Time-harmonic scattering of plane waves from an infinite periodically inhomogeneous medium

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Abstract

We propose a new radiation condition for an infinite inhomogeneous two-dimensional medium which is periodic in the vertical direction and remains invariant in the horizontal direction. The classical Rayleigh-expansion radiation condition does not apply to our case, because this would require the medium to be inhomogeneous in a half plane. We utilize the Floquet theory to derive upward/downward wave modes and define radiation conditions by expansions w.r.t. these modes. The downward radiation conditions leads to a downward Dirichlet-to-Neumann map which can be used to truncate the infinite inhomogeneous domain in the vertical direction. So we prove mapping properties of the upward/downward Dirichlet-to-Neumann maps based on the asymptotic behavior of high-order wave modes. Finally, we verify the strong ellipticity of the sesquilinear form corresponding to the new scattering problem and show the unique solvability for all wavenumbers with the exception of a countable set of numbers bounded below by a small positive constant.

Keywords: radiation condition; Helmholtz equation; inhomogeneous medium; uniqueness and existence.

1 Introduction

Time-harmonic scattering problems for periodic gratings have attracted considerable attention in the mathematical community (cf. e.g. [1, 2, 4, 10]). A key issue for the scattering problems in unbounded domains is how to characterize an outgoing radiation condition at infinity. A physical-meaningful radiation condition should guarantee well-posedness of the mathematical model. Another motivation for studying radiation conditions is the design of efficient numerical schemes and the convergence analysis. With the help of radiation conditions, one can construct an appropriate Dirichlet-to-Neumann map to reduce the unbounded physical domain to a bounded computational domain. In periodic structures, the classical Rayleigh-expansion radiation condition applies to scattering of plane waves in homogeneous media. However, inhomogeneous media play an important role in practical applications, such as photonic crystals [9] and periodic waveguides, etc. The purpose of this work is to derive radiation conditions in an open periodic waveguide lying above an infinitely inhomogeneous medium and to prove solvability results for the scattering of plane waves by such kind of periodic media.

We consider the time-harmonic scattering of plane waves by a two-dimensional and horizontally periodic grating structure between a homogeneous cover and a substrate, which is periodically inhomogeneous w.r.t. the vertical direction (see Figure 1). Plane wave incidence together with the periodicity of the medium in horizontal direction gives rise to the quasi-periodicity of the wave fields. A challenging problem is to handle the infinity of the inhomogeneous medium in the substrate. Similarly to the generalized plane-wave modes in the derivation of the classical Rayleigh expansion, we can obtain wave modes by solving an ordinary differential equation with periodic coefficients. Then we can define the upward and downward radiation conditions by choosing outgoing bounded wave modes. Using these radiation conditions, we construct a downward Dirichlet-to-Neumann (DtN) map and formulate the boundary value problem in a periodic cell. We show some mapping properties of the DtN map and prove that the sesquilinear form in the variational formulation, corresponding to our boundary value problem, is strongly elliptic. Furthermore, uniqueness and existence of weak solutions are proved for all incident angles if the positive wavenumber is sufficiently small or if it is not in a countable set of exceptional wavenumbers with the only accumulating point at infinity. If the refractive index in the substrate depends only on the horizontal coordinate, upward and downward radiating modes can be derived by solving a one-dimensional Sturm-Liouville eigenvalue problem for an ODE in matrix form (see the authors' previous work [8]). This current work together with [8] provides a first insight into the well-posedness of scattering problems in an infinitely bi-periodic inhomogeneous medium.

In closed periodic waveguides [7], Fliss and Joly use the Floquet-Bloch theory and dispersion relations to classify the wave modes propagating into two different directions, under the assumption of non-vanishing group velocity for dispersion curves. Then outgoing radiation conditions are obtained by applying the Limiting Absorption Principle (LAP). Comparing [7] with the current work, we can define an explicit DtN operator without using LAP and with more mapping properties in Sobolve spaces. One reason for this lies in the fact that, due to plane-wave incidence, the solution modes depend explicitly on the the horizontal coordinate. In a series of works by Kirsch and coauthors [12, 11, 13], radiation conditions for open periodic waveguides with local perturbations are derived mostly motivated by the LAP arguments of [7]. However, these are confined to homogeneous background media. Further, uniqueness and existence of solutions caused by a compactly supported source term are verified in those papers. In contrast, here we consider open periodic waveguides, but restrict our attention to scattering problems for plane-wave incidence into an infinite and inhomogeneous medium, without using LAP arguments. The mathematical setting of this work is close to that of Lamacz and Schweizer [14], who derive a radiation condition for photonic crystals in a bi-periodic medium. Based on Bloch expansions and the Poynting vector, they construct an outgoing wave condition which only contains outgoing Bloch waves. Altogether, all of the above works extend the Rayleigh-expansion radiation condition from infinite homogeneous periodic settings to more complicated periodic materials. The advantage of our research methodology lies in its ability to obtain explicit wave modes and prove stronger solvability results by the DtN method.

This paper is organized as follows. In Section 2, we introduce the medium, which is 2π-periodic in vertical direction. We use the Floquet theory to get the wave modes and then define the radiation condition in Section 3. In Section 4, we construct the Dirichlet-to-Neumann map based on the new radiation condition. Then a boundary value problem for a grating between a homogeneous and an inhomogeneous periodic medium is formulated. We apply the variational method to discuss the solvability of the problem. Under a few technical conditions, we show the existence of a unique solution for the boundary value problem for any wavenumber k not contained in an at most countable set of exceptional wavenumbers. In other words, consider a horizontically periodic grating structure above a substrate, the refractive index of which is periodic in vertical and constant in horizontal direction. Then we prove that (cf. Theorem 4.4), with the exception of countable wavenumbers, the problem of plane waves scattered by the grating has a unique solution.

2 Quasiperiodic boundary value problem in an inhomogeneous half space

We first introduce the geometry of the problem, as shown in Figure 1. Choose real numbers b and d with $d > b$ and the two lines, $\Gamma_d := \{x = (x_1, x_2)^{\mathrm{T}} \in \mathbb{R}^2 \colon x_2 = d\}$ and $\Gamma_b := \{x = (x_1, x_2)^{\mathrm{T}} \in \mathbb{R}^2 \colon x_2 = b\}$, which divide $\mathbb{R}^2$ into the three regions

$$\begin{aligned}
\Omega_d^+ &:= \{(x_1, x_2)^{\mathrm{T}} \in \mathbb{R}^2 \colon x_2 > d\},\\
\Omega &:= \{(x_1, x_2)^{\mathrm{T}} \in \mathbb{R}^2 \colon b < x_2 < d\},\\
\Omega_b^- &:= \{(x_1, x_2)^{\mathrm{T}} \in \mathbb{R}^2 \colon x_2 < b\}.
\end{aligned}$$

The medium in $\mathbb{R}^2$ is characterized by the refraction index $\tilde{q}(x_1, x_2) \in L^\infty(\mathbb{R}^2)$ such that

$$\tilde{q}(x_1, x_2) = \begin{cases} 1, & \text{in } \Omega_d^+,\\ q_0(x_1, x_2), & \text{in } \Omega,\\ q(x_2), & \text{in } \Omega_b^-. \end{cases}$$

Here the first function $x = (x_1, x_2)^{\mathrm{T}} \mapsto q_0(x_1, x_2)$ is supposed to be $\mathtt{p}$-periodic w.r.t. x_1 ($\mathtt{p} > 0$) and bounded w.r.t. x_2 in Ω. The second function $x_2 \mapsto q(x_2)$ is real-valued and bounded w.r.t. $x_2 \in (-\infty, b]$. Furthermore, we assume $\operatorname{Im} q_0(x_1, x_2) \geqslant 0$, $\operatorname{Re} q_0(x_1, x_2) > 0$ for all $x \in \Omega$ and $q(x_2) > 0$ for all $x_2 < b$. Let $u^{\mathrm{in}}(x_1, x_2) := e^{i\hat{\alpha}x_1 - i\beta x_2}$ be the field incident from the region Ω_d^+, where $\hat{\alpha} := k \sin\theta$, $\beta := k\cos\theta$, k is the positive wavenumber, and $\theta \in (-\pi/2, \pi/2)$ the angle of incidence. Since the medium in Ω_d^+ is homogeneous, u^{in} satisfies the Helmholtz equation

$$\Delta u^{\mathrm{in}} + k^2 u^{\mathrm{in}} = 0 \text{ in } \Omega_d^+.$$

The infinite region Ω_b^- is supposed to be filled by an infinitely periodic medium characterized by the 2π-periodic refractive index $q(x_2)$. Then the total field u can be written as

$$u = \begin{cases} u^{\mathrm{in}} + u^{\mathrm{sc}} & \text{in } \Omega_d^+,\\ u & \text{in } \Omega,\\ u^{\mathrm{tr}} & \text{in } \Omega_b^-, \end{cases}$$

where u^{sc} is the scattered and u^{tr} the transmitted field. The time-harmonic acoustic wave propagation in $\mathbb{R}^2$ is governed by the Helmholtz equation

$$\Delta u(x_1, x_2) + k^2 \tilde{q}(x_1, x_2) u(x_1, x_2) = 0 \;, (x_1, x_2)^{\mathrm{T}} \in \mathbb{R}^2,$$

where u denotes the pressure of an acoustic wave or a transverse field component of a polarized electromagnetic wave.

