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Agnes Lamacz, Ben Schweizer

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Fakultät für Mathematik
Technische Universität Dortmund
Vogelpothsweg 87
44227 Dortmund

tu-dortmund.de/MathPreprints

Outgoing wave conditions in photonic crystals and transmission properties at interfaces

A. Lamacz, B. Schweizer*

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Abstract

We analyze the propagation of waves in unbounded photonic crystals, the waves are described by a Helmholtz equation with x-dependent coefficients. The scattering problem must be completed with a radiation condition at infinity, which was not available for x-dependent coefficients. We develop an outgoing wave condition with the help of a Bloch wave expansion. Our radiation condition admits a (weak) 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 derive 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.

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

MSC: 35Q60, 35P25, 35B27

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. Several interesting effects can be observed, we are interested here in the effect of negative refraction at the interface between free space and a photonic crystal. 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 [22].

*Technische Universität Dortmund, Fakultät für Mathematik, Vogelpothsweg 87, D-44227 Dortmund, Germany. agnes.lamacz@tu-dortmund.de, ben.schweizer@tu-dortmund.de

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

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

which must be solved for u in a domain Ω, $x = (x_1, x_2) \in \Omega$. Here, we are interested in the unbounded rectangle $\Omega := \mathbb{R} \times (0, h) \subset \mathbb{R}^2$ (our methods can be used also 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 x-dependent coefficient a 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. that $K = h/\varepsilon \in \mathbb{N}$. 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.

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

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

To guarantee that U_{inc} is a solution to (1.1) on the left, we assume $\omega^2 = 4\pi^2|k|^2$. Since the Helmholtz-equation models a time-harmonic situation, we should think here of a solution of the wave equation in the form $\hat{U}_{\text{inc}}(x,t) = U_{\text{inc}}(x)e^{-i\omega t} = \exp(i[2\pi k\cdot x - \omega t])$. We always consider $k_1 > 0$ such that U_{inc} represents a right-going wave. In addition, we assume that the incident wave respects the periodicity condition in vertical direction, i.e. $e^{2\pi i k_2 h} = 1$ or, equivalently, $k_2 h \in \mathbb{Z}$.

With the incident wave U_{inc} at hand we can now describe – at least formally – the boundary conditions for solutions u of (1.1) as $x_1 \to \pm\infty$. We seek for u such that (i) u satisfies an outgoing wave condition as $x_1 \to \infty$ and (ii) $u - U_{\text{inc}}$ satisfies an outgoing wave condition for $x_1 \to -\infty$. This leads us to our first question:

> **Question 1:** How can we prescribe an outgoing wave condition in a periodic medium?

The answer to Question 1 is intricate and requires a detailed study. We will use Bloch expansions and Bloch projections to formulate our new outgoing wave condition in Definition 3.3. In order to motivate our choice, we sketch some background in the next subsection.

Once we have a precise formulation of the scattering problem, we can turn to the application: What can be said about the transmission problem? When an incident wave U_{inc} lights the interface, it creates waves inside the photonic crystal, described by u on $\{x_1 > 0\}$. What can we say about these waves? Performing a Bloch expansion, we write u as a superposition of Bloch waves. In this superposition, we expect that only those

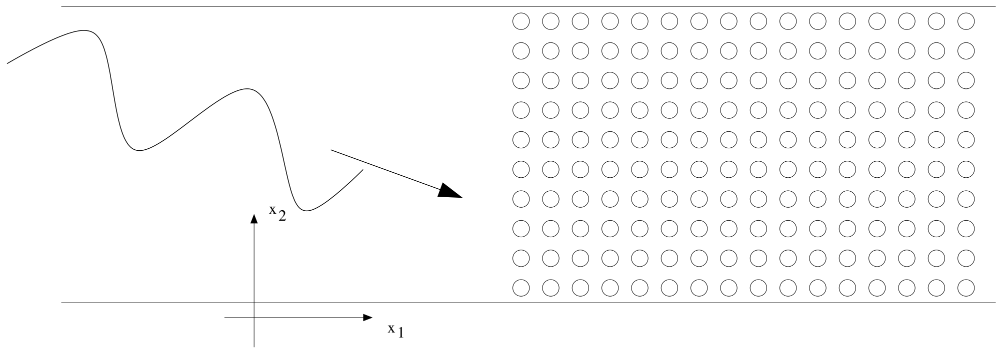

Figure 1: The geometry of the transmission problem for $K = 10$ (number of cells in vertical direction). An incoming wave hits the boundary of a photonic crystal. We are interested in the waves that are generated in the photonic crystal.

waves appear, which satisfy two requirements: (a) the Bloch frequency coincides with the frequency ω. (b) the vertical wave number of the Bloch wave is k_2 ("conservation of the vertical wave number").

> **Question 2:** Let u be the solution of the transmission problem for the incoming wave U_{inc}. Does the Bloch expansion of u in the right half plane respect requirements (a) and (b), i.e.: Is the frequency condition satisfied and is the vertical wave number conserved?

A positive answer to Questions 2 provides information on the negative refraction phenomenon. The requirements (a) and (b) are used in [22] to explain negative refraction without referring to a negative index material: Denoting the m-th Bloch eigenvalue for the wave-vector $j \in Z := [0,1]^2$ as $\mu_m(j)$, the photonic crystal can have the property that the three conditions (a) $\mu_0(j) = \omega^2$, (b) $j_2 = k_2$, and the additional condition (c) $e_1 \cdot \nabla_j \mu_0(j) > 0$ (the group velocity has a positive x_1-component), determine j uniquely. For an appropriately chosen field a, an appropriate frequency ω and an appropriate incoming wave vector k, we have the following situation: $e_2 \cdot k = k_2$ is negative, but the solution j satisfies $e_2 \cdot \nabla_j \mu_0(j) > 0$. This means that a light beam that hits the interface from above (k_2 negative in free space implies that the vertical group velocity is negative) produces a light beam in the photonic crystal that is directed towards the top (vertical group velocity is positive, $e_2 \cdot \nabla_j \mu_0(j) > 0$). With this mechanism, the conditions (a)–(b) can lead to negative refraction. This is outlined in [22], where a specific photonic crystal is described and the negative refraction effect is supported by numerical results. We note that a quite different interpretation is given in [12].

We will answer the above Questions 1 and 2. The precise answers are more complex than one might expect at first sight (we sketch some of the principal difficulties in the next two subsections). We define the outgoing wave conditions in Definition 3.3. We assure that these conditions are *good* conditions by providing a uniqueness result: Theorem 1.2 yields, in a weak sense, the uniqueness of solutions in terms of the Bloch measure. Question 2 is answered with Theorem 1.3: If u is a solution that satisfies the outgoing wave condition, then the corresponding Bloch measure is concentrated in those frequencies that respect (a)–(b). In Section 1.3 we present the mathematical description of our results.

1.1 Outgoing wave conditions

Although we use our results to analyze negative refraction, the core of our mathematical theory is more general: We develop an outgoing wave condition for the Helmholtz equation in a periodic medium. In this section, we sketch some background concerning radiation conditions, mainly in free space. Our aim is to demonstrate the importance of radiation conditions, to show the intimate link between radiation conditions and uniqueness results, and to motivate our mathematical approach.

