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Transmission through a thick periodic slab ^{*}

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Abstract

For the scalar wave equation in periodic structures, we establish rigorously the emergence of a spectral bandgap as a frequency interval of exponentially small transmission of energy through a slab of the crystal when the thickness of the slab tends to infinity. We extend the result to slabs that contain a planar defect for frequencies that do not coincide with guided mode frequencies for the defect. For one-dimensional crystals, we prove that the transmission approaches a nonzero value at guided mode frequencies and give an explicit formula for the transmission. The main analytical tool in the multidimensional case is the Calderón boundary integral projectors for the Helmholtz equation.

Key words. Photonic crystals; periodic structures; Helmholtz equation; Green functions; potential theory; Calderón projector

AMS Subject Classification. 35B27, 35B34, 78M35

1 Introduction

The subject of this work is a rigorous study of the attenuation of linear scalar waves as they travel through a thick slab of a lossless periodic medium at frequencies for which propagation is prohibited. It is known that certain periodic media prohibit the propagation of waves in certain frequency intervals, known as spectral gaps or “bandgaps”. Thus, if a steady harmonic plane wave is incident upon the left side of the slab, it is expected that one will observe spatial attenuation of the field across the slab, resulting in low transmission of energy to the right side. The presence of defects in the structure, however, may lead to resonance at certain frequencies, leading to the transmission of a significant amount of energy.

^{*}This work started while the second author was visiting the Institut Elie Cartan de Nancy as an invited Professor.

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Our investigations pertain to acoustic waves in three-dimensional periodic structures, and also to polarized electromagnetic waves in the two-dimensional reduction, in which the material properties are constant in one direction. We analyze the problem using a partial Floquet-Bloch transform, which decomposes harmonic fields into fields that are pseudo-periodic in the directions parallel to the slab. Thus our problem has as parameters the frequency and the two-dimensional Bloch wave vector parallel to the slab. The governing equation is

$$(\Delta + \omega^2 \varepsilon(x))u(x) = 0,$$

in which ω is the normalized frequency.

These are the main ideas:

- (i) Perfect periodic media filling all of space can exhibit gaps in their acoustic and electromagnetic spectra, that is, frequency intervals for which wave propagation is prohibited. It has been proved rigorously that there exist periodic structures (other than one-dimensional structures) that admit spectral gaps [7].
- (ii) If a periodic structure is truncated to a slab of finite width in one dimension, remaining periodic in the other directions, a spectral gap is manifest as a frequency interval in which the amount of energy of a plane wave, incident on one side of the slab, that is transmitted to the other side is very small. As the thickness of the slab increases, the spectral gap of the infinite structure emerges as an interval of zero transmission. This has been demonstrated rigorously for one-dimensional structures in Ref. [8] and numerically for higher dimensions in many works, such as Ref. [15].
- (iii) Suppose a planar defect is introduced into the untruncated periodic medium. This means that the medium is modified within a finite interval in one direction but periodicity is retained in the other directions (as two half-spaces of a crystal separated by a wall of air). This can cause the emergence of guided modes at frequencies in a spectral gap for the perfect structure. These are fields that are essentially localized to the defect, decaying exponentially with the distance from the defect. Existence of these modes was proved in Ref. [10] in a more general (not necessarily periodic) setting than ours; their mathematical and numerical treatment in the periodic setting, including dispersion relations, is given in Ref. [2].
- (iv) When a periodic structure with a planar defect is truncated parallel to the defect, transmission resonances emerge at the frequencies of the guided modes for the untruncated defective structure. These are spikes in the graph of the transmitted energy as a function of frequency, centered about the frequencies of the guided modes. They become sharper as the thickness of the slab increases, and the transmission tends to zero at neighboring frequencies. Detailed numerical investigations of these resonances are performed in Ref. [15].

The purpose of this work is to establish rigorously points (ii) and (iv) for lossless media. We prove exponential decay to zero of the transmission through a slab for frequencies in a spectral gap as the (integral) number of periods across the slab increases to infinity. We also prove this exponential decay for slabs with planar defects, away from guided-mode

frequencies for the untruncated defective structure, as discussed in point (iv). As suggested also in point (iv), the transmission at a guided mode frequency should converge to a nonzero number. We are able to establish this rigorously only for one-dimensional structures, in which explicit calculations using transfer matrices can be carried out. We find that the transmission at waveguide frequencies exponentially approaches a percentage strictly greater than 0 as the thickness of the slab grows, and that this is not necessarily 100%. The difficulty in constructing a proof for multidimensional crystals is the lack of precise knowledge of the rate of decay of the Green functions for the periodic medium in a spectral gap.

Intimately related to anomalous transmission of plane wave source fields near a guided mode frequency for a slab with a planar defect is the resonant scattering of the field inside the defect. These scattering states approximate the bound state when the slab becomes very thick. This bears resemblance to the related phenomenon in which a bound state localized inside a bounded defect in a periodic medium is approximated by extended (Bloch) states in a structure whose period consists of N^2 periods of the original structure, with a defect in the middle. As a technique to compute eigenvalues of the defect, this is known as the “supercell” method; exponential spectral convergence as N tends to infinity was proved in Ref. [14].

Our aim is different from that of Ref. [14]: we are interested in the scattering states in their own right, in particular the transmission coefficient, a quantity that does not have an analog in the supercell problem. Although it is clear that transmission resonance is intimately related to the perturbation of a bound state by truncation of a periodic structure to a finite slab, we cannot yet give a satisfactory description of the mechanism. The direct calculations possible in one-dimensional structures do not seem to provide enlightenment. This is a very subtle point that may be best approached by trying to relate the resonances to the poles of a resolvent function as in Ref. [12] or [13].

We make a number of assumptions:

- (a) Positivity of the material constants;
- (b) The periodic structure can be truncated by a periodic surface such that, in a small vicinity of the surface, the slab is homogeneous;
- (c) Nonresonance assumption: that there exist no modes residing on the surface of the semi-infinite periodic structure.

Assumption (b) enables us to use the classical tools of potential theory, and more especially the jump relations for the single and double layer potentials (Section 2.3). This includes crystals consisting of a matrix with periodic inclusions of a contrasting material. The nonresonance assumption (c), discussed later on (cf. Remark 2.10), is reasonable in the context of the problem of scattering by the slab.

The paper is organized as follows:

- i. Section 2 lays down the foundations of the Calderón boundary-integral projectors that form the main tool in proving the theorems.
- ii. In Section 3, we derive properties of the Green function for the slab structure and use them to prove the exponential decay of transmission for gap frequencies as the number of periods of the slab tends to infinity.

- iii. This result is extended in to slabs with a planar defect in Section 4 for gap frequencies that do not coincide with frequencies of guided modes of the defect.
- iv. The connection between guided defect modes and transmission anomalies is established in Section 5 for one-dimensional structures. An exact formula for the transmission is obtained.

2 Boundary data and the Calderón projectors

Given an orthonormal system of coordinates (Ox_1, Ox_2, Ox_3) , consider a three-dimensional periodic structure characterized by a material parameter $\varepsilon^{\text{per}}(x) = \varepsilon^{\text{per}}(x_1, x_2, x_3)$ in $L^\infty(\mathbb{R}^3)$, that is uniformly bounded from above and below,

$$\varepsilon_+ > \varepsilon^{\text{per}}(x) > \varepsilon_- > 0,$$

and has period 1 in all three variables,

$$\varepsilon^{\text{per}}(x_1 + 1, x_2, x_3) = \varepsilon^{\text{per}}(x_1, x_2 + 1, x_3) = \varepsilon^{\text{per}}(x_1, x_2, x_3 + 1) = \varepsilon^{\text{per}}(x) \quad \forall x \in \mathbb{R}^3.$$

Denote by \mathcal{S} the strip

$$\mathcal{S} = \mathbb{R} \times (0, 1) \times (0, 1),$$

and let x be decomposed into variables $x_1 \in \mathbb{R}$ and $x' = (x_2, x_3) \in (0, 1)^2$:

$$x = (x_1, x_2, x_3) = (x_1, x').$$

Throughout the paper, we assume that the frequency ω is in an interval $J = [\omega_1, \omega_2]$ contained in a spectral gap for the infinite periodic structure. This is to ensure that ω is bounded away from the spectrum.

We also assume that $\varepsilon^{\text{per}}(x)$ is constant in a neighborhood of the graph of a certain smooth function $x_1 = f(x_2, x_3)$, periodic in x_2 and x_3 , whose intersection with S we denote by Γ_0 . For simplicity of notation, we take $f(x_2, x_3) = 0$, although all of the analysis, particularly involving the Calderón boundary integral projectors, is valid for an arbitrary smooth periodic function (Fig. 2.1).

2.1 Green kernels

Let $\mathcal{G}^{\text{per}}(\omega; x, y)$ denote the Green function of the operator $\Delta + \omega^2 \varepsilon^{\text{per}}$ in \mathbb{R}^3 . Since ω is supposed to be in a gap, $\mathcal{G}^{\text{per}}(\omega; x, y)$ decays exponentially with $|x - y|$ (see Ref. [6]). For $\theta \in (0, 2\pi)^2$, we define the pseudo-periodic Green function $G^{\text{per}}(\omega, \theta; x, y)$ as the partial Floquet transform[12, 16, 3] of $\mathcal{G}^{\text{per}}(\omega; x, y)$ in the y_2 and y_3 directions:

$$G^{\text{per}}(\omega, \theta; x, y) = \sum_{n \in \mathbb{Z}^2} \mathcal{G}^{\text{per}}(\omega; x, y + (0, n)) e^{-in \cdot \theta}. \quad (2.1)$$

Here, $(0, n)$ refers to the vector $(0, n_1, n_2)$, where $n = (n_1, n_2)$. Using the properties of \mathcal{G}^{per} , one can verify that

$$(\Delta_y + \omega^2 \varepsilon^{\text{per}}(y)) G^{\text{per}}(\omega, \theta; x, y) = \sum_{n \in \mathbb{Z}^2} \delta_{(x_1, x'_1 + n)}(y) e^{in \cdot \theta}, \quad (2.2)$$

$$G^{\text{per}}(\omega, \theta; x, y + (0, n)) = e^{in \cdot \theta} G^{\text{per}}(\omega, \theta; x, y), \quad (2.3)$$

$$|G^{\text{per}}(\omega, \theta; x, y)| \rightarrow 0 \quad \text{as } |x_1 - y_1| \rightarrow 0. \quad (2.4)$$

The pseudo-periodicity condition (2.3) shows the main advantage of using the Green function $G^{\text{per}}(\omega, \theta; x, y)$: it allows us to study the scattering problem by the photonic slab in the strip $\mathcal{S} = \mathbb{R} \times (0, 1)^2$ instead of the whole space. For each integer $M > 0$, let us then define the following subsets of \mathcal{S} :

$$\begin{aligned} \Omega_M &= \{x = (x_1, x_2, x_3) \in \mathcal{S}; |x_1| < M\}, \\ \Omega_M^c &= \{x = (x_1, x_2, x_3) \in \mathcal{S}; |x_1| > M\}, \end{aligned}$$

and the vertical boundary (for all $M \in \mathbb{R}$):

$$\Gamma_M = \{x = (x_1, x_2, x_3) \in \mathcal{S}; x_1 = M\}.$$

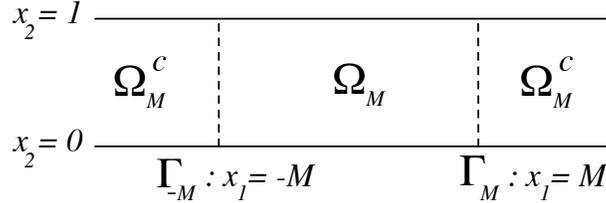


Figure 1: Reference strip $\mathcal{S} = \mathbb{R} \times (0, 1)^2$, projected to the x_1x_2 -plane

To study the periodic slab, we also need to define the pseudo-periodic outgoing Green function $G^0(\omega, \theta; x, y)$ of the homogeneous medium with constant material parameter $\varepsilon(x) = \varepsilon^0$. More precisely, let $\mathcal{P} = \mathcal{P}(\omega, \theta)$ denote the finite set of “propagating Fourier harmonics”:

$$\mathcal{P} = \{m \in \mathbb{Z}^2 \mid \beta_m^2 := \omega^2 \varepsilon^0 - |2\pi m + \theta|^2 > 0\}, \quad (2.5)$$

and assume that $\beta_m \neq 0$ for all $m \in \mathbb{Z}^2$. In the context of the slab, the outgoing radiation condition is given by the well-known Rayleigh principle, stating that an outgoing field can be decomposed into modes propagating towards infinity and evanescent (exponentially decreasing) modes. More precisely, with the convention that $\beta_m > 0$ for $m \in \mathcal{P}$, we have the following definition.