Remark 2.1. A radiation condition needs to be imposed at infinity to ensure the well-posedness of the diffraction problem. We recall that, in the case $q(x_2) \equiv 1$ in Ω_b^-, the solution u satisfies the downward radiating (outgoing) classical Rayleigh-expansion radiation condition if u admits a Rayleigh expansion

$$u(x) = \sum_{n \in \mathbb{Z}} u_n e^{i(\alpha_n x_1 - \beta_n (x_2 - b))}, \; u_n \in \mathbb{C}, \; x_2 < b, \tag{2.1}$$

where $i = \sqrt{-1}$ and

$$\alpha_n := \hat{\alpha} + \frac{2\pi}{\mathtt{p}} n, \; \beta_n := \begin{cases} \sqrt{k^2 - \alpha_n^2} & \text{if } \alpha_n^2 \le k^2,\\ i\sqrt{\alpha_n^2 - k^2} & \text{if } \alpha_n^2 > k^2. \end{cases} \tag{2.2}$$

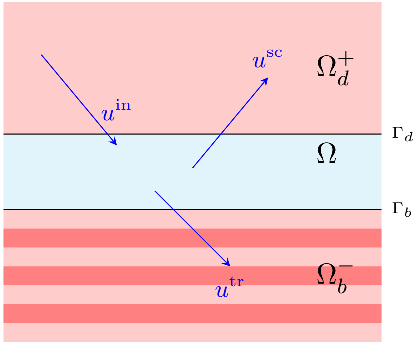

Figure 1: Geometry of the diffraction problem.

For Ω_b^-, we shall define generalized upward and downward propagating radiation conditions later. These new radiation conditions will generalize the above Rayleigh-expansion radiation condition from the infinite homogeneous medium to an infinite medium, the refractive index q of which is periodic in the vertical direction but remains invariant in the horizontal direction.

Definition 2.1. The wave function u is called $\hat{\alpha}$-quasi-periodic in x_1 with the parameter $\hat{\alpha} := k\sin\theta$, $\theta \in (-\pi/2, \pi/2)$, if $x_1 \mapsto u(x_1, x_2)e^{-i\hat{\alpha}x_1}$ is p-periodic for any fixed x_2.

Define the quasi-periodic Sobolev spaces on Ω_d^+, Ω_b^-, and $\mathbb{R}$ by

$$\begin{aligned} H^1_{\hat{\alpha}}(\Omega_d^+) &:= \{u \in H^1_{loc}(\Omega_d^+) : u \text{ is } \hat{\alpha}\text{-quasi-periodic in } x_1\}, \\ H^1_{\hat{\alpha}}(\Omega_b^-) &:= \{u \in H^1_{loc}(\Omega_b^-) : u \text{ is } \hat{\alpha}\text{-quasi-periodic in } x_1\}, \\ H^{1/2}_{\hat{\alpha}}(\mathbb{R}) &:= \{f \in H^{1/2}_{loc}(\mathbb{R}) : e^{-i\hat{\alpha}x_1}f(x_1) \text{ is } \mathsf{p}\text{-periodic in } x_1\}, \\ H^{-1/2}_{\hat{\alpha}}(\mathbb{R}) &:= \{f \in H^{-1/2}_{loc}(\mathbb{R}) : e^{-i\hat{\alpha}x_1}f(x_1) \text{ is } \mathsf{p}\text{-periodic in } x_1\}. \end{aligned}$$

Consider the Dirichlet boundary value problem in an inhomogeneous half space: For given Dirichlet data $f \in H^{1/2}_{\hat{\alpha}}(\mathbb{R})$, seek a solution $u \in H^1_{\hat{\alpha}}(\Omega_b^-)$ such that

$$\begin{cases} \Delta u(x_1, x_2) + k^2 q(x_2) u(x_1, x_2) = 0, & (x_1, x_2)^{\rm T} \in \Omega_b^-, \\ u(x_1, b) = f(x_1), & x_1 \in \mathbb{R}. \end{cases} \tag{2.3}$$

To ensure the well-posedness of (2.3), u is required to satisfy an appropriate downward propagating radiation condition to be discussed within this paper.

We may expand the Dirichlet data $u\big|_{\Gamma_b} = f$ into the Fourier series

$$f(x_1) = \sum_{n\in\mathbb{Z}} f_n e^{i\alpha_n x_1},$$

where the coefficients $f_n \in \mathbb{C}$ satisfy $\sum_{n\in\mathbb{Z}}(1 + |n|^2)^{1/2}|f_n|^2 < \infty$. Indeed, since u is α-quasi-periodic, it admits the Fourier expansion

$$e^{-i\hat{\alpha}x_1}u(x_1, x_2) = \sum_{n\in\mathbb{Z}} u_n(x_2)e^{i\frac{2\pi}{\mathsf{p}}nx_1}, \ x_2 < b,$$

or equivalently,

$$u(x_1, x_2) = \sum_{n\in\mathbb{Z}} u_n(x_2)e^{i\alpha_n x_1}, \ x_2 < b. \tag{2.4}$$

Inserting (2.4) into the Helmholtz equation, we find that

$$\sum_{n\in\mathbb{Z}} \left[u_n''(x_2) + (k^2 q(x_2) - \alpha_n^2) u_n(x_2)\right] e^{i\alpha_n x_1} = 0. \tag{2.5}$$

Below we shall confine our studies to a real-valued index function $q(x_2)$ for $x_2 < b$. By (2.5), we need to look for solutions u_n to the Hill's equations

$$u_n''(x_2) + (k^2 q(x_2) - \alpha_n^2) u_n(x_2) = 0,\ x_2 < b,\ n \in \mathbb{Z},$$

for which the functions $(x_1, x_2) \mapsto u_n(x_2)e^{i\alpha_n x_1}$ with $n \in \mathbb{Z}$ physically represent downward and upward wave modes. We will use the Floquet theory (cf. Appendix A) to find an outgoing solution to the above Hill's equation in $x_2 < b$ for every fixed $n \in \mathbb{Z}$, which represents the downward propagating wave mode as $x_2 \to \infty$.

3 Downward radiation condition for $q = q(x_2)$ in $x_2 < b$.

3.1 Downward and upward radiation conditions in $\mathbb{R}^2$.

In this section we extend $q(x_2)$ from $x_2 < b$ to $x_2 \in \mathbb{R}$ by the 2π-periodicity extension. Consider the one-dimensional ordinary differential equations

$$u_n''(x_2) + (k^2 q(x_2) - \alpha_n^2) u_n(x_2) = 0,\ x_2 \in \mathbb{R},\ n \in \mathbb{Z}. \tag{3.1}$$

We need to find two linearly independent solutions to (3.1), in order to classify the downward and upward wave modes for each $n \in \mathbb{Z}$. Let $w_{n,1}$ and $w_{n,2}$ be the linearly independent solutions of (3.1), which satisfy the "initial" value conditions

$$\begin{aligned} &w_{n,1}(0) = 1,\ w_{n,1}'(0) = 0; \\ &w_{n,2}(0) = 0,\ w_{n,2}'(0) = 1. \end{aligned} \tag{3.2}$$

Consider the matrix

$$W_n := \begin{pmatrix} w_{n,1}(2\pi) & w_{n,2}(2\pi) \\ w_{n,1}'(2\pi) & w_{n,2}'(2\pi) \end{pmatrix} \in \mathbb{C}^{2\times 2}.$$

Using Liouville's formula for the Wronskian [16, Lemma 3.11], we have

$$\det W_n = 1. \tag{3.3}$$

Definition 3.1. The eigenvalues $\lambda_{n,1}$, $\lambda_{n,2}$ of W_n are called the characteristic multipliers of (3.1). The numbers $\mu_{n,1}$, $\mu_{n,2}$ satisfying $-1/2 < \operatorname{Im}\mu_{n,j} \leqslant 1/2$ and $e^{2\pi\mu_{n,j}} = \lambda_{n,j}$, $j = 1, 2$, are called the characteristic exponents of (3.1).

It follows from (3.3) that

$$\lambda_{n,j}^2 - \eta_n \lambda_{n,j} + 1 = 0,\ j = 1, 2,\ n \in \mathbb{Z}, \tag{3.4}$$

$$\eta_n := w_{n,1}(2\pi) + w_{n,2}'(2\pi) \in \mathbb{C}. \tag{3.5}$$

Consequently, we have

Lemma 3.1. The characteristic multipliers and exponents of (3.1) satisfy the relations

$$\lambda_{n,1}\lambda_{n,2} = 1,\ \mu_{n,1} + \mu_{n,2} \in \{0, i\},\ \text{for all } n \in \mathbb{Z}.$$

Without loss of generality we suppose that $|\lambda_{n,1}| \geqslant |\lambda_{n,2}|$. Applying the Floquet theory we shall derive two linearly independent solutions of (3.1).

Now suppose $q(x_2)$ is real-valued. Then the $w_{n,j}$ and η_n are all real-valued.

Lemma 3.2. There are two linearly independent solutions $\xi_{n,j}$, $j = 1, 2$ of (3.1) expressed with the help of two 2π-periodic functions $v_{n,j}$, $j = 1, 2$, where these expressions depend on the number η_n as follows.

