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OUTGOING WAVE CONDITIONS IN PHOTONIC CRYSTALS AND TRANSMISSION PROPERTIES AT INTERFACES

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Abstract. We analyze the propagation of waves in unbounded photonic crystals. Waves are described by a Helmholtz equation with x-dependent coefficients, the scattering problem must be completed with a radiation condition at infinity. We develop an outgoing wave condition with the help of a Bloch wave expansion. Our radiation condition admits a uniqueness result, formulated in terms of the Bloch measure of solutions. We use the new radiation condition to analyze the transmission problem where, at fixed frequency, a wave hits the interface between free space and a photonic crystal. We show that the vertical wave number of the incident wave is a conserved quantity. Together with the frequency condition for the transmitted wave, this condition leads (for appropriate photonic crystals) to the effect of negative refraction at the interface.

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1. Introduction

Photonic crystals are optical devices that allow to mold the propagation properties of light. They usually have a periodic structure and are operated with light at a fixed frequency ω. Due to their spectral properties (band gap structure), light of certain frequencies can travel in the photonic crystal, but, at other frequencies, the crystal is opaque. A large body of literature is available on this aspect of photonic crystals. Most contributions study a periodic medium, possibly with a compactly supported perturbation of the periodic structure. In contrast, we are interested in the interface between a photonic crystal and free space.

An interesting effect of such an interface is negative refraction. A recent discussion in the physical literature concerns the following question: Is negative refraction always the result of a negative index of the photonic crystal, or can negative refraction also occur at the interface between air and a photonic crystal with positive index? Our mathematical results confirm the latter: The conservation of the transversal wave number can lead to negative refraction between two materials with positive index, as suggested in [27]. For a numerical confirmation see [11].

In mathematical terms, the light intensity is determined by the Helmholtz equation

$$-\nabla \cdot (a(x)\nabla u(x)) = \omega^2\, u(x)\,, \tag{1.1}$$

Keywords and phrases: Helmholtz equation, radiation, waveguide, Bloch analysis, outgoing wave condition, photonic crystal, transmission problem, negative refraction.

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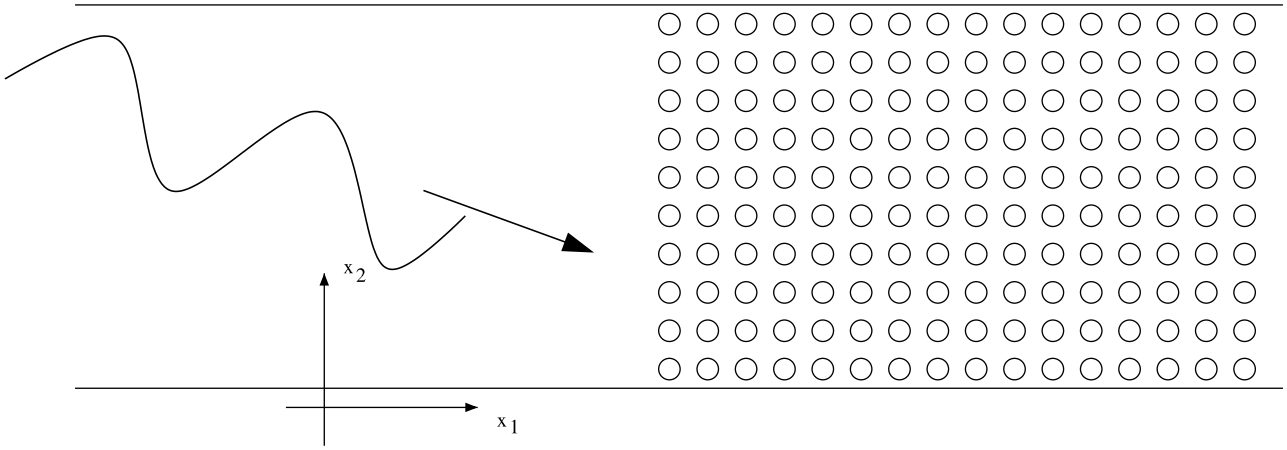

FIGURE 1. The geometry of the transmission problem for $K = 10$ (number of cells in vertical direction). An incoming wave hits the boundary of a photonic crystal. We are interested in the waves that are generated in the photonic crystal.

which must be solved for u in a domain Ω, $u = u(x)$, $x = (x_1, x_2) \in \Omega$. Here, we restrict our analysis to an unbounded rectangle $\Omega := \mathbb{R} \times (0, h) \subset \mathbb{R}^2$, but note that our methods can also be used in higher dimension, *e.g.* for $\Omega := \mathbb{R} \times (0, h_2) \times (0, h_3) \subset \mathbb{R}^3$. In (1.1), $\omega > 0$ is a prescribed frequency and $a = a(x)$ is the inverse permittivity of the medium. In an x_3-independent geometry and with polarized light, the time-harmonic Maxwell's equations reduce to (1.1) and $u = u(x)$ is the out-of-plane component of the magnetic field.

The coefficient $a = a(x)$ describes the medium. We assume that the right half space $\{x = (x_1, x_2) \in \Omega | x_1 > 0\}$ is occupied by a periodic photonic crystal with periodicity length $\varepsilon > 0$. Using the unit cube $Y = (0, 1)^2$ and the scaled cube $Y_\varepsilon = \varepsilon Y = (0, \varepsilon)^2$, we therefore assume that the coefficient $a = a^\varepsilon$ is Y_ε-periodic for $x_1 > 0$. We make the assumption that an integer number K of cells fits vertically in the domain, *i.e.* $K = h/\varepsilon \in \mathbb{N}$. On the left half space $\{x = (x_1, x_2) \in \Omega | x_1 < 0\}$, we set $a = a^\varepsilon \equiv 1$. With $a = a^\varepsilon$ and ω given, problem (1.1) is an equation for u, but it must be accompanied by boundary conditions (Fig. 1).

We impose periodic boundary conditions in the vertical direction, *i.e.* we identify the lower boundary $\{x = (x_1, x_2) | x_2 = 0\}$ with the upper boundary $\{x = (x_1, x_2) | x_2 = h\}$. In order to analyze scattering properties of the interface, we assume that the interface is lit by a planar wave. We consider, for a fixed wave-vector $k \in \mathbb{R}^2$, the incident wave

$$U_{\text{inc}}(x) = e^{2\pi i k \cdot x/\varepsilon}. \tag{1.2}$$

To guarantee that U_{inc} is a solution to (1.1) on the left, we assume $\omega^2 = 4\pi^2 |k|^2/\varepsilon^2$. We think of time-dependent solutions of the form $\hat{U}_{\text{inc}}(x, t) = U_{\text{inc}}(x) e^{-i\omega t} = \exp(i[2\pi k \cdot x/\varepsilon - \omega t])$. We always consider $k_1 > 0$ such that U_{inc} represents a right-going wave. To satisfy the periodicity condition in vertical direction, we demand $e^{2\pi i k_2 h/\varepsilon} = 1$ or, equivalently, $k_2 h \in \varepsilon\mathbb{Z}$.

For a given incident wave U_{inc} we seek for solutions u of (1.1) such that u satisfies a radiation condition as $x_1 \to \infty$, and $u - U_{\text{inc}}$ satisfies a radiation condition for $x_1 \to -\infty$.

Question 1: How can we prescribe radiation conditions in periodic media?

The answer to Question 1 requires a detailed study. We will use Bloch expansions and Bloch projections to formulate our new outgoing wave condition in Definition 3.3. Our choice is further motivated in the next section.

We now turn to the transmission problem. When an incident wave U_{inc} lights the interface, it creates waves inside the photonic crystal. These waves are described by u on $\{x_1 > 0\}$, our aim is to characterize this solution.

Question 2: Let u be the solution of the transmission problem for the incoming wave U_{inc}. Does the Bloch expansion of u on the right contain only waves that correspond to the frequency ω and to the vertical wave number k_2?

A positive answer to Question 2 provides information on the negative refraction phenomenon: They support the line of argument of [27] which explains negative refraction without referring to a negative index material (note that a quite different interpretation is given in [12]).

This article attempts to provide answers to the above Questions 1 and 2, which turn out to be more delicate than one might expect at first sight (see next two sections). We provide a radiation condition in Definition 3.3 and show that it is a reasonable condition by proving a (weak) uniqueness result in Theorem 1.3. Question 2 is answered with Theorem 1.6: If u is a solution of the transmission problem, then the Bloch measure of u is concentrated on waves that correspond to ω and k_2. The mathematical description of our results is given in Section 1.3.

1.1. Outgoing wave conditions

The Helmholtz equation (1.1) has been studied already by Euler and Lagrange, but Helmholtz was the first who expressed solutions in bounded domains with a representation formula [18]. Regarding the unbounded domain $\mathbb{R}^3$, Sommerfeld was the first to introduce a radiation condition in [35], today named after him:

$$|x|^{(n-1)/2}(\partial_{|x|}u - i\omega u)(x) \to 0 \quad \text{as } |x| \to \infty\,. \tag{1.3}$$

The condition can be understood by considering the two fundamental solutions of the Helmholtz equation in $\mathbb{R}^3$,

$$u_{\text{out}}(x) := \frac{1}{|x|}e^{i\omega|x|} \quad \text{and} \quad u_{\text{inc}}(x) := \frac{1}{|x|}e^{-i\omega|x|}\,. \tag{1.4}$$

With the time-dependence $e^{-i\omega t}$, u_{out} represents an outgoing wave and u_{inc} an incoming wave. And, indeed, u_{out} satisfies (1.3) and is therefore admissible, u_{inc} does not satisfy (1.3) and is not accepted as a solution. Sommerfeld justified his radiation condition with a uniqueness proof: Prescribing boundary data on an obstacle (the scatterer) and the radiation condition (1.3) at infinity, the Helmholtz equation has at most one solution. Actually, Sommerfeld demanded two further properties to guarantee uniqueness, but the results of Rellich (today known as "Rellich Lemma") showed that the additional assumptions are not necessary [32], see [33] for the historical background.

We cannot use the Sommerfeld radiation condition in the periodic wave guide. One reason is that we consider x-dependent coefficients a. The second is that we study a vertically periodic situation such that our situation is neither one- nor two-dimensional. Our aim is therefore to design a radiation condition for wave guides which implies a uniqueness result. The underlying idea is simple: We demand that the Bloch-expansion of solutions contains only outgoing waves as $|x_1| \to \infty$. This has a strong resemblance to the classical approach where one demands that solutions are superpositions of the outgoing waves of (1.4), compare [10].

1.1.1. On radiation in waveguides and photonic crystals

An important contribution is the recent work of Fliss and Joly [16], which is also concerned with outgoing wave conditions and the existence and the uniqueness of solutions for periodic wave-guides. Essentially, the outgoing wave condition of [16] for $x_1 \to +\infty$ reads

$$u(x) = \sum_{\lambda \in N(\omega)} \alpha_\lambda^+ U_\lambda^+(x) + w^+(x)\,, \tag{1.5}$$

where $N(\omega)$ is a finite index set, α_λ^+ are real coefficients, U_λ^+ are right-going Bloch waves and $w^+(x)$ is exponentially small for $x_1 \to +\infty$. The setting of the problem differs in one important point from ours: [16] studies a medium which is identical at the far left and at the far right, which allows to use global Floquet–Bloch transformations; this is not possible in our setting. Below we give a more detailed comparison of our results to those of [16].

Another radiation condition in a waveguide is the "modal radiation condition", formulated in Definition 2.4 of [6]. The modal radiation condition is expressed with a Fourier transform and it is restricted to media that have variations only in transversal direction. The radiation of waves in a photonic crystal (including an interface with free space) is investigated also in [5], but there the frequency ω is assumed to lie in a band-gap of the photonic crystal.

For numerical calculations, one is interested in replacing the unbounded domain by a bounded domain. In this case, one asks for appropriate boundary conditions that must be imposed on the boundary of the bounded domain. This point of view leads to the construction of Dirichlet-to-Neumann maps or similar ideas [14, 15, 17, 21]. Other key-words are perfectly matched layers [23] or transparent boundary conditions, but these approaches are not suited for periodic media.

1.2. Uniqueness properties

It is an essential feature of the Helmholtz equation that, even without source terms and with homogeneous boundary conditions, solutions may be nontrivial. The bounded domain $\Omega = (0,1) \subset \mathbb{R}^1$ with $u(x) = \sin(\pi x)$ for $\omega = \pi$ provides an example. A more relevant example in higher space dimension is the Helmholtz resonator, compare [34]. A positive result is that, for regular exterior domains, the Sommerfeld condition implies uniqueness, but this result concerns only the operator with constant coefficients. Neglecting radiation conditions, we observe: In full space, the problem with periodic coefficients admits multiple solutions whenever the frequency ω is not in a band-gap.

In our case of non-constant and (looking globally) non-periodic coefficients, there can be nontrivial solutions to the homogeneous Helmholtz equation satisfying also a radiation condition, *e.g.* in the form of localized modes. An example are standing waves in a photonic crystals with a point defect, compare *e.g.* Chapter 5 in [22]. In the case of a line defect (or in our situation of an interface between free space and photonic crystal), one expects nontrivial solutions travelling along the interface, see *e.g.* [28, 29]. Concerning the mathematical analysis of defects in a photonic crystal and the possibility that they support modes (and hence act as a waveguide) see [4, 13]. On the other hand, for the vertically periodic setting it was shown in [20] that a line defect cannot support bounded modes.

The strong uniqueness result of [16] fits in the picture: In a situation where the surrounding medium is perfectly periodic, a radiation condition implies uniqueness for non-singular frequencies. Transversal waves in the crystal are excluded by the non-singularity assumption, waves along a line defect and localized waves are excluded by the absence of defects.

In contrast, we cannot expect uniqueness in the standard sense in our situation: The interface can support nontrivial solutions. Our uniqueness result states: Imposing the new radiation condition, for non-singular frequencies every homogeneous solution has a vanishing Bloch measure. Loosely speaking: the solution vanishes far away from the interface. For general frequencies, the radiating solution may contain vertical waves. See Theorem 1.3 for both results.

Bloch measures (see *e.g.* [1], p. 182) must be used in the limit analysis for the following reason: A periodic Bloch expansion of the solution uses a discrete set of frequencies j. In general, not even the elementary frequency condition $\mu_0(j) = \omega^2$ (the Bloch wave frequency coincides with ω) can be satisfied in the discrete set of frequencies j. For this reason, we cannot expect that the Bloch expansion of u (at a finite distance) satisfies conditions such as $\mu_0(j) = \omega^2$. Instead, we must introduce a limiting object (the Bloch measure) that describes the solution u for large $|x|$. Our results describe this limiting object.

Regarding other mathematical approaches to related problems, we mention [2, 3], where the authors investigate diffraction effects in time-dependent equations. In [1], the spectrum of an elliptic operator in a periodic medium is investigated; we use methods of this contribution, the Bloch measure and the pre-Bloch expansion.

This work was motivated by the effect of negative refraction, which can be a consequence of a negative index, see [30] for the effect and [7, 8, 26] for rigorous results, obtained with the tools of homogenization theory. In [12], negative refraction is explained with a negative index. But negative refraction can also occur without a negative index material, see [27], which analyzes the same material as [12]. With the work at hand we support the line of argument of [27]. In [11] we furthermore demonstrate with numerical results that the negative refraction effect (for that specific material) is only a result of the conservation of the vertical wave number. The numerics of [11] are based on the methods developed here and demonstrate the applicability of the approach.

1.3. Main results

Throughout this article we consider the following parameters as fixed: The frequency $\omega > 0$, the height $h > 0$ of the waveguide, the periodicity length $\varepsilon > 0$ with $K = h/\varepsilon \in \mathbb{N}$, and the wave number $k \in \mathbb{R}^2$ of the incident wave with $k_2 h \in \varepsilon\mathbb{Z}$, $k_1 > 0$ and $4\pi^2|k|^2/\varepsilon^2 = \omega^2$. The underlying domain is $\Omega := \mathbb{R} \times (0, h)$ and the coefficient field is $a = a^\varepsilon : \Omega \to \mathbb{R}$. We assume $0 < a_* \le a(x) \le a^* < \infty \ \forall x \in \Omega$ and $a \equiv 1$ on $\{x_1 < 0\}$, but the latter assumption is not essential. We demand $a \in C^1$ with ε-periodicity with respect to x_1 and x_2 on $\{x_1 > 0\}$. This requirement could be relaxed, but in our proof we need solutions of class H^2 in order to apply Lemma 3.4 or Lemma A.4.

We use Bloch expansions of the solution; the superscript "$\pm$" distinguishes right and left part, $\pm x_1 > 0$. The Bloch expansion uses two indices, $m \in \mathbb{N}_0 = \{0, 1, 2, ...\}$ numbers the eigenfunctions in the periodicity cell, the Bloch number $j \in Z := [0, 1]^2$ measures the phase shift along one periodicity cell. We collect the two indices in one as $\lambda := (j, m) \in I := Z \times \mathbb{N}_0$. To every $\lambda \in I$ we associate a Poynting number $P_\lambda^\pm \in \mathbb{R}$, see (3.1). For the Bloch wave $U_\lambda^\pm$ with index λ, the number $P_\lambda^\pm$ is a measure for the flux of energy in positive x_1-direction.

We introduce the outgoing wave condition (on the right)

$$\fint_{RY_\varepsilon} \left|\Pi_{<0}^+(u_R^+)\right|^2 \to 0 \quad \text{as} \quad R \to \infty\,. \tag{1.6}$$

Here u_R^+ is, up to periodic extensions, the function $u_R^+(x_1, x_2) = u(R\varepsilon + x_1, x_2)$. The map $\Pi_{<0}^+$ is a projection onto those Bloch waves that correspond to an energy flux to the left (*i.e.* incoming waves, $P_\lambda^+ < 0$). The precise description is given in Definition 3.3. The outgoing condition on the left is analogous.

Our results are formulated with the help of index sets. Waves with vertical energy flux (or without energy flux) correspond to $\lambda \in I := Z \times \mathbb{N}_0$ in

$$I_{=0}^\pm := \left\{\lambda \in I \,|\, P_\lambda^\pm = 0\right\}\,.$$

For fixed $m \in \mathbb{N}_0$, we also use the corresponding j-values,

$$J_{=0,m}^\pm := \left\{j \in Z \,|\, P_{(j,m)}^\pm = 0\right\} = \left\{j \in Z \,|\, (j, m) \in I_{=0}^\pm\right\}\,.$$

The statements below are meaningful for general frequencies $\omega > 0$. Unfortunately, we are only able to prove theorems for moderate frequencies, as expressed in the following assumption. It demands that the frequency of the wave is below the energy band corresponding to the index $m = 1$ (below the second band).