Definition 2.1. *Given $M > 0$, let v be a solution of*

$$\left. \begin{aligned} (\Delta + \omega^2 \varepsilon^0)v(y) &= 0 \\ v(y_1, y'_1 + n) &= e^{in \cdot \theta} v(y_1, y'_1) \end{aligned} \right\}, \quad |y_1| > M.$$

Then, v is outgoing as $y_1 \rightarrow \pm\infty$ if and only if there exist complex coefficients A_m^\pm , $m \in \mathcal{P}$, such that

$$\lim_{y_1 \rightarrow \pm\infty} \left| v(y) - \sum_{m \in \mathcal{P}} A_m^\pm e^{\pm i\beta_m y_1} e^{i(2\pi m + \theta) \cdot y'} \right| = 0. \quad (2.6)$$

Let

$$\mathcal{G}^0(\omega; x, y) = -\frac{1}{4\pi} \frac{1}{|y - x|} e^{ik|y-x|}, \quad (2.7)$$

where $k = \sqrt{\varepsilon^0} \omega$, be the outgoing Green function of the operator $\Delta + \omega^2 \varepsilon^0$ in \mathbb{R}^3 . For $\theta \in (0, 2\pi)^2$, we define the pseudo-periodic Green function $G^0(\omega, \theta; x, y)$ as the partial Floquet transform $\mathcal{G}^0(\omega; x, y)$ in y' ,

$$G^0(\omega, \theta; x, y) = \sum_{n \in \mathbb{Z}^2} \mathcal{G}^0(\omega; x, y + (0, n)) e^{-in \cdot \theta}, \quad (2.8)$$

and we can once again check that $G^0(\omega, \theta; x, y)$ satisfies for all $x \in \mathcal{S}$:

$$(\Delta_y + \omega^2 \varepsilon^0) G^0(\omega, \theta; x, y) = \sum_{n \in \mathbb{Z}^2} \delta_{(x_1, x'_1 + n)}(y) e^{in \cdot \theta} \quad (2.9)$$

$$G^0(\omega, \theta; x, y + (0, n)) = e^{in \cdot \theta} G^0(\omega, \theta; x, y), \quad (2.10)$$

$$G^0(\omega, \theta; x, \cdot) \text{ is outgoing as } y_1 \rightarrow \pm\infty \text{ (in the sense of Definition 2.1)}. \quad (2.11)$$

When no confusion is possible, we will write $G^0(x, y)$ (resp. $G^{\text{per}}(x, y)$) instead of $G^0(\omega, \theta; x, y)$ (resp. $G^{\text{per}}(\omega, \theta; x, y)$). We collect some of the useful properties of the Green functions in the following Proposition.

Proposition 2.2 (Properties of the Green functions). *Let G denote either of the Green functions G^0 or G^{per} . Then G satisfies the following properties ($n \in \mathbb{Z}^2$):*

$$G(\omega, \theta; x + (0, n), y + (0, n)) = G(\omega, \theta; x, y), \quad (\text{translation}) \quad (2.12)$$

$$G(\omega, \theta; x + (0, n), y) = e^{-in \cdot \theta} G(\omega, \theta; x, y), \quad (\text{pseudo-periodicity in } x) \quad (2.13)$$

$$G(\omega, \theta; x, y + (0, n)) = e^{in \cdot \theta} G(\omega, \theta; x, y), \quad (\text{pseudo-periodicity in } y) \quad (2.14)$$

$$G(\omega, \theta; x, y) = G(\omega, -\theta; y, x), \quad (\text{symmetry}) \quad (2.15)$$

$$G(\omega, \theta; x, y) + \frac{1}{4\pi} \frac{1}{|x - y|} \text{ is continuous in } y \text{ at } y = x. \quad (\text{singularity}) \quad (2.16)$$

If $[\omega_1, \omega_2]$ is contained in a gap for ε^{per} , then there exist constants $C_1, C_2 > 0$ such that, for all $\omega \in [\omega_1, \omega_2]$,

$$\begin{aligned} |G^{\text{per}}(\omega, \theta; x, y)| &\leq C_1 e^{-C_2|x_1 - y_1|} \\ |\nabla G^{\text{per}}(\omega, \theta; x, y)| &\leq C_1 e^{-C_2|x_1 - y_1|} \end{aligned} \quad \text{for } |x_1 - y_1| \text{ sufficiently large.} \quad (2.17)$$

From (2.15) and the defining properties (2.9) and (2.2), it follows that for $y \in \mathbb{R}^3$,

$$(\Delta_x + \omega^2 \varepsilon^0) G^0(\omega, \theta; x, y) = \sum_{n \in \mathbb{Z}} \delta_{(y_1, y_2 + n)}(x) e^{-in \cdot \theta}, \quad (2.18)$$

$$(\Delta_x + \omega^2 \varepsilon^{\text{per}}(x)) G^{\text{per}}(\omega, \theta; x, y) = \sum_{n \in \mathbb{Z}} \delta_{(y_1, y_2 + n)}(x) e^{-in \cdot \theta}. \quad (2.19)$$

Proof. The translation property follows from the definition of the pseudo-periodic Green functions through the Floquet transform (see (2.1) and (2.8)).

The pseudo-periodicity in the second spatial variable follows from (2.3). Its counterpart in the first spatial variable is a consequence of the pseudo-periodicity in the second one and the translation property. The symmetry property (2.15) is proved by integration by parts: Let G denote either G^0 or G^{per} and ε either ε^0 or ε^{per} , and let x and y lie within the strip $\mathcal{S} = \mathbb{R} \times (0, 1)^2$. Then we can write that for all $M > 0$ such that $x, y \in \Omega_M$:

$$\begin{aligned}
G(\omega, -\theta; y, x) - G(\omega, \theta; x, y) &= \int_{\Omega_M} [\delta_x(z)G(\omega, -\theta; y, z) - \delta_y(z)G(\omega, \theta; x, z)] \, dV(z) \\
&= \int_{\Omega_M} \{ [(\Delta_z + \omega^2\varepsilon(z))G(\omega, \theta; x, z)] G(\omega, -\theta; y, z) \\
&\quad - [(\Delta_z + \omega^2\varepsilon(z))G(\omega, -\theta; y, z)] G(\omega, \theta; x, z) \} \, dV(z) \\
&= \int_{\partial\Omega_M} \{ [\partial_{n(z)}G(\omega, \theta; x, z)] G(\omega, -\theta; y, z) \\
&\quad - [\partial_{n(z)}G(\omega, -\theta; y, z)] G(\omega, \theta; x, z) \} \, dA(z) \\
&= 0.
\end{aligned}$$

The integral over the top and bottom parts of $\partial\Omega_M$ vanishes due to the pseudo-periodicity of the Green function. Since the integral is independent of M , one lets M tend to infinity, and a simple calculation using the outgoing condition (2.11) for G^0 or the decay condition for G^{per} shows that the integral over each of the sides vanishes separately. One now uses the pseudo-periodicity in both spatial variables to extend the result to x and y not necessarily in \mathcal{S} .

The singular behavior (2.16) of G^{per} is derived in Lemma 2 of Ref. [2]. The exponential decay property (2.17) follows from the exponential decay of the single-source Green function of a periodic operator in a spectral gap and the definition of G^{per} through the Floquet transform (see Lemma 4 of Ref. [2]). \square

2.2 Functional spaces

We introduce the following function spaces.

Definition 2.3. *Let $\theta \in (0, 2\pi)^2$ and Ω be open subset of \mathcal{S} .*

- $\mathcal{C}^{\infty, \theta}(\mathbb{R}^3)$ denotes the set of all functions $v \in \mathcal{C}^\infty(\mathbb{R}^3)$ satisfying the following conditions:
 - $\text{Supp}(u) \subseteq \{x \in \mathbb{R}^3 \mid |x_1| < \rho\}$ for some $\rho > 0$,
 - u is pseudo-periodic : $u(x + (0, n)) = e^{in \cdot \theta} u(x)$.
- $\mathcal{C}^{\infty, \theta}(\Omega)$ consists of the restrictions to Ω of the functions of $\mathcal{C}^{\infty, \theta}(\mathbb{R}^3)$.
- $H^{1, \theta}(\Omega)$ denotes the closure of $\mathcal{C}^{\infty, \theta}(\Omega)$ in $H^1(\Omega)$.
- $H_{\text{loc}}^{1, \theta}(\Omega)$ denotes the set of functions u such that $\chi u \in H^{1, \theta}(\Omega)$, for all $\chi \in \mathcal{C}^\infty(\Omega)$.

Define then the following spaces of functions (called \mathcal{L} -spaces in the sequel):

$$\mathcal{L}_{M^+}^0 = \{u \in H_{\text{loc}}^{1, \theta}(\{x_1 > M\}) : (\Delta + \omega^2\varepsilon^0)u = 0, u \text{ is outgoing as } x_1 \rightarrow \infty\}, \quad (2.20)$$

$$\mathcal{L}_{M^-}^0 = \{u \in H_{\text{loc}}^{1, \theta}(\{x_1 < M\}) : (\Delta + \omega^2\varepsilon^0)u = 0, u \text{ is outgoing as } x_1 \rightarrow -\infty\}, \quad (2.21)$$

$$\mathcal{L}_{\Omega_M^c}^0 = \{u \in H_{\text{loc}}^{1, \theta}(\Omega_M^c) : (\Delta + \omega^2\varepsilon^0)u = 0, u \text{ is outgoing as } |x_1| \rightarrow \infty\}, \quad (2.22)$$

$$\mathcal{L}_{M^+}^{\text{per}} = \{u \in H_{\text{loc}}^{1,\theta}(\{x_1 > M\}) : (\Delta_x + \omega^2 \varepsilon^{\text{per}}(x))u = 0, u \rightarrow 0 \text{ as } x_1 \rightarrow \infty\}, \quad (2.23)$$

$$\mathcal{L}_{M^-}^{\text{per}} = \{u \in H_{\text{loc}}^{1,\theta}(\{x_1 < M\}) : (\Delta_x + \omega^2 \varepsilon^{\text{per}}(x))u = 0, u \rightarrow 0 \text{ as } x_1 \rightarrow -\infty\}, \quad (2.24)$$

$$\mathcal{L}_{\Omega_M}^{\text{per}} = \{u \in H^{1,\theta}(\Omega_M) : (\Delta_x + \omega^2 \varepsilon^{\text{per}}(x))u = 0\}, \quad (2.25)$$

$$\mathcal{L}_{\Omega_M^c}^{\text{per}} = \{u \in H_{\text{loc}}^{1,\theta}(\Omega_M^c) : (\Delta_x + \omega^2 \varepsilon^{\text{per}}(x))u = 0, u \rightarrow 0 \text{ as } |x_1| \rightarrow \infty\}. \quad (2.26)$$