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 [15]. In unbounded domains, one faces the problem of boundary conditions at infinity. We recall that two fundamental solutions of the Helmholtz equation for $x \in \mathbb{R}^3$ are given by

$$u_+(x) := \frac{1}{|x|} e^{i\omega|x|} \quad \text{and} \quad u_-(x) := \frac{1}{|x|} e^{-i\omega|x|} . \tag{1.3}$$

With the time-dependence $e^{-i\omega t}$, the solution u_+ represents an outgoing wave, u_- an incoming wave. Outgoing waves are expected to be the building stones of solutions of scattering problems, incoming waves should not be present in the expansion of solutions. We note that both elementary solutions decay for $|x| \to \infty$ (even at the same rate), it is therefore not reasonable to demand only a decay property of solutions.

Sommerfeld introduced in [31] for dimension $n = 3$ a radiation condition; until today, it is the standard outgoing wave condition in free space and is named after him:

$$|x|^{(n-1)/2} (\partial_{|x|} u - i\omega u)(x) \to 0 \quad \text{as } |x| \to \infty . \tag{1.4}$$

The solution u_+ satisfies (1.4) and is therefore an admissible building block, u_- does not satisfy (1.4) and is therefore 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 (1.4) 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 [28]. We refer to the overview article [29] for the historical background.

For two reasons, we cannot use the Sommerfeld radiation condition. The obvious point is that we consider x-dependent coefficients a. The interest in x-dependent coefficients is not new: Sommerfeld himself studied the case that a takes two different values in two disjoint half-spaces. In [16], Jäger studied coefficients a that stabilize to constant coefficients for $|x| \to \infty$. Our situation is different, since a is periodic in the right half plane.

The second point is that our situation is neither one- nor two-dimensional. The elementary solution in a strip $\mathbb{R} \times (0, 1)$ with constant coefficients is $e^{i\kappa \cdot x}$ with $\kappa = (\kappa_1, \kappa_2)$ and $|\kappa|^2 = \omega$, which is right-going for $\kappa_1 > 0$ and left-going for $\kappa_1 < 0$. The solution has no decay (similar to the one-dimensional case), but the expression $\partial_{x_1} u - i\omega u$ does not vanish for right-going waves due to the presence of κ_2.

It is not at all clear how to formulate a condition for non-constant coefficients in infinite strips. In our approach, we demand that (at the far right) the projection of

u onto left-going Bloch-waves vanishes. To make the condition precise, we have to deal with the fact that u is not periodic; for this reason, we must consider u on large domains, for large values x_1, and study the corresponding Bloch expansion.

We emphasize that, even though the conditions become more technical, we follow the historical pathway: The expression in (1.4) can be understood as a projection of the solution u onto incoming waves since outgoing waves are filtered out. It is demanded that the projection is small for large radii. We my also formulate our outgoing wave condition (3.6) as follows: At the far right, the solution u can be expanded in a Bloch series that contains only right-going waves. With this requirement, we follow once more Sommerfeld who writes in [31]: "at infinity u must be representable as a sum (or integral) of waves of the divergent traveling type." For more material concerning the situation of a homogeneous material we refer to [11].

On radiation in waveguides and photonic crystals

A radiation condition in a waveguide with varying index in transversal direction is studied in [6]. The "modal radiation condition", formulated in Definition 2.4 of [6], demands for solutions u of the Helmholtz equation that

$$(\mathcal{F}u(x,.))(\lambda) = \hat{\alpha}_\lambda^{\pm} e^{-\sqrt{\lambda}|x|} \qquad \text{for } \pm x > a$$

holds for every λ. Here, $\mathcal{F}$ denotes a generalized Fourier transform and x is the longitudinal independent variable. As in our radiation condition, it is demanded that only outgoing waves ($e^{-\sqrt{\lambda}|x|}$ instead of $e^{+\sqrt{\lambda}|x|}$) are present. The new feature of our approach is that it covers media with oscillations also in longitudinal direction. We cannot use methods that rely on separation of variables and the Fourier transform must be replaced by a Bloch transform.

Also in [4], the radiation of waves inside a photonic crystal is investigated. The connection to our work is even closer since, more precisely, the interface between a photonic crystal and free space is investigated. The fundamental difference to our work is that the underlying frequency ω is assumed to lie in a band-gap of the photonic crystal. For this reason, in [4], waves are found to decay exponentially in the photonic crystal (and no explicit radiation condition must be formulated).

We mention [25] and the references therein for other approaches to radiation conditions, also based on Poynting vectors and incoming and outgoing waves. The time dependent wave-guide problem (using a photonic crystal with a defect) is studied in [21]. The authors show that the dynamics can be approximately described by a nonlinear Schrödinger equation.

We do not relate here our new outgoing wave condition to the approaches that are more oriented to numerics, such as perfectly matched layers or transparent boundary conditions [14, 18].

1.2 Uniqueness and negative refraction

Sommerfeld introduced his radiation condition together with a uniqueness result. We follow his example and provide a uniqueness statement for our outgoing wave condition in photonic crystals. With this result, we can treat the application on negative refraction. Several problems must be tackled in this process and the uniqueness result is, unfortunately, not as strong and simple as one would like it to be.

It is an essential feature of the Helmholtz equation that, even without source terms and with homogeneous boundary conditions, the solution may be nontrivial. One example on a bounded domain is $\Omega = (0, 1) \subset \mathbb{R}^1$ with the solution $u(x) = \sin(\pi x)$ for $\omega = \pi$. A more relevant example in higher dimension (2 or 3) is the Helmholtz resonator: When ω coincides with the resonance frequency, there is a nontrivial solution to homogeneous boundary conditions, see [30]. For regular exterior domains, the Sommerfeld condition implies uniqueness (the Helmholtz operator has only a continuous spectrum and no point spectrum), but this is true only for the original Helmholtz equation with constant coefficients.

In our case of non-constant and (looking globally) non-periodic coefficients, there might be nontrivial surface wave solutions to the Helmholtz equation, which satisfy the radiation condition. An example of such a case are standing wave solutions in photonic crystals with a point defect, compare e.g. [17], Chapter 5. Also in our situation of an interface between free space and photonic crystal, one expects nontrivial solutions, see e.g. [23, 24]. Concerning the mathematical analysis of defects in a photonic crystal and the possibility that they support modes (and hence act as a waveguide) see [5, 13]. Our uniqueness result in the transmission problem must deal with the fact that there might be solutions that are concentrated at the interface or solutions that correspond to waves in the vertical direction. As a consequence, our uniqueness result can provide only the following: Imposing the new radiation condition in photonic crystals:

1. the radiating solution has certain properties *far away from the interface*

2. the radiating solution consists of outgoing waves at infinity, *but may contain additionally waves in vertical direction*

These two points imply that our uniqueness statement has only a weak form. 1. We characterize in Theorem 1.2 only the Bloch measure of solutions, which means that solutions are studied only for large values of $|x_1|$. 2. Given two solutions u and $\tilde{u}$ and their difference $v := u - \tilde{u}$, we cannot show that the Bloch measure of v vanishes; we can only show that the Bloch measure of v is supported on vertically travelling waves.