Assumption 1.1 (Smallness of the frequency)**.** We assume on the coefficient a and the frequency ω that

$$\omega^2 < \inf_{j \in Z,\, m \ge 1} \mu_m^+(j)\,, \tag{1.7}$$

and $\omega^2 < \inf_{j\in Z,\, m\geq 1} \mu_m^-(j)$, where $\mu_m^\pm(j)$ are the Bloch-eigenvalues.

Our results concern solutions u of the transmission problem, specified as follows.

Problem 1.2 (Transmission problem)**.** We say that $u \in H^1_{\mathrm{loc}}(\Omega)$ solves the scattering problem if it satisfies the Helmholtz equation (1.1) in $\Omega = \mathbb{R}\times(0,h)$ with $h = K\varepsilon$ and periodic boundary conditions in the x_2-variable. We furthermore assume that it is generated by the incoming wave U_{inc} of (1.2) in the following sense: u satisfies the outgoing wave condition (3.6) on the right and the difference $u - U_{\mathrm{inc}}$ satisfies the outgoing wave condition (3.7) on the left.

Our uniqueness result characterizes the Bloch measures $\nu^\pm_{l,\infty}$ of a difference of two solutions (the Bloch measures are introduced in Def. 4.2). The theorem below yields that, for large values of $|x_1|$, the difference of two solutions does not contain Bloch waves with an eigenvalue index larger than 0. Furthermore, only those waves can appear that satisfy all of the following three requirements: They correspond to the imposed frequency ω, they correspond to vertically periodic waves, they transport energy in vertical direction.

Theorem 1.3 (Uniqueness)**.** *Let Assumption 1.1 on the frequency ω be satisfied. Let v be a solutions of the transmission Problem 1.2 without incoming wave, $U_{\mathrm{inc}} \equiv 0$. For $l \in \mathbb{N}_0$, let $\nu^\pm_{l,\infty}$ be the Bloch measures that are generated by v. Then:*

$$\nu^\pm_{l,\infty} = 0 \quad \text{for } l \geq 1\,, \tag{1.8}$$

$$\operatorname{supp}(\nu^\pm_{0,\infty}) \subset \left\{ j \in Z \,|\, \mu_0^\pm(j) = \omega^2\,,\ j_2 \in \mathbb{Z}/K \right\} \cap J^\pm_{=0,0}\,. \tag{1.9}$$

An immediate consequence of Theorem 1.3 is the following result for frequencies ω that do not support vertical waves.

Corollary 1.4 (Uniqueness for non-singular frequencies)**.** *Let the situation be as in Theorem 1.3 and let the frequency ω be non-singular in the sense that $\left\{ j \in Z \,|\, \mu_0^\pm(j) = \omega^2\,,\ j_2 \in \mathbb{Z}/K \right\} \cap J^\pm_{=0,0} = \emptyset$. Then the solution v of the transmission Problem 1.2 without incident wave has a vanishing Bloch measure.*

Theorem 1.3 implies the following uniqueness result for solutions to inhomogeneous Helmholtz equations.

Corollary 1.5 (Uniqueness for inhomogeneous equations)**.** *Let Assumption 1.1 be satisfied, let $f \in L^2(\Omega)$ be a source and let U_{inc} be an incoming wave. Let u and $\tilde{u}$ be solutions to the transmission problem with right hand side f,* i.e.

$$-\nabla\cdot(a(x)\nabla u(x)) - \omega^2\, u(x) = f(x)\,.$$

holds for $x \in \Omega$ and the radiation conditions are satisfied. Then the Bloch measures $\nu^\pm_{l,\infty}$ that are generated by the difference $v := u - \tilde{u}$ satisfy (1.8) and (1.9).

Indeed, the difference $v := u - \tilde{u}$ solves the homogeneous transmission problem without incoming wave and thus Theorem 1.3 can be applied to v.

Our second main result shows that the transmission of an incoming wave occurs in such a way that two quantities are conserved: The vertical wave number and the energy.

Theorem 1.6 (Transmission conditions)**.** *Let Assumption 1.1 be satisfied, let k be the wave vector of the incoming wave U_{inc}. Let u be a solution of the transmission problem 1.2 and let $\nu^\pm_{l,\infty}$, with $l \in \mathbb{N}_0$, be the Bloch measures that are generated by u. Then $\nu^\pm_{l,\infty} = 0$ for $l \geq 1$ and*

$$\operatorname{supp}(\nu^\pm_{0,\infty}) \;\subset\; \left\{ j \in Z \,|\, \mu_0^\pm(j) = \omega^2\,,\ j_2 \in \mathbb{Z}/K \right\} \bigcap \left(\{ j \in Z \,|\, j_2 = k_2 \} \;\cup\; J^\pm_{=0,0} \right)\,. \tag{1.10}$$

As above, we have the following corollary for non-singular frequencies.

Corollary 1.7 (Transmission condition for non-singular frequencies)**.** *Let the situation be as in Theorem 1.6 and let the frequency ω be non-singular. Then the Bloch measure $\nu^{\pm}_{0,\infty}$ of u satisfies*

$$\operatorname{supp}(\nu^{\pm}_{0,\infty}) \ \subset \ \left\{ j \in Z \,|\, \mu^{\pm}_0(j) = \omega^2 \text{ and } j_2 = k_2 \right\} . \tag{1.11}$$

1.4. Further comments on the main results

1.4.1. On the uniqueness result

We recall that we expect the existence of solutions that are supported on the interface between photonic crystal and free space. For this reason, uniqueness results can only provide information "far away from the interface", *i.e.* information on the Bloch measure.

A weakness of our uniqueness results concerns Assumption 1.1: Our results are proven under the assumption that the underlying frequency ω is in the first band (more precisely: below the second band). Our conjecture is that our uniqueness result remains valid for arbitrary frequencies, stating that $\operatorname{supp}(\nu^{\pm}_{l,\infty}) \subset \left\{ j |\, \mu^{\pm}_l(j) = \omega^2, j_2 \in \mathbb{Z}/K \right\} \cap J^{\pm}_{=0,l}$ for every $l \geq 0$. Due to a lack of orthogonality properties in the sesquilinear form b (see Sect. 4), we must exploit the frequency assumption in our uniqueness proof.

Singular frequencies in Corollaries 1.4 and 1.7: A frequency ω is singular on the right (superscript "+") if there exists a wave vector $j \in Z$ that satisfies three conditions, $\mu^{+}_0(j) = \omega^2$, $j_2 \in \mathbb{Z}/K$, and $P^{+}_{(j,0)} = 0$, *i.e.*: j has the right frequency, the right vertical wave number, and a group velocity with vanishing horizontal component. Such wave vectors j exist only for a discrete set of ω's, see Theorem 5 in [16].

1.4.2. Relations to Fliss and Joly [16]

The contribution [16] contains strong results: (1) A uniqueness result in the classical form (due to the absence of an interface that can support waves and due to the restriction to non-singular frequencies). (2) An existence result, based on a limiting absorption principle. We note that also the existence result of [16] uses global Floquet–Bloch transformations and is therefore not easily adaptable to our setting. We remark that our outgoing wave condition is weaker than the one of [16], see Lemma 3.8. This means that, apart from the problems due to the non-periodic geometry, an existence proof should be simpler for our outgoing wave condition.

We mention at this place that our outgoing wave condition differs in one point with all existing radiation conditions: Our condition does not use explicitly the frequency ω. We regard this as an advantage: our condition might be applicable also in time-dependent problems.

1.4.3. A possible scaling in $\varepsilon > 0$

In all our theorems we keep the length scale $\varepsilon > 0$ fixed. In other words: the wave-length $1/\omega$ and the periodicity length ε are both of order 1. It is very interesting to analyze the behavior of light in small micro-structures, *i.e.* to analyze the limit $\varepsilon \to 0$. The limit can be performed in two settings: In the classical homogenization problem, one keeps ω (and hence the wave-length) fixed and analyzes the behavior of solutions $u = u^{\varepsilon}$ as $\varepsilon \to 0$. This approach was carried out *e.g.* in [7–9, 25, 26].

The second setting regards the limit $\varepsilon \to 0$ in a situation where the wave-length of the incoming wave is also of order ε. This is the scaling that is suggested by our notation in (1.2), which corresponds to a frequency $\omega = \omega^{\varepsilon} = \varepsilon^{-1}\omega^*$. Loosely speaking, our Theorem 1.6 yields in this scaling: Solutions u^{ε} to the scattering problem with incoming wave (1.2) for fixed k consist, at a fixed distance $x_1 > 0$ from the interface and in the limit $\varepsilon \to 0$, only of Bloch waves that correspond to the frequency ω^{ε} and to the wave number k_2 (up to vertical waves).

1.4.4. Outline of this contribution

Bloch expansions are described in Section 2. In Section 3 we define energy flux numbers and corresponding index sets; these are used to define the new outgoing wave condition. In Section 4 we define Bloch measures, Theorems 1.3 and 1.6 are shown in Section 4.3.

2. Bloch expansions

2.1. Pre-Bloch expansions

We start our analysis with a discrete expansion. This discrete expansion is the first stage of a Bloch expansion and closely related to the Floquet–Bloch transform. We apply it to the h-periodic function $u(x_1,\cdot)$. The subsequent result appears as Lemma 4.9 in [1].

Lemma 2.1 (Vertical pre-Bloch expansion)**.** *Let $K\in\mathbb{N}$ be the number of periodicity cells and let $h=\varepsilon K$ be the height of the strip $\mathbb{R}\times(0,h)$. Let $u\in L^2_{\mathrm{loc}}(\mathbb{R}\times(0,h);\mathbb{C})$ be a function. Then u can be expanded uniquely in periodic functions with phase-shifts: With the finite index set $Q_K:=\{0,\frac{1}{K},\frac{2}{K},\dots,\frac{K-1}{K}\}$ we find*

$$u(x_1,x_2)=\sum_{j_2\in Q_K}\Phi_{j_2}(x_1,x_2)\,e^{2\pi i j_2 x_2/\varepsilon}\,, \tag{2.1}$$

where each function $\Phi_{j_2}(x_1,\cdot)$ is ε-periodic. The equality (2.1) holds in $L^2_{\mathrm{loc}}(\mathbb{R}\times(0,h);\mathbb{C})$.

Sketch of proof. We sketch a proof (different from the one chosen in [1]), considering only $u=u(x_2)$ and $h=1$. Expanding u in a Fourier series, we may write

$$u(x_2)=\sum_{k_2\in\varepsilon\mathbb{Z}}\beta_{k_2}\,e^{2\pi i k_2 x_2/\varepsilon}\,. \tag{2.2}$$

For every $j_2\in\varepsilon\mathbb{N}_0$ with $j_2<1$ (*i.e.* for every $j_2\in Q_K$) we set

$$\Phi_{j_2}(x_2):=\sum_{k_2\in j_2+\mathbb{Z}}\beta_{k_2}\,e^{2\pi i(k_2-j_2)x_2/\varepsilon}\,. \tag{2.3}$$

With this choice, each Φ_{j_2} is ε-periodic and (2.1) is satisfied. □

For the above pre-Bloch expansion we define the projection on a vertical wave number k_2 as follows.

Definition 2.2 (Vertical pre-Bloch projection $\Pi^{\mathrm{vert}}_{k_2}$)**.** Let $u\in L^2_{\mathrm{loc}}(\mathbb{R}\times(0,h);\mathbb{C})$ with $h=\varepsilon K$ be a function on a strip and let $k_2\in Q_K$ be a vertical wave number. Then, expanding u as in (2.1), we set

$$\Pi^{\mathrm{vert}}_{k_2}u(x_1,x_2):=\Phi_{k_2}(x_1,x_2)\,e^{2\pi i k_2 x_2/\varepsilon}\,. \tag{2.4}$$

The projection is an orthogonal projection: For ε-periodic functions Φ and $\tilde\Phi$ and indices $k_2\neq\tilde k_2$ there holds $\int_0^h\overline{\Phi(x_2)}e^{-2\pi i\tilde k_2 x_2/\varepsilon}\tilde\Phi(x_2)e^{2\pi i k_2 x_2/\varepsilon}\,\mathrm{d}x_2=0$ by Lemma A.1.

We will later use the following fact: If u is a solution of the scattering problem with incident vertical wave number k_2, then also the projection $\Pi^{\mathrm{vert}}_{k_2}u$ is a solution of the scattering problem. Together with a uniqueness result for solutions, we can conclude from this fact that the vertical wave number is conserved in the photonic crystal.

Below, we have to deal with the following situation: For a function u on a strip with height h, we can perform a pre-Bloch expansion. We may also extend u periodically in the vertical direction and perform a pre-Bloch expansion of the extended function on a wider strip. We find that both constructions yield the same result.

Remark 2.3 (Vertical pre-Bloch expansion of a periodically extended function)**.** Let $K = h/\varepsilon \in \mathbb{N}$ denote the number of periodicity cells in vertical direction and let $u \in L^2_{\mathrm{loc}}(\mathbb{R} \times (0,h))$ be a function with vertical pre-Bloch expansion

$$u(x_1,x_2) = \sum_{j_2 \in Q_K} \Phi_{j_2}(x_1,x_2)\, e^{2\pi i j_2 x_2/\varepsilon}.$$

Let $R \in \mathbb{N}$ be a multiple of K and let $\tilde{u}$ be the periodic extension of u to the interval $(0,\varepsilon R)$ in x_2-direction. Then $\tilde{u} \in L^2_{\mathrm{loc}}(\mathbb{R} \times (0,\varepsilon R))$ has the vertical pre-Bloch expansion

$$\tilde{u}(x_1,x_2) = \sum_{\tilde{j}_2 \in Q_R} \tilde{\Phi}_{\tilde{j}_2}(x_1,x_2)\, e^{2\pi i \tilde{j}_2 x_2/\varepsilon}, \tag{2.5}$$

where the coefficients according to the finer grid Q_R satisfy

$$\tilde{\Phi}_{\tilde{j}_2}(x) = \begin{cases} 0 & \text{if } \tilde{j}_2 \notin Q_K\,, \\ \Phi_{\tilde{j}_2}(x) & \text{if } \tilde{j}_2 \in Q_K\,. \end{cases}$$

The statement follows immediately from the uniqueness of the pre-Bloch expansion. Remark 2.3 explains our choice concerning scalings: Given a sequence of functions u_R, defined on a sequence of increasing domains, at first sight, one might find it natural to rescale u_R to a standard domain and to analyze the sequence of rescaled functions. Instead, we work with the sequence u_R on increasing domains. In this way, one index $j \in Z$ always refers to the same elementary wave, which allows to investigate the Bloch measure limit.

2.1.1. Pre-Bloch expansion in two variables

For a function u that is defined on a rectangle and that is periodic in both directions, the pre-Bloch expansion in two variables can be defined by expanding first in one variable and then in the other.

For functions u on $\mathbb{R} \times (0,h)$ the situation is more difficult, since u is not periodic in x_1-direction. In order to expand in both directions, we truncate u with a cut-off function $\eta : \mathbb{R} \times [0,h]$ with compact support. For convenience, we assume that the support of η is contained in the square $[0,h] \times [0,h]$.

The truncation of u is defined as $w(x) := u(x)\,\eta(x)$. We expand w (on the square $[0,h] \times [0,h]$) in both directions in a pre-Bloch expansion, using the vector $j = (j_1,j_2) \in Q_K \times Q_K$ and $x = (x_1,x_2)$:

$$w(x) = \sum_{j \in Q_K \times Q_K} \Phi_j(x)\, e^{2\pi i j\cdot x/\varepsilon}\,. \tag{2.6}$$

The functions $\Phi_j = \Phi_{(j_1,j_2)}$ are now ε-periodic in both variables. Due to orthogonality there holds ($h = \varepsilon K$)

$$\frac{1}{(\varepsilon K)^2}\|w\|^2_{L^2(KY_\varepsilon)} = \sum_{j \in Q_K \times Q_K} \fint_{Y_\varepsilon} |\Phi_j|^2\,,$$

where $\fint_{Y_\varepsilon} |\Phi_j|^2 := \frac{1}{|Y_\varepsilon|}\int_{Y_\varepsilon} |\Phi_j|^2$ denotes the mean value.

2.2. Bloch expansion

With the help of the pre-Bloch expansion we construct now the Bloch expansion. This step consists in developing each of the periodic functions Φ_j for $j = (j_1,j_2)$ in terms of eigenfunctions of the operator

$$\mathcal{L}^+_j := -\left(\nabla + 2\pi i j/\varepsilon\right)\cdot\left(a^\varepsilon(x)\left(\nabla + 2\pi i j/\varepsilon\right)\right)\,. \tag{2.7}$$

The operator $\mathcal{L}_j^+$ acts on complex-valued functions on the cell Y_ε with periodic boundary conditions. It appears in the analysis of (1.1) for the following reason: Let Ψ_j^+ be an eigenfunction of $\mathcal{L}_j^+$ with eigenvalue $\mu^+(j)$; then there holds

$$-\nabla\cdot\left(a^\varepsilon(x)\nabla[\Psi_j^+ e^{2\pi ij\cdot x/\varepsilon}]\right) = [\mathcal{L}_j^+\Psi_j^+]e^{2\pi ij\cdot x/\varepsilon} = \mu^+(j)\,[\Psi_j e^{2\pi ij\cdot x/\varepsilon}]\,.$$

We see that $\Psi_j^+ e^{2\pi ij\cdot x/\varepsilon}$ is a solution of the Helmholtz equation on the right half-plane if and only if $\mu^+(j)=\omega^2$.

We have to distinguish between $x_1>0$ and $x_1<0$. On the right, the expansion is performed with $\mathcal{L}_j^+$ as above, with the periodic coefficient $a^\varepsilon = a^\varepsilon(x)$. On the left, expansions are performed according to $a^\varepsilon\equiv 1$ with the operator $\mathcal{L}_j^- := -(\nabla+2\pi ij/\varepsilon)\cdot(\nabla+2\pi ij/\varepsilon)$. The result is a classical Fourier expansion of the solution.