The \mathcal{L} -spaces have well-defined traces on Γ_M that are of class $H^{\frac{1}{2}}$ and normal derivatives that are of class $H^{-\frac{1}{2}}$ (see for example Lemma 3.1 of Ref. [5]). Thus we define the space

$$\mathcal{H}_M = H^{\frac{1}{2}}(\Gamma_M) \oplus H^{-\frac{1}{2}}(\Gamma_M),$$

and the spaces of the corresponding Cauchy data of the above \mathcal{L} spaces are

$$\begin{aligned} \mathcal{B}_{M^+}^0 &= \left\{ \xi = \begin{bmatrix} u|_{\Gamma_M} \\ \partial_n u|_{\Gamma_M} \end{bmatrix} \in \mathcal{H}_M; u \in \mathcal{L}_{M^+}^0 \right\}, \\ \mathcal{B}_{M^-}^0 &= \left\{ \xi = \begin{bmatrix} u|_{\Gamma_M} \\ \partial_n u|_{\Gamma_M} \end{bmatrix} \in \mathcal{H}_M; u \in \mathcal{L}_{M^-}^0 \right\}, \\ \mathcal{B}_{\Omega_M^c}^0 &= \left\{ \xi = \begin{bmatrix} u|_{\Gamma_M \cup \Gamma_M} \\ \partial_n u|_{\Gamma_M \cup \Gamma_M} \end{bmatrix} \in \mathcal{H}_{-M} \oplus \mathcal{H}_M; u \in \mathcal{L}_{\Omega_M^c}^0 \right\} = \mathcal{B}_{-M^-}^0 \oplus \mathcal{B}_{M^+}^0, \\ \mathcal{B}_{M^+}^{\text{per}} &= \left\{ \xi = \begin{bmatrix} u|_{\Gamma_M} \\ \partial_n u|_{\Gamma_M} \end{bmatrix} \in \mathcal{H}_M; u \in \mathcal{L}_{M^+}^{\text{per}} \right\}, \\ \mathcal{B}_{M^-}^{\text{per}} &= \left\{ \xi = \begin{bmatrix} u|_{\Gamma_M} \\ \partial_n u|_{\Gamma_M} \end{bmatrix} \in \mathcal{H}_M; u \in \mathcal{L}_{M^-}^{\text{per}} \right\}, \\ \mathcal{B}_{\Omega_M}^{\text{per}} &= \left\{ \xi = \begin{bmatrix} u|_{\Gamma_M \cup \Gamma_M} \\ \partial_n u|_{\Gamma_M \cup \Gamma_M} \end{bmatrix} \in \mathcal{H}_{-M} \oplus \mathcal{H}_M; u \in \mathcal{L}_{\Omega_M}^{\text{per}} \right\}, \\ \mathcal{B}_{\Omega_M^c}^{\text{per}} &= \left\{ \xi = \begin{bmatrix} u|_{\Gamma_M \cup \Gamma_M} \\ \partial_n u|_{\Gamma_M \cup \Gamma_M} \end{bmatrix} \in \mathcal{H}_{-M} \oplus \mathcal{H}_M; u \in \mathcal{L}_{\Omega_M^c}^{\text{per}} \right\} = \mathcal{B}_{-M^-}^{\text{per}} \oplus \mathcal{B}_{M^+}^{\text{per}}. \end{aligned}$$

2.3 Integral operators

Given a distribution ϕ on Γ_M , we define the single-layer potentials

$$\left(\tilde{S}_M^0 \phi \right) (x) = \int_{\Gamma_M} G^0(\omega, \theta; y, x) \phi(y) \, dA(y), \quad (2.27)$$

$$\left(\tilde{S}_M^{\text{per}} \phi \right) (x) = \int_{\Gamma_M} G^{\text{per}}(\omega, \theta; y, x) \phi(y) \, dA(y), \quad (2.28)$$

and the double-layer potentials

$$\left(\tilde{K}_M^0 \phi \right) (x) = \int_{\Gamma_M} \partial_{n(y)} G^0(\omega, \theta; y, x) \phi(y) \, dA(y), \quad (2.29)$$

$$\left(\tilde{K}_M^{\text{per}} \phi \right) (x) = \int_{\Gamma_M} \partial_{n(y)} G^{\text{per}}(\omega, \theta; y, x) \phi(y) \, dA(y), \quad (2.30)$$

where n denotes here the unit normal to Γ_M directed towards the right: $\partial_n = \frac{\partial}{\partial x_1}$.

A form of the usual Green theorem allows us to represent a function u in any of the spaces \mathcal{L} as a combination of the single- and double-layer potentials applied to the boundary data of u :

Lemma 2.4 (Integral representation formula). *Let $u \in \mathcal{L}_{M+}^0$ or $u \in \mathcal{L}_{M-}^0$. Then*

$$u(x) = \operatorname{sgn}(M - x_1) \left[(\tilde{K}_M^0 u|_{\Gamma_M})(x) - \tilde{S}_M^0 \partial_n u|_{\Gamma_M}(x) \right].$$

Similarly, let $u \in \mathcal{L}_{M+}^{\text{per}}$ or $u \in \mathcal{L}_{M-}^{\text{per}}$. Then

$$u(x) = \operatorname{sgn}(M - x_1) \left[(\tilde{K}_M^{\text{per}} u|_{\Gamma_M})(x) - (\tilde{S}_M^{\text{per}} \partial_n u|_{\Gamma_M})(x) \right].$$

Proof. The proof is accomplished in the standard way using integration by parts. For $u \in \mathcal{L}_{M+}^0$, for example, one integrates over the part of the strip with $M < x_1 < M'$. As in the proof of Lemma 2.2, the integral over the top and bottom parts of the boundary of \mathcal{S} vanish, as does the integral over $\Gamma_{M'}$ as M' tends to infinity, thanks to the outgoing radiation condition. \square

Remark 2.5. *Observe that the representation formula involves integrals over Γ_M alone, even for values of x exterior to Ω_M . This is accomplished by choosing Green functions that are pseudoperiodic and outgoing (for the homogeneous material) or decaying (for the periodic material). In short, the Green function should possess the boundary behavior (including behavior at infinity) of the functions that are represented by the formula. See, for example, similar representation formulas for outgoing fields exterior to a bounded obstacle in Refs. [4] and [11], and for fields that are pseudoperiodic in all directions, as equation (2.13) in Ref. [1].*

Next, we introduce the boundary-integral operators that give the boundary data on Γ_M for the single- and double-layer potentials. Given a regular function ϕ defined on Γ_M , we set for $x \in \Gamma_M$

$$(S_M^0 \phi)(x) = \int_{\Gamma_M} G^0(\omega, \theta; y, x) \phi(y) \, dA(y), \quad (2.31)$$

$$(K_M^0 \phi)(x) = \int_{\Gamma_M} \partial_{n(y)} G^0(\omega, \theta; y, x) \phi(y) \, dA(y), \quad (2.32)$$

$$(K_M^{\prime 0} \phi)(x) = \int_{\Gamma_M} \partial_{n(x)} G^0(\omega, \theta; y, x) \phi(y) \, dA(y), \quad (2.33)$$

$$(D_M^0 \phi)(x) = \partial_n (\tilde{K}_M^0 \phi)(x). \quad (2.34)$$

The corresponding operators for the periodic medium, S_M^{per} , K_M^{per} , $K_M^{\prime \text{per}}$, and D_M^{per} , are defined by replacing G^0 with G^{per} .

Lemma 2.6 (Boundary data of potentials). *Let $\xi = (\xi, \eta)^t \in \mathcal{H}_M$. Then the potentials $\tilde{S}_M^0 \eta$ and $\tilde{K}_M^0 \xi$ (resp. $\tilde{S}_M^{\text{per}} \eta$ and $\tilde{K}_M^{\text{per}} \xi$) belong to \mathcal{L}_{M+}^0 (resp. $\mathcal{L}_{M+}^{\text{per}}$) for $x_1 > M$ and to \mathcal{L}_{M-}^0 (resp. $\mathcal{L}_{M-}^{\text{per}}$) for $x_1 < M$ and*

$$\begin{aligned} (\tilde{K}_M^0 \xi)|_{\Gamma_M} &= (K_M^0 \pm \frac{1}{2}I) \xi, & (\tilde{S}_M^0 \eta)|_{\Gamma_M} &= S_M^0 \eta, \\ \partial_n (\tilde{K}_M^0 \xi)|_{\Gamma_M} &= D_M^0 \xi, & \partial_n (\tilde{S}_M^0 \eta)|_{\Gamma_M} &= (K_M^{\prime 0} \mp \frac{1}{2}I) \eta, \end{aligned}$$

in which the upper sign holds if $x_1 \rightarrow M$ from the left and the lower sign if $x_1 \rightarrow M$ from the right. The analogous formulas hold for the boundary values of the periodic potentials $\tilde{S}_M^{\text{per}}\eta$ and $\tilde{K}_M^{\text{per}}\xi$.

Proof. The above trace formulas essentially follow from the fact that the singularity of the Green kernels G^0 and G^{per} behave as $1/|x-y|$ as in the free space case (see (2.16)). Therefore, the proof is a direct adaptation of the classical jump conditions from potential theory (for more details see for instance Ref. [4] for the case of homogeneous media and Lemma 3.8 of Ref. [5] for the case of transmission problems). \square

The following theory regarding boundary data and the Calderón boundary integral projectors (see Ref. [11]) is justified by suitable modifications of the exposition of Ref. [5], Section 3.

We define the following singular integral operators in \mathcal{H}_M in matrix form with respect to this decomposition:

$$C_M^0 = \begin{bmatrix} K_M^0 & -S_M^0 \\ D_M^0 & -K_M^0 \end{bmatrix}, \quad C_M^{\text{per}} = \begin{bmatrix} K_M^{\text{per}} & -S_M^{\text{per}} \\ D_M^{\text{per}} & -K_M^{\text{per}} \end{bmatrix} : \mathcal{H}_M \rightarrow \mathcal{H}_M. \quad (2.35)$$

In addition, we will make use of two regular integral operators that couple the boundary data \mathcal{H}_M and \mathcal{H}_{-M} :

$$\begin{aligned} C^{-+} : \mathcal{H}_M &\rightarrow \mathcal{H}_{-M}, & C^{+-} : \mathcal{H}_{-M} &\rightarrow \mathcal{H}_M, \\ C_M^{-+} \begin{bmatrix} \xi \\ \eta \end{bmatrix} (x) &= \begin{bmatrix} \tilde{K}_M^{\text{per}} & -\tilde{S}_M^{\text{per}} \\ \partial_{n(x)}\tilde{K}_M^{\text{per}} & -\partial_{n(x)}\tilde{S}_M^{\text{per}} \end{bmatrix} \begin{bmatrix} \xi \\ \eta \end{bmatrix} (x) && \text{for } x \in \Gamma_{-M}, \\ C_M^{+-} \begin{bmatrix} \xi \\ \eta \end{bmatrix} (x) &= \begin{bmatrix} \tilde{K}_M^{\text{per}} & -\tilde{S}_M^{\text{per}} \\ \partial_{n(x)}\tilde{K}_M^{\text{per}} & -\partial_{n(x)}\tilde{S}_M^{\text{per}} \end{bmatrix} \begin{bmatrix} \xi \\ \eta \end{bmatrix} (x) && \text{for } x \in \Gamma_M. \end{aligned}$$

In these operators, the integration is performed at a distance from the point of influence x , and we can write them in integral form:

$$C_M^{-+} \begin{bmatrix} \xi \\ \eta \end{bmatrix} (x) = \begin{bmatrix} \int_{\Gamma_M} (\partial_{n(y)}G^{\text{per}}(x,y)\xi(y) - G^{\text{per}}(x,y)\eta(y)) \, dA(y) \\ \int_{\Gamma_M} (\partial_{n(x)}\partial_{n(y)}G^{\text{per}}(x,y)\xi(y) - \partial_{n(x)}G^{\text{per}}(x,y)\eta(y)) \, dA(y) \end{bmatrix}, \quad x \in \Gamma_{-M}, \quad (2.36)$$

$$C_M^{+-} \begin{bmatrix} \xi \\ \eta \end{bmatrix} (x) = \begin{bmatrix} \int_{\Gamma_{-M}} (\partial_{n(y)}G^{\text{per}}(x,y)\xi(y) - G^{\text{per}}(x,y)\eta(y)) \, ds(y) \\ \int_{\Gamma_{-M}} (\partial_{n(x)}\partial_{n(y)}G^{\text{per}}(x,y)\xi(y) - \partial_{n(x)}G^{\text{per}}(x,y)\eta(y)) \, ds(y) \end{bmatrix}, \quad x \in \Gamma_M. \quad (2.37)$$

In terms of these operators, we define two operators on $\mathcal{H}_{-M} \oplus \mathcal{H}_M$:

$$L_M := \begin{bmatrix} -C_{-M}^{\text{per}} & C_M^{-+} \\ -C_M^{+-} & C_M^{\text{per}} \end{bmatrix} : \mathcal{H}_{-M} \oplus \mathcal{H}_M \rightarrow \mathcal{H}_{-M} \oplus \mathcal{H}_M, \quad (2.38)$$

$$R_M := \begin{bmatrix} -C_{-M}^0 & 0 \\ 0 & C_M^0 \end{bmatrix} : \mathcal{H}_{-M} \oplus \mathcal{H}_M \rightarrow \mathcal{H}_{-M} \oplus \mathcal{H}_M. \quad (2.39)$$

Remark 2.7. Let us emphasize that the operator L_M is nothing but the counterpart of the operator C_M^{per} when the domain under consideration is no longer one-sided (i.e. of the form $\{x_1 < M\}$ or $\{x_1 > M\}$) but two-sided (i.e. of the form $\{-M < x_1 < M\}$).