A second and more technical problem will accompany us on our way to a radiation condition and to the uniqueness result: The geometry is not globally periodic and the solution u is not periodic (and u is, in general, not periodic on any rectangle in the right half plane). For this reason, neither a Bloch transformation of u nor a periodic Bloch expansion of u are meaningful as such. We will have to truncate u on large squares at the far right and consider the Bloch expansion of the result. We must use large squares in order to acchieve that the truncation of u introduces only small errors.

Bloch measures (as used e.g. in [1]) are the appropriate tool for the limit analysis, which is necessary for the following reason: A periodic Bloch expansion uses a discrete set of frequences j. In general, not even the elementary frequency condition $\mu_0(j) = \omega^2$ (the Bloch wave frequency coincides with the frequency of the Helmholtz equation) can be satisfied in a discrete set of frequencies j. For this reason, we cannot expect that the Bloch expansion of u (at a finite distance) satisfies certain conditions (such as the frequency condition), but we must introduce a limiting object (in our case the Bloch measure). Our aim is to derive properties of 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 some methods of [1], in particular in our pre-Bloch expansion. Moreover, the above mentioned problem of waves that are concentrated at the interface of the photonic crystal has a counterpart in [1]: The part of the spectrum that is related to the boundary layer cannot be characterized explicitly (in the sense of [1], where the sequence $\varepsilon_i \to 0$ is fixed, and in contrast to [9], where the sequence $\varepsilon_i \to 0$ is chosen appropriately).

We close this section with more references to negative refraction effects. Negative refraction can be a consequence of a negative index material, see [26] for the effect and [7, 8, 10, 19, 20] for rigorous results, obtained with the tools of homogenization theory. In [12, 27], the negative refraction effect is explained in the spirit of negative index materials. But negative refraction can also occur without a negative index material, see [22]. We note that the photonic crystals in [12] and in [22] are identical and that they do not have a negative effective index in the sense of homogenization. With the work at hand we support the line of argument of [22].

1.3 Main results

Throughout this article we consider the following parameters as fixed: The frequency $\omega > 0$, the height $h > 0$, 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 $k_2 h \in \mathbb{Z}$, $k_1 > 0$ and $4\pi^2|k|^2 = \omega$. The underlying domain is $\Omega := \mathbb{R} \times (0, h)$ and the coefficient field is $a = a^\varepsilon : \Omega \to \mathbb{R}$. We assume $0 < a_* \le a(x) \le a^* < \infty\ \forall x \in \Omega$, $a \equiv 1$ on $\{x_1 < 0\}$, and $a \in C^1$ with ε-periodicity with respect to x_1 and x_2 on $\{x_1 > 0\}$.

We use Bloch expansions of the solution. Let us give a description of our results, focussing on the situation at the far right (the superscript "+" indicates that we study $x_1 > 0$). The Bloch expansion uses two indices, $m \in \mathbb{N}_0 = \{0, 1, 2, ...\}$ numbers the eigenfunctions in the periodicity cell and $j \in Z := [0, 1]^2$ measures the phase shift along one periodicity cell. We collect the two indices in one index as $\lambda := (j, m) \in I := Z \times \mathbb{N}_0$.

To every $\lambda \in I$ we associate a Poynting number $P_\lambda^+ \in \mathbb{R}$, see (3.1). For the Bloch wave with index λ, the number P_λ^+ is a measure for the flux of energy in positive x_1-direction. Our outgoing wave condition demands (in some quantitative form, see Definition 3.3), that the solution does not contain left-going waves on the far right (waves with $P_\lambda^+ < 0$). Our results are formulated with the help of subsets of indices. Waves with vertical energy flux (or no energy flux) correspond to $\lambda \in I$ in

$$I_{=0}^+ := \left\{ \lambda \in I \,|\, P_\lambda^+ = 0 \right\} \subset I := Z \times \mathbb{N}_0 \,,$$

and the set of corresponding $j \in Z$ (for a given $m \in \mathbb{N}_0$) is

$$J_{=0,m}^+ := \left\{ j \in Z \,|\, P_{(j,m)}^+ = 0 \right\} = \left\{ j \in Z \,|\, (j, m) \in I_{=0}^+ \right\} \subset Z = [0, 1]^2 \,.$$

Our results are meaningful for general frequencies $\omega > 0$. Unfortunately, we are only able to prove results 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 $m = 1$.

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

$$\omega^2 < \inf_{j\in Z,\, m\geq 1} \mu_m^+(j)\,, \tag{1.5}$$

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

Our main results concern solutions u of the scattering problem, which we specify as follows: 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 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 $\nu_{l,\infty}^\pm$ of a difference of two solutions (the Bloch measures are introduced in Definition 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 which transport energy in vertical direction.

Theorem 1.2 (Uniqueness up to vertical waves). *Let Assumption 1.1 on the frequency ω be satisfied. For the incoming wave U_{inc} with wave vector k, let u and $\tilde{u}$ be two solutions of the scattering problem. With the difference $v := u - \tilde{u}$, let $\nu_{l,\infty}^\pm$, with $l \in \mathbb{N}_0$, be Bloch measures that are generated by v. Then there holds*

$$\nu_{l,\infty}^\pm = 0 \quad \text{for } l \geq 1\,, \tag{1.6}$$

$$\mathrm{supp}(\nu_{0,\infty}^\pm) \subset J_{=0,0}^\pm\,. \tag{1.7}$$

Our second main results 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 1.3 (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 scattering problem and $\nu_{l,\infty}^\pm$, with $l \in \mathbb{N}_0$, the Bloch measures that are generated by u. Then $\nu_{l,\infty}^\pm = 0$ for $l \geq 1$ and*

$$\mathrm{supp}(\nu_{0,\infty}^\pm) \;\subset\; \left\{ j\in Z \,|\, \mu_0^\pm(j) = \omega^2 \right\} \cap \left(\{ j \in Z \,|\, j_2 = k_2 \} \;\cup\; J_{=0,0}^\pm \right)\,. \tag{1.8}$$

1.4 Further comments on the main results

On the uniqueness result. The uniqueness result of Theorem 1.2 has two weaknesses: The first is related to the presence of vertical waves and of surface waves; these have been discussed above. The second weakness concerns Assumption 1.1: We can derive our results under the assumption that the underlying frequency ω is small; it must lie below the second band of the Bloch energy landscape. Our conjecture is that our results remain valid for arbitrary frequencies (in the form $\mathrm{supp}(\nu_{l,\infty}^\pm) \subset J_{=0,l}^\pm$ for every $l \geq 0$). But due to a lack of orthogonality properties in the bilinear form b (see Section 4), we must exploit the frequency assumption in our uniqueness proof.

A possible scaling in $\varepsilon > 0$. In all our theorems we keep the length scale $\varepsilon > 0$ fixed. In other words: wave-length $1/\omega$ and periodicity length ε are of order 1 and are thus related by a factor of order 1.

