightarrow \infty$,

if and only if

1. v is the natural extension to \mathbb{R}^3 of a solution to the following eigenvalue problem on $\Omega \cap \mathcal{S}$

$$v(x, y, z) = \lambda \int_{\Omega \cap \mathcal{S}} H(x - x', y - y', z - z') v(x', y', z') dV(x', y', z'), \quad (2.14)$$

where $\lambda = \omega^2(\epsilon_1 - \epsilon_0)$;

- 2.

$$\int_{\Omega \cap \mathcal{S}} e^{-i\mu_{mn}z'} e^{-i(mx'+ny')} v(x', y', z') dV(x', y', z') = 0, \quad (2.15)$$

$$\int_{\Omega \cap \mathcal{S}} e^{i\mu_{mn}z'} e^{-i(mx'+ny')} v(x', y', z') dV(x', y', z') = 0, \quad (2.16)$$

for all m, n such that $\epsilon_0\omega^2 - (m + \kappa_1)^2 - (n + \kappa_2)^2 > 0$.

Let $\langle H \rangle$ denote the convolution operator from $L^2(\Omega \cap \mathcal{S})$ into itself with integral kernel $H(x - x', y - y', z - z')$:

$$\langle H \rangle : L^2(\Omega \cap \mathcal{S}) \rightarrow L^2(\Omega \cap \mathcal{S})$$

$\langle H \rangle$ is compact and self-adjoint. In fact, $H(r)$ (where $r = (x, y, z)$) differs from

$$\frac{r}{|r|^2} e^{i\omega\sqrt{\epsilon_0}|r|}$$

by a regular function of r so that $\langle H \rangle$ is compact. H is conjugate-symmetric in r , that is, $H(r) = \overline{H(-r)}$, making $\langle H \rangle$ self-adjoint. Therefore there exists a sequence of real eigenvalues $\{\lambda_i\}_{i=1}^\infty$ of the problem (2.14) with $|\lambda_i| \rightarrow \infty$ and corresponding eigenfunctions $\{v_i\}$ that form an orthonormal Hilbert-space basis for $L^2(\Omega \cap \mathcal{S})$.

Suppose first that the values of ϵ_0 , ω , κ_1 , and κ_2 admit no propagating Fourier harmonics, that is,

$$\epsilon_0\omega^2 < (m + \kappa_1)^2 + (n + \kappa_2)^2 \quad \text{for all } m, n \in \mathbb{Z}.$$

This is the case discussed in the Introduction, in which $(\kappa_1, \kappa_2, \omega)$ lies outside of the light cone (or ‘‘sound cone’’) for the exterior material, assuming (κ_1, κ_2) lies in the first Brillouin zone of the structure, that is, $|\kappa_1| < 1/2$ and $|\kappa_2| < 1/2$. Each eigenvalue λ_i gives rise to an interior material coefficient

$$\epsilon_{1i} = \frac{\lambda_i}{\omega^2} + \epsilon_0,$$

for which there exists a bound state at the given frequency ω traveling along the periodic slab with Bloch wave vector (κ_1, κ_2) . Indeed, the extension of the eigenfunctions to \mathbb{R}^3 automatically decay as $|z| \rightarrow \infty$ because there are no propagating harmonics; the second condition in the Corollary is trivially satisfied. The time dependent fields are

$$|v(x, y, z)| \cos(\theta(x, y, z) + \kappa_1 x + \kappa_2 y - \omega t),$$

where $\theta(x, y, z) = \arg v(x, y, z)$.

Consider next the case in which $\kappa_1 = \kappa_2 = 0$ and $\epsilon_0\omega^2 < 1$. In this case, the Green function has exactly one propagating harmonic,

$$e^{\pm i\mu_{00}z}, \quad \mu_{00} = \omega\sqrt{\epsilon_0}.$$

The conditions that an eigenfunction v_i of $\langle H \rangle$ (extended to \mathbb{R}^3) be a bound state are given by (2) of the Corollary and reduce in this case to

$$\int_{\Omega \cap \mathcal{S}} e^{\pm i\mu_{00}z} v_i(x, y, z) dx dy dz = 0.$$

Under the assumption that Ω is symmetric about a plane parallel to the xz -plane or the yz -plane, we have an infinite sequence of interior coefficients ϵ_1 that support bound states, as stated in the following theorem. As $\kappa_1 = \kappa_2 = 0$, these are standing waves.