(a) If $\eta_n > 2$, then

$$\xi_{n,1}(x_2) = e^{\mu_{n,1}x_2} v_{n,1}(x_2),\ \xi_{n,2}(x_2) = e^{-\mu_{n,1}x_2} v_{n,2}(x_2),$$

where $\mu_{n,1}$ is a positive real number such that $e^{2\pi\mu_{n,1}} = \lambda_{n,1}$.

(b) If $\eta_n < -2$, then

$$\xi_{n,1}(x_2) = e^{\left(\tilde{\mu}_{n,1}+\frac{i}{2}\right)x_2} v_{n,1}(x_2),\ \xi_{n,2}(x_2) = e^{\left(-\tilde{\mu}_{n,1}+\frac{i}{2}\right)x_2} v_{n,2}(x_2),$$

where $\tilde{\mu}_{n,1}$ is a positive real number such that $e^{2\pi\tilde{\mu}_{n,1}} = |\lambda_{n,1}|$.

(c) If $|\eta_n| < 2$, then

$$\xi_{n,1}(x_2) = e^{-i\theta_n x_2} v_{n,1}(x_2),\ \xi_{n,2}(x_2) = e^{i\theta_n x_2} v_{n,2}(x_2),$$

where $\theta_n = \mu_{n,1}$ is a real number and $\theta_n \in (0, 1/2)$ such that $e^{i2\pi\theta_n} = \lambda_{n,1}$.

(d) If $\eta_n = 2$, then there are two sub-cases as follows:

case (i): For $\operatorname{rank}(W_n - I) = 0$, we have

$$\xi_{n,1}(x_2) = v_{n,1}(x_2),\ \xi_{n,2}(x_2) = v_{n,2}(x_2),$$

case (ii): For $\operatorname{rank}(W_n - I) \neq 0$, we have

$$\xi_{n,1}(x_2) = v_{n,1}(x_2),\ \xi_{n,2}(x_2) = x_2 v_{n,1}(x_2) + v_{n,2}(x_2).$$

(e) If $\eta_n = -2$, then there are two sub-cases:

case (i): For $\operatorname{rank}(W_n + I) = 0$, we have

$$\xi_{n,1}(x_2) = e^{i\frac{x_2}{2}} v_{n,1}(x_2),\ \xi_{n,2}(x_2) = e^{i\frac{x_2}{2}} v_{n,2}(x_2),$$

case (ii): For $\operatorname{rank}(W_n + I) \neq 0$, we have

$$\xi_{n,1}(x_2) = e^{i\frac{x_2}{2}} v_{n,1}(x_2),\ \xi_{n,2}(x_2) = e^{i\frac{x_2}{2}} (x_2 v_{n,1}(x_2) + v_{n,2}(x_2)).$$

Proof. (a) Since $\eta_n > 2$ and $\lambda_{n,1}\lambda_{n,2} = 1$, $\lambda_{n,1}$ and $\lambda_{n,2}$ are distinct positive real numbers and $0 < \lambda_{n,2} < 1 < \lambda_{n,1}$. By Definition 3.1, there exists a positive real number $\mu_{n,1}$ such that

$$e^{2\pi\mu_{n,1}} = \lambda_{n,1},\ e^{-2\pi\mu_{n,1}} = \lambda_{n,2}.$$

Thus, by part (1) of Theorem A.2,

$$\xi_{n,1}(x_2) = e^{\mu_{n,1}x_2} v_{n,1}(x_2),\ \xi_{n,2}(x_2) = e^{-\mu_{n,1}x_2} v_{n,2}(x_2),$$

where $v_{n,1}$ and $v_{n,2}$ are 2π-periodic functions.

(b) Since $\eta_n < -2$ and $\lambda_{n,1}\lambda_{n,2} = 1$, $\lambda_{n,1}$ and $\lambda_{n,2}$ are both negative real numbers and $\lambda_{n,1} < -1 < \lambda_{n,2} < 0$. There exists a positive real number $\tilde{\mu}_{n,1}$ such that

$$e^{2\pi\tilde{\mu}_{n,1}} = |\lambda_{n,1}|,\ e^{-2\pi\tilde{\mu}_{n,1}} = |\lambda_{n,2}|.$$

By part (1) of Theorem A.2, we get

$$\xi_{n,1}(x_2) = e^{\left(\tilde{\mu}_{n,1}+\frac{i}{2}\right)x_2} v_{n,1}(x_2),\ \xi_{n,2}(x_2) = e^{\left(-\tilde{\mu}_{n,1}+\frac{i}{2}\right)x_2} v_{n,2}(x_2),$$

where $v_{n,1}$ and $v_{n,2}$ are 2π-periodic functions.

(c) If $|\eta_n| < 2$, then $\lambda_{n,1}$ and $\lambda_{n,2}$ are complex conjugates. Additionally, $\lambda_{n,1}\lambda_{n,2} = |\lambda_{n,1}|^2 = 1$. We assume that $\lambda_{n,1}$ lies in the upper half plane. There is a real number $\theta_n \in (0, 1/2)$ such that

$$e^{i2\pi\theta_n} = \lambda_{n,1},\ e^{-i2\pi\theta_n} = \lambda_{n,2}.$$

Therefore, by part (1) of Theorem A.2,

$$\xi_{n,1}(x_2) = e^{-i\theta_n x_2} v_{n,1}(x_2),\ \xi_{n,2}(x_2) = e^{i\theta_n x_2} v_{n,2}(x_2),$$

where $v_{n,1}$ and $v_{n,2}$ are 2π-periodic functions.

(d) If $\eta_n = 2$, then we have $\lambda_{n,1} = \lambda_{n,2} = 1$. Under this condition, we need to compute the rank of $W_n - I \in \mathbb{C}^{2\times 2}$ to decide which part of Theorem A.2 is applicable.

case (i): $w_{n,2}(2\pi) = w'_{n,1}(2\pi) = 0$.
Then

$$\det\begin{pmatrix} w_{n,1}(2\pi) & w'_{n,1}(2\pi) \\ w_{n,2}(2\pi) & w'_{n,2}(2\pi) \end{pmatrix} = \det\begin{pmatrix} w_{n,1}(0) & w'_{n,1}(0) \\ w_{n,2}(0) & w'_{n,2}(0) \end{pmatrix} = 1.$$

We have $w_{n,1}(2\pi)w'_{n,2}(2\pi) = 1$ and

$$\eta_n = w_{n,1}(2\pi) + w'_{n,2}(2\pi) = 2.$$

Hence $w_{n,1}(2\pi) = w'_{n,2}(2\pi) = 1$, which implies $\operatorname{rank}(W_n - I) = 0$, i.e., there are two linearly independent solutions of (3.1). Now we may apply part (1) of Theorem A.2. Since $\lambda_{n,1} = \lambda_{n,2} = 1$, we get $\mu_{n,1} = \mu_{n,2} = 0$ and

$$\xi_{n,1}(x_2) = v_{n,1}(x_2),\ \xi_{n,2}(x_2) = v_{n,2}(x_2),$$

where $v_{n,1}$ and $v_{n,2}$ are 2π-periodic functions.

case (ii): $w_{n,2}(2\pi), w'_{n,1}(2\pi)$ not both zero
In this case $\operatorname{rank}(W_n - I) \neq 0$. Applying part (2) of Theorem A.2 gives $\mu_{n,1} = \mu_{n,2} = 0$ and

$$\xi_{n,1}(x_2) = v_{n,1}(x_2),\ \xi_{n,2}(x_2) = x_2 v_{n,1}(x_2) + v_{n,2}(x_2),$$

where $v_{n,1}$ and $v_{n,2}$ are 2π-periodic functions.

(e) Similar to the assertion (d), we consider the following two cases.

case (i): $w_{n,2}(2\pi) = w'_{n,1}(2\pi) = 0$.
We have that $\operatorname{rank}(W_n + I) = 0$. By part (1) of Theorem A.2, one obtains $\mu_{n,1} = \mu_{n,2} = i/2$ and

$$\xi_{n,1}(x_2) = e^{i\frac{x_2}{2}} v_{n,1}(x_2),\ \xi_{n,2}(x_2) = e^{i\frac{x_2}{2}} v_{n,2}(x_2),$$

where $v_{n,1}$ and $v_{n,2}$ are 2π-periodic functions.

case (ii): $w_{n,2}(2\pi), w'_{n,1}(2\pi)$ not both zero.
Here $\operatorname{rank}(W_n + I) \neq 0$. Again using part (2) of Theorem A.2, we get $\mu_{n,1} = \mu_{n,2} = i/2$ and

$$\xi_{n,1}(x_2) = e^{i\frac{x_2}{2}} v_{n,1}(x_2),\ \xi_{n,2}(x_2) = e^{i\frac{x_2}{2}} (x_2 v_{n,1}(x_2) + v_{n,2}(x_2)),$$

where $v_{n,1}$ and $v_{n,2}$ are 2π-periodic functions.

$\square$

Remark 3.1. In Lemma 3.2, the functions $\xi_{n,j}$ are periodic in cases (d) (i) and anti-periodic in cases (e) (i).

According to Lemma 3.2, we can now define the upward modes $u_n^+(x_2)e^{i\alpha_n x_1}$ (that is, modes decaying for $x_2 \to +\infty$ or modes propagating upwards) and downward modes $u_n^-(x_2)e^{i\alpha_n x_1}$ (modes decaying for $x_2 \to -\infty$ or modes propagating downwards), where $u_n^\pm(x_2)$ are defined as follows.