We collect in the next Theorem some useful properties satisfied by the above operators.

Theorem 2.8 (Calderón projectors).

i. The operators

$$C_M^0 : \mathcal{H}_M \rightarrow \mathcal{H}_M \quad C_M^{\text{per}} : \mathcal{H}_M \rightarrow \mathcal{H}_M$$

are uniformly bounded with respect to the integer M .

ii. There exists $d_1 > 0$ and $d_2 > 0$ such that the operators

$$C_M^{-+} : \mathcal{H}_M \rightarrow \mathcal{H}_{-M} \quad C_M^{+-} : \mathcal{H}_{-M} \rightarrow \mathcal{H}_M,$$

satisfy, for M sufficiently large,

$$\|C_M^{-+}\|_{\mathcal{L}(\mathcal{H}_M, \mathcal{H}_{-M})} + \|C_M^{+-}\|_{\mathcal{L}(\mathcal{H}_M, \mathcal{H}_{-M})} < d_1 e^{-d_2 M}.$$

iii. The operators $\frac{1}{2}I \pm C_M^0$ (resp. $\frac{1}{2}I \pm C_M^{\text{per}}$) are complementary projections with images $\mathcal{B}_{M^\mp}^0$ (resp. $\mathcal{B}_{M^\mp}^{\text{per}}$):

$$\begin{aligned} \mathcal{B}_{M^\pm}^0 &= \text{Ran} \left(\frac{1}{2}I \mp C_M^0 \right) = \text{Null} \left(\frac{1}{2}I \pm C_M^0 \right), \\ \mathcal{B}_{M^\pm}^{\text{per}} &= \text{Ran} \left(\frac{1}{2}I \mp C_M^{\text{per}} \right) = \text{Null} \left(\frac{1}{2}I \pm C_M^{\text{per}} \right). \end{aligned}$$

iv. The operator $\frac{1}{2}I + R_M$ is a projection with image $\mathcal{B}_{-M^+}^0 \oplus \mathcal{B}_{M^-}^0$, and its complementary projection $\frac{1}{2}I - R_M$ has image $\mathcal{B}_{\Omega_M^c}^0 = \mathcal{B}_{-M^-}^0 \oplus \mathcal{B}_{M^+}^0$:

$$\begin{aligned} \mathcal{B}_{-M^+}^0 \oplus \mathcal{B}_{M^-}^0 &= \text{Ran} \left(\frac{1}{2}I + R_M \right) = \text{Null} \left(\frac{1}{2}I - R_M \right), \\ \mathcal{B}_{\Omega_M^c}^0 &= \text{Ran} \left(\frac{1}{2}I - R_M \right) = \text{Null} \left(\frac{1}{2}I + R_M \right). \end{aligned}$$

v. The operator $\frac{1}{2}I + L_M$ is a projection with image $\mathcal{B}_{\Omega_M}^{\text{per}}$, and its complementary projection $\frac{1}{2}I - L_M$ has image $\mathcal{B}_{\Omega_M^c}^{\text{per}} = \mathcal{B}_{-M^-}^{\text{per}} \oplus \mathcal{B}_{M^+}^{\text{per}}$:

$$\begin{aligned} \mathcal{B}_{\Omega_M}^{\text{per}} &= \text{Ran} \left(\frac{1}{2}I + L_M \right) = \text{Null} \left(\frac{1}{2}I - L_M \right) \\ \mathcal{B}_{\Omega_M^c}^{\text{per}} &= \text{Ran} \left(\frac{1}{2}I - L_M \right) = \text{Null} \left(\frac{1}{2}I + L_M \right). \end{aligned}$$

Proof. *i.* The boundedness of the integral operators C_M^0 and C_M^{per} is straightforward, since the singularities of their kernels is as $1/|x - y|$ (for more details, see for instance Lemma 3.9 of Ref. [5]). The fact that the bounds are uniform with respect to M is a direct consequence of the translation property (2.12) satisfied by G^0 and G^{per} .

ii. The exponential decay of the norms of C_M^{-+} and C_M^{+-} follows from the decay property of the Green function G^{per} (see (2.17)).

iii. To prove, for example, that $\frac{1}{2}I + C_M^0$ is a projection onto $\mathcal{B}_{M^-}^0$, we observe first that $\frac{1}{2}I + C_M^0$ has image in $\mathcal{B}_{M^-}^0$. Indeed, for all $[\xi, \eta]^t \in \mathcal{H}_M$, the potential $u = \tilde{K}_M^0 \xi - \tilde{S}_M^0 \eta$ in $\mathcal{L}_{M^-}^0$ has, by Lemma 2.6, boundary data equal to

$$\left(\frac{1}{2}I + C_M^0\right) \begin{bmatrix} \xi \\ \eta \end{bmatrix} = \begin{bmatrix} u|_{\Gamma_M} \\ \partial_n u|_{\Gamma_M} \end{bmatrix} \in \mathcal{B}_{M^-}^0.$$

Second, if $[\xi, \eta]^t \in \mathcal{B}_{M^-}^0$, then $[\xi, \eta] = [u|_{\Gamma_M}, \partial_n u|_{\Gamma_M}]$ for some $u \in \mathcal{L}_{M^-}^0$, and the integral representation formula of Lemma 2.4 together with Lemma 2.6 give us that

$$\left(\frac{1}{2}I + C_M^0\right) \begin{bmatrix} \xi \\ \eta \end{bmatrix} = \begin{bmatrix} \xi \\ \eta \end{bmatrix}.$$

These two observations prove that $\frac{1}{2}I + C_M^0$ is a projection onto $\mathcal{B}_{M^-}^0$. The proofs for the other three operators are analogous.

iv. The projection properties concerning $\frac{1}{2}I \pm R_M$ follow immediately from those of $\frac{1}{2}I \pm C_M^0$.

v. That $\frac{1}{2}I + L_M$ is a projection onto $\mathcal{B}_{\Omega_M}^{\text{per}}$ is proved using a combination of potentials produced by data on Γ_{-M} and Γ_M arising from the modified representation formula for $u \in \mathcal{L}_{\Omega_M}^{\text{per}}$:

$$u(x) = \left[(\tilde{K}_M^{\text{per}} u|_{\Gamma_M})(x) - (\tilde{S}_M^{\text{per}} \partial_n u|_{\Gamma_M})(x) \right] - \left[(\tilde{K}_{-M}^{\text{per}} u|_{\Gamma_{-M}})(x) - (\tilde{S}_{-M}^{\text{per}} \partial_n u|_{\Gamma_{-M}})(x) \right]. \quad (2.40)$$

The images of their complements are obtained similarly. \square

We shall assume the following nonresonance condition for the periodic structure in the half plane:

Condition 2.9 (Nonresonance condition). *For each integer M and $\omega \in [\omega_1, \omega_2]$, the following pairs have only the trivial solution:*

$$\left\{ \begin{array}{l} \left(\frac{1}{2}I - C_M^0\right)\boldsymbol{\xi} = \mathbf{0} \\ \left(\frac{1}{2}I + C_M^{\text{per}}\right)\boldsymbol{\xi} = \mathbf{0} \end{array} \right\}, \quad \left\{ \begin{array}{l} \left(\frac{1}{2}I + C_M^0\right)\boldsymbol{\xi} = \mathbf{0} \\ \left(\frac{1}{2}I - C_M^{\text{per}}\right)\boldsymbol{\xi} = \mathbf{0} \end{array} \right\}. \quad (2.41)$$

By the translation property of the Green functions, this condition is equivalent to the simpler condition that

$$\left\{ \begin{array}{l} \left(\frac{1}{2}I - C_0^0\right)\boldsymbol{\xi} = \mathbf{0} \\ \left(\frac{1}{2}I + C_0^{\text{per}}\right)\boldsymbol{\xi} = \mathbf{0} \end{array} \right\}, \quad \left\{ \begin{array}{l} \left(\frac{1}{2}I + C_0^0\right)\boldsymbol{\xi} = \mathbf{0} \\ \left(\frac{1}{2}I - C_0^{\text{per}}\right)\boldsymbol{\xi} = \mathbf{0} \end{array} \right\}.$$

Remark 2.10. *The Nonresonance Condition, which is needed to prove the existence of a unique outgoing Green function for the slab structure, has a physical meaning. We give a short discussion, excluding the details. According to Theorem 2.8, the first pair in the Condition characterizes boundary data ξ on Γ_M of a Helmholtz field decaying into the periodic medium to the right of Γ_M and decaying into the homogeneous medium to the left. The second pair characterizes boundary data ξ on Γ_M of a Helmholtz field decaying into the periodic medium to the left of Γ_M and decaying into the homogeneous medium to the right. Such fields are “surface waves” at the interface of the periodic and homogeneous media. Now, the existence of a unique Green function for the slab structure extending from $-M$ to M is tantamount to the nonexistence of guided modes in that structure. As $M \rightarrow \infty$, with ω in a spectral gap, a guided mode of the slab becomes concentrated at the left and right surfaces of the slab, thus being approximated by a pair of surface waves. Therefore, the Nonresonance Condition effectively excludes guided modes of the slab in the limit of infinite thickness. Surface waves satisfy dispersion relations relating their wavenumber κ and frequency ω , which give ω as complex functions of κ when G^0 admits propagating Fourier harmonics, as is always the case in the scattering problem. A real pair (κ, ω) will admit a surface wave only at special values when the dispersion relation meets the real subspace of \mathbb{C}^2 . Furthermore, results by Iantchenko[9] show that, at least for one-dimensional crystals, guided modes of a thick slab occur only for frequencies in a propagation band, rendering the Condition superfluous. One should keep in mind that we are referring here to guided modes of the perfect (without defect) crystal slab. The guided modes of a planar defect introduced later occur in a spectral gap.*

Lemma 2.11. *The operator*

$$C_M^0 - C_M^{\text{per}} : \mathcal{H}_M \rightarrow \mathcal{H}_M$$

is compact. Given $\mathbf{f} \in \mathcal{B}_{M^-}^0$ and $\mathbf{g} \in \mathcal{B}_{M^+}^{\text{per}}$, respectively $\mathbf{f} \in \mathcal{B}_{M^+}^0$ and $\mathbf{g} \in \mathcal{B}_{M^-}^{\text{per}}$, the nonresonance condition implies that the pairs

$$\begin{cases} (\frac{1}{2}I + C_M^0)\xi = \mathbf{f} \\ (\frac{1}{2}I - C_M^{\text{per}})\xi = \mathbf{g} \end{cases}, \quad \begin{cases} (\frac{1}{2}I - C_M^0)\xi = \mathbf{f} \\ (\frac{1}{2}I + C_M^{\text{per}})\xi = \mathbf{g} \end{cases}, \quad (2.42)$$

are equivalent, respectively, to

$$(I + C_M^0 - C_M^{\text{per}})\xi = \mathbf{f} + \mathbf{g}, \quad (I - C_M^0 + C_M^{\text{per}})\xi = \mathbf{f} + \mathbf{g} \quad (2.43)$$

and that the latter have unique solutions for all integers M and $\omega \in [\omega_1, \omega_2]$. Finally, the operators $I + C_M^0 - C_M^{\text{per}}$ and $I - C_M^0 + C_M^{\text{per}}$ are bounded from below uniformly for integers M and $\omega \in [\omega_1, \omega_2]$.