Definition 2.4 (Bloch eigenfunctions)**.** Let $j\in[0,1]^2$ be a fixed wave vector. We denote by $\left(\Psi_{j,m}^+\right)_{m\in\mathbb{N}_0}$ the family of eigenfunctions of the operator $\mathcal{L}_j^+$ of (2.7). The labelling is such that the corresponding eigenvalues $\mu_m^+(j)$ are ordered, $\mu_{m+1}(j)\geq\mu_m(j)$ for all $m\in\mathbb{N}_0$. Similarly, $\left(\Psi_{j,m}^-\right)_{m\in\mathbb{N}_0}$ is the family of eigenfunctions of the operator $\mathcal{L}_j^-$ and $\mu_m^-(j)$ are the corresponding eigenvalues. We normalize with $⨍_{Y_\varepsilon}|\Psi_{j,m}^\pm|^2=1$.

A standard symmetry argument yields that, after an appropriate orthonormalization procedure for multiple eigenvalues, all functions $\Psi_{j,m}^\pm(x)\,e^{2\pi ij\cdot x/\varepsilon}$ with $j\in Q_K$ are orthonormal in the space $L^2_\sharp(KY_\varepsilon;\mathbb{C})=L^2(KY_\varepsilon;\mathbb{C})$ (the sharp symbol is sometimes used to indicate that one thinks of periodic functions, but, of course, in the case of L^2, the periodicity does not alter the function space). On the left hand side (*i.e.* for $x_1<0$, denoted with the superscript "$-$"), the Bloch eigenfunctions are harmonic waves and the Bloch expansion coincides with a Fourier expansion. We collect properties on the left half-domain in Remark 3.6.

Lemma 2.5 (Bloch expansion)**.** *Let $K\in\mathbb{N}$ be the number of cells in each direction, let $u\in L^2(KY_\varepsilon;\mathbb{C})$ be a function on the square $(0,K\varepsilon)\times(0,K\varepsilon)$. Expanding u in a pre-Bloch expansion and then expanding each Φ_j in eigenfunctions $\Psi_{j,m}^+$ we obtain, with coefficients $\alpha_{j,m}^+\in\mathbb{C}$,*

$$u(x)=\sum_{j\in Q_K\times Q_K}\sum_{m=0}^{\infty}\alpha_{j,m}^+\Psi_{j,m}^+(x)\,e^{2\pi ij\cdot x/\varepsilon}\,,$$

and similarly, for an expansion corresponding to constant coefficients $a^\varepsilon\equiv 1$,

$$u(x)=\sum_{j\in Q_K\times Q_K}\sum_{m=0}^{\infty}\alpha_{j,m}^-\Psi_{j,m}^-(x)\,e^{2\pi ij\cdot x/\varepsilon}\,.$$

To shorten notation, we will use the multi-index $\lambda=(j,m)$ in the index-set $I_K:=\{(j,m)|j\in Q_K\times Q_K,\ m\in\mathbb{N}_0\}\subset I:=Z\times\mathbb{N}_0$. Abbreviating additionally

$$U_\lambda^\pm(x):=\Psi_\lambda^\pm(x)\,e^{2\pi ij\cdot x/\varepsilon}\,, \tag{2.8}$$

we may write the formulas of Lemma 2.5 as

$$u(x)=\sum_{\lambda=(j,m)\in I_K}\alpha_\lambda^\pm\Psi_\lambda^\pm(x)\,e^{2\pi ij\cdot x/\varepsilon}=\sum_{\lambda\in I_K}\alpha_\lambda^\pm U_\lambda^\pm(x)\,. \tag{2.9}$$

The expansion holds for the basis functions U_λ^+ with coefficients α_λ^+ and for the basis functions U_λ^- with coefficients α_λ^-. Moreover, due to L^2-orthonormality of the functions $U_\lambda^\pm$, with $h = \varepsilon K$ and $KY_\varepsilon = (0,h)\times(0,h)$,

$$\frac{1}{(\varepsilon K)^2}\|u\|^2_{L^2(KY_\varepsilon)} = \sum_{\lambda\in I_K} |\alpha_\lambda^\pm|^2 . \tag{2.10}$$

3. Outgoing wave condition

3.1. Poynting numbers and projections

Let $\lambda = (j,m) \in I$ be an index and let $U_\lambda^\pm$ be the corresponding Bloch function. Denoting by $e_1 = (1,0) \in \mathbb{R}^2$ the first unit vector, we connect to $\lambda \in I$ the real numbers

$$\begin{aligned} P_\lambda^+ &:= \operatorname{Im} \fint_{Y_\varepsilon} \bar U_\lambda^+(x)\, e_1 \cdot \left[a^\varepsilon(x)\nabla U_\lambda^+(x)\right] \mathrm{d}x\,, \\ P_\lambda^- &:= \operatorname{Im} \fint_{Y_\varepsilon} \bar U_\lambda^-(x)\, e_1 \cdot \nabla U_\lambda^-(x)\, \mathrm{d}x\,. \end{aligned} \tag{3.1}$$

The number P_λ^+ is related to the Poynting vector of the Bloch eigenfunction U_λ^+. It corresponds (up to a positive constant) to the horizontal group velocity of this eigenfunction and measures its energy flux in horizontal direction: In the case $P_\lambda^+ > 0$, the energy of the wave is travelling to the right, in the case $P_\lambda^+ < 0$, the energy of the wave is travelling to the left.

Let us point out the relation to Maxwell's equations: If u denotes the out-of-plane magnetic field, *i.e.* $H = (0,0,u)$, then the electric field is $(E_1, E_2, 0)$ with $E_1 = (-i\omega\epsilon)^{-1}\partial_2 u$ and $E_2 = (i\omega\epsilon)^{-1}\partial_1 u$ where ϵ is the permittivity of the medium. The complex Poynting vector is $P = \frac{1}{2}E \times \bar H$, so the real part of its horizontal component is $\operatorname{Re}(e_1 \cdot P) = \operatorname{Re}(\frac{1}{2}\bar H_3 E_2) = (2\omega)^{-1}\operatorname{Re}(-i\,\bar u\,\epsilon^{-1}\partial_1 u) = (2\omega)^{-1}\operatorname{Im}(\bar u\, a\partial_1 u)$, where we used that the coefficient $a = \epsilon^{-1}$ is the inverse permittivity. Our expression in (3.1) coincides up to the factor 2ω with an integral of this expression. Since P represents a local energy flux, the physical quantity of a total energy flux is a surface integral over P. In fact, for solutions U_λ of a Helmholtz equation, the surface integral is independent of the position of the surface. Hence our volume integral in (3.1) indeed coincides with the physical quantity of a surface integral.

The index set for λ: In our construction, we fix the height $h > 0$ of the domain and the periodicity length $\varepsilon = h/K$, the Bloch expansion is performed in this fixed geometry. As a consequence, we consider only indices $\lambda = (j,m) \in I_K$, the frequency parameter j must lie in the discrete set $Q_K \times Q_K \subset Z$. On the other hand, for arbitrary $j \in Z$, we can still consider the functions $\Psi_{j,m}^\pm$ and $U_\lambda^\pm$. They do not depend on K, hence also the values $P_\lambda^\pm$ are independent of K.

Definition 3.1 (Index sets and projections)**.** We define the set of indices corresponding to right-going waves in $x_1 > 0$ as

$$I_{>0}^+ := \left\{\lambda \in I \mid P_\lambda^+ > 0\right\} . \tag{3.2}$$

The index sets $I_{>0}^-$, $I_{<0}^\pm$, $I_{\geq 0}^\pm$, $I_{\leq 0}^\pm$, $I_{=0}^\pm$ are defined accordingly.

For $K \in \mathbb{N}$ we define the projections $\Pi_{>0}^\pm$ as follows: Let $u \in L^2(KY_\varepsilon;\mathbb{C})$ be a function with the discrete Bloch expansion

$$u(x) = \sum_{\lambda\in I_K} \alpha_\lambda^\pm U_\lambda^\pm(x)\,.$$

Then we set

$$\Pi^{\pm}_{>0} u(x) := \sum_{\lambda \in I_K \cap I^{\pm}_{>0}} \alpha^{\pm}_{\lambda} U^{\pm}_{\lambda}(x)\,.$$

With this definition, $\Pi^{\pm}_{>0}$ are the projections onto right-going Bloch-waves. The projections $\Pi^{\pm}_{<0}, \Pi^{\pm}_{\geq 0}$, $\Pi^{\pm}_{\leq 0}$, and $\Pi^{\pm}_{=0}$ are defined accordingly.

For $k_2 \in Q_K$ and $l \in \mathbb{N}_0$, the "vertical" projection $\Pi^{\mathrm{vert},\pm}_{k_2}$ and the "eigenvalue" projection $\Pi^{\mathrm{ev},\pm}_{l}$ are defined by

$$\Pi^{\mathrm{vert},\pm}_{k_2} u(x) := \sum_{\lambda \in \{(j,m) \in I_K \,|\, j_2 = k_2\}} \alpha^{\pm}_{\lambda} U^{\pm}_{\lambda}(x)\,,$$
$$\Pi^{\mathrm{ev},\pm}_{l} u(x) := \sum_{\lambda \in \{(j,m) \in I_K \,|\, m = l\}} \alpha^{\pm}_{\lambda} U^{\pm}_{\lambda}(x)\,.$$

Note that the projections $\Pi^{\mathrm{vert},\pm}_{k_2}$ of the discrete Bloch expansion indeed coincide with the projection $\Pi^{\mathrm{vert}}_{k_2}$ of the corresponding vertical pre-Bloch expansion of Definition 2.2. The vertical projection is independent of K in the sense that a periodically extended u with a larger value of K has the same projection, compare Remark 2.3.

3.2. Bloch expansion at infinity and outgoing wave condition

We can now formulate the outgoing wave condition for a solution u of the Helmholtz equation (1.1). The loose description of our outgoing wave condition (on the right) is: The Bloch expansion of u does not contain Bloch waves that transport energy to the left.

For a rigorous definition we must deal with the problem that u is not necessarily periodic in x_1-direction. Our solution to this problem is to consider u on large domains (which reduces the effects of non-periodicity) and to employ a truncation procedure. Furthermore, we want to formulate a condition that characterizes u for large values of x_1. For these two reasons, we consider $u(x_1, x_2)$ for $x_1 \in (R\varepsilon, 2R\varepsilon)$ with a large natural number $R >> K$.

In order to construct a function on a large domain, we consider the periodic extension of u in vertical direction and restrict afterwards the function to a large rectangle. For convenience of notation, we restrict our analysis to squares.

Definition 3.2 (Bloch expansion far away from the interface)**.** Let $u \in L^2_{\mathrm{loc}}(\mathbb{R} \times (0,h); \mathbb{C})$ be a function on the infinite strip with height $h = \varepsilon K$. Let $R \in \mathbb{N}K$ be a multiple of K. We define $\tilde{u} : \mathbb{R}^2 \to \mathbb{C}$ as the h-periodic extension of u in x_2-direction. We furthermore define functions $u^{\pm}_R : RY_\varepsilon \to \mathbb{C}$ by

$$u^{+}_R(x_1, x_2) := \tilde{u}(R\varepsilon + x_1, x_2)\,, \tag{3.3}$$
$$u^{-}_R(x_1, x_2) := \tilde{u}(-2R\varepsilon + x_1, x_2)\,. \tag{3.4}$$

We use the discrete Bloch expansions of the functions $u^{\pm}_R \in L^2_\sharp(RY_\varepsilon; \mathbb{C})$,

$$u^{\pm}_R(x) = \sum_{\lambda \in I_R} \alpha^{\pm}_{\lambda,R} U^{\pm}_{\lambda}(x)\,. \tag{3.5}$$

The coefficients $(\alpha^{\pm}_{\lambda,R})_{\lambda \in I}$ encode the behavior of u for large values of $|x_1|$.

We are now in the position to define the outgoing wave condition for a solution u to the Helmholtz equation, using the short notation $⨍_{RY_\varepsilon} f := \frac{1}{|RY_\varepsilon|}\int_{RY_\varepsilon} f$ for averages of functions.

Definition 3.3 (Outgoing wave condition)**.** For $K \in \mathbb{N}$, $h = K\varepsilon$, and $R \in \mathbb{N}K$, we consider $u \in L^2_{\mathrm{loc}}(\mathbb{R} \times (0,h);\mathbb{C})$. We say that u satisfies the outgoing wave condition on the right if the following two conditions are satisfied: $\int_0^h \int_L^{L+1} |u|^2$ is bounded, independently of $L \geq 0$, and

$$⨍_{RY_\varepsilon} \left|\Pi^+_{<0}(u^+_R)\right|^2 \to 0 \text{ as } R \to \infty\,. \tag{3.6}$$

Accordingly, we say that u satisfies the outgoing wave condition on the left, if $\int_0^h \int_{L-1}^{L} |u|^2$ is bounded, independently of $L \leq 0$, and if

$$⨍_{RY_\varepsilon} \left|\Pi^-_{>0}(u^-_R)\right|^2 \to 0 \text{ as } R \to \infty\,. \tag{3.7}$$

Let us repeat the idea of condition (3.6): The function u is considered at the far right by construcing u^+_R as in Definition 3.2. This function is projected onto the space of left-going waves. We demand that the L^2-averages of the resulting functions $\Pi^+_{<0}(u^+_R)$ vanish in the limit $R \to \infty$.

With the expansion (3.5) we can write condition (3.6) equivalently as:

$$\sum_{\lambda \in I_R \cap I^+_{<0}} |\alpha^+_{\lambda,R}|^2 \to 0 \text{ as } R \to \infty\,. \tag{3.8}$$

Our aim is to show that this definition of an outgoing wave condition implies uniqueness properties for the scattering problem.

We note that the uniform L^2-bounds for large values of $|L|$ imply, for solutions u of the Helmholtz equation, also uniform bounds for gradients, see Lemma A.3 in Appendix A.

3.3. Truncations and $m \geq 1$-projections

In the outgoing wave condition, we study the limit $|x_1| \sim R \to \infty$ and the functions $u^\pm_R$ on large squares $W_R := RY_\varepsilon = (0, R\varepsilon)^2$ with $|W_R| = (\varepsilon R)^2$. As a measure for typical values of a function v we use L^2-averages on W_R and the corresponding scalar product,

$$\langle v, w\rangle_R := ⨍_{W_R} v \cdot \bar{w}\,. \tag{3.9}$$

In the following we denote by $\mathcal{L}_0 = \mathcal{L}^+_0 = -\nabla\cdot(a^\varepsilon\nabla)$ the elliptic operator of (2.7). As above, we denote cubes by $W_R = RY_\varepsilon$ and, by slight abuse of notation, we write $W_{R-1} := \varepsilon(1, R-1)^2$ for a smaller cube that has the point $\varepsilon(1,1)$ as its bottom left corner and $\varepsilon(R-1, R-1)$ as its top right corner. We use a family of smooth cut-off functions $\eta := \eta_R$ with the properties

$$\eta_R \in C^\infty(W_R;\mathbb{R}), \quad \eta_R = 1 \text{ on } W_{R-1}, \quad \|\nabla\eta_R\|_\infty \leq C_0, \quad \|\nabla^2\eta_R\|_\infty \leq C_0 \tag{3.10}$$

for some R-independent constant C_0 ($\varepsilon > 0$ is fixed), and with compact support in $(0, R\varepsilon) \times (0, R\varepsilon)_\sharp$, where $(0, R\varepsilon)_\sharp$ indicates the interval with identified end points. The latter requirement admits sequences η with compact support in $(0, R\varepsilon) \times (0, R\varepsilon)$, but also sequences of vertically periodic functions η, in particular functions $\eta = \eta(x_1)$. In the subsequent proofs we do not indicate the R-dependence of η_R and write only η. We furthermore

omit the superscripts $\pm$, the eigenvalue corresponding to $\lambda = (j, m)$ is denoted by $\mu_\lambda = \mu_m(j)$. Constants are allowed to depend on $\varepsilon > 0$.