Theorem 2.3.

1. If the parameters ω , κ_1 , κ_2 , and ϵ_0 admit no propagating Fourier harmonics, or

2. if $\epsilon_0\omega^2 < 1$, and
 either $\kappa_1 = 0$ and Ω is symmetric about a plane parallel to the yz -plane,
 or $\kappa_2 = 0$ and Ω is symmetric about a plane parallel to the xz -plane,

then there exists a sequence of coefficients ϵ_{1i} in Ω , such that $\epsilon_{1i} \rightarrow \infty$, for which the periodic structure admits a bound slab mode.

PROOF. We have already proved the first case in the discussion above. For the second, let Ω be symmetric about the yz -plane and $\kappa_1 = 0$; symmetry about the xz -plane and $\kappa_2 = 0$ is handled similarly. Symmetry about planes parallel to these two is handled by shifting the domain Ω so that the plane of symmetry is one of the coordinate planes. Formula (2.1) shows that $H(x, y, z) = H(-x, y, z)$ when $\kappa_1 = 0$. By the symmetry of H and Ω about the yz -plane, $\langle H \rangle$ acts invariantly on the closed subspace $L^2_{\text{odd}}(\Omega \cap \mathcal{S})$ consisting of those elements of $L^2(\Omega \cap \mathcal{S})$ that are odd with respect to the x -variable. Therefore there exists an infinite sequence of eigenvalues $\{\lambda_i\}$ such that $|\lambda_i| \rightarrow \infty$ and eigenfunctions v_i (that are odd in x). It follows from the symmetry of Ω and antisymmetry of the v_i in x that

$$\int_{\Omega \cap \mathcal{S}} e^{\pm i\mu_{00}z} v_i(x, y, z) dx dy dz = 0,$$

thereby satisfying condition 2 of Corollary 2 that an eigenfunction be a bound state. The sequence $\epsilon_{1i} = \lambda_i/\omega^2 - \epsilon_0$ is the sequence we seek.

3. Numerical Example. A class of acoustic and photonic bandgap structures used commonly in experiments and applications consists of periodic arrays of vertical rods. These are special cases of two-dimensional acoustic or photonic crystals. High-contrast dielectric arrays tend to exhibit wide bandgaps that are complete, that is, intervals of frequencies at which polarized electromagnetic waves at all angles of propagation perpendicular to the rods are prohibited.

Fig. 1 shows (one period of) a numerical simulation of a bound mode on a slab consisting of an array of penetrable rods, four rods thick, with a high contrast in the material constant ϵ between the rods and the ambient space. The mode is non-robust, and its frequency lies within a region for which very little energy of plane wave sources is transmitted through the slab, indicating a bandgap for the corresponding infinite array of rods. It is captured by a ‘‘surface defect’’ in the crystal, produced by the enlargement of the first rod in each row of four comprising each period of the slab. The mode is periodic ($\kappa = 0$), and represents those nonrobust modes described in Theorem 2.3 that arise due to the symmetry of the structure. The mode disappears from the bandgap altogether as κ is perturbed from zero.

The simulation was produced using a boundary-integral numerical code developed in [5] and [6]. Other simulations of slab modes in similar rod structures are shown in [7].

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FIGURE 1. One period of a nonrobust guided Helmholtz mode; the full slab mode is visualized by repeating the figure periodically in the vertical direction. A level-set diagram of the amplitude is shown, with black indicating zero amplitude and white indicating maximal amplitude. The white circles are superimposed to indicate the locations of the circular rods, in which $\epsilon_1 = 10$; outside the rods, $\epsilon_0 = 1$. The reduced frequency of the mode is $\omega \approx 0.3997$, and $\kappa = 0$.

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