Definition 3.2. (a) If $\eta_n > 2$, then

$$u_n^+(x_2) := e^{-\mu_{n,1}x_2} v_{n,2}(x_2),\ u_n^-(x_2) := e^{\mu_{n,1}x_2} v_{n,1}(x_2),$$

where $v_{n,1}$ and $v_{n,2}$ are the 2π-periodic functions of Lemma 3.2 (a).

(b) If $\eta_n < -2$, then

$$u_n^+(x_2) := e^{\left(-\tilde{\mu}_{n,1}+\frac{i}{2}\right)x_2} v_{n,2}(x_2),\ u_n^-(x_2) := e^{\left(\tilde{\mu}_{n,1}+\frac{i}{2}\right)x_2} v_{n,1}(x_2),$$

where $v_{n,1}$ and $v_{n,2}$ are the 2π-periodic functions of Lemma 3.2 (b).

(c) If $|\eta_n| < 2$, then

$$u_n^+(x_2) := e^{i\theta_n x_2} v_{n,2}(x_2),\ u_n^-(x_2) := e^{-i\theta_n x_2} v_{n,1}(x_2),$$

where $v_{n,1}$ and $v_{n,2}$ are the 2π-periodic functions of Lemma 3.2 (c).

(d) If $\eta_n = 2$, then

case (i):
$$u_n^+(x_2) = u_n^-(x_2) := (v_{n,1}(x_2), v_{n,2}(x_2))^{\mathrm{T}},$$

case (ii):
$$u_n^+(x_2) = u_n^-(x_2) := v_{n,1}(x_2),$$

where $v_{n,1}$ and $v_{n,2}$ are the 2π-periodic functions of Lemma 3.2 (d).

(e) If $\eta_n = -2$, then

case (i):
$$u_n^+(x_2) = u_n^-(x_2) := e^{i\frac{x_2}{2}} (v_{n,1}(x_2), v_{n,2}(x_2))^{\mathrm{T}},$$

case (ii):
$$u_n^+(x_2) = u_n^-(x_2) := e^{i\frac{x_2}{2}} v_{n,1}(x_2),$$

where $v_{n,1}$ and $v_{n,2}$ are the 2π-periodic functions of Lemma 3.2 (e).
Note that $u_n^\pm$ are vectorial functions in cases (d) (i) and (e) (i).

With the help of Definition 3.2, we can define the upward and downward radiation conditions by a possible representation as a superposition of upward and downward modes, respectively.

Definition 3.3 (Radiation Conditions)**.** Consider $\hat{\alpha}$-quasiperiodic solutions to the Helmholtz equation $\Delta u(x_1, x_2) + k^2 q(x_2) u(x_1, x_2) = 0$. The solution u is called an upward radiating solution if there exist an $a^+ \in \mathbb{R}$ and coefficients C_n^+ such that

$$u(x_1, x_2) = \sum_{n \in \mathbb{Z}} C_n^+ \cdot u_n^+(x_2)\, e^{i\alpha_n x_1} \qquad \text{in } x_2 > a^+, \tag{URC}$$

where $C_n^+ \in \mathbb{C}^2$ in case (d) (i) or (e) (i) and $C_n^+ \in \mathbb{C}$ otherwise.

The solution u is called an downward radiating solution if there exist an $a^- \in \mathbb{R}$ and coefficients C_n^- such that

$$u(x_1, x_2) = \sum_{n \in \mathbb{Z}} C_n^- \cdot u_n^-(x_2)\, e^{i\alpha_n x_1} \qquad \text{in } x_2 < a^-, \tag{DRC}$$

where $C_n^- \in \mathbb{C}^2$ in case (d) (i) or (e) (i) and $C_n^- \in \mathbb{C}$ otherwise.

3.2 Special instance: $q(x_2) \equiv 1$

It is natural to ask how do the new radiation conditions of Definition 3.3 generalize the classical Rayleigh-expansion radiation conditions. Below we show that the Rayleigh-expansion condition in the homogeneous case that $q(x_2) \equiv 1$ is a special instance of Definition 3.3. Consider $u_n''(x_2) + (k^2 - \alpha_n^2) u_n(x_2) = 0$. Here, α_n and β_n have been defined in (2.2).

(1) If $k^2 > \alpha_n^2$, then there are two linearly independent solutions

$$\xi_1(x_2) = e^{i\sqrt{k^2 - \alpha_n^2} x_2}, \ \xi_2(x_2) = e^{-i\sqrt{k^2 - \alpha_n^2} x_2}.$$

This corresponds to part (1) of Theorem A.2 with $m_1 = i\sqrt{k^2 - \alpha_n^2}$, $m_2 = -i\sqrt{k^2 - \alpha_n^2}$ and $v_1 = v_2 = 1$, that is, case (c) in Lemma 3.2.

(2) If $k^2 < \alpha_n^2$, then there are two linearly independent solutions

$$\xi_1(x_2) = e^{\sqrt{\alpha_n^2 - k^2} x_2}, \ \xi_2(x_2) = e^{-\sqrt{\alpha_n^2 - k^2} x_2}.$$

This corresponds to part (1) of Theorem A.2 with $m_1 = \sqrt{\alpha_n^2 - k^2}$, $m_2 = -\sqrt{\alpha_n^2 - k^2}$ and $v_1 = v_2 = 1$, that is, case (a) in Lemma 3.2.

(3) If $k^2 = \alpha_n^2$, then there are two linearly independent solutions

$$\xi_1(x_2) = a, \ \xi_2(x_2) = a x_2 + b, \ \text{for some } a, b \in \mathbb{C}.$$

This corresponds to part (2) of Theorem A.2 with $m = 0$, $v_1 = a$ and $v_2 = b$, that is, case (ii) in Lemma 3.2 (d).

Furthermore, we can also compute η_n for each case above. Solving two initial value problems for the ODE

$$\begin{cases} w_{n,1}''(x_2) + \beta_n^2 w_{n,1}(x_2) = 0, \\ w_{n,1}(0) = 1, \ w_{n,1}'(0) = 0, \end{cases} \qquad \begin{cases} w_{n,2}''(x_2) + \beta_n^2 w_{n,2}(x_2) = 0, \\ w_{n,2}(0) = 0, \ w_{n,2}'(0) = 1, \end{cases} \tag{3.6}$$

we get solutions for (3.6) as below:

$$
\begin{aligned}
w_{n,1}(x_2) &= \frac{1}{2}\left(e^{i\beta_n x_2} + e^{-i\beta_n x_2}\right), \\
w'_{n,1}(x_2) &= \frac{i\beta_n}{2}\left(e^{i\beta_n x_2} - e^{-i\beta_n x_2}\right), \\
w_{n,2}(x_2) &= \frac{1}{2i\beta_n}\left(e^{i\beta_n x_2} - e^{-i\beta_n x_2}\right) = \frac{1}{(i\beta_n)^2} w'_{n,1}(x_2), \\
w'_{n,2}(x_2) &= \frac{1}{2}\left(e^{i\beta_n x_2} + e^{-i\beta_n x_2}\right) = w_{n,1}(x_2).
\end{aligned}
$$

Then we can compute η_n as

$$\eta_n = w_{n,1}(2\pi) + w'_{n,2}(2\pi) = e^{i2\pi\beta_n} + e^{-i2\pi\beta_n}.$$

(1) If $k^2 > \alpha_n^2$, then $\eta_n = 2\cos(2\pi\beta_n)$ and $|\eta_n| < 2$. This corresponds to case (c) in Lemma 3.2. We can define the upward mode $u_n^+(x_2)e^{i\alpha_n x_1}$ and the downward mode $u_n^-(x_2)e^{i\alpha_n x_1}$, where

$$u_n^+(x_2) = e^{i\beta_n x_2} \text{ and } u_n^-(x_2) = e^{-i\beta_n x_2}.$$

(2) If $k^2 < \alpha_n^2$, then $\beta_n = i|\beta_n|$ and $\eta_n = e^{-2\pi|\beta_n|} + e^{2\pi|\beta_n|} > 2$. This corresponds to case (a) in Lemma 3.2. We can define the upward mode $u_n^+(x_2)e^{i\alpha_n x_1}$ and the downward mode $u_n^-(x_2)e^{i\alpha_n x_1}$, where

$$u_n^+(x_2) = e^{-|\beta_n| x_2} \text{ and } u_n^-(x_2) = e^{|\beta_n| x_2}.$$

(3) If $k^2 = \alpha_n^2$, then $\beta_n = 0$ and $\eta_n = 2$. Check the two initial value problems

$$
\begin{cases} w''_{n,1} = 0, \\ w_{n,1}(0) = 1,\ w'_{n,1}(0) = 0, \end{cases}
\qquad
\begin{cases} w''_{n,2} = 0, \\ w_{n,2}(0) = 0,\ w'_{n,2}(0) = 1. \end{cases}
$$

We have $w_{n,1} = 1,\ w_{n,2} = x_2$, and

$$W_n = \begin{pmatrix} w_{n,1}(2\pi) & w'_{n,1}(2\pi) \\ w_{n,2}(2\pi) & w'_{n,2}(2\pi) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 2\pi & 1 \end{pmatrix},$$

rank$(W_n - I) = 1$. This corresponds to part (ii) of case (d) in Lemma 3.2 with $v_{n,1}(x_2) \equiv 1$. We can only define the outgoing bounded wave mode $u_n^\pm(x) := e^{i\alpha_n x_1}$.