Lemma 3.4 (The effect of truncations)**.** *For $R \in \mathbb{N}$ let $\eta = \eta_R$ be a family of cut-off functions satisfying (3.10). Let v_R and w_R be sequences of functions in $L^2(W_R; \mathbb{C})$ with $v_R \in H^2(W_R; \mathbb{C})$. We assume that certain averages over boundary strips are bounded:*

$$\frac{1}{R}\int_{W_R \setminus W_{R-1}} |v_R|^2 + |\nabla v_R|^2 \le C_0\,, \qquad \frac{1}{R}\int_{W_R \setminus W_{R-1}} |w_R|^2 \le C_0\,, \tag{3.11}$$

with C_0 independent of R. Then, with a constant C that is independent of R:

1. *Application of $\mathcal{L}_0$ to a truncated function:*

$$⨍_{W_R} |\mathcal{L}_0(v_R)\eta - \mathcal{L}_0(v_R\eta)|^2 = ⨍_{W_R} \left|\mathcal{L}_0(v_R)\eta - \sum_{\lambda\in I_R} \mu_\lambda \langle v_R\eta, U_\lambda\rangle_R\, U_\lambda\right|^2 \le \frac{C}{R}\,. \tag{3.12}$$

2. *If Π is one of the projections of Definition 3.1, then*

$$⨍_{W_R} |\Pi(w_R) - \Pi(w_R\,\eta)|^2 \le ⨍_{W_R} |w_R - w_R\,\eta|^2 \le \frac{C}{R}\,. \tag{3.13}$$

Proof. In the following, the letter C denotes different constants, possibly varying from one line to the next, but always independent of R. To prove (3.12), we expand the L^2-function $\mathcal{L}_0(v_R)\eta$ in Bloch-waves. The following calculation uses several times integration by parts; due to the η-factor, no boundary integrals occur. In the first equation we use that the coefficient α_λ in the expansion of $\mathcal{L}_0(v_R)\eta$ is obtained by taking the scalar product with U_λ (orthonormality of the U_λ).

$$\begin{aligned}
\mathcal{L}_0(v_R)\eta &= \sum_{\lambda\in I_R} \langle \mathcal{L}_0(v_R)\eta, U_\lambda\rangle_R\, U_\lambda = \sum_{\lambda\in I_R} \langle v_R, \mathcal{L}_0(\eta U_\lambda)\rangle_R\, U_\lambda \\
&= \sum_{\lambda\in I_R} \left(\langle v_R\eta, \mathcal{L}_0 U_\lambda\rangle_R + \langle v_R\mathcal{L}_0(\eta), U_\lambda\rangle_R - 2\,\langle v_R\, a^\varepsilon\nabla\eta, \nabla U_\lambda\rangle_R\right) U_\lambda \\
&= \sum_{\lambda\in I_R} \left(\mu_\lambda\,\langle v_R\eta, U_\lambda\rangle_R - \langle v_R\mathcal{L}_0(\eta), U_\lambda\rangle_R + 2\,\langle \nabla v_R\cdot a^\varepsilon\nabla\eta, U_\lambda\rangle_R\right) U_\lambda \\
&= \left(\sum_{\lambda\in I_R} \mu_\lambda\,\langle v_R\eta, U_\lambda\rangle_R\, U_\lambda\right) - v_R\mathcal{L}_0(\eta) + 2a^\varepsilon\nabla v_R\cdot\nabla\eta\,,
\end{aligned}$$

where in the third equality we exploited $\mathcal{L}_0 U_\lambda = \mu_\lambda U_\lambda$ and $\mu_\lambda \in \mathbb{R}$. The contribution of the last two terms can be estimated by

$$\begin{aligned}
&⨍_{W_R} |v_R\,\mathcal{L}_0(\eta)|^2 + |2a^\varepsilon\nabla v_R\cdot\nabla\eta|^2 \\
&\quad\le \|\mathcal{L}_0(\eta)\|^2_{L^\infty(W_R)} ⨍_{W_R} |v_R|^2 1_{\{\mathrm{supp}(\nabla\eta)\}} + \|2a^\varepsilon\nabla\eta\|^2_{L^\infty(W_R)} ⨍_{W_R} |\nabla v_R|^2 1_{\{\mathrm{supp}(\nabla\eta)\}} \\
&\quad\le \frac{C}{R^2}\left(\int_{W_R\setminus W_{R-1}} |v_R|^2 + \int_{W_R\setminus W_{R-1}} |\nabla v_R|^2\right) \le \frac{C}{R}\,.
\end{aligned}$$

In the second inequality we exploited $\operatorname{supp}(\nabla\eta) \subset (W_R \setminus W_{R-1})$, in the last inequality we used the uniform bounds (3.11). This proves the inequality in (3.12).

Regarding the equality in (3.12) we have to verify that the formal equality $\mathcal{L}_0 w = \sum_\lambda \mu_\lambda \langle w, U_\lambda\rangle_R U_\lambda$ holds for functions $w \in H^2(W_R)$ with vanishing boundary data. We find this from

$$\langle \mathcal{L}_0 w, U_\lambda\rangle \overset{(!)}{=} \langle w, \mathcal{L}_0 U_\lambda\rangle = \mu_\lambda \langle w, U_\lambda\rangle\,, \tag{3.14}$$

where we used in the marked equality that boundary terms vanish.

Inequality (3.13) is a direct consequence of linearity and norm-boundedness of the projections:

$$\fint_{W_R} |\Pi w_R - \Pi(w_R\,\eta)|^2 = \fint_{W_R} |\Pi(w_R(1-\eta))|^2 \le \fint_{W_R} |w_R(1-\eta)|^2 \le \frac{C}{R^2}\int_{W_R\setminus W_{R-1}} |w_R|^2 \le \frac{C}{R}\,.$$

This concludes the proof. □

3.3.1. A warning concerning the non-periodicity of truncated solutions

Let u be a vertically periodic solution of the Helmholtz equation on $\mathbb{R}\times(0,h)$ and let u_R^+ be defined as in Definition 3.2. Then u_R^+ is a solution of the Helmholtz equation on the open square $W_R = RY_\varepsilon$. But u_R^+ is not a *periodic solution* on the square (since it is not periodic in horizontal direction).

This fact implies that certain formal calculations are wrong: Let u_R^+ have the Bloch expansion $u_R^+ = \sum_{\lambda\in I_R}\alpha_\lambda U_\lambda^+$ for some coefficients α_λ (every L^2-function possesses such an expansion). Then, in general, the following identity fails to hold:

$$\mathcal{L}_0 \sum_{\lambda\in I_R} \alpha_\lambda U_\lambda^+ \overset{(?)}{=} \sum_{\lambda\in I_R} \alpha_\lambda \mathcal{L}_0(U_\lambda^+).$$

To see this, let us assume that the relation (?) holds. Then the Helmholtz equation provides $\sum_{\lambda\in I_R}\omega^2\alpha_\lambda U_\lambda^+ = \omega^2 u_R^+ = \mathcal{L}_0 u_R^+ = \mathcal{L}_0\sum_{\lambda\in I_R}\alpha_\lambda U_\lambda^+ \overset{(?)}{=} \sum_{\lambda\in I_R}\alpha_\lambda\mathcal{L}_0(U_\lambda^+) = \sum_{\lambda\in I_R}\alpha_\lambda\mu_\lambda^+ U_\lambda^+$. Uniqueness of the Bloch expansion implies $\alpha_\lambda(\omega^2-\mu_\lambda^+)=0$ for every $\lambda\in I_R$, hence $\alpha_\lambda = 0$ for every λ with $\mu_\lambda^+ \neq \omega^2$. We conclude that the Bloch expansion of u_R^+ contains only contributions from those basis functions U_λ^+ with $\mu_\lambda^+ = \omega^2$.

This is a contradiction for general solutions u: Let ω be a frequency such that ω^2 is not contained in the discrete set of $(\mu_\lambda^+)_{\lambda\in I_R}$. Let furthermore u be a non-vanishing Bloch wave for the frequency ω. Then the expansion of u does not use only $\alpha_\lambda = 0$, a contradiction.

Lemma 3.5 (Contributions from energy levels $m \ge 1$)**.** *Let ω satisfy the smallness condition (1.7) of Assumption 1.1. Let $u \in L^2_{\mathrm{loc}}(\mathbb{R}\times(0,h);\mathbb{C})$ be a vertically periodic solution of the Helmholtz equation $\mathcal{L}_0 u = \omega^2 u$ satisfying the uniform L^2-bounds of Definition 3.3. Let $\eta = \eta_R$ be a family of cut-off functions as in (3.10). Then, with a constant C that is independent of R:*

$$\fint_{W_R}\left|\Pi^{\mathrm{ev},\pm}_{m\ge1}(u_R^\pm)\right|^2 \le \frac{C}{R} \quad \text{and} \quad \fint_{W_R}\left|\Pi^{\mathrm{ev},\pm}_{m\ge1}(u_R^\pm\,\eta)\right|^2 \le \frac{C}{R}\,. \tag{3.15}$$

Proof. We perform the proof for the superscript "+". Relation (3.13) applied to u_R^+ provides

$$\fint_{W_R}\left|\Pi^{\mathrm{ev},+}_{m\ge1}(u_R^+) - \Pi^{\mathrm{ev},+}_{m\ge1}(u_R^+\,\eta)\right|^2 \le \frac{C}{R}\,.$$

Indeed, by the uniform L^2-bounds of u, the condition $\frac{1}{R}\int_{W_R\setminus W_{R-1}}|u_R^+|^2 \le C_0$ with C_0 independent of R is satisfied. The above inequality implies that it is sufficient to show only one of the two relations in (3.15), we show the second.

We now exploit Assumption 1.1. Due to (1.7), there exists $\delta>0$ such that $|\omega^2-\mu_\lambda|^2\ge\delta$ for all $\lambda=(j,m)$ with $m\ge 1$. We therefore find

$$\begin{aligned}
&\delta\fint_{W_R}\left|\Pi^{\mathrm{ev},+}_{m\ge1}(u_R^+\eta)\right|^2 = \delta\sum_{\substack{\lambda=(j,m)\in I_R\\ m\ge1}}\left|\langle u_R^+\eta,U_\lambda\rangle_R\right|^2 \le \sum_{\substack{\lambda=(j,m)\in I_R\\ m\ge1}}\left|(\omega^2-\mu_\lambda)\langle u_R^+\eta,U_\lambda\rangle_R\right|^2\\
&\le \sum_{\lambda\in I_R}\left|\langle\omega^2u_R^+\eta,U_\lambda\rangle_R-\langle\mu_\lambda u_R^+\eta,U_\lambda\rangle_R\right|^2 = \sum_{\lambda\in I_R}\left|\langle\mathcal{L}_0(u_R^+)\eta,U_\lambda\rangle_R-\langle\mu_\lambda u_R^+\eta,U_\lambda\rangle_R\right|^2\\
&= \fint_{W_R}\left|\mathcal{L}_0(u_R^+)\eta-\sum_{\lambda\in I_R}\mu_\lambda\langle u_R^+\eta,U_\lambda\rangle_R\,U_\lambda\right|^2 \le \frac{C}{R}\,.
\end{aligned}$$

In the second line we used that $\mathcal{L}_0(u_R^+)=\omega^2u_R^+$ holds pointwise almost everywhere in W_R. In the last inequality we used (3.12), exploiting the uniform H^1-bounds provided by Lemma A.3. This concludes the proof. □

3.4. Other radiation conditions and the sesquilinear form $b_R^\pm$

In this section we discuss how our radiation condition simplifies in the case of a homogeneous medium. We furthermore show that the radiation condition suggested by Fliss and Joly in [16] is formally stronger than our condition: Every solution that satisfies the condition of [16] satisfies also our condition. Finally, we introduce the sesquilinear form $b_R^\pm$, which plays a major role in our proofs. The form $b_R^\pm$ can also be used to introduce an even weaker form of the outgoing wave condition.

3.4.1. In free space, Bloch expansions are Fourier expansions

Let us study the outgoing wave condition in a homogeneous medium. This is our situation for $x_1<0$, indicated with the superscript "−". In a homogeneous medium, the Bloch waves are harmonic waves. This allows to give explicit formulas for some quantities and, in particular, for the outgoing wave condition.

Remark 3.6 (Basis functions and Poynting numbers in a homogeneous medium)**.** The functions $\Psi^-_{j,m}$ are ε-periodic eigenfunctions of the operator $\mathcal{L}_j^- = -(\nabla+2\pi ij/\varepsilon)\cdot(\nabla+2\pi ij/\varepsilon)$. As such, for fixed $j\in Z$, they are harmonic waves, $\{\Psi^-_{j,m}\,|\,m\in\mathbb{N}_0\}=\{e^{2\pi ik\cdot x/\varepsilon}\,|\,k\in\mathbb{Z}^2\}$. More precisely, for every $j\in Z$ and every $m\in\mathbb{N}$, there exists a wave-number $k=k(j,m)\in\mathbb{Z}^2$ such that

$$\Psi^-_{j,m}(x)=e^{2\pi ik\cdot x/\varepsilon}\,,\qquad \mu^-_m(j)=4\pi^2\frac{|k+j|^2}{\varepsilon^2}\,. \tag{3.16}$$

Accordingly, for $\lambda=(j,m)$, we have $U^-_\lambda(x)=e^{2\pi i(k+j)\cdot x/\varepsilon}$, and the Poynting number is

$$P^-_\lambda=\operatorname{Im}\fint_{Y_\varepsilon}\bar U^-_\lambda(x)e_1\cdot\nabla U^-_\lambda(x)\,\mathrm{d}x=\frac{2\pi}{\varepsilon}\,(k_1+j_1)\,.$$

In particular, for the first energy level, $\lambda=(j,0)$, we find

$$k=k(j,0)\in\operatorname*{argmin}_{k\in\mathbb{Z}^2}|k+j|^2\,,$$

and thus, for $j = (j_1, j_2)$ with $j_1 \neq \frac{1}{2}$:

$$\frac{\varepsilon}{2\pi} P^-_{(j,0)} = j_1 + \operatorname*{argmin}_{k_1 \in \mathbb{Z}} |k_1 + j_1|^2 = \begin{cases} j_1 & \text{for } j_1 \in [0, \frac{1}{2}), \\ j_1 - 1 & \text{for } j_1 \in (\frac{1}{2}, 1]. \end{cases} \tag{3.17}$$

The wave $U^-_{(j,0)}$ is right-going in the sense of Definition 3.1 if and only if $j_1 \in [0, \frac{1}{2})$.

Remark 3.7 (Outgoing wave condition in a homogeneous medium)**.** Let u^-_R be as in Definition 3.2. Remark 3.6 implies that, for every index $\lambda = (j, m) \in I_R$, there exists an index $k = k(\lambda) \in \mathbb{Z}^2$ with $U^-_\lambda(x) = e^{2\pi i(k+j)\cdot x/\varepsilon} = e^{2\pi i R(k+j)\cdot x/R\varepsilon}$. Using the shorthand notation $l(\lambda) := R\,(k(\lambda) + j) \in \mathbb{Z}^2$, the Bloch expansion of u^-_R can be rewritten as a Fourier expansion,

$$u^-_R(x) = \sum_{\lambda \in I_R} \alpha^-_{\lambda,R} U^-_\lambda(x) = \sum_{\lambda \in I_R} \alpha^-_{\lambda,R}\, e^{2\pi i l(\lambda)\cdot x/R\varepsilon}\,.$$

By Remark 3.6, the basis function $U^-_\lambda(x)$ is right-going in the sense of Definition 3.1 if and only if $l_1(\lambda) > 0$. This simplifies the radiation condition: The function u with the truncations u^-_R on the left satisfies the outgoing wave condition (3.7) if and only if

$$\sum_{\substack{\lambda \in I_R \\ l_1(\lambda) > 0}} |\alpha^-_{\lambda,R}|^2 \to 0 \quad \text{as } R \to \infty\,. \tag{3.18}$$

We emphasize that, in order to evaluate the radiation condition, the map $l : I_R \to \mathbb{Z}^2$ need not be evaluated (we know that it is bijective). By expanding u^-_R in a classical Fourier series, $u^-_R(x) = \sum_{l \in \mathbb{Z}^2} \beta^-_{l,R}\, e^{2\pi i l\cdot x/R\varepsilon}$ with some coefficients $\beta^-_{l,R}$, the outgoing wave condition (3.18) is equivalent to $\sum_{\substack{l \in \mathbb{Z}^2 \\ l_1 > 0}} |\beta^-_{l,R}|^2 \to 0$ as $R \to \infty$.

3.4.2. Comparison to the outgoing wave condition of Fliss and Joly [16]

We claim that the outgoing wave condition of Fliss and Joly is formally stronger than our condition. More precisely: Every solution u that satisfies the radiation condition (1.5) of [16] satisfies also our radiation condition (3.6) (we restrict the considerations here to the right side $x_1 \to +\infty$). Indeed, let u be as in (1.5), *i.e.* a finite sum of right-going Bloch-waves plus an exponentially decaying remainder $w^+(x)$. In order to check (3.6) for u, it suffices to verify, for each of the finitely many terms, the smallness of its $\Pi^+_{<0}$-projection. The smallness of the projection of $w^+(x)$ is clear because of the exponential decay of $w^+(x)$ and the boundedness of the projection operator. The smallness of the projection for each of the Bloch waves is shown in the subsequent lemma.

Since the expansion (1.5) contains only vertically periodic waves with frequency ω that are outgoing, we restrict our analysis to such Bloch-waves U^+_λ.

Lemma 3.8 (Right-going Bloch waves satisfy the radiation condition)**.** *Let $K \in \mathbb{N}$ denote the number of periodicity cells in vertical direction and let U^+_λ be a Bloch wave with $\lambda = (j, m) \in Z \times \mathbb{N}_0$, $j_2 \in Q_K = \{0, \frac{1}{K}, ..., \frac{K-1}{K}\}$, $\mu^+_m(j) = \omega^2$, and $P^+_\lambda > 0$. We impose that the frequency ω satisfies Assumption 1.1 (hence $m = 0$). Then, as $\mathbb{N}K \ni R \to \infty$:*

$$\fint_{RY_\varepsilon} \left|\Pi^+_{<0}((U^+_\lambda)^+_R)\right|^2 \to 0\,, \tag{3.19}$$

$$\fint_{RY_\varepsilon} \left|\Pi^+_{\geq 0}((U^+_\lambda)^+_R)\right|^2 \to 1\,. \tag{3.20}$$

Proof.
Step 1: Equivalence of (3.19) and (3.20). By L^2-orthogonality of the projections we can calculate

$$1 = \fint_{RY_\varepsilon} |(U_\lambda^+)_R^+|^2 = \fint_{RY_\varepsilon} \left|\Pi_{\geq 0}^+((U_\lambda^+)_R^+)\right|^2 + \fint_{RY_\varepsilon} \left|\Pi_{<0}^+((U_\lambda^+)_R^+)\right|^2 ,$$

which yields the equivalence of (3.19) and (3.20).