It is very interesting to analyze the behavior of light in small micro-structures, i.e. to analyze the limit $\varepsilon \to 0$ (this limit process actually inspired our research). 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, 8, 10, 19, 20]. 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. In this case, the following scaling should be chosen:

$$k^\varepsilon = (k_1^\varepsilon, k_2^\varepsilon) = \frac{1}{\varepsilon}(k_1^*, k_2^*)\,, \qquad \omega^\varepsilon = \varepsilon^{-1}\omega^*\,, \qquad \mu_m^{\varepsilon,\pm}(j) = \varepsilon^{-2}\mu_m^{*,\pm}(j)\,, \tag{1.9}$$

and $U_{\mathrm{inc}}^\varepsilon = e^{2\pi i k^\varepsilon \cdot x}$, which makes the incoming wave of (1.2) ε-dependent. Our methods are adapted to this scaling. Loosely stated, after a rescaling, our Theorem 1.3 yields: The solution u^ε to the scattering problem with incoming wave k^ε consists, at fixed distance $x_1 > 0$ and in the limit $\varepsilon \to 0$, only of Bloch waves that correspond to the frequency ω^* and to the wave number k_2^* (up to vertical waves).

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. Theorem 1.2 is shown in Section 4, Theorem 1.3 is shown in Section 5.

2 Bloch expansions

2.1 Pre-Bloch expansions

We use a discrete expansion which is the first stage of a Bloch expansion (and closely related to the Floquet-Bloch transform). We analyze 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. $\square$

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 $h = K\varepsilon$ 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 $\int_0^h \overline{\Phi(x_2) e^{-2\pi i \tilde{k}_2 x_2/\varepsilon}} \tilde{\Phi}(x_2) e^{2\pi i k_2 x_2/\varepsilon}\, dx_2 = 0$ 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 $K = h/\varepsilon$ denote the number of oscillations 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 an 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.

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 ($h = \varepsilon K$)

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

2.2 Bloch expansion

We now construct the Bloch expansion with the help of the pre-Bloch expansion. This is done by developing each function 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

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

Hence $\Psi^+_j e^{2\pi i j \cdot x/\varepsilon}$ is a solution of the Helmholtz equation on the right half-plane 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 $\mathcal{L}^-_j := -\left(\nabla + 2\pi i j/\varepsilon\right) \cdot \left(\nabla + 2\pi i j/\varepsilon\right)$. 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 increasing in m.*

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 $\fint_{Y_\varepsilon} |\Psi^\pm_{j,m}|^2 = 1$.

A standard symmetry argument yields that all functions $\Psi^\pm_{j,m}(x)\, e^{2\pi i j \cdot x/\varepsilon}$ are orthonormal (at least after an appropriate orthonormalization procedure for multiple eigenvalues). On the left hand side (i.e. for $x_1 < 0$, denoted with the superscript "-"), the Bloch eigenfunctions are exponentials, and the Bloch expansion coincides with a Fourier expansion. We collect properties on the left half-domain in Remark 3.8.

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 $\alpha^+_{j,m} \in \mathbb{R}$,*

$$u(x) = \sum_{j \in Q_K \times Q_K} \sum_{m=0}^{\infty} \alpha^+_{j,m} \Psi^+_{j,m}(x)\, e^{2\pi i j\cdot x/\varepsilon}\,,$$

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

$$u(x) = \sum_{j \in Q_K \times Q_K} \sum_{m=0}^{\infty} \alpha^-_{j,m} \Psi^-_{j,m}(x)\, e^{2\pi i j\cdot x/\varepsilon}\,.$$

To shorten notation, we will use the multi-index $\lambda = (j,m)$ in the index-set $I_K := \{(j,m) | j \in Q_K \times Q_K,\ m \in \mathbb{N}_0\} \subset I := Z \times \mathbb{N}_0$. For a multi-index $\lambda = (j,m)$, the phase shift is extracted with the function $\theta : I \to \mathbb{R}^2$, defined as $\theta((j,m)) := j$. Abbreviating additionally

$$U^\pm_\lambda(x) := \Psi^\pm_\lambda(x)\, e^{2\pi i \theta(\lambda)\cdot x/\varepsilon}\,, \tag{2.8}$$

we may write the formulas of Lemma 2.5 as

$$u(x) = \sum_{\lambda \in I_K} \alpha^\pm_\lambda \Psi^\pm_\lambda(x)\, e^{2\pi i \theta(\lambda)\cdot x/\varepsilon} = \sum_{\lambda \in I_K} \alpha^\pm_\lambda U^\pm_\lambda(x)\,. \tag{2.9}$$

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 $U^\pm_\lambda$, with $h = \varepsilon K$ and $KY_\varepsilon = (0,h) \times (0,h)$,

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

3 Outgoing wave condition

3.1 Poynting numbers and projections

Let $\lambda = (j,m) \in I$ be an index and let $U^\pm_\lambda$ 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

$$\begin{aligned} P^+_\lambda &= \operatorname{Im} ⨍_{Y_\varepsilon} \bar{U}^+_\lambda(x)\, e_1 \cdot \left[a^\varepsilon(x) \nabla U^+_\lambda(x)\right]\, dx\,, \\ P^-_\lambda &= \operatorname{Im} ⨍_{Y_\varepsilon} \bar{U}^-_\lambda(x)\, e_1 \cdot \nabla U^-_\lambda(x)\, dx\,. \end{aligned} \tag{3.1}$$

The number P^+_λ is related to the Poynting vector of the Bloch eigenfunction U^+_λ. It indicates the energy flux of this eigenfunction 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.

The relation to Maxwell's equations is as follows: 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 $\mathrm{Re}(e_1 \cdot P) = \mathrm{Re}(\frac{1}{2}\bar{H}_3 E_2) = (2\omega)^{-1}\mathrm{Re}(-i\,\bar{u}\,\epsilon^{-1}\partial_1 u) = (2\omega)^{-1}\mathrm{Im}(\bar{u}\,a\partial_1 u)$, 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.

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 $\Psi^{\pm}_{j,m}$ and $U^{\pm}_{\lambda}$. They do not depend on K, hence also the values $P^{\pm}_{\lambda}$ 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 $I^{-}_{>0}$, $I^{\pm}_{<0}$, $I^{\pm}_{\geq 0}$, $I^{\pm}_{\leq 0}$, $I^{\pm}_{=0}$ are defined accordingly.

Projections. *For $K \in \mathbb{N}$ we define the projections $\Pi^{\pm}_{>0}$ as follows. For $u \in L^2(KY_\varepsilon;\mathbb{C})$ with discrete Bloch expansion*

$$u(x) = \sum_{\lambda \in I_K} \alpha^{\pm}_{\lambda} U^{\pm}_{\lambda}(x)$$

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

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

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. Indeed, we will later use the projection with $K = R$.

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 fact that u is not periodic in x_1-direction: u cannot be written as a finite sum of Bloch waves. At the same time, we want to formulate a condition that characterizes u for large values of x_1. For these two reasons, we consider u for $x_1 \in (R\varepsilon, 2R\varepsilon)$ with a large natural number $R >> K$.