3.3 Asymptotics of η_n and μ_n as $|n| \to +\infty$.

The purpose of this subsection is to prove the asymptotic behavior of η_n and μ_n as $|n| \to \infty$ through the comparison theorem for initial value problems of an ordinary differential equation, which is stated as below.

Lemma 3.3 (Comparison Theorem)**.** Consider the initial value problem

$$
\begin{cases} u''(t) = f(t, u, u'),\ t \in [t_0, t_1] \\ u(t_0) = u_0,\ u'(t_0) = u'_0. \end{cases} \tag{3.7}
$$

Suppose that

(1) There exist a subsolution $u_{\rm sub}(t)$ and a supersolution $u_{\rm sup}(t)$ such that

$$
\begin{aligned}
&(i)\, u_{\rm sub}(t) \leqslant u_{\rm sup}(t),\ u'_{\rm sub}(t) \leqslant u'_{\rm sup}(t),\ t \in [t_0, t_1];\\
&(ii)\, u_{\rm sub}(t_0) \leqslant u_{\rm sup}(t_0),\ u'_{\rm sub}(t_0) \leqslant u'_{\rm sup}(t_0);\\
&(iii)\, \text{For any } t \in [t_0, t_1]) \text{ and } u \in [u_{\rm sub}(t), u_{\rm sup}(t)],\ \text{we have}\\
&\qquad u''_{\rm sub}(t) \leqslant f(t, u, u'_{\rm sub}(t)),\ u''_{\rm sup}(t) \geqslant f(t, u, u'_{\rm sup}(t)).
\end{aligned}
$$

(2) The function f on the right-hand side of the ODE in (3.7) is continuous on the domain $D = \{(t, u, v)\colon t_0 \leqslant t \leqslant t_1,\ u_{\rm sub}(t) \leqslant u \leqslant u_{\rm sup}(t),\ u'_{\rm sub}(t) \leqslant v \leqslant u'_{\rm sup}(t)\}$.

Then the solution $u(t)$ of the initial value problem (3.7) satisfies $u(t) \in C^2[t_0, t_1]$ and $u_{\rm sub}(t) \leqslant u(t) \leqslant u_{\rm sup}(t)$, $u'_{\rm sub}(t) \leqslant u'(t) \leqslant u'_{\rm sup}(t)$ for any $t \in [t_0, t_1]$.

To define subsolutions and supersolutions of the ODE (3.1), we introduce the upper and lower bound of $q(x_2)$ by

$$
q_{\max} \coloneqq \sup_{x_2 \in [0, 2\pi]} q(x_2), \quad q_{\min} \coloneqq \inf_{x_2 \in [0, 2\pi]} q(x_2),
$$

respectively. Recalling the definition of η_n in (3.5), we estimate η_n for large $|n|$ as follows.

Lemma 3.4. We have $\eta_n > 2$ if $\alpha_n^2 > k^2 q_{\max}$ and $\eta_n = O(e^{2\pi|n|})$ as $|n| \to \infty$.

Proof. Using Lemma 3.3, we can estimate η_n by constructing subsolutions and supersolutions for the ODEs (3.1). The subsolution and supersolution with the initial conditions $w_{n,1}(0) = 1, w'_{n,1}(0) = 0$ are given by

$$
\begin{aligned}
u_{\rm sub}(x_2) &= \frac{1}{2}\left(e^{\beta_n^+ x_2} + e^{-\beta_n^+ x_2}\right),\\
u'_{\rm sub}(x_2) &= \frac{\beta_n^+}{2}\left(e^{\beta_n^+ x_2} - e^{-\beta_n^+ x_2}\right),\\
u_{\rm sup}(x_2) &= \frac{1}{2}\left(e^{\beta_n^- x_2} + e^{-\beta_n^- x_2}\right),\\
u'_{\rm sup}(x_2) &= \frac{\beta_n^-}{2}\left(e^{\beta_n^- x_2} - e^{-\beta_n^- x_2}\right),
\end{aligned}
$$

where $\beta_n^+ = \sqrt{\alpha_n^2 - k^2 q_{\max}}$ and $\beta_n^- = \sqrt{\alpha_n^2 - k^2 q_{\min}}$. Similarly, the subsolution and supersolution with the initial condition $w_{n,2}(0) = 0, w'_{n,2}(0) = 1$ are

$$
\begin{aligned}
u_{\rm sub}(x_2) &= \frac{1}{2\beta_n^+}\left(e^{\beta_n^+ x_2} - e^{-\beta_n^+ x_2}\right),\\
u'_{\rm sub}(x_2) &= \frac{1}{2}\left(e^{\beta_n^+ x_2} + e^{-\beta_n^+ x_2}\right),\\
u_{\rm sup}(x_2) &= \frac{1}{2\beta_n^-}\left(e^{\beta_n^- x_2} - e^{-\beta_n^- x_2}\right),\\
u'_{\rm sup}(x_2) &= \frac{1}{2}\left(e^{\beta_n^- x_2} + e^{-\beta_n^- x_2}\right).
\end{aligned}
$$

By Lemma 3.3, we have that

$$
\begin{aligned}
\frac{1}{2}\left(e^{\beta_n^+ x_2} + e^{-\beta_n^+ x_2}\right) \leqslant w_{n,1}(x_2) \leqslant \frac{1}{2}\left(e^{\beta_n^- x_2} + e^{-\beta_n^- x_2}\right),\\
\frac{1}{2}\left(e^{\beta_n^+ x_2} + e^{-\beta_n^+ x_2}\right) \leqslant w'_{n,2}(x_2) \leqslant \frac{1}{2}\left(e^{\beta_n^- x_2} + e^{-\beta_n^- x_2}\right).
\end{aligned}
$$

For $\alpha_n^2 > k^2 q_{\max}$, the number β_n^+ is real-valued. Hence

$$\begin{aligned}\eta_n &= w_{n,1}(2\pi) + w'_{n,2}(2\pi)\\ &\geqslant e^{2\pi\beta_n^+} + e^{-2\pi\beta_n^+}\\ &> 2.\end{aligned}$$

Furthermore, it follows from Lemma 3.3 with the above subsolutions and supersolutions that $\eta_n = O(e^{2\pi|n|})$ as $|n| \to +\infty$. □

Lemma 3.5. Recall the definition of $\mu_{n,1}$ in Definition 3.1. The sequences $\mu_{n,1}$ and $\mu_{-n,1}$ are monotonically increasing as $|n|$ goes to ∞. Moreover, $|\mu_{n,1}| = O(|n|)$.

Proof. We first prove that $\mu_{n,1}$ is monotonically increasing as n tends to infinity. By (3.4), it suffices to prove that η_n is monotonically increasing as n tends to infinity. We use the same argument as in the proof of Lemma 3.4 to get the upper bound for η_n and the lower bound for η_{n+1}, i.e., $\eta_n \leqslant e^{2\pi\beta_n^-} + e^{-2\pi\beta_n^-}$ and $\eta_{n+1} \geqslant e^{2\pi\beta_{n+1}^+} + e^{-2\pi\beta_{n+1}^+}$. If $e^{2\pi\beta_{n+1}^+}$ is greater than $e^{2\pi\beta_n^-}$, i.e., n is greater than $\left(k^2(q_{\max} - q_{\min}) - 2\alpha - 1\right)/2$, then η_n is monotonically increasing. With the help of Definition 3.1 and (3.4), we can show that $\mu_{n,1}$ is monotonically increasing. Similarly, if n approaches the negative infinity, then we may have the upper bound for η_n and the lower bound for η_{n-1}, i.e., $\eta_n \leqslant e^{2\pi\beta_n^-} + e^{-2\pi\beta_n^-}$ and $\eta_{n-1} \geqslant e^{2\pi\beta_{n-1}^+} + e^{-2\pi\beta_{n-1}^+}$. Hence, if n is less than $(k^2(q_{\min} - q_{\max}) - 2\alpha + 1)/2$, then $\mu_{n,1}$ is monotonically decreasing. By equation (3.4) and $e^{2\pi\mu_{n,1}} = \lambda_{n,1}$, we know that $|\mu_{n,1}| = O(|n|)$. □

More precise estimates of η_n and $\mu_{n,1}$ will be shown in the proof of Lemma 4.1 below. These asymptotics enable us to justify the pointwise convergence of the proposed upward and downward radiation conditions.

Theorem 3.1 (Pointwise Convergence)**.** If $u \in H^1_{loc}(\mathbb{R}^2)$, then the infinite series on the right-hand side of (URC) (resp. (DRC)) in Definition 3.3 is pointwisely convergent.

Proof. Without loss of generality, we only prove the theorem for the upward radiation condition. It suffices to prove that the radiation condition converges pointwisely in $x_2 > d$ for n sufficiently large.