Step 2: Proof of (3.19). Let $\lambda = (j,m) = (j,0)$ be as in the lemma. Arguing exactly as in Lemma 3.5 we conclude that contributions from energy levels $m \geq 1$ are negligible,

$$\fint_{RY_\varepsilon} \left|\Pi_{m\geq 1}^{\mathrm{ev},+}((U_\lambda^+)_R^+)\right|^2 \to 0 \quad \text{as } R \to \infty.$$

Consequently, for the weighted L^2-norm of $\Pi_{<0}^+((U_\lambda^+)_R^+)$ we calculate

$$\begin{aligned}\fint_{RY_\varepsilon} \left|\Pi_{<0}^+((U_\lambda^+)_R^+)\right|^2 &= \sum_{\tilde\lambda \in I_R \cap I_{<0}^+} \left|\langle (U_\lambda^+)_R^+, U_{\tilde\lambda}\rangle_R\right|^2 = \sum_{\substack{\tilde\lambda \in I_R \cap I_{<0}^+ \\ \tilde m = 0}} \left|\langle (U_\lambda^+)_R^+, U_{\tilde\lambda}\rangle_R\right|^2 + o(1) \\ &= \sum_{\substack{\tilde\lambda \in I_R \cap I_{<0}^+ \\ \tilde m = 0,\ \tilde j_2 = j_2}} \left|\langle (U_\lambda^+)_R^+, U_{\tilde\lambda}\rangle_R\right|^2 + o(1) \quad \text{as } R \to \infty.\end{aligned}$$

In the last line we exploited that due to $j_2 \in Q_R$ all scalar products with $\tilde j_2 \neq j_2$ vanish. Next we show that there exists a constant $C = C(\lambda) > 0$ such that

$$\left|\langle (U_\lambda^+)_R^+, U_{\tilde\lambda}\rangle_R\right| \leq \frac{C}{R} \tag{3.21}$$

for all $\tilde\lambda = (\tilde j, 0) \in I_R \cap I_{<0}^+$ with $\tilde j_2 = j_2$. Indeed, a direct calculation analogous to that of Lemma A.1 yields

$$\langle (U_\lambda^+)_R^+, U_{\tilde\lambda}\rangle_R = e^{-2\pi i j_1 R}\, \frac{C(\lambda,\tilde\lambda)}{R}\, \frac{1 - e^{2\pi i(\tilde j_1 - j_1)R}}{1 - e^{2\pi i(\tilde j_1 - j_1)}}$$

with $C(\lambda,\tilde\lambda) := \fint_{(0,\varepsilon)^2} \Psi_\lambda^+ \bar\Psi_{\tilde\lambda}^+ e^{2\pi i(\tilde j_1 - j_1)y_1/\varepsilon} \mathrm{d}y$. In particular $|C(\lambda,\tilde\lambda)| \leq 1$ and therefore

$$\left|\langle (U_\lambda^+)_R^+, U_{\tilde\lambda}\rangle_R\right| \leq \frac{1}{R} \left|\frac{1 - e^{2\pi i(\tilde j_1 - j_1)R}}{1 - e^{2\pi i(\tilde j_1 - j_1)}}\right| \leq \frac{1}{R} \frac{2}{\left|1 - e^{2\pi i(\tilde j_1 - j_1)}\right|}. \tag{3.22}$$

We now exploit $P_\lambda^+ > 0$. The eigenvalue $\mu_0^+(j)$ is simple, hence the Poynting number $P_\lambda^+ = P_{(j,0)}^+$ is continuous in the wave number j. One thus finds a positive constant $\delta = \delta(\lambda) > 0$ such that

$$\left|1 - e^{2\pi i(\tilde j_1 - j_1)}\right| > \delta$$

for all $\tilde\lambda = (\tilde j, 0) \in I_R \cap I_{<0}^+$ with $\tilde j_2 = j_2$. Together with (3.22) this yields the claim (3.21) with $C = \frac{2}{\delta}$.

With estimate (3.21) at hand we conclude

$$\fint_{RY_\varepsilon} \left|\Pi^+_{<0}((U^+_\lambda)^+_R)\right|^2 \le \frac{C^2}{R^2}\left|\left\{\tilde\lambda = (\tilde j, 0) \in I_R \cap I^+_{<0} \text{ with } \tilde j_2 = j_2\right\}\right| + o(1) \le \frac{C^2}{R} + o(1) \to 0 \quad \text{as } R \to \infty\,,$$

which was the claim. □

3.4.3. The sesquilinear form $b^\pm_R$

Let $\eta = \eta_R$ be a family of cut-off functions as in (3.10). In view of Relation (3.13) of Lemma 3.4, the outgoing wave conditions (3.6) and (3.7) are equivalent to outgoing wave conditions for the truncated functions $u^\pm_{R,\eta} := u^\pm_R\,\eta$. More precisely, they are equivalent to the conditions

$$\fint_{W_R} \left|\Pi^+_{<0}(u^+_{R,\eta})\right|^2 \to 0 \quad \text{and} \quad \fint_{W_R} \left|\Pi^-_{>0}(u^-_{R,\eta})\right|^2 \to 0 \quad \text{as} \quad R \to \infty\,. \tag{3.23}$$

In the proof of our uniqueness result we will use (3.23) instead of the original conditions (3.6) and (3.7). In fact, even a weaker form of the conditions is sufficient and we discuss this relaxation in the following.

Corresponding to the energy flux definition in (3.1), we associate to a function $w \in H^1(W_R;\mathbb{C})$ on $W_R = RY_\varepsilon$ the Poynting number

$$B^+_R(w) := \operatorname{Im} \fint_{W_R} \bar w(x) e_1 \cdot [a^\varepsilon(x)\nabla w(x)]\,\mathrm{d}x\,. \tag{3.24}$$

The quadratic expression B^-_R is defined analogously, with $a^\varepsilon(x)$ replaced by 1.

Definition 3.9 (Weaker form of the outgoing wave condition)**.** For $K, R \in \mathbb{N}$ with $R \in K\mathbb{N}$ we consider $u \in H^1_{\mathrm{loc}}(\mathbb{R}\times(0,\varepsilon K);\mathbb{C})$ and $u^\pm_{R,\eta}$ as in (3.23). We say that u satisfies the energetic outgoing wave condition on the right, if

$$B^+_R\left(\Pi^+_{<0}\Pi^{\mathrm{ev},+}_{m=0}(u^+_{R,\eta})\right) \to 0 \text{ as } R \to \infty\,. \tag{3.25}$$

Accordingly, we say that u satisfies the energetic outgoing wave condition on the left, if

$$B^-_R\left(\Pi^-_{>0}\Pi^{\mathrm{ev},-}_{m=0}(u^-_{R,\eta})\right) \to 0 \text{ as } R \to \infty\,. \tag{3.26}$$

In two respects, the condition (3.25) is similar to the condition (3.23): the function u is considered at the far right since only $u^+_{R,\eta}$ is used. In view of Lemma 3.5, contributions from energy levels $m \ge 1$ can be neglected and we consider only $\Pi^{\mathrm{ev},+}_{m=0}(u^+_{R,\eta})$. Furthermore, this function is projected to left-going waves, *i.e.* only $\Pi^+_{<0}\Pi^{\mathrm{ev},+}_{m=0}(u^+_{R,\eta})$ is studied. The main difference between the two conditions is that, instead of looking at the weighted L^2-norm, one demands in (3.25) a decay property for the energy-flux quantity B^+_R. At the end of this section, we will see that condition (3.23) (together with the uniform L^2-bounds and the solution property) implies (3.25).

The definition of B_R^+ in (3.24) suggests to introduce additionally the (nonsymmetric) sesquilinear forms $b_R^\pm : L^2(W_R;\mathbb{C}) \times H^1(W_R;\mathbb{C}) \to \mathbb{C}$,

$$b_R^+(u,v) := \fint_{W_R} \bar{u}(x)\, e_1 \cdot [a^\varepsilon(x)\nabla v(x)]\, \mathrm{d}x\,,$$
$$b_R^-(u,v) := \fint_{W_R} \bar{u}(x)\, e_1 \cdot \nabla v(x)\, \mathrm{d}x\,. \tag{3.27}$$

The definition is tailored to calculate energy fluxes. The energy flux of the left-going contributions of $u_{R,\eta}^+$ (in the right half-plane) is quantified by

$$B_R^+(\Pi_{<0}^+ u_{R,\eta}^+) = \operatorname{Im} b_R^+\left(\Pi_{<0}^+ u_{R,\eta}^+, \Pi_{<0}^+ u_{R,\eta}^+\right) = \operatorname{Im} \fint_{W_R} \overline{\Pi_{<0}^+ u_{R,\eta}^+(x)} e_1 \cdot \left[a^\varepsilon(x)\nabla(\Pi_{<0}^+ u_{R,\eta}^+)(x)\right]\, \mathrm{d}x\,.$$

The connection to $P_\lambda^\pm$ is given by

$$P_\lambda^\pm = B_R^\pm(U_\lambda^\pm) = \operatorname{Im} b_R^\pm\left(U_\lambda^\pm, U_\lambda^\pm\right)\,. \tag{3.28}$$

Let us collect some properties of the sesquilinear forms $b_R^\pm$.

Lemma 3.10 (Properties of the sesquilinear form $b_R^\pm$)**.** *For $R \in \mathbb{N}$, the following holds:*

1. Orthogonality property of $b_R^\pm$. *Let $\lambda, \tilde\lambda \in I_R$ be such that $\lambda = (j,m)$, $\tilde\lambda = (\tilde j, \tilde m)$ with $j \neq \tilde j$. Then $U_\lambda^\pm, U_{\tilde\lambda}^\pm$ of (2.8) satisfy*

$$b_R^\pm(U_\lambda^\pm, U_{\tilde\lambda}^\pm) = 0\,. \tag{3.29}$$

2. Convergence property of $b_R^\pm$. *Sequences $u_R \in L^2(W_R;\mathbb{C})$ and $v_R \in H^1(W_R;\mathbb{C})$ be such that*

$$\fint_{W_R} |u_R|^2 + |\nabla v_R|^2 \leq C_0 \tag{3.30}$$

with C_0 independent of R. Let either $\fint_{W_R} |u_R|^2 \to 0$ or $\fint_{W_R} |\nabla v_R|^2 \to 0$ as $R \to \infty$. Then there holds

$$b_R^\pm(u_R, v_R) \to 0\,. \tag{3.31}$$

Proof. 1. We prove (3.29) for $U_\lambda^+, U_{\tilde\lambda}^+$, the argument for $U_\lambda^-, U_{\tilde\lambda}^-$ is analogous. We have to show that

$$b_R^+(U_\lambda^+, U_{\tilde\lambda}^+) = \fint_{W_R} \overline{U_\lambda^+}(x)\, e_1 \cdot \left[a^\varepsilon(x)\nabla U_{\tilde\lambda}^+(x)\right]\, \mathrm{d}x \stackrel{!}{=} 0\,.$$

By definition of U_λ^+ and $U_{\tilde\lambda}^+$ there holds

$$\overline{U_\lambda^+}(x) = \overline{\Psi_\lambda^+}(x) e^{-i2\pi j\cdot x/\varepsilon},$$
$$\nabla U_{\tilde\lambda}^+(x) = \left[\nabla\Psi_{\tilde\lambda}^+(x) + (i2\pi\tilde j/\varepsilon)\,\Psi_{\tilde\lambda}^+(x)\right] e^{i2\pi\tilde j\cdot x/\varepsilon}$$

with ε-periodic functions Ψ_λ^+, $\Psi_{\tilde\lambda}^+$, and $\nabla\Psi_{\tilde\lambda}^+$. Due to the ε-periodicity of a^ε and since $j, \tilde j \in Q_R$ satisfy $j \neq \tilde j$, we can apply Lemma A.1 of Appendix A, which yields the claim.

2. We show the claim for b_R^+, the argument for b_R^- is analogous. The Cauchy–Schwarz inequality allows to calculate

$$\left|b_R^+(u_R, v_R)\right| = \left| \fint_{W_R} \bar{u}_R(x)\, e_1 \cdot [a^\varepsilon(x) \nabla v_R(x)]\, \mathrm{d}x \right| \leq \|a^\varepsilon\|_\infty \left(\fint_{W_R} |u_R|^2 \right)^{1/2} \left(\fint_{W_R} |\nabla v_R|^2 \right)^{1/2} \to 0 \text{ as } R \to \infty\,,$$

which concludes the proof. □

Lemma 3.10 shows that the outgoing wave condition (3.23) together with the L^2-bounds of Definition 3.3 imply (3.25). Indeed, by (3.23), there holds

$$\fint_{W_R} \left| \Pi_{<0}^+ \Pi_{m=0}^{\mathrm{ev},+}(u_{R,\eta}^+) \right|^2 \leq \fint_{W_R} \left| \Pi_{<0}^+ (u_{R,\eta}^+) \right|^2 \to 0 \text{ as } R \to \infty\,.$$

Moreover, $\Pi_{<0}^+ \Pi_{m=0}^{\mathrm{ev},+}(u_{R,\eta}^+)$ satisfies $\fint_{W_R} |\nabla \left(\Pi_{<0}^+ \Pi_{m=0}^{\mathrm{ev},+}(u_{R,\eta}^+) \right)|^2 \leq C$ with C independent of R due to Lemma A.3 and Lemma A.4 of Appendix A. Lemma 3.10 provides

$$B_R^+ \left(\Pi_{<0}^+ \Pi_{m=0}^{\mathrm{ev},+}(u_{R,\eta}^+) \right) = \operatorname{Im} b_R^+ \left(\Pi_{<0}^+ \Pi_{m=0}^{\mathrm{ev},+}(u_{R,\eta}^+), \Pi_{<0}^+ \Pi_{m=0}^{\mathrm{ev},+}(u_{R,\eta}^+) \right) \to 0 \text{ as } R \to \infty\,,$$

and hence (3.25).

Remark 3.11 (On the sesquilinear form $b_R^\pm$)**.** Another choice of a bilinear form is

$$\tilde{b}_R^+(u, v) := \frac{1}{2} \fint_{W_R} \left\{ \bar{u}(x)\, e_1 \cdot [a^\varepsilon(x) \nabla v(x)] - v(x)\, e_1 \cdot [a^\varepsilon(x) \nabla \bar{u}(x)] \right\} \mathrm{d}x\,. \tag{3.32}$$

With this choice, the energy flux $B_R^\pm$ can be calculated as before, since $\operatorname{Im} b_R^+(u, u) = \operatorname{Im} \tilde{b}_R^+(u, u)$ holds for every u. The properties of Lemma 3.10 remain also unchanged, the only additional requirement would be an H^1-bound also for u_R in (3.30).

The advantage of $\tilde{b}_R^+(u, v)$ is that more orthogonality can be expected for $\tilde{b}_R^+$ than for b_R^+. Essentially, the bilinear form q of (27) in [16] coincides with $\tilde{b}_R^+$ (up to a factor 2, our coefficient a^ε, and the fact that we use a volume integral for the averaging). In Theorem 3 of [16], an orthogonality property is shown for q, which resembles our orthogonality relation (3.29), stating that orthogonality holds also for $\lambda = (j, m)$ and $\tilde{\lambda} = (j, \tilde{m})$ with $m \neq \tilde{m}$. Unfortunately, such an orthogonality is only true for basis functions corresponding to the same frequency ω, while our analysis of an interface would require orthogonality independent of the frequency.

4. Bloch measures and uniqueness properties

Our aim is to show uniqueness properties of the transmission Problem 1.2 with incoming wave U_{inc} and outgoing wave conditions. Following the standard procedure of uniqueness proofs, we consider two solutions u and $\tilde{u}$ of the problem. Due to linearity of the system, the difference $v := u - \tilde{u}$ satisfies again (1.1). Furthermore, it satisfies outgoing wave conditions on the left and on the right according to Definition 3.3, without any incoming wave U_{inc}. At this point, we have exploited the triangle inequality: Certain projections of u and $\tilde{u}$ tend to zero in a weighted L^2-norm, hence also the projections of v tend to zero. We can not show that v vanishes (indeed, as explained in the introduction, we expect that there exist nontrivial solutions for vanishing U_{inc}). But we can show that the functions $v_R^\pm$ consist, in the limit $R \to \infty$, only of vertical waves. The right object to study is the *Bloch measure* associated with $v_R^\pm$.

We recall that the frequency assumption (1.7) implies that, in the limit $R \to \infty$, the discrete Bloch expansions of $u_R^\pm$ contain only modes corresponding to $\lambda = (j, m)$ with $m = 0$, see Lemma 3.5.

4.1. Bloch measures

In the definition of Bloch measures we use the space of all Radon measures on the unit square Z, which we denote as $\mathcal{M}(Z)$. It is the dual of the space of continuous functions on Z and accordingly equipped with the topology of weak-$*$ convergence. This means, in particular, that every bounded sequence in $\mathcal{M}(Z)$ has a convergent subsequence.

Definition 4.1 (Discrete Bloch measure)**.** Let $u_R \in L^2(W_R;\mathbb{C})$ be a sequence of functions with discrete Bloch-expansions

$$u_R(x) = \sum_{\lambda\in I_R} \alpha_\lambda^\pm U_\lambda^\pm(x)\,,$$

where $\alpha_\lambda^\pm = \alpha_\lambda^\pm(R)$ depend on $R \in \mathbb{N}$. Given these coefficients, for fixed $l \in \mathbb{N}_0$, we define the l-th discrete Bloch-measure $\nu_{l,R}^\pm \in \mathcal{M}(Z)$ by

$$\nu_{l,R}^\pm := \sum_{\lambda=(j,l)\in I_R} |\alpha_\lambda^\pm|^2\ \delta_j\,, \tag{4.1}$$

where δ_j denotes the Dirac measure at the frequency $j \in Z$.

For u_R fixed, $\nu_{l,R}^\pm$ is a non-negative Radon measure on $Z = [0,1]^2$. There holds

$$\sum_{l=0}^{\infty} \int_Z d\nu_{l,R}^\pm = \sum_{\lambda\in I_R} |\alpha_\lambda^\pm|^2 = \fint_{W_R} |u_R|^2\,. \tag{4.2}$$

Our aim is to study the limiting behavior $R \to \infty$ of the discrete Bloch measures $\nu_{l,R}^\pm$.

Definition 4.2 (Bloch measure)**.** For $\varepsilon > 0$, $K \in \mathbb{N}$ and $h = K\varepsilon$, let u be a function $u \in L^2_{\mathrm{loc}}(\mathbb{R}\times(0,h);\mathbb{C})$. We consider a sequence $\mathbb{N}K \ni R \to \infty$. We extract $u_{R,\eta}^\pm := u_R^\pm\,\eta$ according to Definition 3.2 with a sequence of cut-off functions $\eta = \eta_R$ as in (3.10). For $l \in \mathbb{N}_0$, let $\nu_{l,R}^\pm$ be the discrete Bloch measures associated with $u_{R,\eta}^\pm$.

We say that the measure $\nu_{l,\infty}^\pm \in \mathcal{M}(Z)$ is a Bloch measure generated by u if there holds, along a subsequence $R \to \infty$, in the sense of measures (*i.e.* weak-$*$),

$$\nu_{l,R}^\pm \to \nu_{l,\infty}^\pm\,. \tag{4.3}$$

Relation (4.3) is equivalent to the following: for every test-function $\phi \in C(Z)$ on $Z = [0,1]^2$ there holds

$$\sum_{\lambda=(j,l)\in I_R} \phi(j)|\alpha_\lambda^\pm|^2 = \int_Z \phi\, d\nu_{l,R}^\pm \to \int_Z \phi\, d\nu_{l,\infty}^\pm \quad \text{as } R\to\infty\,.$$

The methods of Section 4.3 force us to work with cut-off functions, *i.e.* with $u_{R,\eta}^\pm$ and with $\nu_{l,R}^\pm$. Nevertheless, one may also study the discrete Bloch measures $\tilde\nu_{l,R}^\pm$ associated to $u_R^\pm$ (without cut-off function). In the limit $R \to \infty$, the two measures coincide,

$$\nu_{l,R}^\pm - \tilde\nu_{l,R}^\pm \to 0$$

in the sense of measures. In particular, the Bloch measure generated by $u_{R,\eta}^\pm$ is independent of the choice of η.