Proof. The compactness of $C_M^0 - C_M^{\text{per}}$ is due to the cancellation of the leading singularities in the Green function. We refer to the discussion on page 331 of Ref. [13]. The equivalence statement is essentially Theorems 4.3 and 4.4 in Ref. [13]. The first equation in (2.43) (the second is proved similarly) implies

$$\begin{cases} (\frac{1}{2}I + C_M^0)\xi = \mathbf{f} + \mathbf{h}, \\ (\frac{1}{2}I - C_M^{\text{per}})\xi = \mathbf{g} - \mathbf{h}, \end{cases}$$

for some \mathbf{h} . Since $\mathbf{f} \in \mathcal{B}_{M^-}^0 = \text{Ran}(\frac{1}{2}I + C_M^0)$ and $\mathbf{g} \in \mathcal{B}_{M^+}^{\text{per}} = \text{Ran}(\frac{1}{2}I - C_M^{\text{per}})$, the above relations imply that

$$\mathbf{h} \in \text{Ran}(\frac{1}{2}I + C_M^0) \cap \text{Ran}(\frac{1}{2}I - C_M^{\text{per}}) = \text{Null}(\frac{1}{2}I - C_M^0) \cap \text{Null}(\frac{1}{2}I + C_M^{\text{per}}), \quad (2.44)$$

which, by the first pair of the nonresonance condition, implies that $\mathbf{h} = 0$. This proves the equivalence.

We see that the nullspace of $I + C_M^0 - C_M^{\text{per}}$ is trivial by setting \mathbf{f} and \mathbf{g} equal to zero and using the equivalence just proved and the first pair of the nonresonance condition.

Since $C_M^0 - C_M^{\text{per}}$ is compact, $I + C_M^0 - C_M^{\text{per}}$ is surjective whenever if and only if it is injective, and we conclude that $(I + C_M^0 - C_M^{\text{per}})\boldsymbol{\xi} = \mathbf{f} + \mathbf{g}$ has a unique solution $\boldsymbol{\xi}$. Since this is true for all M and $\omega \in [\omega_1, \omega_2]$, the compactness and translation properties of $C_M^0 - C_M^{\text{per}}$, as well as continuity in ω , imply that $I + C_M^0 - C_M^{\text{per}}$ has a lower bound that is uniform over integers M and $\omega \in [\omega_1, \omega_2]$. \square

3 Fields in a thick PC slab

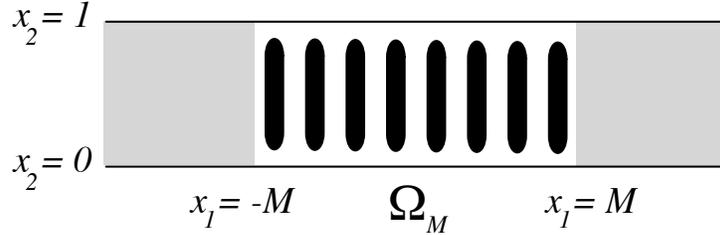


Figure 2: Thick PC slab.

We consider the problem of transmission of plane waves scattered by a thick photonic crystal slab characterized by the dielectric permittivity

$$\varepsilon_M^{\text{per}}(x) = \begin{cases} \varepsilon^{\text{per}}(x), & |x_1| \leq M, \\ \varepsilon^0, & |x_1| > M. \end{cases}$$

We take the source field to be a plane wave incident on the slab from the left. The incident field has a wave number in the x_1 -direction given by some β_n for $n \in \mathcal{P}$ (see equation (2.5)). The associated scattering problem can be formulated as follows:

Problem 3.1 (Scattering by a perfect slab). *Given an incident field*

$$u^{\text{inc}}(x) = e^{i\bar{m}x_1} e^{i(2\pi\bar{m}+\theta)\cdot x'}, \quad \bar{m} \in \mathcal{P},$$

find a function u that satisfies the following conditions:

$$(\Delta + \omega^2 \varepsilon_M^{\text{per}}(x))u(x) = 0, \quad (3.1.a)$$

$$u(x + (0, n)) = e^{in\cdot\theta} u(x), \quad (3.1.b)$$

$$u - u^{\text{inc}} \text{ is outgoing as } x_1 \rightarrow \pm\infty. \quad (3.1.c)$$

The outgoing radiation condition (3.1.c) is to be understood in the sense of Definition 2.1.

We begin our analysis of the transmission problem in a thick photonic crystal slab with a study of the *outgoing pseudo-periodic Green function* $G_M^{\text{per}}(\omega, \theta; x, y)$ for the slab structure. By definition, G_M^{per} satisfies

$$(\Delta_y + \omega^2 \varepsilon_M^{\text{per}}(y)) G_M^{\text{per}}(\omega, \theta; x, y) = \sum_{n \in \mathbb{Z}} \delta_{(x_1, x'_1 + n)}(y) e^{in \cdot \theta}, \quad (3.2.a)$$

$$G_M^{\text{per}}(\omega, \theta; x, y + (0, n)) = e^{in \cdot \theta} G_M^{\text{per}}(\omega, \theta; x, y), \quad (3.2.b)$$

$$G_M^{\text{per}}(\omega, \theta; x, \cdot) \text{ is outgoing as } y_1 \rightarrow \pm\infty. \quad (3.2.c)$$

Lemma 3.2. *For all $x \notin \Gamma_{-M} \cup \Gamma_M$, set*

$$\xi_x = \begin{bmatrix} \xi_x^- \\ \xi_x^+ \end{bmatrix} = \text{Cauchy data on } \Gamma_{-M} \cup \Gamma_M \text{ of } G_M^{\text{per}}(x, \cdot).$$

Then, we have:

i. For $|x_1| < M$:

$$\begin{cases} \left(\frac{1}{2}I + R_M \right) \xi_x = \mathbf{0}, \\ \left(\frac{1}{2}I - L_M \right) \xi_x = \gamma_x, \end{cases} \quad (3.3)$$

where

$$\gamma_x = \begin{bmatrix} \gamma_x^- \\ \gamma_x^+ \end{bmatrix} = \text{Cauchy data on } \Gamma_{-M} \cup \Gamma_M \text{ of } G^{\text{per}}(x, \cdot).$$

ii. for $|x_1| > M$:

$$\begin{cases} \left(\frac{1}{2}I - L_M \right) \xi_x = \mathbf{0}, \\ \left(\frac{1}{2}I + R_M \right) \xi_x = \gamma_x^0, \end{cases} \quad (3.4)$$

where we have set

$$\gamma_x^0 = \begin{cases} \begin{bmatrix} \gamma_x^{0,-} \\ 0 \end{bmatrix} & \text{for } x_1 < -M, \\ \begin{bmatrix} 0 \\ \gamma_x^{0,+} \end{bmatrix} & \text{for } x_1 > M. \end{cases}$$

and where $\begin{bmatrix} \gamma_x^{0,-} \\ \gamma_x^{0,+} \end{bmatrix} = \text{Cauchy data on } \Gamma_{-M} \cup \Gamma_M \text{ of } G^0(x, \cdot).$

Proof.

i. Since for $|x_1| < M$ we have $G_M^{\text{per}}(x, \cdot) \in \mathcal{L}_{\Omega_M^c}^0$, it follows that

$$\xi_x \in \mathcal{B}_{\Omega_M^c}^0 = \text{Null} \left(\frac{1}{2}I + R_M \right).$$

To show the second relation, let us introduce the function

$$g(x, \cdot) = G_M^{\text{per}}(x, \cdot) - G^{\text{per}}(x, \cdot)$$

Then, we clearly have $g(x, \cdot) \in \mathcal{L}_{\Omega_M}^{\text{per}}$. Thus, if we denote by $\boldsymbol{\eta}_x = \boldsymbol{\xi}_x - \boldsymbol{\gamma}_x$ the Cauchy data of $g(x, \cdot)$, we have

$$\boldsymbol{\eta}_x \in \mathcal{B}_{\Omega_M}^{\text{per}} = \text{Null} \left(\frac{1}{2}I - L_M \right).$$

On the other hand, $G^{\text{per}}(x, \cdot) \in \mathcal{L}_{\Omega_M^c}^{\text{per}}$ yields

$$\boldsymbol{\gamma}_x \in \mathcal{B}_{\Omega_M^c}^{\text{per}} = \text{Ran} \left(\frac{1}{2}I - L_M \right).$$

Consequently

$$\left(\frac{1}{2}I - L_M \right) \boldsymbol{\xi}_x = \left(\frac{1}{2}I - L_M \right) (\boldsymbol{\eta}_x + \boldsymbol{\gamma}_x) = \boldsymbol{\gamma}_x.$$

ii. Since $|x_1| > M$, we have $G_M^{\text{per}}(x, \cdot) \in \mathcal{L}_{\Omega_M}^{\text{per}}$ and thus

$$\boldsymbol{\xi}_x \in \mathcal{B}_{\Omega_M}^{\text{per}} = \text{Null} \left(\frac{1}{2}I - L_M \right).$$

To prove the last relation, we first note that

$$\left(\frac{1}{2}I + R_M \right) \boldsymbol{\xi}_x = \begin{bmatrix} \left(\frac{1}{2} - C_{-M}^0 \right) \boldsymbol{\xi}_x^- \\ \left(\frac{1}{2} + C_M^0 \right) \boldsymbol{\xi}_x^+ \end{bmatrix}. \quad (3.5)$$

Let us assume that $x_1 > M$, the proof being exactly similar for $x_1 < -M$. Then, we have $G_M^{\text{per}}(x, \cdot) \in \mathcal{L}_{-M^-}^0$ and consequently $\boldsymbol{\xi}_x^- \in \mathcal{B}_{-M^-}^0$, or equivalently by Theorem 2.8,

$$\left(\frac{1}{2}I - C_{-M}^0 \right) \boldsymbol{\xi}_x^- = 0. \quad (3.6)$$

On the other hand, if we set

$$g^0(x, \cdot) = G_M^{\text{per}}(x, \cdot) - G^0(x, \cdot)$$

then it can be easily checked that $g^0(x, \cdot) \in \mathcal{L}_{M^+}^0$ and thus, if we denote by $\boldsymbol{\eta}_x^{0,+} = \boldsymbol{\xi}_x^+ - \boldsymbol{\gamma}_x^{0,+}$ the Cauchy data of $g^0(x, \cdot)$ on Γ_M , there holds

$$\boldsymbol{\eta}_x^{0,+} \in \mathcal{B}_{M^+}^0 = \text{Null} \left(\frac{1}{2}I + C_M^0 \right).$$

But since $G^0(x, \cdot) \in \mathcal{L}_{M^-}^0$, we have on the other hand that

$$\boldsymbol{\gamma}_x^{0,+} \in \mathcal{B}_{M^-}^0 = \text{Ran} \left(\frac{1}{2}I + C_M^0 \right).$$

Therefore, we have

$$\left(\frac{1}{2}I + C_M^0 \right) \boldsymbol{\xi}_x^+ = \left(\frac{1}{2}I + C_M^0 \right) (\boldsymbol{\eta}_x^{0,+} + \boldsymbol{\gamma}_x^{0,+}) = \boldsymbol{\gamma}_x^{0,+}. \quad (3.7)$$

The claimed result follows then from relations (3.5),(3.6) and (3.7). \square

Corollary 3.3. *Let the Nonresonance Condition be satisfied. With the notation of Lemma 3.2, the pairs of equations (3.3) and (3.4) satisfied by the Cauchy data $\boldsymbol{\xi}_x$ of G_M^{per} are respectively equivalent to the two single equations:*

$$(I + R_M - L_M)\boldsymbol{\xi}_x = \boldsymbol{\gamma}_x \quad \text{for } |x_1| < M, \quad (3.8)$$

and

$$(I + R_M - L_M)\boldsymbol{\xi}_x = \boldsymbol{\gamma}_x^0 \quad \text{for } |x_1| > M. \quad (3.9)$$

If M is sufficiently large, then equation (3.8) has a unique solution that is the boundary data on $\Gamma_{-M} \cup \Gamma_M$ of a solution $G_M^{\text{per}}(\omega, \theta; x, \cdot)$ of equations (3.2).