For any fixed $(x_1, x_2)^{\mathrm{T}} \in \Omega_d^+$, there is a real number $\sigma \in (0, 2\pi]$ such that $v_{n,2}(x_2) = v_{n,2}(d+\sigma)$ for any $n \in \mathbb{Z}$. If $x_2 > d+\sigma$, then we can decompose the upward mode into two parts. Namely, applying Young's inequality and Parseval's equality yields the estimate

$$\begin{aligned}&2\left|\sum_{\eta_n>2} C_n^+ e^{-\mu_{n,1}x_2} v_{n,2}(x_2) e^{i\alpha_n x_1}\right|\\ \leqslant &\sum_{\eta_n>2} 2\left|C_n^+ e^{-\mu_{n,1}(d+\sigma)} v_{n,2}(x_2) e^{i\alpha_n x_1} e^{-\mu_{n,1}(x_2-d-\sigma)}\right|\\ \leqslant &\sum_{\eta_n>2}\left|C_n^+ e^{-\mu_{n,1}(d+\sigma)} v_{n,2}(x_2) e^{i\alpha_n x_1}\right|^2 + \sum_{\eta_n>2}\left|e^{-\mu_{n,1}(x_2-d-\sigma)}\right|^2\\ = &\sum_{\eta_n>2}\left|C_n^+ e^{-\mu_{n,1}(d+\sigma)} v_{n,2}(d+\sigma) e^{i\alpha_n x_1}\right|^2 + \sum_{\eta_n>2}\left|e^{-\mu_{n,1}(x_2-d-\sigma)}\right|^2\\ \leqslant &\frac{1}{\mathrm{p}}\int_0^{\mathrm{p}} |u(x_1, d+\sigma)|^2 dx_1 + \sum_{\eta_n>2}\left|e^{-\mu_{n,1}(x_2-d-\sigma)}\right|^2\\ < &\infty,\end{aligned}$$

where the second term of the last inequality is convergent since $\mu_{n,1}$ is monotonically increasing and $|\mu_{n,1}| = O(|n|)$ (cf. the proof of Lemma 3.5).

If $x_2 \in (d, d+\sigma]$, then we choose an appropriate ϵ such that $d < \epsilon < x_2$ and $v_{n,2}(\epsilon) \neq 0$ (see Remark 4.1). Using Parseval's equality and the asymptotic behavior of $v_{n,2}(x_2)$ in Lemma 4.1 yields that

$$
\begin{aligned}
& 2\Big|\sum_{\eta_n>2} C_n^+ e^{-\mu_{n,1}x_2} v_{n,2}(x_2) e^{i\alpha_n x_1}\Big| \\
\leqslant & \sum_{\eta_n>2} 2\Big|C_n^+ e^{-\mu_{n,1}\epsilon} v_{n,2}(x_2) e^{i\alpha_n x_1} e^{-\mu_{n,1}(x_2-\epsilon)}\Big| \\
\leqslant & \sum_{\eta_n>2} \Big|C_n^+ e^{-\mu_{n,1}\epsilon} v_{n,2}(\epsilon) e^{i\alpha_n x_1}\Big|^2 \Big|\frac{v_{n,2}(x_2)}{v_{n,2}(\epsilon)}\Big|^2 + \sum_{\eta_n>2} \Big|e^{-\mu_{n,1}(x_2-\epsilon)}\Big|^2.
\end{aligned}
$$

Indeed, in view of the subsequent (4.16), we get $|\frac{v_{n,2}(x_2)}{v_{n,2}(\epsilon)}|^2 < C$ for $|n| > n_a$ with sufficiently large n_a.

$$
\begin{aligned}
& 2\Big|\sum_{|n|>n_a} C_n^+ e^{-\mu_{n,1}x_2} v_{n,2}(x_2) e^{i\alpha_n x_1}\Big| \\
\leqslant & \frac{C}{\mathrm{p}} \int_0^{\mathrm{p}} |u(x_1,\epsilon)|^2 dx_1 + \sum_{|n|>n_a} \Big|e^{-\mu_{n,1}(x_2-\epsilon)}\Big|^2 < \infty.
\end{aligned}
$$

This completes the proof. □

4 Uniqueness and existence results

The aim of this section is to prove well-posedness of the diffraction problem described in Section 2 complemented with the classical upward Rayleigh expansion in $x_2 > d$ and the new downward radiation condition (DRC) defined in Definition 3.3 in $x_2 < b$. In Subsection 4.1 we carefully define the DtN maps on Γ_b and Γ_d, allowing us to truncate the physical domain to a bounded periodic cell. In Subsection 4.2 we prove the Fredholm property of the resulting sesquilinear form and then in Subsection 4.3 the uniqueness and existence of our diffraction problem. The solvability results depend on a well-defined downward DtN mapping for the infinite inhomogeneous medium $q(x_2)$ and the mapping properties for its real and imaginary parts.

4.1 Dirichlet-to-Neumann (DtN) maps

We first recall the classical $\hat{\alpha}$-quasiperiodic (upward) DtN map T for $q \equiv 1$.

Definition 4.1 (Classical upward DtN map)**.** Given a quasi-periodic function f over Γ_d, which has a Fourier series expansion

$$
f(x_1) = \sum_{n\in\mathbb{Z}} f_n e^{i\alpha_n x_1}, \quad f_n := \frac{1}{\mathrm{p}} \int_0^{\mathrm{p}} f(x_1) e^{-i\alpha_n x_1} dx_1. \tag{4.1}
$$

The classical upward DtN map T in a homogeneous medium (that is, $q(x_2) \equiv 1$) is defined as

$$
(Tf)(x_1) = \sum_{n\in\mathbb{Z}} i\beta_n f_n \, e^{i\alpha_n x_1}, \tag{4.2}
$$

such that the relation $\partial_{x_2} u = Tu$ is equivalent with the classical upward Rayleigh-expansion condition for u in $x_2 > d$. Note that this classical upward Rayleigh-expansion condition is (2.1) with $-\beta_n$ replaced by $+\beta_n$ if the domain is Ω_b^- instead of Ω_d^+.

Next we define the upward DtN map T^+ for the inhomogeneous periodic medium $q(x_2)$. The downward DtN map T^- can be treated similarly. In the remaining part of this paper we make the following assumption on $q(x_2)$:

Assumption A: If there holds $\eta_n = 2$ for η_n in (3.5) and some $n \in \mathbb{Z}$, then the condition of Case (d) (ii) in Lemma 3.2 is fulfilled. Similarly, if there holds $\eta_n = -2$ for some $n \in \mathbb{Z}$, then the condition of Case (e) (ii) is fulfilled. In other words, Case (d) (i) for $\eta_n = 2$ and Case (e) (i) for $\eta_n = -2$ are excluded.

Note that Assumption A is always satisfied if $q(x_2) \equiv 1$.

Consider the Dirichlet boundary value problem

$$\begin{cases} \Delta u(x_1, x_2) + k^2 q(x_2) u(x_1, x_2) = 0 & \text{in } \Omega_d^+, \\ u = f \in H_{\hat{\alpha}}^{1/2}(\mathbb{R}) & \text{on } \Gamma_d, \\ u \text{ satisfies the (URC) in Definition 3.3.} \end{cases} \tag{4.3}$$

The DtN map T^+ maps the Dirichlet value f to the Neumann value of the solution u of (4.3), i.e.,

$$T^+ \colon f \longmapsto \left. \frac{\partial u(x_1, x_2)}{\partial x_2} \right|_{\Gamma_d}.$$

Since u satisfies the (URC) and $f \in H_{\hat{\alpha}}^{1/2}(\mathbb{R})$, we have that (cf. (4.1))

$$u(x_1, d) = \sum_{n \in \mathbb{Z}} C_n^+ u_n^+(d) e^{i\alpha_n x_1} = f(x_1) = \sum_{n \in \mathbb{Z}} f_n e^{i\alpha_n x_1} \quad \text{for all } x_1 \in \mathbb{R}.$$

If $u_n^+(d) \neq 0$ for all n, then we can compute $C_n^+ = f_n / u_n^+(d)$ and formally rewrite the unique solution $u(x_1, x_2)$ as

$$u(x_1, x_2) = \sum_{n \in \mathbb{Z}} \frac{f_n}{u_n^+(d)} u_n^+(x_2) e^{i\alpha_n x_1}. \tag{4.4}$$

Taking the derivative of (4.4) w.r.t. x_2 on Γ_d, we get

$$\left. \frac{\partial u(x_1, x_2)}{\partial x_2} \right|_{\Gamma_d} = \sum_{n \in \mathbb{Z}} \frac{{u_n^+}'(d)}{u_n^+(d)} f_n \, e^{i\alpha_n x_1}.$$

Remark 4.1. (i) It is possible to choose $d \in \mathbb{R}$ such that $u_n^+(d) \neq 0$ for all $n \in \mathbb{N}$. For this purpose we need to consider the zeros of solutions of equation (3.1). Property 4.1.2 in [5, Section 4.1] asserts that any solution of (3.1) has a finite number of zeros only in any bounded closed interval. Furthermore, Theorem 4.23 in [5, Section 4.2] shows that if n is sufficiently large such that $k^2 q(x_2) - \alpha_n^2 \leqslant 0$, then no solutions of (3.1) has more than one zero. Let $\mathcal{Z}$ denote the set of all zeros of solutions to (3.1) for all $n \in \mathbb{N}$. Then $\mathcal{Z}$ is a countable set. Hence, we can always find an appropriate $d \in \mathbb{R} \backslash \mathcal{Z}$ such that $u_n^+(d) \neq 0$ for all $n \in \mathbb{Z}$. Below we shall assume that $u_n^+(d) \neq 0$ for all $n \in \mathbb{Z}$. If $u_n^+(d) = 0$ but if there exists the finite limit $\lim_{0<\varepsilon\to 0} \frac{{u_n^+}'(d+\varepsilon)}{u_n^+(d+\varepsilon)}$, then $\frac{{u_n^+}'(d)}{u_n^+(d)}$ in (4.5) can be replaced by $\lim_{0<\varepsilon\to 0} \frac{{u_n^+}'(d+\varepsilon)}{u_n^+(d+\varepsilon)}$.