4.2. Energy estimates and consequences for the Bloch measure

Up to this point (with the exception of Lem. 3.5), our considerations have been completely abstract in the following sense: Given a function $u \in L^2_{\mathrm{loc}}(\mathbb{R} \times (0,h);\mathbb{C})$, we have constructed restrictions of u to large boxes, projections of these restrictions, and finally discrete and limiting Bloch measures corresponding to u. Except for regularity properties, we have not exploited the Helmholtz equation. In this section, we will derive relations that express a physical law: energy conservation. This will eventually lead us to the uniqueness properties which are expressed with the Bloch measures.

The subsequent result states that, while left-going waves on the right vanish by the outgoing wave condition, right-going waves vanish by energy conservation.

Proposition 4.3. *Let Assumption 1.1 on $\omega > 0$ be satisfied and let v be a solution to the scattering problem (1.1), periodic in vertical direction, satisfying outgoing wave conditions on the left and on the right according to Definition 3.3, without incoming wave,* i.e. $U_{\mathrm{inc}} \equiv 0$. *For a sequence of cut-off functions $\eta = \eta_R$ as in (3.10) we consider $v^{\pm}_{R,\eta} := v^{\pm}_R\, \eta_R = \sum_{\lambda \in I_R} \alpha^{\pm}_{\lambda,R} U^{\pm}_{\lambda}$, c.f. Definition 3.2. Then, as $\mathbb{N}K \ni R \to \infty$,*

$$\sum_{\substack{\lambda=(j,0)\\ \lambda \in I_R \cap I^-_{\leq 0}}} |\alpha^-_{\lambda,R}|^2\, P^-_\lambda \to 0 \quad \textit{and} \quad \sum_{\substack{\lambda=(j,0)\\ \lambda \in I_R \cap I^+_{\geq 0}}} |\alpha^+_{\lambda,R}|^2\, P^+_\lambda \to 0\,. \tag{4.4}$$

Proof.
Step 1: Energy flux equality. For $h = \varepsilon K$ and $R \in \mathbb{N}K$, we consider the special cut-off function $\vartheta(x) = \vartheta_R(x)$, defined for $x = (x_1, x_2)$ as

$$\vartheta(x) := \begin{cases} 1 & \text{if } |x_1| \leq \varepsilon R\,, \\ 2 - \frac{|x_1|}{\varepsilon R} & \text{if } \varepsilon R < |x_1| < 2\varepsilon R\,, \\ 0 & \text{if } |x_1| \geq 2\varepsilon R\,. \end{cases}$$

We multiply the Helmholtz equation (1.1) with coefficients $a = a^\varepsilon$ and solution v by the test-function $\vartheta(x)\,\overline{v}(x)$. An integration over $\mathbb{R} \times (0,h)$ and integration by parts yields (no boundary terms appear due to periodicity in x_2-direction and compact support):

$$\int_{\mathbb{R}} \int_0^h \left\{ a^\varepsilon\, \vartheta\, |\nabla v|^2 + a^\varepsilon\, \partial_{x_1}\vartheta\; \overline{v}\; \partial_{x_1} v \right\} = \omega^2 \int_{\mathbb{R}} \int_0^h \vartheta\, |v|^2\,.$$

Due to the special choice of ϑ and $a^\varepsilon(x) = 1$ for $x_1 < 0$, this equation reads

$$⨍_{-2R\varepsilon}^{-R\varepsilon} \int_0^h \overline{v}\, \partial_{x_1} v - ⨍_{R\varepsilon}^{2R\varepsilon} \int_0^h \overline{v}\, a^\varepsilon \partial_{x_1} v = \int_{\mathbb{R}} \int_0^h \left\{ \omega^2 \vartheta\, |v|^2 - a^\varepsilon\, \vartheta\; |\nabla v|^2 \right\}.$$

On the left-hand side, we recognize the sesquilinear forms $b^{\pm}_R$ of (3.27). Because of periodicity in x_2-direction, we may write

$$h\;\left[b^-_R\left(v^-_R, v^-_R\right) - b^+_R\left(v^+_R, v^+_R\right)\right] = \int_{\mathbb{R}} \int_0^h \left\{ \omega^2 \vartheta\, |v|^2 - a^\varepsilon\, \vartheta\; |\nabla v|^2 \right\}. \tag{4.5}$$

Since the right hand side is real, taking the imaginary part of (4.5) yields

$$\operatorname{Im} b^-_R\left(v^-_R, v^-_R\right) - \operatorname{Im} b^+_R\left(v^+_R, v^+_R\right) = 0\,. \tag{4.6}$$

Relation (4.6) is an energy conservation: The energy flux into the domain from the left must coincide with the energy flux out of the domain at the right.

Step 2: Truncations and $(m \geq 1)$-waves. We start this part of the proof with an observation regarding the cut-off functions; we want to have them in the argument of the sesquilinear form. Due to Lemma A.3 and the properties of the cut-off functions $\eta = \eta_R$ we have

$$\int_{W_R} |v_R^\pm - v_{R,\eta}^\pm|^2 + |\nabla v_R^\pm - \nabla v_{R,\eta}^\pm|^2 \leq \frac{C}{R}\,, \tag{4.7}$$

and therefore, by Lemma 3.10,

$$b_R^\pm\left(v_R^\pm, v_R^\pm\right) - b_R^\pm\left(v_{R,\eta}^\pm, v_{R,\eta}^\pm\right) = b_R^\pm\left(v_R^\pm - v_{R,\eta}^\pm, v_R^\pm\right) + b_R^\pm\left(v_{R,\eta}^\pm, v_R^\pm - v_{R,\eta}^\pm\right) \to 0 \quad \text{as } R \to \infty\,.$$

The energy conservation (4.6) therefore implies that, as $R \to \infty$,

$$\operatorname{Im} b_R^-\left(v_{R,\eta}^-, v_{R,\eta}^-\right) - \operatorname{Im} b_R^+\left(v_{R,\eta}^+, v_{R,\eta}^+\right) \to 0\,. \tag{4.8}$$

We next decompose the sesquilinear forms $b_R^\pm$ according to the projections of Definition 3.1, and suppress the superscript "$\pm$" in the projection. We exploit sesquilinearity of b_R^+ in both arguments and write

$$\begin{aligned}\operatorname{Im} b_R^+\left(v_{R,\eta}^+, v_{R,\eta}^+\right) &= \operatorname{Im} b_R^+\left(\Pi_{m\geq 1}^{\mathrm{ev}}\left(v_{R,\eta}^+\right), v_{R,\eta}^+\right) + \operatorname{Im} b_R^+\left(\Pi_{m=0}^{\mathrm{ev}}\left(v_{R,\eta}^+\right), \Pi_{m\geq 1}^{\mathrm{ev}}\left(v_{R,\eta}^+\right)\right)\\ &\quad + \operatorname{Im} b_R^+\left(\Pi_{m=0}^{\mathrm{ev}}\left(v_{R,\eta}^+\right), \Pi_{m=0}^{\mathrm{ev}}\left(v_{R,\eta}^+\right)\right)\,.\end{aligned} \tag{4.9}$$

We want to exploit the smallness of $m \geq 1$-contributions of Lemma 3.5. The regularity result of Lemma A.3 together with the properties of the sesquilinear form b_R^+ of Lemma 3.10 yield that the first term on the right hand side of (4.9) vanishes in the limit as $R \to \infty$. For the second term we apply Lemma A.4, which provides that also the gradient of $\Pi_{m\geq 1}^{\mathrm{ev}}\left(v_{R,\eta}^+\right)$ is small; Lemma 3.10 implies

$$b_R^+\left(\Pi_{m=0}^{\mathrm{ev}}\left(v_{R,\eta}^+\right), \Pi_{m\geq 1}^{\mathrm{ev}}\left(v_{R,\eta}^+\right)\right) \to 0 \quad \text{as } R \to \infty\,,$$

i.e. also the second term on the right hand side of (4.9) vanishes in the limit. We find that, as $R \to \infty$,

$$\operatorname{Im} b_R^+\left(v_{R,\eta}^+, v_{R,\eta}^+\right) = \operatorname{Im} b_R^+\left(\Pi_{m=0}^{\mathrm{ev}}\left(v_{R,\eta}^+\right), \Pi_{m=0}^{\mathrm{ev}}\left(v_{R,\eta}^+\right)\right) + o(1)\,. \tag{4.10}$$

Step 3: Energy flux and outgoing wave conditions. In this step we decompose $\operatorname{Im} b_R^+\left(\Pi_{m=0}^{\mathrm{ev}}\left(v_{R,\eta}^+\right), \Pi_{m=0}^{\mathrm{ev}}\left(v_{R,\eta}^+\right)\right)$ as follows:

$$\begin{aligned}\operatorname{Im} b_R^+\left(\Pi_{m=0}^{\mathrm{ev}}\left(v_{R,\eta}^+\right), \Pi_{m=0}^{\mathrm{ev}}\left(v_{R,\eta}^+\right)\right) &= \operatorname{Im} b_R^+\left(\Pi_{<0}^+\Pi_{m=0}^{\mathrm{ev}}\left(v_{R,\eta}^+\right), \Pi_{<0}^+\Pi_{m=0}^{\mathrm{ev}}\left(v_{R,\eta}^+\right)\right)\\ &\quad + \operatorname{Im} b_R^+\left(\Pi_{<0}^+\Pi_{m=0}^{\mathrm{ev}}\left(v_{R,\eta}^+\right), \Pi_{\geq 0}^+\Pi_{m=0}^{\mathrm{ev}}\left(v_{R,\eta}^+\right)\right) + \operatorname{Im} b_R^+\left(\Pi_{\geq 0}^+\Pi_{m=0}^{\mathrm{ev}}\left(v_{R,\eta}^+\right), \Pi_{\geq 0}^+\Pi_{m=0}^{\mathrm{ev}}\left(v_{R,\eta}^+\right)\right)\\ &\quad + \operatorname{Im} b_R^+\left(\Pi_{\geq 0}^+\Pi_{m=0}^{\mathrm{ev}}\left(v_{R,\eta}^+\right), \Pi_{<0}^+\Pi_{m=0}^{\mathrm{ev}}\left(v_{R,\eta}^+\right)\right) = \operatorname{Im} b_R^+\left(\Pi_{<0}^+\Pi_{m=0}^{\mathrm{ev}}\left(v_{R,\eta}^+\right), \Pi_{<0}^+\Pi_{m=0}^{\mathrm{ev}}\left(v_{R,\eta}^+\right)\right)\\ &\quad + \operatorname{Im} b_R^+\left(\Pi_{\geq 0}^+\Pi_{m=0}^{\mathrm{ev}}\left(v_{R,\eta}^+\right), \Pi_{\geq 0}^+\Pi_{m=0}^{\mathrm{ev}}\left(v_{R,\eta}^+\right)\right)\,,\end{aligned} \tag{4.11}$$

where the last equality holds, since for $\lambda = (j, m = 0) \in I^+_{<0}$ and $\tilde\lambda = (\tilde j, m = 0) \in I^+_{\geq 0}$ one always has $j \neq \tilde j$ and thus the mixed sesquilinear forms vanish due to orthogonality in the wave number, *cf.* Lemma 3.10. Exploiting the outgoing wave condition (3.23) on the right or, better, the weaker expression (3.25), we find that the first term on the right hand side of (4.11) vanishes in the limit $R \to \infty$. Hence

$$\operatorname{Im} b^+_R\left(\Pi^{\mathrm{ev}}_{m=0}\left(v^+_{R,\eta}\right), \Pi^{\mathrm{ev}}_{m=0}\left(v^+_{R,\eta}\right)\right) = \operatorname{Im} b^+_R\left(\Pi^+_{\geq 0}\Pi^{\mathrm{ev}}_{m=0}\left(v^+_{R,\eta}\right), \Pi^+_{\geq 0}\Pi^{\mathrm{ev}}_{m=0}\left(v^+_{R,\eta}\right)\right) + o(1) \quad \text{as } R \to \infty\,. \tag{4.12}$$

We emphasize that we only used the energetic outgoing wave condition (3.25) in this calculation.

Combining (4.10) with (4.12) we finally obtain, as $R \to \infty$,

$$\operatorname{Im} b^+_R\left(v^+_{R,\eta}, v^+_{R,\eta}\right) = \operatorname{Im} b^+_R\left(\Pi^+_{\geq 0}\Pi^{\mathrm{ev}}_{m=0}\left(v^+_{R,\eta}\right), \Pi^+_{\geq 0}\Pi^{\mathrm{ev}}_{m=0}\left(v^+_{R,\eta}\right)\right) + o(1)\,. \tag{4.13}$$

Step 4: Consequences for outgoing waves. We analyze (4.13) further, exploiting the discrete Bloch expansion of $v^\pm_{R,\eta} = \sum_{\lambda\in I_R} \alpha^\pm_{\lambda,R} U^\pm_\lambda$:

$$\begin{aligned}\operatorname{Im} b^+_R\left(\Pi^+_{\geq 0}\Pi^{\mathrm{ev}}_{m=0}\left(v^+_{R,\eta}\right), \Pi^+_{\geq 0}\Pi^{\mathrm{ev}}_{m=0}\left(v^+_{R,\eta}\right)\right) &= \operatorname{Im} \sum_{\lambda=(j,0)\in I_R\cap I^+_{\geq 0}} \sum_{\tilde\lambda=(\tilde j,0)\in I_R\cap I^+_{\geq 0}} \bar\alpha^+_{\lambda,R}\,\alpha^+_{\tilde\lambda,R}\; b^+_R\left(U^+_\lambda, U^+_{\tilde\lambda}\right)\\ &= \sum_{\lambda=(j,0)\in I_R\cap I^+_{\geq 0}} |\alpha^+_{\lambda,R}|^2 \operatorname{Im} b^+_R\left(U^+_\lambda, U^+_\lambda\right) = \sum_{\lambda=(j,0)\in I_R\cap I^+_{\geq 0}} |\alpha^+_{\lambda,R}|^2\, P^+_\lambda\,.\end{aligned}$$

In the last line we again exploited the orthogonality of the sesquilinear form b^+_R in the wave number j, see Lemma 3.10, and the relation (3.28) for $P^\pm_\lambda$. We may therefore write (4.13) as

$$\operatorname{Im} b^+_R\left(v^+_{R,\eta}, v^+_{R,\eta}\right) = \sum_{\lambda=(j,0)\in I_R\cap I^+_{\geq 0}} |\alpha^+_{\lambda,R}|^2\, P^+_\lambda + o(1)\,.$$

On the left, we find similarly

$$\operatorname{Im} b^-_R\left(v^-_{R,\eta}, v^-_{R,\eta}\right) = \sum_{\lambda=(j,0)\in I_R\cap I^-_{\leq 0}} |\alpha^-_{\lambda,R}|^2\, P^-_\lambda + o(1)\,.$$

The energy relation (4.6) together with the sign properties $P^+_\lambda \geq 0$ for $\lambda \in I^+_{\geq 0}$ and $P^-_\lambda \leq 0$ for $\lambda \in I^-_{\leq 0}$ allows to conclude (4.4). □

4.3. Proof of Theorems 1.3 and 1.6

We study solutions to the Helmholtz equation (1.1). In order to prove Theorems 1.3 and 1.6, we have to check conditions that are satisfied by the support of Bloch measures of solutions. We recall the notation

$$J^\pm_{=0,l} = \{j \in Z = [0,1]^2 \mid P^\pm_\lambda = 0 \text{ for } \lambda = (j,l)\}$$

for the index set corresponding to vertical waves.

Proof of Theorem 1.3. In the following, we consider solutions to the transmission Problem 1.2. We are interested in a solution to the problem without incoming wave. □

Proposition 4.4 (Solutions in absence of incoming waves)**.** *Let Assumption 1.1 on $\omega > 0$ be satisfied and let v be a solution to the scattering problem (1.1), periodic in vertical direction, satisfying outgoing wave conditions on the left and on the right according to Definition 3.3, without incoming wave. Let $\nu^\pm_{l,\infty}$, with $l \in \mathbb{N}_0$, be Bloch measures that are generated by v. Then*

$$\nu^\pm_{l,\infty} = 0 \qquad \textit{for } l \geq 1, \tag{4.14}$$

$$\operatorname{supp}(\nu^\pm_{0,\infty}) \subset J^\pm_{=0,0}\,. \tag{4.15}$$

Proof. We only show the statement for the limiting Bloch measures $\nu^+_{l,\infty}$, the argument for $\nu^-_{l,\infty}$ is analogous. Let $v^+_{R,\eta} = \sum_{\lambda\in I_R} \alpha^+_{\lambda,R} U^+_\lambda$ be the expansion of the truncated solution. Then the corresponding discrete Bloch measures are given by

$$\nu^+_{l,R} = \sum_{\lambda=(j,l)\in I_R} |\alpha^+_{\lambda,R}|^2 \, \delta_j \,.$$

The case $l \geq 1$: From (3.15) we know that

$$\fint_{W_R} \left|\Pi^{\mathrm{ev}}_{m\geq 1}(v^+_{R,\eta})\right|^2 = \sum_{\substack{\lambda=(j,m)\in I_R \\ m\geq 1}} |\alpha^+_{\lambda,R}|^2 \leq \frac{C}{R} \,,$$

and hence

$$\int_Z d\nu^+_{l,R} = \sum_{\lambda=(j,l)\in I_R} |\alpha^+_{\lambda,R}|^2 \to 0 \quad \text{as } R\to\infty \,.$$

This shows $\nu^+_{l,\infty} = 0$ for every $l \geq 1$.