Proof. Let us detail the proof for $|x_1| < M$. To show that the pair in (3.3) is equivalent to (3.8), assume that $\boldsymbol{\xi}_x$ satisfies (3.8). Then,

$$\mathbf{h} := \left(\frac{1}{2}I + R_M \right) \boldsymbol{\xi}_x \in \text{Ran} \left(\frac{1}{2}I + R_M \right) \cap \text{Ran} \left(\frac{1}{2}I - L_M \right),$$

which also reads, by Theorem 2.8,

$$\mathbf{h} = \begin{bmatrix} \mathbf{h}^- \\ \mathbf{h}^+ \end{bmatrix} \in (\mathcal{B}_{-M^+}^0 \oplus \mathcal{B}_{M^-}^0) \cap \mathcal{B}_{\Omega_M^c}^{\text{per}}.$$

The above relation is equivalent to

$$\mathbf{h}^- \in \mathcal{B}_{-M^+}^0 \cap \mathcal{B}_{-M^-}^{\text{per}} \quad \mathbf{h}^+ \in \mathcal{B}_{M^-}^0 \cap \mathcal{B}_{M^+}^{\text{per}}$$

and thus, by the Nonresonance Condition, we have $\mathbf{h}^- = \mathbf{h}^+ = \mathbf{0}$, and we have proved equivalence of (3.3) and (3.8).

To prove that (3.8) has a unique solution, we write the operator in matrix form with respect to the decomposition $\mathcal{H}_{-M} \oplus \mathcal{H}_M$:

$$I + R_M - L_M = \begin{bmatrix} I + C_{-M}^{\text{per}} - C_{-M}^0 & -C_M^{-+} \\ C_M^{+-} & I - C_M^{\text{per}} + C_M^0 \end{bmatrix}.$$

From Lemma 2.11, we know that the operators on the diagonal are bounded uniformly from below for integers M and $\omega \in [\omega_1, \omega_2]$. From the integral expressions (2.36) and (2.37), we see that, for $|M|$ sufficiently large, the off-diagonal operators are small enough so that $I + R_M - L_M$ is also uniformly bounded from below, and thus equation (3.8) has a unique solution, which is nothing but the Cauchy boundary data on $\Gamma_{-M} \cup \Gamma_M$ of the Green function $G_M^{\text{per}}(\omega, \theta; x, \cdot)$. \square

Theorem 3.4 (Green function of a PC slab). *Let the Nonresonance Condition be satisfied.*

- i.* Let $M_0 > 0$ be fixed. There exist numbers $c_1 > 0$ and $c_2 > 0$ such that, for $M > M_0$ sufficiently large,

$$\begin{aligned} |G_M^{\text{per}}(x, y) - G^{\text{per}}(x, y)| &< c_1 e^{-c_2 M}, \quad |x_1| < M_0, |y_1| < M, \\ |G_M^{\text{per}}(x, y)| &< c_1 e^{-c_2 |y_0 - x|}, \quad |x_1| < M_0, \end{aligned}$$

where $y_0 = \min(|y_1|, M)\text{sgn}(y_1)$.

ii. There exist numbers $d_1 > 0$ and $d_2 > 0$ such that, if M is sufficiently large, $|x_1| > M$, $|y_1| > M$, and $x_1 y_1 < 0$, then

$$|G_M^{\text{per}}(\omega, \theta; x, y)| < d_1 e^{-d_2 M}.$$

Proof. To prove part (i), let M_0 be given, with $|x_1| < M_0$. Then $\|\gamma\| < A_1 e^{A_2 |M - M_0|}$. For M sufficiently large, the operator $I + R_M - L_M$ is bounded from below, say by δ , and we have $\delta \|\xi\| < \|\gamma\|$. Using the representation (2.40) applied to the boundary data $\xi - \gamma$, we obtain the exponential estimates for g_x and thus also for G_M^{per} .

For part (ii), since $x_1 < -M$ (the case $x_1 > M$ is handled similarly), we must solve

$$\begin{bmatrix} I + C_{-M}^{\text{per}} - C_{-M}^0 & -C_M^{-+} \\ C_M^{+-} & I - C_M^{\text{per}} + C_M^0 \end{bmatrix} \begin{bmatrix} \xi_- \\ \xi_+ \end{bmatrix} = \begin{bmatrix} \gamma_- \\ \mathbf{0} \end{bmatrix}. \quad (3.10)$$

Since $I + R_M - L_M$ is bounded below by δ , we obtain (by first using $[\xi_-, 0]^t$ and then $[0, \xi_+]^t$ in place of $\xi = [\xi_-, \xi_+]^t$ in (3.10))

$$\delta \|\xi_-\| < \|\gamma_-\| \quad \text{and} \quad \delta \|\xi_+\| < \|(I - C_M^{\text{per}} + C_M^0)\xi_+\|.$$

By using the representation formulas (2.36) and (2.37), we see that there are constants a_1 and a_2 such that

$$\|C_M^\pm\| < a_1 e^{-a_2 M}.$$

These estimates together with the second equation in the system (3.10) yield

$$\delta \|\xi_+\| \leq \|(I - C_M^{\text{per}} + C_M^0)\xi_+\| \leq \|C_M^{+-}\| \|\xi_-\| < a_1 e^{-a_2 M} \|\gamma_-\| / \delta,$$

from which we obtain a bound on the trace ξ_+ , of G_M^{per} on Γ_+ ,

$$\|\xi_+\| < c_1 e^{-c_2 M} \|\gamma_-\| / (\delta^2),$$

which then yields the result through the representation formula from Lemma 2.4. \square

Theorem 3.5 (Transmission). *There exist constants $c_1 > 0$ and $c_2 > 0$ such that, for M sufficiently large, the scattering Problem 3.1 has a unique solution u , and*

$$|u(x)| < c_1 e^{-c_2 M} \quad \text{for } x_1 > M.$$

Proof. Let m be a fixed number such that $m < -M$. We introduce the function space

$$\mathcal{L}_{m+}^* = \{u \in H_{\text{loc}}^1(\{x_1 > m\}) : (\Delta + \omega^2 \varepsilon_M^{\text{per}}(x)) u = 0, u \text{ is outgoing}\}$$

with boundary data on Γ_m

$$\mathcal{B}_{m+}^* = \left\{ \begin{bmatrix} \xi \\ \eta \end{bmatrix} \in \mathcal{H}_m : \exists u \in \mathcal{L}_{m+}^* \text{ with } \xi = u|_{\Gamma_m}, \eta = \partial_n u|_{\Gamma_m} \right\}.$$

One can define single- and double-layer potentials \tilde{S}_m^* , etc., using the Green function G_M^{per} that are analogous to those defined for G^0 and G^{per} in equations (2.27)–(2.30) and a representation formula for $u \in \mathcal{L}_{m+}^*$ as in Lemma 2.4, as well as the boundary integral operators

S_m^* analogous to (2.31–2.34). The singular integral operator C_m^* is then defined in \mathcal{H}_m , analogously to (2.35). Ultimately, we obtain the complementary Calderón projectors $\frac{1}{2}I \pm C_m^*$, whose properties are proved similarly to those of C_m^0 . In particular, the nullspace of $\frac{1}{2}I + C_m^*$ is equal to $\mathcal{B}_{m^+}^*$, and we recall from Theorem 2.8 that $\frac{1}{2}I - C_m^0$ has nullspace $\mathcal{B}_{m^-}^0$ and image $\mathcal{B}_{m^+}^0$.

For a function u that solves Problem 3.1, let

$$\boldsymbol{\xi} = \begin{bmatrix} u|_{\Gamma_m} \\ \partial_n u|_{\Gamma_m} \end{bmatrix}, \quad \boldsymbol{\gamma} = \begin{bmatrix} u^{\text{inc}}|_{\Gamma_m} \\ \partial_n u^{\text{inc}}|_{\Gamma_m} \end{bmatrix}.$$

Since $u^{\text{inc}} \in \mathcal{L}_{m^+}^0$, we have $\boldsymbol{\gamma} \in \mathcal{B}_{m^+}^0$. We conclude that u solves Problem 3.1 if and only if $\boldsymbol{\xi}$ solves the pair

$$\begin{aligned} \left(\frac{1}{2}I + C_m^*\right)\boldsymbol{\xi} &= \mathbf{0}, \\ \left(\frac{1}{2}I - C_m^0\right)\boldsymbol{\xi} &= \boldsymbol{\gamma}. \end{aligned} \tag{3.11}$$

As before, we find that pair is equivalent to the sum of the two equations

$$(I + C_m^* - C_m^0)\boldsymbol{\xi} = \boldsymbol{\gamma} \tag{3.12}$$

if there exists only the trivial solution to the pair

$$\begin{aligned} \left(\frac{1}{2}I - C_m^*\right)\mathbf{f} &= \mathbf{0}, \\ \left(\frac{1}{2}I + C_m^0\right)\mathbf{f} &= \mathbf{0}. \end{aligned}$$

To see that this is indeed the case, we observe that the nullspace of $\frac{1}{2}I - C_m^*$ coincides with that of $\frac{1}{2}I - C_m^0$, namely $\mathcal{B}_{m^-}^0$, and that the nullspace of $\frac{1}{2}I + C_m^0$ is $\mathcal{B}_{m^+}^0$. A vector \mathbf{f} that is in both of these spaces is equal to the trace on Γ_m of a solution of $\Delta u + \omega^2 \varepsilon^0 u = 0$ that is outgoing (in both directions), which means that u and therefore \mathbf{f} must vanish. Thus (3.11) is equivalent to (3.12).

We have, as before, that $C_m^* - C_m^0$ is compact, and we observe as follows that there exists a unique solution $\boldsymbol{\xi}$: A solution \mathbf{g} to the homogeneous equation $(I + C_m^* - C_m^0)\mathbf{g} = 0$ is the boundary data of an outgoing solution to $\Delta u + \omega^2 \varepsilon_M^{\text{per}} u = 0$, which must be zero by the Nonresonance Assumption. Finally, we apply a representation theorem analogous to that of Lemma 2.4, using G_M^{per} , to the unique solution $\boldsymbol{\xi}$ of (3.11), and the estimate in (iii) of Theorem 3.4 yields the result. \square

4 Scattering by a defective slab

We now investigate the scattering of plane waves by a defective PC slab described by the dielectric permittivity

$$\varepsilon_M^{\text{def}} = \begin{cases} \varepsilon_M^{\text{per}} + q & \text{for } x \in \Omega_0 := \Omega_m \\ \varepsilon_M^{\text{per}} & \text{for } x \notin \Omega_0. \end{cases}$$

We seek then a θ -pseudoperiodic solution of the Helmholtz equation

$$(\Delta + \omega \varepsilon_M^{\text{def}}(x)) u_M^{\text{tot}}(x) = 0$$

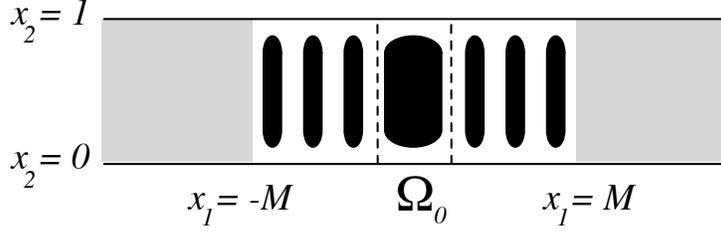


Figure 3: Defective slab.

such that the scattered field $u_M^{\text{tot}} - u^{\text{inc}}$ is outgoing. It is convenient to view the scattering process in two steps. First the incident field u^{inc} is scattered by the perfect slab and we obtain the total field u from Problem 3.1. We then use this field u as a source field for the defective slab and denote it by v_M^{inc} . It is scattered by the defect in the slab, producing a total field u_M^{tot} and outgoing scattered field v_M^{sc} :

$$u_M^{\text{tot}} = v_M^{\text{inc}} + v_M^{\text{sc}}.$$

Problem 4.1 (Scattering by a defective slab). *Given the solution $v_M^{\text{inc}} = u$ (for M sufficiently large) of the scattering Problem 3.1, find a function u_M^{tot} that satisfies the following conditions:*

$$(\Delta + \omega \varepsilon_M^{\text{def}}(x))u_M^{\text{tot}}(x) = 0, \quad (4.1.a)$$

$$u_M^{\text{tot}}(x + (0, n)) = e^{in \cdot \theta} u_M^{\text{tot}}(x), \quad (4.1.b)$$

$$u_M^{\text{tot}} - v_M^{\text{inc}} \text{ is outgoing.} \quad (4.1.c)$$

We can similarly state the problem of a bound state supported by the defect in the slab by removing incident field and demanding that the solution of the Helmholtz equation be decaying.