Definition 3.2 (Bloch expansion far away from the interface)**.** *Let $u \in L^2_{\rm loc}(\mathbb{R} \times (0,h);\mathbb{C})$ 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 $u_R^\pm : RY_\varepsilon \to \mathbb{C}$ by*

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

The functions $u_R^\pm \in L^2(RY_\varepsilon;\mathbb{C})$ have discrete Bloch expansions

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

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.

Definition 3.3 (Outgoing wave condition)**.** *For $K \in \mathbb{N}$, $R \in \mathbb{N}K$ and $h = K\varepsilon$, we consider $u \in L^2_{\rm loc}(\mathbb{R} \times (0,h);\mathbb{C})$. 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*

$$\frac{1}{(\varepsilon R)^2} \int_{RY_\varepsilon} \left|\Pi^+_{<0}(u_R^+)\right|^2 \to 0 \text{ as } R \to \infty\,. \tag{3.6}$$

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

$$\frac{1}{(\varepsilon R)^2} \int_{RY_\varepsilon} \left|(\Pi^-_{>0}(u_R^-)\right|^2 \to 0 \text{ as } R \to \infty\,. \tag{3.7}$$

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 weighted L^2-norm of the resulting function $\Pi^+_{<0}(u_R^+)$ vanishes in the limit $R \to \infty$.

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

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

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 the appendix.

In equation (3.6) we use the projection $\Pi^+_{<0}$. It is not clear if this is the natural choice, one might as well use $\Pi^+_{\le 0}$, which means that vertical waves are also suppressed for $R \to \infty$. Unfortunately, even with that stronger requirement, we could not rule out the appearance of vertical waves in our uniqueness result. We therefore stick with the weaker requirement of (3.6).

3.3 Truncations and $m \ge 1$-projections

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

$$\fint_{W_R} |v|^2 := \frac{1}{|W_R|} \int_{W_R} |v|^2 \,, \qquad \langle v, w\rangle_R := \frac{1}{|W_R|} \int_{W_R} v \cdot \bar{w} \,. \tag{3.8}$$

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. We use a family of smooth cut-off functions $\eta := \eta_R$ with the properties

$$\eta_R \in C^\infty(W_R; \mathbb{R}), \quad \eta_R = 1 \text{ on } W_{R-1}, \quad \|\nabla \eta_R\|_\infty \le 2, \quad \|\nabla^2 \eta_R\|_\infty \le C_0 \tag{3.9}$$

for some R-independent constant C_0, 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 superscipts $\pm$, the eigenvalue corresponding to $\lambda = (j, m)$ is denoted by $\mu_\lambda = \mu_m(j)$. We recall that $\varepsilon > 0$ is fixed.

Lemma 3.4 (The effect of truncations). *For $R \in \mathbb{N}$ let $\eta = \eta_R$ be a family of cut-off functions satisfying* (3.9)*. 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,*

$$\frac{1}{R} \int_{W_R \setminus W_{R-1}} |v_R|^2 + |\nabla v_R|^2 \le C_0 \,, \qquad \frac{1}{R} \int_{W_R \setminus W_{R-1}} |w_R|^2 \le C_0 \,, \tag{3.10}$$

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:*

$$\fint_{W_R} |\mathcal{L}_0(v_R)\eta - \mathcal{L}_0(v_R\eta)|^2 = \fint_{W_R} \left| \mathcal{L}_0(v_R)\eta - \sum_{\lambda \in I_R} \mu_\lambda \langle v_R \eta, U_\lambda \rangle_R \, U_\lambda \right|^2 \le \frac{C}{R} \,. \tag{3.11}$$

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

$$\fint_{W_R} |\Pi(w_R) - \Pi(w_R\,\eta)|^2 \le \fint_{W_R} |w_R - w_R\,\eta|^2 \le \frac{C}{R}\,. \tag{3.12}$$

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 (3.11), 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.

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

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

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

In the second inequality we exploited $\mathrm{supp}(\nabla\eta) \subset (W_R \setminus W_{R-1})$, in the last inequality we used the uniform bounds (3.10). This proves the inquality in (3.11).

Regarding the equality in (3.11) 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

$$\langle \mathcal{L}_0 w, U_\lambda\rangle \overset{(!)}{=} \langle w, \mathcal{L}_0 U_\lambda\rangle = \mu_\lambda \langle w, U_\lambda\rangle\,, \tag{3.13}$$

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

Inequality (3.12) is a direct consequence of linearity and norm-boundedness of the projections:

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

This concludes the proof. $\square$

Remark concerning the need of truncations. One of the fundamental problems of our approach lies in the periodicity conditions of $u_R^\pm$, or, better: the absence of periodicity in x_1-direction. It is for this problem that we have to use large squares and truncations of u_R.

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

To illustrate the point, let us assume that u_R^+ is indeed a periodic solution. In this case, its Bloch expansion reads $u_R^+ = \sum_{\lambda\in I_R}\alpha_\lambda U_\lambda^+$, and the equation provides $\omega^2 u_R^+ = \mathcal{L}_0\sum_{\lambda\in I_R}\alpha_\lambda U_\lambda^+ \overset{(?)}{=} \sum_{\lambda\in I_R}\alpha_\lambda \mathcal{L}_0(U_\lambda^+) = \sum_{\lambda\in I_R}\alpha_\lambda\mu_\lambda^+ U_\lambda^+$. Comparing coefficients with the Bloch expansion of u_R^+ we conclude, by uniqueness of the Bloch coefficients, that $\alpha_\lambda = 0$ for those $\lambda\in I_R$ with $\mu_\lambda^+ \neq \omega^2$: The Bloch expansion of u_R^+ contains only contributions from the basis functions U_λ^+ with $\mu_\lambda^+ = \omega^2$. In particular, we find the following: If the discrete set of $(\mu_\lambda^+)_{\lambda\in I_R}$ does not contain ω^2, then u_R^+ necessarily vanishes.

In the above argument, the equality marked with (?) holds for functions with compact support or, more generally, for periodic functions. For a non-periodic solution, in general, there holds $\mathcal{L}_0\sum_{\lambda\in I_R}\alpha_\lambda U_\lambda \neq \sum_{\lambda\in I_R}\alpha_\lambda\mathcal{L}_0(U_\lambda)$.

Lemma 3.5 (Contributions from energy levels $m\geq 1$)**.** *Let ω satisfy the smallness* (1.5) *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* (3.9)*. Then, with a constant C that is independent of R:*

$$\fint_{W_R}\left|\Pi^{\mathrm{ev},\pm}_{m\geq 1}(u_R^\pm)\right|^2 \leq \frac{C}{R} \qquad \textit{and} \qquad \fint_{W_R}\left|\Pi^{\mathrm{ev},\pm}_{m\geq 1}(u_R^\pm\,\eta)\right|^2 \leq \frac{C}{R}\,. \tag{3.14}$$

Proof. We perform the proof for the superscript "+". Relation (3.12) applied to u_R^+ provides

$$\fint_{W_R}\left|\Pi^{\mathrm{ev},+}_{m\geq 1}(u_R^+) - \Pi^{\mathrm{ev},+}_{m\geq 1}(u_R^+\,\eta)\right|^2 \leq \frac{C}{R}\,.$$

Indeed, by the uniform L^2-bounds of u, the condition $\frac{1}{R}\int_{W_R\setminus W_{R-1}}|u_R^+|^2 \leq C_0$ 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 (3.14), we show the second.