The case $l = 0$: We have to show $\mathrm{supp}(\nu^+_{0,\infty}) \subset J^+_{=0,0}$. To this end, we consider an arbitrary test function $\phi \in C(Z)$ with

$$\mathrm{supp}(\phi) \subset \{j \in Z \,|\, \lambda = (j,0) \in I^+_{<0} \cup I^+_{>0}\} \,.$$

The outgoing wave condition (3.6) and Proposition 4.3 yield, in the limit $R\to\infty$,

$$\sum_{\lambda=(j,0)\in I_R\cap I^+_{<0}} |\alpha^+_{\lambda,R}|^2 \to 0 \quad \text{and} \quad \sum_{\lambda=(j,0)\in I_R\cap I^+_{>0}} |\alpha^+_{\lambda,R}|^2 \, P^+_\lambda \to 0 \,.$$

In the following we assume that $\mathrm{supp}(\phi) \cap \{j \in Z \,|\, \lambda = (j,0) \in I^+_{>0}\} \neq \emptyset$, otherwise the proof simplifies. We find

$$c_1 := \inf_{\substack{\lambda=(j,0)\in I^+_{>0} \\ j\in\mathrm{supp}(\phi)}} P^+_\lambda > 0 \,.$$

Without loss of generality, we assume $\phi \geq 0$ (otherwise we consider absolute values). For the limit $R\to\infty$ we calculate

$$\begin{aligned}\int_Z \phi \, d\nu^+_{0,R} &= \sum_{\substack{\lambda=(j,0)\in I^+_{<0}\cap I_R \\ j\in\mathrm{supp}(\phi)}} |\alpha^+_{\lambda,R}|^2 \phi(j) + \sum_{\substack{\lambda=(j,0)\in I^+_{>0}\cap I_R \\ j\in\mathrm{supp}(\phi)}} |\alpha^+_{\lambda,R}|^2 \phi(j) \\ &\leq \|\phi\|_\infty \sum_{\lambda=(j,0)\in I_R\cap I^+_{<0}} |\alpha^+_{\lambda,R}|^2 + \|\phi\|_\infty \, \frac{1}{c_1} \sum_{\lambda=(j,0)\in I_R\cap I^+_{>0}} |\alpha^+_{\lambda,R}|^2 \, P^+_\lambda \to 0 \,.\end{aligned}$$

This shows (4.15) for "+", since ϕ with support outside $J^+_{=0,0}$ was arbitrary. The argument for "−" is analogous. □

We next prove that, far away from the interface, solutions to the transmission problem contain only waves that satisfy the frequency condition and the vertical periodicity.

Proposition 4.5 (Bloch measures and frequency condition)**.** *Let Assumption 1.1 on $\omega > 0$ be satisfied and let v be a solution to the scattering problem (1.1), periodic in vertical direction, satisfying outgoing wave conditions on the left and on the right according to Definition 3.3, with incoming wave U_{inc} or without incoming wave. Let $\nu^{\pm}_{0,\infty}$ be the Bloch measure to $l = 0$ that is generated by v. Then*

$$\operatorname{supp}(\nu^{\pm}_{0,\infty}) \subset \left\{ j \in Z | \mu^{\pm}_0(j) = \omega^2 \,,\ j_2 \in \mathbb{Z}/K \right\} . \tag{4.16}$$

Proof. Remark 2.3 implies that the discrete Bloch measures $\nu^{\pm}_{l,R}$ are supported on $\{j \in Z |\, j_2 \in \mathbb{Z}/K\}$. This implies that also the limit measure $\nu^{\pm}_{l,\infty}$ are supported on this set.

In order to show (4.16), it remains to check the frequency condition; we proceed as in the last proof. Let $\phi : Z \to \mathbb{R}$ be continuous and bounded with $\operatorname{supp}(\phi) \cap \{j | \mu_0(j) = \omega^2\} = \emptyset$. Arguing with decompositions of the domain of integration, we can consider separately a test-function $\phi \geq 0$ with the property $\phi(j) > 0 \Rightarrow \mu_0(j) > \omega^2$ and a test-function $\tilde{\phi} \geq 0$ with the property $\tilde{\phi}(j) > 0 \Rightarrow \mu_0(j) < \omega^2$. The arguments are analogous and we consider here only ϕ as above.

By continuity of ϕ we find some $\delta > 0$ such that $\mu_0(j) - \omega^2 \geq \delta$ for every $j \in \operatorname{supp}(\phi)$. Our aim is to show that $\int_Z \phi \, d\nu^{+}_{0,\infty} = 0$. By definition of the Bloch measure $\nu^{+}_{0,\infty}$ we have, as $R \to \infty$,

$$0 \leq \delta \int_Z \phi \, d\nu^{+}_{0,\infty} \leftarrow \delta \int_Z \phi \, d\nu^{+}_{0,R} = \delta \sum_{\lambda=(j,0)\in I_R} |\alpha^{+}_{\lambda,R}|^2 \phi(j) \leq \sum_{\lambda=(j,0)\in I_R} (\mu_0(j) - \omega^2) |\alpha^{+}_{\lambda,R}|^2 \phi(j) \,. \tag{4.17}$$

The result $\int_Z \phi \, d\nu^{+}_{0,\infty} = 0$ is shown once we prove that the right hand side of (4.17) vanishes in the limit $R \to \infty$. In order to show this fact, we recall that the coefficients $\alpha^{+}_{\lambda,R}$ are obtained from a Bloch-expansion of the solution at the far right, *i.e.* $\alpha^{+}_{\lambda,R} = \langle u^{+}_{R,\eta}, U^{+}_{\lambda} \rangle_R$. We calculate

$$\begin{aligned}
\sum_{\lambda=(j,0)\in I_R} (\mu_0(j) - \omega^2) |\alpha^{+}_{\lambda,R}|^2 \phi(j) &\overset{(1)}{=} \sum_{\lambda=(j,0)\in I_R} \phi(j) \, \overline{\alpha^{+}_{\lambda,R}} \left[\langle u^{+}_{R,\eta}, \mu_0(j) U^{+}_{\lambda} \rangle_R - \langle \omega^2 \, u^{+}_{R,\eta}, U^{+}_{\lambda} \rangle_R \right] \\
&\overset{(2)}{=} \sum_{\lambda=(j,0)\in I_R} \phi(j) \, \overline{\alpha^{+}_{\lambda,R}} \left[\langle u^{+}_{R,\eta}, \mathcal{L}_0 U^{+}_{\lambda} \rangle_R - \langle \omega^2 \, u^{+}_{R,\eta}, U^{+}_{\lambda} \rangle_R \right] \overset{(3)}{=} \sum_{\lambda=(j,0)\in I_R} \phi(j) \, \overline{\alpha^{+}_{\lambda,R}} \, \langle \mathcal{L}_0 u^{+}_{R,\eta} - \omega^2 \, u^{+}_{R,\eta}, U^{+}_{\lambda} \rangle_R \\
&\overset{(4)}{\leq} \|\phi\|_\infty \left(\sum_{\lambda=(j,0)\in I_R} |\alpha^{+}_{\lambda,R}|^2 \right)^{1/2} \left(\sum_{\lambda=(j,0)\in I_R} \left| \langle \mathcal{L}_0 u^{+}_{R,\eta} - \omega^2 \, u^{+}_{R,\eta}, U^{+}_{\lambda} \rangle_R \right|^2 \right)^{1/2} .
\end{aligned}$$

In this calculation we used the following: (1) formula for $\alpha^{+}_{\lambda,R}$, (2) the eigenvalue property of U_λ with eigenvalue $\mu_\lambda = \mu_m(j)$, (3) integration by parts without boundary terms due to the cut-off function η, (4) Cauchy–Schwarz inequality. Using orthonormality of the basis functions $U^{\pm}_{\lambda}$ we obtain

$$\begin{aligned}
\sum_{\lambda=(j,0)\in I_R} (\mu_0(j) - \omega^2) |\alpha^{+}_{\lambda,R}|^2 \phi(j) &\leq \|\phi\|_\infty \left(\fint_{W_R} \left| \Pi^{\mathrm{ev}}_{m=0} u^{+}_{R,\eta} \right|^2 \right)^{1/2} \left(\fint_{W_R} \left| \Pi^{\mathrm{ev}}_{m=0} \left(\mathcal{L}_0 u^{+}_{R,\eta} - \omega^2 \, u^{+}_{R,\eta} \right) \right|^2 \right)^{1/2} \\
&\leq \|\phi\|_\infty \left(\fint_{W_R} \left| u^{+}_{R,\eta} \right|^2 \right)^{1/2} \left(\fint_{W_R} \left| \mathcal{L}_0 u^{+}_{R,\eta} - \omega^2 \, u^{+}_{R,\eta} \right|^2 \right)^{1/2} .
\end{aligned}$$

Since $u^{+}_{R,\eta}$ satisfies uniform L^2-bounds and since $\mathcal{L}_0 u^{+}_{R,\eta} = \omega^2 \, u^{+}_{R,\eta}$ holds up to a small L^2-error, the right hand side of (4.17) is small for large $R > 0$. This proves $\int_Z \phi \, d\nu^{+}_{0,\infty} = 0$ and hence (4.16) for "+". The proof for "−" is analogous. □

Proof of Theorem 1.3. Since a solution of the transmission problem without incoming wave satisfies the assumptions of Propositions 4.4 and 4.5, Theorem 1.3 is an immediate consequence of these propositions. □

Proof of Theorem 1.6. We now provide the proof of Theorem 1.6. We therefore assume that: Assumption 1.1 on $\omega > 0$ is satisfied and u is a solution of the scattering problem with incoming wave U_{inc}, which has the wave number $k = (k_1, k_2)$. In particular, u is a vertically periodic solution of (1.1) such that u and $u - U_{\text{inc}}$ satisfy the outgoing wave conditions on the right and on the left. □

Let $\nu^{\pm}_{l,\infty}$ be Bloch measures that are generated by the solution u. The frequency condition (1.7) is satisfied and we can therefore use Lemma 3.5. As in Proposition 4.4, case $l \geq 1$, we conclude from (3.15) (and the analogous result for "−") that $\nu^{\pm}_{l,\infty} = 0$ holds for every $l \geq 1$. Moreover, according to Proposition 4.5 we have that $\operatorname{supp}(\nu^{\pm}_{0,\infty}) \subset \{j \in Z | \mu^{\pm}_0(j) = \omega^2\,,\ j_2 \in \mathbb{Z}/K\}$.

Theorem 1.6 is shown once we verify the following property of the Bloch measure $\nu^{\pm}_{0,\infty}$:

$$\operatorname{supp}(\nu^{\pm}_{0,\infty}) \subset \{j \in Z | j_2 = k_2\} \cup J^{\pm}_{=0,0}\,. \tag{4.18}$$

Proof of (4.18). We consider the projection $\Pi^{\text{vert}}_{k_2} u$ of u. This function is again a solution of the scattering problem. Indeed, by Lemma A.2 one has $\Pi^{\text{vert}}_{k_2} u \in H^1_{\text{loc}}(\mathbb{R} \times (0,h); \mathbb{C})$ with periodicity in the x_2-variable, and for arbitrary test functions $\varphi \in C^\infty_c(\mathbb{R} \times (0,h))$ there holds

$$\begin{aligned}
&\int_{\mathbb{R}} \int_0^h \nabla\varphi \cdot a^\varepsilon \nabla \left(\Pi^{\text{vert}}_{k_2} u\right) = \int_{\mathbb{R}} \int_0^h \nabla\varphi \cdot a^\varepsilon \Pi^{\text{vert}}_{k_2} (\nabla u) = \int_{\mathbb{R}} \int_0^h \Pi^{\text{vert}}_{k_2} (\nabla\varphi) \cdot a^\varepsilon \nabla u \\
&= \int_{\mathbb{R}} \int_0^h \nabla \left(\Pi^{\text{vert}}_{k_2} \varphi\right) \cdot a^\varepsilon \nabla u = \omega^2 \int_{\mathbb{R}} \int_0^h \Pi^{\text{vert}}_{k_2} \varphi\, u = \omega^2 \int_{\mathbb{R}} \int_0^h \varphi\, \Pi^{\text{vert}}_{k_2} u\,,
\end{aligned}$$

where we exploited the orthogonality properties of $\Pi^{\text{vert}}_{k_2}$ from Lemma A.1 and the solution property of u.

As a consequence, the difference $v := u - \Pi^{\text{vert}}_{k_2} u$ is a solution of the scattering problem with vanishing incoming wave. The statement of Proposition 4.4 implies: Bloch measures (for $l = 0$) that are generated by v have their support in vertical waves, *i.e.* in $J^{\pm}_{=0,0}$.

On the other hand, the Bloch measure of $\Pi^{\text{vert}}_{k_2} u$ is concentrated on waves with vertical wave number k_2, *i.e.* in $\{j \in Z | j_2 = k_2\}$. This follows immediately from the fact that all coefficients $\alpha_{(j,m)}$ with $j_2 \neq k_2$ in the expansion of $\Pi^{\text{vert}}_{k_2} u$ vanish.

Since the Bloch measure of u can have its support only in the union of the supports corresponding to $\Pi^{\text{vert}}_{k_2} u$ and $u - \Pi^{\text{vert}}_{k_2} u$, the claim (4.18) follows.

Theorem 1.6 is shown.

5. Outlook and conclusions

5.1. Remarks on the existence of solutions

We give some remarks concerning the existence of solutions to the scattering problem. In the end, our radiation condition is "the right one" only if, besides uniqueness, an existence result can be shown.

We formulate the following conjecture: Given a non-singular frequency $\omega > 0$, given coefficients $a = a^\varepsilon$ that are equal to 1 in the left half plane and ε-periodic in the right half plane, strictly positive and bounded, given finally an incoming wave U_{inc} as in (1.2) (possibly with a condition on k), there exists a solution u of the transmission Problem 1.2.

The idea for an existence proof is the limiting absorption principle (see *e.g.* [19, 24, 31] for recent contributions): For a positive artificial damping parameter $\delta > 0$, we consider the equation

$$-\nabla\cdot((1-i\delta)a(x)\nabla u^\delta(x)) = \omega^2 u^\delta(x) \tag{5.1}$$

for $x \in \Omega = \mathbb{R}\times(0,h)$. Due to the strictly negative imaginary part of the coefficient $(1-i\delta)a(x)$, this equation admits a unique solution u^δ in the Beppo-Levi space $\dot{H}^1(\Omega)$ as can be shown with the Lax-Milgram Lemma.

To proceed, two properties must be shown. The first is: The sequence u^δ satisfies estimates in some function space, uniformly in $\delta > 0$. Once this is shown, one can consider the distributional limit u of the sequence u^δ as $\delta \to 0$. As a consequence of distributional convergence, the limit u is a solution of the Helmholtz equation with coefficients a.

The other part of this approach is to show: The limit u satisfies the outgoing wave condition. We do not see a straightforward argument that yields this condition.

5.2. Our outgoing wave condition in a numerical scheme

The radiation condition of Definition 3.3 can be used for numerical purposes: Instead of demanding that limits $R \to \infty$ vanish, we demand that, for some fixed distance R, the left hand side of (3.6) vanishes. In the numerical scheme, this amounts to imposing that a finite number of projections to left-going waves vanishes. Results with such a scheme are presented in [11].

5.3. Conclusions

We have investigated transmission properties at the boundary of a photonic crystal. Our theorems justify the following: An incoming wave generates, inside the photonic crystal, only those Bloch waves, for which the eigenvalue coincides with the (squared) frequency of the incoming wave. Furthermore, only those Bloch waves can be generated that have the same vertical wave number as the incoming wave; this latter statement is true up to vertical waves. Conservation of the vertical wave number is essential for negative refraction without a negative index.

Our results rely on a new outgoing wave condition in photonic crystals. The new radiation condition is based on Bloch expansions. It is accompanied by a (weak) uniqueness result, which is expressed with Bloch-measures. The uniqueness result is the basis for the analysis of the transmission problem.

Appendix A. Orthogonality and regularity properties

Lemma A.1 (Orthogonality with periodic weight)**.** *Let $f : \mathbb{R} \to \mathbb{C}$ be ε-periodic and integrable, let $R \in \mathbb{N}$ be an integer.*

1. Orthogonality of exponentials. *Let $j, \tilde{j} \in Q_R$ with $j \neq \tilde{j}$. Then*

$$\int_0^{\varepsilon R} f(y) e^{2\pi i j y/\varepsilon} e^{-2\pi i \tilde{j} y/\varepsilon}\,\mathrm{d}y = 0\,. \tag{A.1}$$

2. Orthogonality of the vertical pre-Bloch projection. *Let $u, v \in L^2_{\mathrm{loc}}(\mathbb{R}\times(0,\varepsilon R);\mathbb{C})$ and let $k_2 \in Q_R$. Then there holds*

$$\int_0^{\varepsilon R} f(y)\, u(x_1,y)\,\overline{\Pi^{\mathrm{vert}}_{k_2} v(x_1,y)}\,\mathrm{d}y = \int_0^{\varepsilon R} f(y)\Pi^{\mathrm{vert}}_{k_2} u(x_1,y)\,\overline{\Pi^{\mathrm{vert}}_{k_2} v(x_1,y)}\,\mathrm{d}y\,. \tag{A.2}$$

Proof.