Problem 4.2 (Bound state). *Find a function ψ that satisfies the following conditions:*

$$(\Delta + \omega \varepsilon_M^{\text{def}}(x))\psi(x) = 0, \quad (4.2.a)$$

$$\psi(x + (0, n)) = e^{in \cdot \theta} \psi(x), \quad (4.2.b)$$

$$\psi \rightarrow 0 \text{ as } |x_1| \rightarrow \infty. \quad (4.2.c)$$

The decaying condition is technically equivalent in this case to the outgoing condition expressed by (2.11). Indeed, if a function ψ satisfies Problem 4.2 with the decay condition replaced with the outgoing condition, then it follows by conservation of energy, or integration by parts, that all the coefficients in (2.11) for ψ are equal to zero, so that ψ is indeed decays exponentially and is therefore square integrable over one period of the defective slab structure.

We reformulate the scattering and bound state problems as a (stationary) Lippman-Schwinger integral equation posed in the domain Ω_0 , in which the defect is localized. The Helmholtz equation is first rewritten as an equation for the scattered field v_M^{sc} :

$$(\Delta v_M^{\text{sc}} + \omega^2 \varepsilon_M^{\text{per}} v_M^{\text{sc}}) = \omega^2 q v_M^{\text{sc}} + f_M, \quad f_M = \omega^2 q v_M^{\text{inc}},$$

then we use the Green function G_M^{per} for the perfect slab to write an integral equation for v_M^{sc} restricted to Ω_0 :

$$v_M^{\text{sc}}(x) = \omega^2 \int_{\Omega_0} G_M^{\text{per}}(\omega, \theta; y, x) [q(y)v_M^{\text{sc}}(y) + f_M] dy, \quad x \in \Omega_0. \quad (4.3)$$

Similarly, a solution of Problem 4.2 satisfies the homogeneous Lippman-Schwinger equation

$$\psi(x) = \omega^2 \int_{\Omega_0} G_M^{\text{per}}(\omega, \theta; y, x) q(y)\psi(y) dy, \quad x \in \Omega_0. \quad (4.4)$$

It is straightforward to verify the equivalence of the differential and integral forms of the scattering and bound-state problems:

Lemma 4.3. *Let u_M^{tot} solve Problem 4.1. Then the scattered field $v_M^{\text{sc}} = u_M^{\text{tot}} - v_M^{\text{inc}}$ satisfies equation 4.3. Conversely, if v_M^{sc} satisfies 4.3 (in Ω_0), then the extension of this field to the plane*

$$v_M^{\text{sc}}(x) = \omega^2 \int_{\Omega_0} G_M^{\text{per}}(\omega, \theta; y, x) [q(y)v_M^{\text{sc}}(y) + f_M] dy, \quad x \in \mathbb{R}^2,$$

is a solution of Problem 4.1.

A solution ψ of Problem 4.2 satisfies equation 4.4. Conversely, if ψ satisfies 4.4 (in Ω_0), then the extension of this field to the plane

$$\psi(x) = \omega^2 \int_{\Omega_0} G_M^{\text{per}}(\omega, \theta; y, x) q(y)\psi(y) dy, \quad x \in \mathbb{R}^2,$$

is a solution of Problem 4.2.

Let $\widehat{G}_M^{\text{per}}$ denote the integral operator in Ω_0 with kernel G_M^{per} in (4.3), so that the Lippman-Schwinger equation (4.3) takes the form

$$v_M^{\text{sc}}(x) - \omega^2 \widehat{G}_M^{\text{per}}(q v_M^{\text{sc}})(x) = F_M(x), \quad F_M = \omega^2 \widehat{G}_M^{\text{per}}(q v_M^{\text{inc}}). \quad (4.5)$$

Let us consider a gap frequency ω for which the defective structure admits no bound state. This is equivalent to assuming that the operator $I - \omega^2 \widehat{G}_M^{\text{per}} q \cdot$ has a trivial nullspace. Since $\widehat{G}_M^{\text{per}}$ is compact, $I - \omega^2 \widehat{G}_M^{\text{per}} q \cdot$ is bounded from below. Moreover, since, by Lemma 3.5, v_M^{inc} decays exponentially in M in the domain Ω_0 , we find that v_M^{sc} decays exponentially on Ω_0 . We can then conclude that, away from bound-state frequencies for the infinite defective structure, the transmission of plane waves through a defective slab decays exponentially as the width of the slab tends to infinity. We state this in the following theorem:

Theorem 4.4. *Suppose that Problem 4.2 has no solution for ω . Then Problem 4.2 has a unique solution u_M^{tot} and there exist constants $c_1 > 0$ and $c_2 > 0$ such that, for integers M sufficiently large,*

$$|u_M^{\text{tot}}(x)| < c_1 e^{-c_2 M} \quad \text{for } x_1 > M.$$

5 The one-dimensional problem and resonance.

For one-dimensional periodic structures, that is, those that have invariant properties in all spatial directions except for, say, the x_1 -direction, the simple form of the transfer matrix allows us to compute the transmission through a thick slab exactly. In fact, even for a structure with a (one-dimensional) defect, the calculations reveal the resonant behavior of the transmission at characteristic frequencies of the infinite defective structure. We find that, at resonant parameters, *the transmission approaches a positive number which is not in general 1, as the width M of the slab tends to infinity.*

We begin with the Helmholtz equation

$$\nabla \cdot \frac{1}{\mu} \nabla u + \omega^2 \varepsilon u = 0, \quad (5.1)$$

considered in the distributional sense, in which ε and μ are positive functions of x_1 alone:

$$\begin{cases} \varepsilon(x) = \varepsilon^{\text{per}}(x_1), \\ \mu(x) = \mu^{\text{per}}(x_1), \end{cases} \quad \text{for } m \leq |x_1| \leq M$$

and

$$\varepsilon(x) = \mu(x) = 1, \quad \text{otherwise.}$$

Both ε^{per} and μ^{per} are bounded functions of x_1 alone, with period 1. The periodic slab extends from $-M$ to M , and the defect, consisting of the same medium as that to the left and right of the slab, extends from $-m$ to m . We think of M as being very large compared to m . We shall take both M and m to be integers in the subsequent calculations.

We consider solutions to the Helmholtz equation that are pseudoperiodic in the other spatial variables $x' = (x_2, x_3)$; in fact, because of the invariance of the structure in these two variables, we may restrict our attention to separable solutions:

$$u = \phi(x_1) e^{i\kappa x'}.$$

The ordinary differential equation for ϕ is

$$\left(\frac{1}{\mu} \phi'\right)' + \left(\omega^2 \varepsilon - \frac{1}{\mu} |\kappa|^2\right) \phi = 0. \quad (5.2)$$

Observe that the *Cauchy data* $[\phi(x_1), \mu^{-1} \phi'(x_1)]^t$ of a solution ϕ to (5.2) is continuous, even if μ is not.

5.1 Preliminary results: the transfer matrices

Outside the slab and in the defect, using $\varepsilon = \mu = 1$, we see that ϕ satisfies

$$\phi'' + \varpi^2 \phi = 0, \quad \text{for } |x_1| < m \text{ and } |x_1| > M \quad (5.3)$$

in which we assume that $\varpi^2 := \omega^2 - |\kappa|^2 > 0$. In addition, *we assume that ω is in a gap for the one-dimensional problem (5.2) in the variable x_1 for the given wave vector κ parallel to the slab.* This means that the matrix Q_1 that transfers the Cauchy data $[\phi(x_1), \mu^{-1} \phi'(x_1)]^t$

of a solution $\phi(x_1)$ to (5.2) in the periodic slab from an integer point $x_1 = n$ to the point $x_1 = n + 1$ has two real eigenvalues $\lambda_1 = e^k$ and $\lambda_2 = e^{-k}$ or $\lambda_1 = -e^k$ and $\lambda_2 = -e^{-k}$ for some $k > 0$. To see this, we observe that Q_1 is equal to the generalized Wronskian matrix $Q(x_1)$ of two real solutions $\psi_1(x_1)$ and $\psi_2(x_1)$ of (5.2), evaluated at $x_1 = 1$, for which $[\psi_1(0), \mu^{-1}\psi_1'(0)] = [1, 0]$ and $[\psi_2(0), \mu^{-1}\psi_2'(0)] = [0, 1]$:

$$Q_1 = Q(1) = \begin{bmatrix} \psi_1(1) & \psi_2(1) \\ \mu^{-1}\psi_1'(1) & \mu^{-1}\psi_2'(1) \end{bmatrix}.$$

From (5.2), we find that the Wronskian W is constant:

$$W(x_1) = \text{constant}.$$

Thus we learn that the determinant of the real matrix Q_1 is unity. This means that the product of its eigenvalues is 1 and that they are either conjugate unitary numbers (indicating that ϖ is in a propagation band for κ) or reciprocal real numbers (indicating that ϖ is in a gap for κ). We assume that the latter case holds, and therefore we can take the eigenvalues to be $\lambda_1 = e^k$ and $\lambda_2 = e^{-k}$ or $\lambda_1 = -e^k$ and $\lambda_2 = -e^{-k}$ for some real $k > 0$.

Let corresponding eigenvectors be given by $[1, \alpha_1]^t$ and $[1, -\alpha_2]^t$, to which correspond an exponentially increasing eigensolution $\phi_1(x_1) = \psi_1(x_1) + \alpha_1\psi_2(x_1)$ and an exponentially decreasing eigensolution $\phi_2(x_1) = \psi_1(x_1) - \alpha_2\psi_2(x_1)$ of (5.2) satisfying:

$$\begin{bmatrix} \phi_1(n) \\ \mu^{-1}\phi_1'(n) \end{bmatrix} = (\lambda_1)^n \begin{bmatrix} 1 \\ \alpha_1 \end{bmatrix} \quad \begin{bmatrix} \phi_2(n) \\ \mu^{-1}\phi_2'(n) \end{bmatrix} = (\lambda_2)^n \begin{bmatrix} 1 \\ -\alpha_2 \end{bmatrix}.$$

The general solution of (5.2) inside the slab then has the form $\phi(x_1) = A_1\phi_1(x_1) + A_2\phi_2(x_1)$, and the general solution outside the slab has the form $\psi(x_1) = A_1e^{i\varpi x_1} + A_2e^{-i\varpi x_1}$. Let us break the calculations down into several steps.