We now exploit Assumption 1.1. Due to (1.5), there exists $\delta > 0$ such that $|\omega^2 - \mu_\lambda|^2 \geq \delta$ for all $\lambda = (j,m)$ with $m\geq 1$. We therefore find

$$\begin{aligned}
\delta\fint_{W_R}\left|\Pi^{\mathrm{ev},+}_{m\geq 1}(u_R^+\,\eta)\right|^2 &= \delta\sum_{\substack{\lambda=(j,m)\in I_R\\ m\geq 1}}\left|\left\langle u_R^+\,\eta, U_\lambda\right\rangle_R\right|^2 \leq \sum_{\substack{\lambda=(j,m)\in I_R\\ m\geq 1}}\left|(\omega^2-\mu_\lambda)\langle u_R^+\,\eta, U_\lambda\rangle_R\right|^2\\
&\leq \sum_{\lambda\in I_R}\left|\left\langle \omega^2 u_R^+\,\eta, U_\lambda\right\rangle_R - \left\langle \mu_\lambda u_R^+\,\eta, U_\lambda\right\rangle_R\right|^2 = \sum_{\lambda\in I_R}\left|\left\langle \mathcal{L}_0(u_R^+)\,\eta, U_\lambda\right\rangle_R - \left\langle \mu_\lambda u_R^+\,\eta, U_\lambda\right\rangle_R\right|^2\\
&= \fint_{W_R}\left|\mathcal{L}_0(u_R^+)\eta - \sum_{\lambda\in I_R}\mu_\lambda\langle u_R^+\eta, U_\lambda\rangle_R\, U_\lambda\right|^2 \leq \frac{C}{R}\,.
\end{aligned}$$

In the second line we used that $\mathcal{L}_0(u_R^+) = \omega^2 u_R^+$ holds pointwise almost everywhere in W_R. In the last inequality we used (3.11), exploiting the uniform H^1-bounds provided by Lemma A.3. This concludes the proof. $\square$

3.4 Other forms of the outgoing wave condition

Let $\eta = \eta_R$ be a family of cut-off functions as in (3.9). In view of Relation (3.12) of Lemma 3.4, the outgoing wave conditions (3.6) and (3.7) are equivalent to outgoing wave conditions for the truncated functions $u_{R,\eta}^\pm := u_R^\pm \eta$. More precisely, they are equivalent to the conditions

$$\fint_{W_R} \left|\Pi_{<0}^+(u_{R,\eta}^+)\right|^2 \to 0 \quad \text{and} \quad \fint_{W_R} \left|(\Pi_{>0}^-(u_{R,\eta}^-)\right|^2 \to 0 \quad \text{as} \quad R \to \infty\,. \tag{3.15}$$

In the proof of our uniqueness result we will use (3.15) 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

$$B_R^+(w) := \operatorname{Im} \fint_{W_R} \bar{w}(x) e_1 \cdot [a^\varepsilon(x)\nabla w(x)]\ dx\,. \tag{3.16}$$

The quadratic expression B_R^- is defined by the same expression, with the only difference that $a^\varepsilon(x)$ is replaced by 1.

Definition 3.6 (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 $u_{R,\eta}^\pm$ as in* (3.15). *We say that u satisfies the energetic outgoing wave condition on the right, if*

$$B_R^+\left(\Pi_{<0}^+ \Pi_{m=0}^{\mathrm{ev},+}(u_{R,\eta}^+)\right) \to 0 \text{ as } R \to \infty\,. \tag{3.17}$$

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

$$B_R^-\left(\Pi_{>0}^- \Pi_{m=0}^{\mathrm{ev},-}(u_{R,\eta}^-)\right) \to 0 \text{ as } R \to \infty\,. \tag{3.18}$$

In two respects, the condition (3.17) is similar to the condition (3.15): 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 $m \geq 1$ can be neglected and we consider only $\Pi_{m=0}^{\mathrm{ev},+}(u_{R,\eta}^+)$. Furthermore, this function is projected to left-going waves, i.e. only $\Pi_{<0}^+ \Pi_{m=0}^{\mathrm{ev},+}(u_{R,\eta}^+)$ is studied. The main difference between the two conditions is that, instead of looking at the weighted L^2-norm, one demands in (3.17) a decay property for the energy-flux quantity B_R^+. At the end of this section, we will see that condition (3.15) (together with the uniform L^2-bounds and the solution property) implies (3.17).

The definition of B_R^+ in (3.16) suggests to introduce additionally the (nonsymmetric) sesquilinear forms $b_R^\pm : L^2(W_R;\mathbb{C}) \times H^1(W_R;\mathbb{C}) \to \mathbb{C}$,

$$\begin{aligned} b_R^+(u,v) &:= \fint_{W_R} \bar{u}(x)\, e_1 \cdot [a^\varepsilon(x)\nabla v(x)]\ dx\,, \\ b_R^-(u,v) &:= \fint_{W_R} \bar{u}(x)\, e_1 \cdot \nabla v(x)\, dx\,. \end{aligned} \tag{3.19}$$

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

$$\begin{aligned} B^+_R(\Pi^+_{<0}u^+_{R,\eta}) &= \operatorname{Im} b^+_R\left(\Pi^+_{<0}u^+_{R,\eta}, \Pi^+_{<0}u^+_{R,\eta}\right) \\ &= \operatorname{Im} \fint_{W_R} \overline{\Pi^+_{<0}u^+_{R,\eta}(x)} e_1 \cdot \left[a^\varepsilon(x)\nabla(\Pi^+_{<0}u^+_{R,\eta})(x)\right] \, dx\,. \end{aligned}$$

The connection to $P^\pm_\lambda$ is given by

$$P^\pm_\lambda = B^\pm_R(U^\pm_\lambda) = \operatorname{Im} b^\pm_R\left(U^\pm_\lambda, U^\pm_\lambda\right)\,. \tag{3.20}$$

Let us collect some properties of the sesquilinear forms $b^\pm_R$.