1. By dividing the interval $(0, \varepsilon R)$ into subintervals of length ε, we obtain

$$\begin{aligned}\int_0^{\varepsilon R} f(y) e^{2\pi i j y/\varepsilon} e^{-2\pi i \tilde{j} y/\varepsilon}\,\mathrm{d}y &= \sum_{k=0}^{R-1} \int_{k\varepsilon}^{(k+1)\varepsilon} f(y) e^{2\pi i (j-\tilde{j}) y/\varepsilon}\,\mathrm{d}y \\ &= \sum_{k=0}^{R-1} \int_0^{\varepsilon} f(y+k\varepsilon) e^{2\pi i (j-\tilde{j})(y+k\varepsilon)/\varepsilon}\,\mathrm{d}y = \sum_{k=0}^{R-1} e^{2\pi i (j-\tilde{j})k} \int_0^{\varepsilon} f(y) e^{2\pi i (j-\tilde{j}) y/\varepsilon}\,\mathrm{d}y\,,\end{aligned}$$

   where in the last equality we exploited the periodicity of the weight f. By setting $C(j,\tilde{j}) := \int_0^{\varepsilon} f(y) e^{2\pi i (j-\tilde{j}) y/\varepsilon}\,\mathrm{d}y$ we conclude

$$\int_0^{\varepsilon R} f(y) e^{2\pi i j y/\varepsilon} e^{-2\pi i \tilde{j} y/\varepsilon}\,\mathrm{d}y = C(j,\tilde{j}) \sum_{k=0}^{R-1} \left(e^{2\pi i (j-\tilde{j})}\right)^k = C(j,\tilde{j}) \frac{1 - e^{2\pi i (j-\tilde{j}) R}}{1 - e^{2\pi i (j-\tilde{j})}} = 0\,.$$

   In the last step we used $j, \tilde{j} \in Q_R$, which implies $R(j-\tilde{j}) \in \mathbb{Z}$ and $j, \tilde{j} < 1$, and exploited $j \neq \tilde{j}$.
2. Let u, v have vertical pre-Bloch expansions

$$u(x_1,x_2) = \sum_{j_2 \in Q_R} \Phi_{j_2}(x_1,x_2)\, e^{2\pi i j_2 x_2/\varepsilon}\,, \quad v(x_1,x_2) = \sum_{\tilde{j}_2 \in Q_R} \tilde{\Phi}_{\tilde{j}_2}(x_1,x_2)\, e^{2\pi i \tilde{j}_2 x_2/\varepsilon}\,.$$

   Then the left hand side of (A.2) reads

$$\int_0^{\varepsilon R} f(y) u(x_1,y)\, \overline{\Pi_{k_2}^{\mathrm{vert}} v(x_1,y)}\,\mathrm{d}y = \sum_{j_2 \in Q_R} \int_0^{\varepsilon R} f(y) \Phi_{j_2}(x_1,y)\, e^{2\pi i j_2 y/\varepsilon}\, \overline{\tilde{\Phi}_{k_2}(x_1,y)}\, e^{-2\pi i k_2 y/\varepsilon}\,\mathrm{d}y\,.$$

   Since the function $f(\cdot)\Phi_{j_2}(x_1,\cdot)\overline{\tilde{\Phi}_{k_2}(x_1,\cdot)}$ is ε-periodic, we can apply the orthogonality (A.1) of Item 1. The sum on the right hand side collapses to $j_2 = k_2$ and we find (A.2).

□

Lemma A.2 (Vertical pre-Bloch projection and gradients)**.** *Let $K \in \mathbb{N}$, $h = \varepsilon K$, and $k_2 \in Q_K$. Let $u \in H^1_{\mathrm{loc}}(\mathbb{R} \times (0,h); \mathbb{C})$ be periodic in the x_2-variable. Then the function $\Pi_{k_2}^{\mathrm{vert}} u \in H^1_{\mathrm{loc}}(\mathbb{R} \times (0,h); \mathbb{C})$ is periodic in x_2 and there holds*

$$\nabla \left(\Pi_{k_2}^{\mathrm{vert}} u\right) = \Pi_{k_2}^{\mathrm{vert}} \left(\nabla u\right)\,. \tag{A.3}$$

Proof. Let u have the pre-Bloch expansion $u(x_1,x_2) = \sum_{j_2 \in Q_K} \Phi_{j_2}(x_1,x_2)\, e^{2\pi i j_2 x_2/\varepsilon}$. Due to the periodicity of u in the x_2-variable, each Φ_{j_2} in the above (finite) sum has H^1-regularity, and thus

$$\begin{aligned}\nabla u(x_1,x_2) &= \sum_{j_2 \in Q_K} \nabla \left(\Phi_{j_2}(x_1,x_2)\, e^{2\pi i j_2 x_2/\varepsilon}\right) \\ &= \sum_{j_2 \in Q_K} \left[\nabla \Phi_{j_2}(x_1,x_2) + 2\pi i j_2/\varepsilon\, \Phi_{j_2}(x_1,x_2) e_2\right] e^{2\pi i j_2 x_2/\varepsilon}\,,\end{aligned} \tag{A.4}$$

where $e_2 = (0,1) \in \mathbb{R}^2$ denotes the second unit vector. Since the expression in the squared brackets is ε-periodic, (A.4) is an expansion of ∇u; uniqueness of the pre-Bloch expansion implies

$$\begin{aligned}\Pi^{\mathrm{vert}}_{k_2}\left(\nabla u\right)(x_1,x_2) &= \left(\nabla \Phi_{k_2}(x_1,x_2) + 2\pi i k_2/\varepsilon\, \Phi_{k_2}(x_1,x_2) e_2\right) e^{2\pi i k_2 x_2/\varepsilon} \\ &= \nabla\left(\Phi_{k_2}(x_1,x_2)\, e^{2\pi i k_2 x_2/\varepsilon}\right) = \nabla\left(\Pi^{\mathrm{vert}}_{k_2} u\right)(x_1,x_2)\,,\end{aligned}$$

which proves (A.3). □

Lemma A.3 (Caccioppoli estimate)**.** *Let $u \in L^2_{\mathrm{loc}}(\mathbb{R}\times(0,h))$ be a vertically periodic solution of the Helmholtz equation $\mathcal{L}_0 u = \omega^2 u$. Let u satisfy the uniform L^2-bounds of Definition 3.3. Then there holds*

$$\frac{1}{R}\int_{W_R\setminus W_{R-1}} |u_R^{\pm}|^2 + |\nabla u_R^{\pm}|^2 \le C \quad \text{and} \quad \fint_{W_R} |u_R^{\pm}|^2 + |\nabla u_R^{\pm}|^2 \le C \tag{A.5}$$

with C independent of R.

Proof. The proof is, up to translations and a summation, analogous to the proof of the standard Caccioppoli estimate: On a rectangle $(L-1,L+2)\times(0,h)$ we use a cut-off function θ with compact support that depends only on x_1 and which is identical 1 on $(L,L+1)\times(0,h)$. Testing the equation with $\theta^2\bar{u}$ provides

$$\int_{L-1}^{L+2}\int_0^h \omega^2|u|^2\theta^2 = \int_{L-1}^{L+2}\int_0^h \mathcal{L}_0 u(\theta^2\bar{u}) = \int_{L-1}^{L+2}\int_0^h \left\{a^\varepsilon|\nabla u|^2\theta^2 + 2a^\varepsilon(\nabla u\theta)\cdot(\nabla\theta\bar{u})\right\}.$$

The Cauchy–Schwarz inequality is used to treat the last term, the first factor is absorbed with Young's inequality in the gradient term, the other consists (up to bounded factors) only of the L^2-norm of u. We conclude that a bound for the L^2-norm on $(L-1,L+2)\times(0,h)$ implies a bound for the L^2-norm of the gradient on $(L,L+1)\times(0,h)$. A summation over many squares yields the result. □

Lemma A.4 (Regularity of eigenvalue projections Π^{ev})**.** *Let $(v_R)_{\mathbb{R}\in\mathbb{N}}$ be a sequence of functions with H^2-regularity and vanishing boundary data,* i.e. *$v_R \in H^2_0(W_R;\mathbb{C})$. We assume that*

$$\fint_{W_R} |v_R|^2 + |\nabla v_R|^2 + |\mathcal{L}_0(v_R)|^2 \le C_0 \tag{A.6}$$

holds for $\mathcal{L}_0 = -\nabla\cdot(a^\varepsilon\nabla)$ with some R-independent constant C_0.

1. *Let Π be any of the projections of Definition 3.1. Then there exists an R-independent constant C such that*

$$\fint_{W_R} \left|\nabla\left(\Pi^{\mathrm{ev},\pm}_{m=0} v_R\right)\right|^2 + \left|\nabla\left(\Pi^{\mathrm{ev},\pm}_{m\ge1} v_R\right)\right|^2 + \left|\nabla\left(\Pi\left(\Pi^{\mathrm{ev},\pm}_{m=0} v_R\right)\right)\right|^2 \le C\,. \tag{A.7}$$

2. *If, additionally, $\fint_{W_R}\left|\Pi^{\mathrm{ev},\pm}_{m\ge1} v_R\right|^2 \to 0$ as $R\to\infty$, then there holds*

$$\fint_{W_R}\left|\nabla\left(\Pi^{\mathrm{ev},\pm}_{m\ge1} v_R\right)\right|^2 \to 0 \quad \text{as } R\to\infty\,. \tag{A.8}$$

Proof.

1. We omit the superscripts $\pm$. Concerning (A.7) we note that, because of $\Pi^{\mathrm{ev}}_{m\geq 1} v_R = v_R - \Pi^{\mathrm{ev}}_{m=0} v_R$, the estimate for $\Pi^{\mathrm{ev}}_{m\geq 1} v_R$ follows directly from the estimate for $\Pi^{\mathrm{ev}}_{m=0} v_R$ and Assumption (A.6).
Since $\Pi^{\mathrm{ev}}_{m=0} v_R = \sum_{\lambda=(j,0)\in I_R} \alpha_\lambda U_\lambda$ is a finite sum of periodic functions, we find that $\Pi^{\mathrm{ev}}_{m=0} v_R$ is periodic in W_R. This allows to calculate, with $0 < a_* \leq \inf a^\varepsilon$,

$$\begin{aligned} a_* \fint_{W_R} \left|\nabla \left(\Pi^{\mathrm{ev}}_{m=0} v_R\right)\right|^2 &\leq \fint_{W_R} a^\varepsilon \nabla \left(\Pi^{\mathrm{ev}}_{m=0} v_R\right) \cdot \overline{\nabla \left(\Pi^{\mathrm{ev}}_{m=0} v_R\right)} \\ &\overset{(1)}{=} \fint_{W_R} \mathcal{L}_0 \left(\Pi^{\mathrm{ev}}_{m=0} v_R\right) \overline{\Pi^{\mathrm{ev}}_{m=0} v_R} \overset{(2)}{=} \fint_{W_R} \Pi^{\mathrm{ev}}_{m=0} \left(\mathcal{L}_0 v_R\right) \overline{\Pi^{\mathrm{ev}}_{m=0} v_R} \\ &\leq \left(\fint_{W_R} \left|\Pi^{\mathrm{ev}}_{m=0} \left(\mathcal{L}_0 v_R\right)\right|^2\right)^{1/2} \left(\fint_{W_R} \left|\Pi^{\mathrm{ev}}_{m=0} v_R\right|^2\right)^{1/2} \leq \left(\fint_{W_R} \left|\mathcal{L}_0 v_R\right|^2\right)^{1/2} \left(\fint_{W_R} \left|v_R\right|^2\right)^{1/2} \leq C_0 \,. \end{aligned}$$

In (1) we exploited the periodicity of $\Pi^{\mathrm{ev}}_{m=0} v_R$ to perform integration by parts without boundary terms. In (2), we used the periodicity of v_R, which yields $\mathcal{L}_0 \left(\Pi^{\mathrm{ev}}_{m=0} v_R\right) = \Pi^{\mathrm{ev}}_{m=0} \left(\mathcal{L}_0 v_R\right)$, as shown in (3.14). In the last line we exploited the norm-boundedness of projections. The claim for $\Pi \left(\Pi^{\mathrm{ev}}_{m=0} v_R\right)$ is shown analogously, using again periodicity. This concludes the proof of Relation (A.7).

2. The proof of Relation (A.8) is similar and can be interpreted as an interpolation between function spaces. Once more, we exploit that v_R has vanishing (and thus periodic) boundary data and that $\Pi^{\mathrm{ev}}_{m=0} v_R$ is periodic as a finite sum (see Item 1.). Therefore also the difference $\Pi^{\mathrm{ev}}_{m\geq 1} v_R = v_R - \Pi^{\mathrm{ev}}_{m=0} v_R$ is periodic. Arguing as above we obtain, as $R \to \infty$,

$$a_* \fint_{W_R} \left|\nabla \left(\Pi^{\mathrm{ev}}_{m\geq 1} v_R\right)\right|^2 \leq \left(\fint_{W_R} \left|\mathcal{L}_0 v_R\right|^2\right)^{1/2} \left(\fint_{W_R} \left|\Pi^{\mathrm{ev}}_{m\geq 1} v_R\right|^2\right)^{1/2} \to 0 \,. \tag{A.9}$$

This shows (A.8) and concludes the proof.

□

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References

[1] G. Allaire and C. Conca, Bloch wave homogenization and spectral asymptotic analysis. *J. Math. Pure Appl.* **77** (1998) 153–208.
[2] G. Allaire, M. Palombaro and J. Rauch, Diffractive behavior of the wave equation in periodic media: weak convergence analysis. *Ann. Mat. Pura Appl.* **188** (2009) 561–589.
[3] G. Allaire, M. Palombaro and J. Rauch, Diffractive geometric optics for Bloch wave packets. *Arch. Ration. Mech. Anal.* **202** (2011) 373–426.
[4] H. Ammari and F. Santosa, Guided waves in a photonic bandgap structure with a line defect. *SIAM J. Appl. Math.* **64** (2004) 2018–2033.
[5] H. Ammari, N. Béreux and E. Bonnetier, Analysis of the radiation properties of a planar antenna on a photonic crystal substrate. *Math. Methods Appl. Sci.* **24** (2001) 1021–1042.
[6] A.-S. Bonnet-Ben Dhia, G. Dakhia, C. Hazard and L. Chorfi, Diffraction by a defect in an open waveguide: a mathematical analysis based on a modal radiation condition. *SIAM J. Appl. Math.* **70** (2009) 677–693.
[7] G. Bouchitté and D. Felbacq, Negative refraction in periodic and random photonic crystals. *New J. Phys.* **7** (2005).
[8] G. Bouchitté and B. Schweizer, Homogenization of Maxwell's equations in a split ring geometry. *Multiscale Model. Simul.* **8** (2010) 717–750.
[9] Y. Chen and R. Lipton, Tunable double negative band structure from non-magnetic coated rods. *New J. Phys.* **12** (2010) 083010.
[10] D. Colton and R. Kress, Inverse Acoustic and Electromagnetic Scattering Theory. Vol. 93 of *Applied Mathematical Sciences*, 2nd edn. Springer-Verlag, Berlin (1998).
[11] T. Dohnal and B. Schweizer, A Bloch wave numerical scheme for scattering problems in periodic wave-guides. *SIAM J. Numer. Anal.* **56** (2018) 1848–1870.

[12] A. Efros and A. Pokrovsky, Dielectric photonic crystal as medium with negative electric permittivity and magnetic permeability. *Solid State Commun.* **129** (2004) 643–647.
[13] A. Figotin and A. Klein, Midgap defect modes in dielectric and acoustic media. *SIAM J. Appl. Math.* **58** (1998) 1748–1773.
[14] S. Fliss, A Dirichlet-to-Neumann approach for the exact computation of guided modes in photonic crystal waveguides. *SIAM J. Sci. Comput.* **35** (2013) B438–B461.
[15] S. Fliss and P. Joly, Wave propagation in locally perturbed periodic media (case with absorption): numerical aspects. *J. Comput. Phys.* **231** (2012) 1244–1271.
[16] S. Fliss and P. Joly, Solutions of the time-harmonic wave equation in periodic waveguides: asymptotic behaviour and radiation condition. *Arch. Ration. Mech. Anal.* **219** (2016) 349–386.
[17] S. Fliss, D. Klindworth and K. Schmidt, Robin-to-Robin transparent boundary conditions for the computation of guided modes in photonic crystal wave-guides. *BIT* **55** (2015) 81–115.
[18] H. Helmholtz, Theorie der Luftschwingungen in Röhren mit offenen Enden. *J. Reine Angew. Math.* **57** (1860) 1–72.
[19] V. Hoang, The limiting absorption principle for a periodic semi-infinite waveguide. *SIAM J. Appl. Math.* **71** (2011) 791–810.
[20] V. Hoang and M. Radosz, Absence of bound states for waveguides in two-dimensional periodic structures. *J. Math. Phys.* **55** (2014) 033506.
[21] Z. Hu and Y.Y. Lu, Efficient analysis of photonic crystal devices by Dirichlet-to-Neumann maps. *Opt. Express* **16** (2008) 17383–17399.
[22] J. Joannopoulos, S. Johnson, J. Winn and R. Meade, Photonic Crystals – Molding the Flow of Light. Princeton University Press (2008).
[23] P. Joly, An elementary introduction to the construction and the analysis of perfectly matched layers for time domain wave propagation. *SeMA J.* **57** (2012) 5–48.
[24] P. Joly, J.-R. Li and S. Fliss, Exact boundary conditions for periodic waveguides containing a local perturbation. *Commun. Comput. Phys.* **1** (2006).
[25] A. Lamacz and B. Schweizer, Effective Maxwell equations in a geometry with flat rings of arbitrary shape. *SIAM J. Math. Anal.* **45** (2013) 1460–1494.
[26] A. Lamacz and B. Schweizer, A negative index meta-material for Maxwell's equations. *SIAM J. Math. Anal.* **48** (2016) 4155–4174.
[27] C. Luo, S.G. Johnson, J.D. Joannopoulos and J.B. Pendry, All-angle negative refraction without negative effective index. *Phys. Rev. B* **65** (2002) 201104.
[28] R.D. Meade, K.D. Brommer, A.M. Rappe and J.D. Joannopoulos, Electromagnetic Bloch waves at the surface of a photonic crystal. *Phys. Rev. B* **44** (1991) 10961–10964.
[29] E. Moreno, F.J. García-Vidal and L. Martín-Moreno, Enhanced transmission and beaming of light via photonic crystal surface modes. *Phys. Rev. B* **69** (2004) 121402.
[30] J. Pendry, Negative refraction makes a perfect lens. *Phys. Rev. Lett.* **85** (2000).
[31] M. Radosz, New limiting absorption and limit amplitude principles for periodic operators. *Z. Angew. Math. Phys.* **66** (2015) 253–275.
[32] F. Rellich, Über das asymptotische Verhalten der Lösungen von $\Delta u + \lambda u = 0$ in unendlichen Gebieten. *Jber. Deutsch. Math. Verein.* **53** (1943) 57–65.
[33] S.H. Schot, Eighty years of Sommerfeld's radiation condition. *Historia Math.* **19** (1992) 385–401.
[34] B. Schweizer, The low-frequency spectrum of small Helmholtz resonators. *Proc. A* **471** (2015) 20140339.
[35] A. Sommerfeld, Die Greensche Funktion der Schwingungsgleichung. *Jbr. Deutsch. Math.-Verein.* **21** (1912) 309–353.