(ii) If case (d) (i) or case (e) (i) occurs, then the DtN map T^+ is not well-defined, because solutions to the Dirichlet problem (4.3) are not unique. For example, if $f(x_1) = f_n e^{i\alpha_n x_1}$ with $\eta_n = 2$ for some $n \in \mathbb{N}$, then any function of the form $u(x) = (c_1 v_{n,1}(x_2) + c_2 v_{n,2}(x_2))e^{i\alpha_n x_1}$, with coefficients $c_j \in \mathbb{C}$ satisfying $c_1 v_{n,1}(d) + c_2 v_{n,2}(d) = f_n$, is a solution of the Dirichlet problem (4.3).

(iii) The assumption $u_n^+(d) \neq 0$ implies that $v_{n,2}(d) \neq 0$ for the case $|\eta_n| > 2$ (cf. Definition 3.2). If $q(x_2) \equiv 1$, then we have $u_n^+(x_2) = e^{i\beta_n x_2}$ and $u_n^+(d) \neq 0$ for all n and d.

The upward and downward DtN maps $T^\pm$ for an inhomogeneous medium $q(x_2)$ are defined as follows.

Definition 4.2 (DtN maps for $q(x_2)$)**.** Choose $d \in \mathbb{R}$ such that $u_n^+(d) \neq 0$ for all $n \in \mathbb{Z}$. For quasi-periodic functions $f \in H_{\hat{\alpha}}^{1/2}(\Gamma_d)$, we define the DtN map $T^+ \colon H_{\hat{\alpha}}^{1/2}(\Gamma_d) \to H_{\hat{\alpha}}^{-1/2}(\Gamma_d)$ by

$$(T^+ f)(x_1) \coloneqq \sum_{n\in\mathbb{Z}} \frac{{u_n^+}'(d)}{u_n^+(d)} f_n \, e^{i\alpha_n x_1}, \tag{4.5}$$

where $f|_{\Gamma_d}$ has the Fourier series expansion (4.1).

Choosing $b \in \mathbb{R}$ such that $u_n^-(b) \neq 0$ for all $n \in \mathbb{Z}$, we define the downward Dirichlet-to-Neumann map T^- on Γ_b by

$$(T^- f)(x_1) \coloneqq \sum_{n\in\mathbb{Z}} -\frac{{u_n^-}'(b)}{u_n^-(b)} f_n \, e^{i\alpha_n x_1}, \tag{4.6}$$

where $f_n \in \mathbb{C}$ denotes the Fourier coefficients of f on Γ_b.

To get the boundedness of the DtN maps $T^\pm$ we need to investigate the asymptotic behavior of $v_{n,j}$ $(j = 1, 2)$ as $|n| \to \infty$. Below we shall only focus on the upward DtN mapping T^+. By Lemma 3.4, we have $\eta_n > 2$ if $|n|$ is sufficiently large.

Lemma 4.1 (Boundedness)**.** Let $v_{n,2}$ be defined as in Lemma 3.2. There exists $M > 0$ such that $\left|\frac{v_{n,2}'(d)}{v_{n,2}(d)}\right| < M$ for all $\eta_n > 2$.

Proof. The proof consists of three steps:

1. Get the solutions of (3.1) with the initial conditions (3.2).

2. Derive the asymptotic behavior of the characteristic exponents defined in Definition 3.1.

3. Derive the asymptotic behavior of $v_{n,j}$, $j = 1, 2$, according to the modes defined in Definition 3.2.

For simplicity, we abuse notation by dropping the subscript n of α_n, η_n, u_n and $\lambda_{n,j}$ in the following steps.

Step 1: Fundamental solutions. Let ψ be the solutions of $u''(t) - \alpha^2 u(t) = 0$ which satisfy the initial conditions

$$u(0) = 1, \ u'(0) = 0, \tag{4.7}$$

or

$$u(0) = 0, \ u'(0) = 1. \tag{4.8}$$

Hence we have that

$$\psi(t)=\begin{cases}\frac{1}{2}(e^{\alpha t}+e^{-\alpha t}), & \text{with condition (4.7)},\\ \frac{1}{2\alpha}(e^{\alpha t}-e^{-\alpha t}), & \text{with condition (4.8)}.\end{cases}$$

We look for solutions to (3.1) of the form $u(t)=\psi(t)\varphi(t)$. Therefore, $\varphi(t)$ should satisfy the equation

$$\varphi''(t)+H(t)\varphi'(t)+k^2q(t)\varphi(t)=0,$$

where

$$H(t)\coloneqq 2\frac{\psi'(t)}{\psi(t)}=\begin{cases}2\alpha\tanh(\alpha t) & \text{with condition (4.7)},\\ 2\alpha\cosh(\alpha t) & \text{with condition (4.8)}.\end{cases}$$

The initial conditions (4.7) and (4.8) for u are satisfied if and only if φ satisfies the initial conditions $\varphi(0)=1$ and $\varphi'(0)=0$. We get $H(t)=2V'(t)/V(t)$, where

$$V(t)\coloneqq\begin{cases}\cosh(\alpha t) & \text{with condition (4.7)},\\ \sinh(\alpha t) & \text{with condition (4.8)}.\end{cases}$$

By straightforward computation, we have that

$$[V^2(t)\varphi'(t)]'=V^2(t)(\varphi''(t)+H(t)\varphi'(t))=-V^2(t)k^2q(t)\varphi(t).$$

Integrating both sides w.r.t. t from 0 to t, we get

$$\varphi'(t)=-k^2V^{-2}(t)\int_0^t V^2(\tau)q(\tau)\varphi(\tau)\,\mathrm{d}\tau.$$

Integrating $\varphi'(t)$ again w.r.t. t from 0 to t, we obtain

$$\begin{aligned}\varphi(t)&=\varphi(0)+\int_0^t\varphi'(\tau)\,\mathrm{d}\tau\\ &=1-k^2\int_0^t V^{-2}(\tau)\int_0^\tau V^2(\sigma)q(\sigma)\varphi(\sigma)\,\mathrm{d}\sigma\,\mathrm{d}\tau\\ &=1-k^2\int_0^t q(\sigma)V^2(\sigma)\left(\int_\sigma^t V^{-2}(\tau)\,\mathrm{d}\tau\right)\varphi(\sigma)\,\mathrm{d}\sigma\\ &=1-k^2\int_0^t\Big[q(\sigma)V^2(\sigma)(\tilde{H}(t)-\tilde{H}(\sigma))\Big]\varphi(\sigma)\,\mathrm{d}\sigma,\end{aligned}\tag{4.9}$$

where

$$\tilde{H}(t)\coloneqq\frac{1}{\alpha}\begin{cases}\tanh(\alpha t) & \text{with condition (4.7)},\\ \coth(\alpha t) & \text{with condition (4.8)}.\end{cases}$$

From the discussions above, we have an integral operator K with kernel $k(t,s)$ defined by

$$(K\varphi)(t)=\int_0^t k(t,\sigma)\varphi(\sigma)\,\mathrm{d}\sigma,$$

where $k(t,\sigma)=q(\sigma)V^2(\sigma)(\tilde{H}(t)-\tilde{H}(\sigma))$. We note that the expression of the kernel $k(t,\sigma)$ relies on the initial conditions (4.7) and (4.8). Now we can formulate (4.9) as the operator equation

$$\varphi(t)+k^2K\varphi(t)=1.\tag{4.10}$$

An expansion of the solution φ can be established by the Neumann series. Firstly, We need to estimate the norm of the operator K restricted to a finite interval $[0,T]$, $T>2\pi$.

We observe that $|k(t,\sigma)| \leqslant |q(\sigma)|/\alpha$. Indeed, with the condition (4.7), we have that

$$\begin{aligned}|k(t,\sigma)| &\leqslant \frac{1}{4\alpha}|q(\sigma)|(e^{\alpha\sigma}+e^{-\alpha\sigma})^2\left(1-\frac{e^{\alpha\sigma}-e^{-\alpha\sigma}}{e^{\alpha\sigma}+e^{-\alpha\sigma}}\right)\\ &\leqslant \frac{1}{2\alpha}|q(\sigma)|(e^{\alpha\sigma}+e^{-\alpha\sigma})e^{-\alpha\sigma}\\ &\leqslant \frac{1}{\alpha}|q(\sigma)|.\end{aligned}$$

With the condition (4.8), we have that

$$\begin{aligned}|k(t,\sigma)| &\leqslant \frac{1}{4\alpha}|q(\sigma)|(e^{\alpha\sigma}-e^{-\alpha\sigma})^2\left(\frac{e^{\alpha\sigma}+e^{-\alpha\sigma}}{e^{\alpha\sigma}-e^{-\alpha\sigma}}-1\right)\\ &\leqslant \frac{1}{2\alpha}|q(\sigma)|(e^{\alpha\sigma}-e^{-\alpha\sigma})e^{-\alpha\sigma} \leqslant \frac{1}{2\alpha}|q(\sigma)|,\\ |\partial_t k(t,\sigma)| &\leqslant \frac{1}{4\alpha}|q(\sigma)|(e^{\alpha\sigma}-e^{-\alpha\sigma})^2\left|\partial_t\left(\frac{e^{\alpha t}+e^{-\alpha t}}{e^{\alpha t}-e^{-\alpha t}}\right)\right|\\ &\leqslant |q(\sigma)|\left|\frac{e^{\alpha\sigma}-e^{-\alpha\sigma}}{e^{\alpha t}-e^{-\alpha t}}\right|^2 \leqslant |q(\sigma)|\end{aligned}$$

for $0 < s \leqslant t < T$. Hence,

$$\|K\| \leqslant C\sup|k(t,\sigma)| \leqslant C\frac{1}{\alpha}$$

and, for the case (4.8), we get $\|\partial_t K\| \leqslant C$.