Lemma 3.7 (Properties of the sesquilinear form $b^\pm_R$)**.** *For $R \in \mathbb{N}$, the following holds:*

1. Orthogonality property of $b^\pm_R$. *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 $U^\pm_\lambda, U^\pm_{\tilde\lambda}$ of* (2.8) *satisfy*

$$b^\pm_R(U^\pm_\lambda, U^\pm_{\tilde\lambda}) = 0\,. \tag{3.21}$$

2. Convergence property of $b^\pm_R$. *Let sequences $u_R, v_R \in H^1(W_R;\mathbb{C})$ be such that*

$$\fint_{W_R} |u_R|^2 + |\nabla v_R|^2 \le C_0 \tag{3.22}$$

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

$$b^\pm_R(u_R, v_R) \to 0\,.$$

Proof. 1. We prove (3.21) for $U^+_\lambda, U^+_{\tilde\lambda}$, the argument for $U^-_\lambda, U^-_{\tilde\lambda}$ is analogous. We have to show that

$$b^+_R(U^+_\lambda, U^+_{\tilde\lambda}) = \fint_{W_R} \overline{U^+_\lambda}(x)\, e_1 \cdot \left[a^\varepsilon(x)\nabla U^+_{\tilde\lambda}(x)\right] \, dx \overset{!}{=} 0\,.$$

By definition of U^+_λ and $U^+_{\tilde\lambda}$ there holds

$$\begin{aligned} \overline{U^+_\lambda}(x) &= \overline{\Psi^+_\lambda}(x) e^{-i2\pi j\cdot x/\varepsilon}, \\ \nabla U^+_{\tilde\lambda}(x) &= \left[\nabla\Psi^+_{\tilde\lambda}(x) + (i2\pi\tilde j/\varepsilon)\,\Psi^+_{\tilde\lambda}(x)\right] e^{i2\pi\tilde j\cdot x/\varepsilon} \end{aligned}$$

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 the appendix, 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

$$\begin{aligned} \left|b^+_R(u_R, v_R)\right| &= \left|\fint_{W_R} \bar u_R(x)\, e_1 \cdot [a^\varepsilon(x)\nabla v_R(x)] \, dx\right| \\ &\le \|a^\varepsilon\|_\infty \left(\fint_{W_R} |u_R|^2\right)^{1/2} \left(\fint_{W_R} |\nabla v_R|^2\right)^{1/2} \to 0 \quad \text{as } R \to \infty\,, \end{aligned}$$

which concludes the proof. □

Lemma 3.7 shows that the outgoing wave condition (3.15) together with the L^2-bounds of Definition 3.3 imply (3.17). Indeed, by (3.15), there holds

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

Moreover, $\Pi^+_{<0}\Pi^{\mathrm{ev},+}_{m=0}(u^+_{R,\eta})$ satisfies $\fint_{W_R} |\nabla\left(\Pi^+_{<0}\Pi^{\mathrm{ev},+}_{m=0}(u^+_{R,\eta})\right)|^2 \le C$ with C independent of R due to Lemma A.3 and Lemma A.4 of the appendix. Lemma 3.7 provides

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

and hence (3.17).

In free space, Bloch waves are exponentials. We conclude this section with a remark concerning the situation for $x_1 < 0$, indicated with the superscript "-". Here, the Bloch waves are exponential functions and some quantities can be expressed explicitly.

Remark 3.8 (Basis functions and index sets on the left)**.** *The functions $\Psi^-_{j,m}$ are ε-periodic eigenfunctions of the operator $\mathcal{L}^-_j = -(\nabla + 2\pi i j/\varepsilon)\cdot(\nabla + 2\pi i j/\varepsilon)$, hence they are of the form* $\exp(2\pi i k\cdot x/\varepsilon)$*. For fixed j and some numbering $k = k^{(j)} : \mathbb{N}_0 \to \mathbb{Z}^2$:*

$$\Psi^-_{j,m}(x) = e^{2\pi i k(m)\cdot x/\varepsilon}\,, \qquad \mu^-_m(j) = 4\pi^2\frac{|k(m)+j|^2}{\varepsilon^2}\,. \tag{3.23}$$

For $\lambda = (j,m)$ there holds

$$\begin{aligned} U^-_\lambda(x) &= e^{2\pi i (k(m)+j)\cdot x/\varepsilon}\,,\\ P^-_\lambda &= \operatorname{Im}\fint_{Y_\varepsilon} \bar U^-_\lambda(x) e_1\cdot\nabla U^-_\lambda(x)\,dx = \frac{2\pi}{\varepsilon}\left(k_1(m)+j_1\right)\,,\\ I^-_{<0} &= \left\{\lambda\in I \,|\, k_1(m)+j_1 < 0\right\}\,, \end{aligned}$$

and analogous characterizations of other index sets.

4 Uniqueness properties of the system

Our aim is to show uniqueness properties of the scattering problem (1.1) 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 a Cauchy-Schwarz 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 non-trivial solutions for vanishing U_{inc}). But we can show that the functions $v^\pm_R$ consist, in the limit $R\to\infty$, only of vertical waves. It turns out that the right object to study is the *Bloch measure* associated with $v^\pm_R$.

We recall that the frequency assumption (1.5) implies that, in the limit $R\to\infty$, the discrete Bloch expansions of $u^\pm_R$ contain only modes corresponding to $\lambda = (j,m)$ with $m = 0$, see Lemma 3.5.

4.1 Bloch measures

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 (3.9). 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 $R \to \infty$, weakly in the sense of measures,

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

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

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

Instead of using the discrete Bloch measures $\nu_{l,R}^\pm$ associated with $u_{R,\eta}^\pm$, one can equivalently consider the discrete Bloch measures $\tilde\nu_{l,R}^\pm$ associated with $u_R^\pm$ (no cut-off function). Indeed, in the limit $R \to \infty$ one obtains

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

weakly in the sense of measures.

4.2 Uniqueness in the sense of Bloch measures

Up to this point (with the exception of Lemma 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* (3.9) *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 $R \to \infty$,*

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

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

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

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

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

On the left-hand side, we recognize the sesquilinear forms $b^\pm_R$ of (3.19). 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

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

and therefore, by Lemma 3.7,

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

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

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

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 3.7 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 3.7 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:

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

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 3.7. Exploiting the outgoing wave condition (3.15) on the right or, better, the weaker expression (3.17), we find that the first term on the right hand side of (4.11) vanishes in the limit $R \to \infty$. Hence

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

We emphasize that we only used the energetic outgoing wave condition (3.17) 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 the Bloch measures. We analyze (4.13) further, exploiting the discrete Bloch expansion of $v^\pm_{R,\eta} = \sum_{\lambda \in I_R} \alpha^\pm_{\lambda,R} U^\pm_\lambda$:

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

In the last line we again exploited the orthogonality of the sesquilinear form b_R^+ in the wave number j, see Lemma 3.7, and the relation (3.20) 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 Theorem 1.2

In what follows we will show that solutions to the Helmholtz equation (1.1) are unique up to waves with vanishing energy flux to the left and to the right (called vertical waves). We use, for $l \in \mathbb{N}_0$, the index sets

$$J^\pm_{=0,l} := \{ j \in Z = [0,1]^2 \,|\, P^\pm_\lambda = 0 \text{ for } \lambda = (j,l)\}\,. \tag{4.14}$$

We are now in the position to prove our uniqueness result. Loosely speaking, we find that the difference of two solutions can contain only vertical waves at infinity.