The matrix $C_k(n)$ taking the coefficients in the expression $\phi(x_1) = A_1\phi_1(x_1) + A_2\phi_2(x_1)$ to the Cauchy data $[\phi(x_1), \mu^{-1}\phi'(x_1)]^t$ at integer values $x_1 = n$, and its inverse, are

$$C_k(n) = (\pm 1)^n \begin{bmatrix} e^{kn} & e^{-kn} \\ \alpha_1 e^{kn} & -\alpha_2 e^{-kn} \end{bmatrix}, \quad C_k(n)^{-1} = \frac{(\pm 1)^n}{\alpha_1 + \alpha_2} \begin{bmatrix} \alpha_2 e^{-kn} & e^{-kn} \\ \alpha_1 e^{kn} & -e^{kn} \end{bmatrix}.$$

where the factor $(\pm 1)^n$ depends on whether the eigenvalues of Q_1 are positive or negative.

The matrix $C_{i\varpi}(x_1)$ taking the coefficients in the expression $\psi(x_1) = A_1e^{i\varpi x_1} + A_2e^{-i\varpi x_1}$ to the Cauchy data of ψ at x_1 , and its inverse, are

$$C_{i\varpi}(x_1) = \begin{bmatrix} e^{i\varpi x_1} & e^{-i\varpi x_1} \\ i\varpi e^{i\varpi x_1} & -i\varpi e^{-i\varpi x_1} \end{bmatrix}, \quad C_{i\varpi}(x_1)^{-1} = \frac{1}{2i\varpi} \begin{bmatrix} i\varpi e^{-i\varpi x_1} & e^{-i\varpi x_1} \\ i\varpi e^{i\varpi x_1} & -e^{i\varpi x_1} \end{bmatrix}.$$

The matrix taking coefficients in the expression $A_1e^{i\varpi x_1} + A_2e^{-i\varpi x_1}$ to those in $B_1\phi_1(x_1) + B_2\phi_2(x_1)$, assuming equality of their Cauchy data (value and derivative) at integer values $x_1 = n$, is

$$T_{i\varpi,k}(n) = C_k(n)^{-1}C_{i\varpi}(n) = \frac{(\pm 1)^n}{\alpha_1 + \alpha_2} \begin{bmatrix} (\alpha_2 + i\varpi)e^{-(k-i\varpi)n} & (\alpha_2 - i\varpi)e^{-(k+i\varpi)n} \\ (\alpha_1 - i\varpi)e^{(k+i\varpi)n} & (\alpha_1 + i\varpi)e^{(k-i\varpi)n} \end{bmatrix},$$

and the matrix taking coefficients in the expression $B_1\phi_1(x_1)+B_2\phi_2(x_1)$ to those in $A_1e^{i\varpi x_1}+A_2e^{-i\varpi x_1}$ at integer values n of x_1 is

$$T_{k,i\varpi}(n) = C_{i\varpi}(n)^{-1}C_k(n) = \frac{(\pm 1)^n}{2i\varpi} \begin{bmatrix} (\alpha_1 + i\varpi)e^{(k-i\varpi)n} & -(\alpha_2 - i\varpi)e^{-(k+i\varpi)n} \\ -(\alpha_1 - i\varpi)e^{(k+i\varpi)n} & (\alpha_2 + i\varpi)e^{-(k-i\varpi)n} \end{bmatrix}.$$

Set now

$$r_1 + ir_2 = r = (\alpha_1 + i\varpi)(\alpha_2 + i\varpi), \quad s_1 + is_2 = s = (\alpha_1 - i\varpi)(\alpha_2 + i\varpi). \quad (5.4)$$

Notice that, if $\alpha_1 = \alpha_2$, then $s_2 = 0$ so that

$$s = \bar{s} = s_1 = |s| = \alpha^2 + \varpi^2. \quad (\text{when } \alpha_1 = \alpha_2 = \alpha)$$

With the above notation, we have then the following result.

Lemma 5.1. *The transfer matrix for the coefficients in $A_1e^{i\varpi x_1}+A_2e^{-i\varpi x_1}$ across a slab of the photonic crystal from $x_1 = n_1$ to $x_2 = n_2$ and that of the coefficients in $A_1\phi_1(x_1) + A_2\phi_2(x_1)$ across a “slab” of vacuum from n_1 to n_2 are respectively given by the relations*

$$T_{k,i\varpi}(n_2)T_{i\varpi,k}(n_1) = \frac{(\pm 1)^{(n_1+n_2)}}{i\varpi(\alpha_1 + \alpha_2)} \begin{bmatrix} e^{-i\Theta}[r_1 \sinh \Xi + ir_2 \cosh \Xi] & e^{-i\Theta}(s_1 - is_2) \sinh \Xi \\ -e^{i\Theta}(s_1 + is_2) \sinh \Xi & e^{i\Theta}[-r_1 \sinh \Xi + ir_2 \cosh \Xi] \end{bmatrix}$$

$$T_{i\varpi,k}(n_2)T_{k,i\varpi}(n_1) = \frac{(\pm 1)^{(n_1+n_2)}}{\omega(\alpha_1 + \alpha_2)} \begin{bmatrix} e^{-\Xi}[r_1 \sin \Theta + r_2 \cos \Theta] & -e^{-k(n_2+n_1)}(\alpha_2^2 + \omega^2) \sin \Theta \\ e^{k(n_2+n_1)}(\alpha_1^2 + \omega^2) \sin \Theta & e^{\Xi}[-r_1 \sin \Theta + r_2 \cos \Theta] \end{bmatrix}$$

where we have set

$$\Theta = \varpi(n_2 - n_1), \quad \Xi = k(n_2 - n_1).$$

5.2 Application to resonant transmission

Bound states of a defect

Let us first compute the eigenvalues for an infinite periodic structure with a defect extending from $-m$ to m . A bound state (or guided mode when considering the x' -dependence) occurs when a solution with only a growing (as x_1 increases) component to the left of the defect has only a decaying component to the right thereof, and this occurs when the 11-entry of $T_{i\varpi,k}(m)T_{k,i\varpi}(-m)$ vanishes, or when

$$r_1 \sin 2\varpi m + r_2 \cos 2\varpi m = 0. \quad (\text{Resonance Condition})$$

Transmission through a slab

A solution ϕ to (5.2) has the following behavior to the left and right of the slab:

$$\begin{aligned} \phi(x_1) &= ae^{i\varpi x_1} + ce^{-i\varpi x_1}, & x_1 < -M, \\ \phi(x_1) &= de^{i\varpi x_1} + be^{-i\varpi x_1}, & x_1 > M. \end{aligned}$$

The transfer matrix (t_{ij}) takes the coefficients on the left to those on the right, and the scattering matrix (s_{ij}) takes the coefficients of the incoming fields to those of the outgoing fields:

$$\begin{bmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{bmatrix} \begin{bmatrix} a \\ c \end{bmatrix} = \begin{bmatrix} d \\ b \end{bmatrix}, \quad \begin{bmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} c \\ d \end{bmatrix}.$$

These matrices are related by

$$\begin{bmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{bmatrix} = \frac{1}{s_{12}} \begin{bmatrix} -\det S & s_{22} \\ -s_{11} & 1 \end{bmatrix}, \quad \begin{bmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{bmatrix} = \frac{1}{t_{22}} \begin{bmatrix} -t_{21} & 1 \\ \det T & t_{12} \end{bmatrix}.$$

Let us take the transmission \mathcal{T} through a slab to be equal to the square of the magnitude of c assuming that the incoming field from the left is zero ($a = 0$) and that from the right is 1 ($b = 1$). This is just $\mathcal{T} = |s_{12}|^2 = |t_{22}|^{-2}$. Therefore the transmission through a slab extending from $-M$ to M without a defect is the square inverse of the 22-entry of $T_{k,i\varpi}(M)T_{i\varpi,k}(-M)$,

$$\mathcal{T}^{-1} = |t_{22}|^2 = r_1^2 \sinh^2 2kM + r_2^2 \cosh^2 2kM,$$

from which we see that the transmission tends exponentially to zero as $M \rightarrow \infty$.

Transmission through a slab with a defect

Let us now place a defect extending from $-m$ to m within the finite slab. The transfer matrix of coefficients for this structure is

$$T_{k,i\varpi}(M)T_{i\varpi,k}(m)T_{k,i\varpi}(-m)T_{i\varpi,k}(-M) = \frac{1}{i\varpi^2(\alpha_1 + \alpha_2)^2} \times \begin{bmatrix} e^{-2i\varpi M} [(ir_2^2 \cos \Theta + r_1^2 \sin \Theta) \cosh \Xi + r_1 r_2 e^{i\Theta} \sinh \Xi - |r|^2 \sin \Theta] \\ -s [r_2 \cos \Theta \sinh \Xi + r_1 \sin \Theta \cosh \Xi - r_1 \sin \Theta] \\ \bar{s} [r_2 \cos \Theta \sinh \Xi + r_1 \sin \Theta \cosh \Xi - r_1 \sin \Theta] \\ e^{2i\varpi M} [(ir_2^2 \cos \Theta - r_1^2 \sin \Theta) \cosh \Xi - r_1 r_2 e^{-i\Theta} \sinh \Xi + |r|^2 \sin \Theta] \end{bmatrix}, \quad (5.5)$$

in which Θ and Ξ are now redefined as

$$\Theta = 2\varpi m, \quad \Xi = 2k(M - m).$$

Let us take a look at the transmission coefficient $\mathcal{T} = |t_{22}|^{-2}$ for this matrix. We compute that

$$\begin{aligned} r_2^4 \mathcal{T}^{-1} &= r_2^4 |t_{22}|^2 \\ &= (r_2^2 \cos \Theta \cosh \Xi + r_1 r_2 \sin \Theta \sinh \Xi)^2 + (-r_1^2 \sin \Theta \cosh \Xi - r_1 r_2 \cos \Theta \sinh \Xi + |r|^2 \sin \Theta)^2 \\ &= (r_1^4 \sin^2 \Theta + r_2^4 \cos^2 \Theta) \cosh^2 \Xi + (r_1 r_2)^2 \sinh^2 \Xi + 2r_1 r_2 |r|^2 \cos \Theta \sin \Theta \cosh \Xi \sinh \Xi + \\ &\quad - 2r_1 |r|^2 \sin \Theta (r_1 \sin \Theta \cosh \Xi + r_2 \cos \Theta \sinh \Xi) + |r|^4 \sin^2 \Theta. \end{aligned}$$

The first three terms contribute a multiple of $e^{2\Xi}$, and if this multiple is nonzero, then it will dominate the behavior of $r_2^4|t_{22}|^2$ as $M \rightarrow \infty$. We compute this part of the expression:

$$r_2^4\mathcal{T}^{-1} = r_2^4|t_{22}|^2 = |r|^2(r_1 \sin 2\varpi m + r_2 \cos 2\varpi m)^2 e^{4k(M-m)} + \mathcal{O}(e^{2k(M-m)}).$$

This implies that the transmission tends exponentially to zero if the resonance condition is not satisfied. At resonant parameters for the infinite slab, we make the substitution $r_1 \sin 2\varpi m = -r_2 \cos 2\varpi m$, or the other way around, and find that not even the $e^{2k(M-m)}$ terms remain:

$$r_2^4\mathcal{T}^{-1} = r_2^4 \cos^2\Theta (\cosh \Xi - \sinh \Xi)^2 + r_1^4 \sin^2\Theta (\cosh \Xi - \sinh \Xi)^2 + 2|r|^2 \sin^2\Theta r_1^2 (-\cosh \Xi + \sinh \Xi) + r_2^2|r|^2,$$

which implies the exponential convergence

$$\mathcal{T} \rightarrow \frac{r_2^2}{|r|^2} = \frac{\varpi^2(\alpha_1 + \alpha_2)^2}{(\alpha_1^2 + \varpi^2)(\alpha_2^2 + \varpi^2)} \leq 1 \quad \text{as } M \rightarrow \infty. \quad (\text{at resonance})$$

We see that the transmission converges to a positive value (assuming $r_2 = \varpi(\alpha_1 + \alpha_2) \neq 0$), which is 1 if and only if $r_1 = 0$, or $\alpha_1\alpha_2 - \varpi^2 = 0$:

$$\mathcal{T} \rightarrow 1 \quad \text{at resonance if and only if } \alpha_1\alpha_2 = \varpi^2.$$

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