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*

$$\nu^{\pm}_{l,\infty} = 0 \qquad \text{for } l \geq 1, \tag{4.15}$$

$$\operatorname{supp}(\nu^{\pm}_{0,\infty}) \subset J^{\pm}_{=0,0}\,. \tag{4.16}$$

Proof. We will only prove the statement for the limiting Bloch measures $\nu^{+}_{l,\infty}$, the argument for $\nu^{-}_{l,\infty}$ is analogous. Let $v^{+}_{R,\eta} = \sum_{\lambda \in I_R} \alpha^{+}_{\lambda,R} U^{+}_{\lambda}$. Then the corresponding 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 (3.14) 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 therefore

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

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

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

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

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

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

Since the function $Z \ni j \mapsto P^{+}_{\lambda=(j,0)} \in \mathbb{R}$ is continuous, we have

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

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

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

This shows (4.16) for "+", since ϕ with support outside $J^{+}_{=0,0}$ was arbitrary. The argument for "-" is analogous. □

Proof of Theorem 1.2. The difference v of two solutions satisfies the outgoing wave condition without an incident wave. Theorem 1.2 is therefore an immediate consequence of Proposition 4.4. $\square$

5 Proof of Theorem 1.3

In this section we prove Theorem 1.3. We therefore assume from now on that we are in the situation of that theorem: Assumption 1.1 on $\omega > 0$ is satisfied and u is a solution of the scattering problem with incoming wave $U_{\rm inc}$, 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 $u - U_{\rm inc}$ 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 (1.5) is satisfied and we can therefore use Lemma 3.5. As in Proposition 4.4, case $l \geq 1$, we conclude from (3.14) (and the analogous result for "-") that $\nu^\pm_{l,\infty} = 0$ holds for every $l \geq 1$.

Theorem 1.3 is shown once that we verify the following two properties of the Bloch measure $\nu^\pm_{0,\infty}$:

$$\mathrm{supp}(\nu^\pm_{0,\infty}) \subset \{j \in Z | j_2 = k_2\} \cup J^\pm_{=0,0}\,, \tag{5.1}$$

$$\mathrm{supp}(\nu^\pm_{0,\infty}) \subset \left\{j \in Z | \mu^\pm_0(j) = \omega^2\right\}\,. \tag{5.2}$$

We note that, on the left, we have $\mu^-_0(j) = 4\pi^2|j|^2/\varepsilon^2$ by (3.23).

1.) Proof of (5.1). We consider the projection $\Pi^{\rm vert}_{k_2} u$ of u. This function is again a solution of the scattering problem. Indeed, by Lemma A.2 one has $\Pi^{\rm vert}_{k_2} u \in H^1_{\rm loc}(\mathbb{R} \times (0,h); \mathbb{C})$ with periodicity in the x_2-variable, and for arbitrary test functions $\varphi \in C^\infty_c(\mathbb{R} \times (0,h))$ there holds

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

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

As a consequence, the difference $v := u - \Pi^{\rm vert}_{k_2} u$ is a solution of the scattering problem with vanishing incoming wave (just as the difference of two solutions in the proof of Theorem 1.2). The uniqueness 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 $\Pi^{\rm vert}_{k_2} u$ 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 $\Pi^{\rm vert}_{k_2} u$ vanish.

Since the Bloch measure of u can have its support only in the union of the supports corresponding to $\Pi^{\rm vert}_{k_2} u$ and $u - \Pi^{\rm vert}_{k_2} u$, the claim (5.1) follows.

2.) Proof of (5.2). We perform a calculation that is similar to that of the uniqueness proof. Let $\phi : Z \to \mathbb{R}$ be continuous and bounded with $\mathrm{supp}(\phi) \cap \{j | \mu_0(j) = \omega^2\} = \emptyset$.

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 $j \in \mathrm{supp}(\phi)$. 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 $R \to \infty$,

$$\begin{aligned} 0 \leq \delta \int_Z \phi \, d\nu_{0,\infty}^+ \leftarrow \delta \int_Z \phi \, d\nu_{0,R}^+ &= \delta \sum_{\lambda=(j,0)\in I_R} |\alpha_{\lambda,R}^+|^2 \phi(j) \\ \leq \sum_{\lambda=(j,0)\in I_R} (\mu_0(j) - \omega^2) |\alpha_{\lambda,R}^+|^2 \phi(j) \, . \end{aligned} \tag{5.3}$$

The result $\int_Z \phi \, d\nu_{0,\infty}^+ = 0$ is shown once we prove that the right hand side of (5.3) 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 $U_\lambda^\pm$ we obtain

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

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 (5.3) is small for large $R > 0$. This proves $\int_Z \phi \, d\nu_{0,\infty}^+ = 0$ and hence (5.2) for "+". The proof for "-" is analogous, Theorem 1.3 is shown.

6 Outlook and conclusions

On the existence of solutions

We conclude with 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 $\omega > 0$, 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), there exists a solution u of the scattering problem (described before Theorem 1.2).

The idea for an existence proof is the limiting absorption principle: For a positive artificial damping parameter $\delta > 0$, we consider the equation

$$-\nabla \cdot ((1 + i\delta) a(x) \nabla u^\delta(x)) = \omega^2 u^\delta(x) \tag{6.1}$$

for $x \in \Omega = \mathbb{R} \times (0, h)$. Due to the strictly positive 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, we 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 intricate part of this approach is to show the second property: The limit u satisfies the outgoing wave condition. We do not see a straightforward argument that yields this condition.

Conclusions

We have investigated the 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.

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.

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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*

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

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*

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

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

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

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

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

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

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

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 $u \in H^1_{\rm loc}(\mathbb{R} \times (0,h);\mathbb{C})$ be periodic in the x_2-variable. Then the function $\Pi^{\rm vert}_{k_2} u \in H^1_{\rm loc}(\mathbb{R} \times (0,h);\mathbb{C})$ is periodic in x_2 and there holds*

$$\nabla \left(\Pi^{\rm vert}_{k_2} u\right) = \Pi^{\rm vert}_{k_2} \left(\nabla u\right) . \tag{A.3}$$

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

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

which proves (A.3). □

Lemma A.3 (Caccioppoli estimate). *Let $u \in L^2_{\rm loc}(\mathbb{R} \times (0,h))$ 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*

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

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

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

The Cauchy-Schwarz inquality is used to treat the last term, the first factor is absorbed with Young's inquality 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 $\Pi^{\rm ev}$). *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*

$$\fint_{W_R} \left|\nabla\left(\Pi^{\mathrm{ev},\pm}_{m=0} v_R\right)\right|^2 + \left|\nabla\left(\Pi^{\mathrm{ev},\pm}_{m\geq 1} v_R\right)\right|^2 + \left|\nabla\left(\Pi\left(\Pi^{\mathrm{ev},\pm}_{m=0} v_R\right)\right)\right|^2 \leq C\,. \tag{A.7}$$

2. *If, additionally,* $\fint_{W_R} \left|\Pi^{\mathrm{ev},\pm}_{m\geq 1} v_R\right|^2 \to 0$ *as* $R\to\infty$*, then there holds*

$$\fint_{W_R} \left|\nabla\left(\Pi^{\mathrm{ev},\pm}_{m\geq 1} v_R\right)\right|^2 \to 0 \qquad \text{as } R\to\infty\,. \tag{A.8}$$

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 $0 < a_* \leq \inf a^\varepsilon$,

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

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 $\mathcal{L}_0(\Pi^{\mathrm{ev}}_{m=0} v_R) = \Pi^{\mathrm{ev}}_{m=0}(\mathcal{L}_0 v_R)$, as shown in (3.13). In the last line we exploited the norm-boundedness of projections. The claim for $\Pi(\Pi^{\mathrm{ev}}_{m=0} v_R)$ is shown analogously, exploiting 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 $R\to\infty$,

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

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

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