For sufficiently large α, $(I+k^2K)^{-1}$ exists and then

$$\varphi(t) = \sum_{m=0}^{\infty}\big((-k^2K)^m 1\big)(t) = 1 - k^2(K1)(t) + O\bigg(\frac{1}{\alpha^2}\bigg), \quad 0 \leqslant t \leqslant T. \tag{4.11}$$

Similarly, in case of (4.8), we get

$$\varphi'(t) = -k^2(\partial_t K1)(t) + k^4\partial_t K(K1)(t) + O\bigg(\frac{1}{\alpha^2}\bigg), \quad 0 \leqslant t \leqslant T.$$

Step 2: Characteristic exponents. Using the fundamental solutions in Step 1 and (3.5), we have that (ignoring higher order terms)

$$\begin{aligned}\eta &= \frac{1}{2}(e^{2\pi\alpha}+e^{-2\pi\alpha})\left(1-O\bigg(\frac{1}{\alpha}\bigg)\right) + \frac{1}{2}(e^{2\pi\alpha}+e^{-2\pi\alpha})\left(1-O\bigg(\frac{1}{\alpha}\bigg)\right) + O\bigg(\frac{1}{\alpha}\bigg)\\ &= e^{2\pi\alpha}\left(1-O\bigg(\frac{1}{\alpha}\bigg)\right).\end{aligned}$$

Then by (3.4) we can get

$$\begin{aligned}\lambda_1 &= \frac{\eta}{2}+\sqrt{\frac{\eta^2}{4}-1} = e^{2\pi\alpha}\left(1-O\left(\frac{1}{\alpha}\right)\right),\\ \lambda_2 &= \frac{1}{\lambda_1} = e^{-2\pi\alpha}\left(1+O\left(\frac{1}{\alpha}\right)\right).\end{aligned}$$

It follows from Definition 3.1 that the asymptotic behavior of characteristic exponents is

$$\mu_1 = \frac{1}{2\pi}\log\lambda_1 = \alpha + O\left(\frac{1}{\alpha}\right) \text{ and } \mu_2 = -\mu_1 = -\alpha + O\left(\frac{1}{\alpha}\right).$$

Furthermore, we know that

$$\mu_j^2 - \alpha^2 = (\mu_j - \alpha)(\mu_j + \alpha) = O\left(\frac{1}{\alpha}\right) O\left(2\alpha + O\left(\frac{1}{\alpha}\right)\right) = O(1), \text{ for } j = 1, 2.$$

Step 3: Asymptotics of Hill's equation. According to the case (a) in Definition 3.2, we assume that $u(x_2) = e^{-\mu x_2} v(x_2)$, where $v(0) = v(2\pi)$ and $v'(0) = v'(2\pi)$. Substituting this representation of u into equation (3.1), we obtain

$$e^{-\mu t}\left(v''(t) - 2\mu v'(t) + (k^2 q(t) + \mu^2 - \alpha^2) v(t)\right) = 0.$$

Then we have that $(e^{-2\mu t} v'(t))' = -e^{-2\mu t}(k^2 q(t) + \mu^2 - \alpha^2) v(t)$. Hence

$$e^{-2\mu t} v'(t) = v'(0) - \int_0^t e^{-2\mu\tau}(k^2 q(\tau) + \mu^2 - \alpha^2) v(\tau)\, \mathrm{d}\tau, \tag{4.12}$$

$$e^{-4\pi\mu} v'(2\pi) = e^{-2\mu t} v'(t) - \int_t^{2\pi} e^{-2\mu\tau}(k^2 q(\tau) + \mu^2 - \alpha^2) v(\tau)\, \mathrm{d}\tau. \tag{4.13}$$

Multiplying (4.12) by $e^{-4\mu\pi}$ and substituting $v'(2\pi) = v'(0)$ in (4.13), respectively, we get the two identities

$$e^{-4\pi\mu} e^{-2\mu t} v'(t) = e^{-4\pi\mu} v'(0) - e^{-4\pi\mu} \int_0^t e^{-2\mu\tau}(k^2 q(\tau) + \mu^2 - \alpha^2) v(\tau)\, \mathrm{d}\tau \tag{4.14}$$

and

$$e^{-2\mu t} v'(t) = e^{-4\pi\mu} v'(0) + \int_t^{2\pi} e^{-2\mu\tau}[k^2 q(\tau) + \mu^2 - \alpha^2] v(\tau)\, \mathrm{d}\tau. \tag{4.15}$$

Subtracting (4.14) from (4.15) gives

$$\begin{aligned}
v'(t) &= \frac{1}{1 - e^{-4\pi\mu}} \int_t^{2\pi} e^{2\mu(t-\tau)}(k^2 q(\tau) + \mu^2 - \alpha^2) v(\tau)\, \mathrm{d}\tau \\
&\quad + \frac{e^{-4\pi\mu}}{1 - e^{-4\pi\mu}} \int_0^t e^{2\mu(t-\tau)}(k^2 q(\tau) + \mu^2 - \alpha^2) v(\tau)\, \mathrm{d}\tau \\
&= \frac{e^{4\pi\mu}}{e^{4\pi\mu} - 1} \int_t^{2\pi} e^{2\mu(t-\tau)}(k^2 q(\tau) + \mu^2 - \alpha^2) v(\tau)\, \mathrm{d}\tau \\
&\quad + \frac{1}{e^{4\pi\mu} - 1} \int_0^t e^{2\mu(t-\tau)}(k^2 q(\tau) + \mu^2 - \alpha^2) v(\tau)\, \mathrm{d}\tau.
\end{aligned}$$

There are two cases to consider. We first suppose that $v(0) \neq 0$. Without loss of generality, we suppose $v(0)=1$. Then

$$\begin{aligned}
v(t) &= 1+\int_0^t v'(\sigma)\,\mathrm{d}\sigma\\
&= 1+\frac{e^{4\pi\mu}}{e^{4\pi\mu}-1}\int_0^t\int_\sigma^{2\pi} e^{2\mu(\sigma-\tau)}(k^2q(\tau)+\mu^2-\alpha^2)v(\tau)\,\mathrm{d}\tau\,\mathrm{d}\sigma\\
&\quad+\frac{1}{e^{4\pi\mu}-1}\int_0^t\int_0^\sigma e^{2\mu(\sigma-\tau)}(k^2q(\tau)+\mu^2-\alpha^2)v(\tau)\,\mathrm{d}\tau\,\mathrm{d}\sigma\\
&= 1+\frac{e^{4\pi\mu}}{e^{4\pi\mu}-1}\int_0^{2\pi}\int_0^{\min(t,\tau)} e^{2\mu(\sigma-\tau)}\,\mathrm{d}\sigma(k^2q(\tau)+\mu^2-\alpha^2)v(\tau)\,\mathrm{d}\tau\\
&\quad+\frac{1}{e^{4\pi\mu}-1}\int_0^t\int_\tau^t e^{2\mu(\sigma-\tau)}\,\mathrm{d}\sigma(k^2q(\tau)+\mu^2-\alpha^2)v(\tau)\,\mathrm{d}\tau\\
&= 1+\frac{e^{4\pi\mu}}{e^{4\pi\mu}-1}\int_0^{2\pi}\frac{1}{2\mu}(e^{2\mu\min(t-\tau,0)}-e^{-2\mu\tau})(k^2q(\tau)+\mu^2-\alpha^2)v(\tau)\,\mathrm{d}\tau\\
&\quad+\frac{1}{e^{4\pi\mu}-1}\int_0^t\frac{1}{2\mu}(e^{2\mu(t-\tau)}-1)(k^2q(\tau)+\mu^2-\alpha^2)v(\tau)\,\mathrm{d}\tau\\
&= 1+\frac{1}{2\mu}\int_0^{2\pi}\left(e^{2\mu\min(t-\tau,0)}+\frac{e^{2\mu(t-\tau)}-e^{2\mu(2\pi-\tau)}}{e^{4\pi\mu}-1}\right)(k^2q(\tau)+\mu^2-\alpha^2)v(\tau)\,\mathrm{d}\tau.
\end{aligned}$$

We define an integral operator L by

$$(Lv)(t):=\int_0^{2\pi} l(t,\tau)v(\tau)\,\mathrm{d}\tau,$$

where the kernel $l(t,\tau)$ is defined by

$$l(t,\tau)=\frac{1}{2}\left(e^{2\mu\min(t-\tau,0)}+\frac{e^{2\mu(t-\tau)}-e^{2\mu(2\pi-\tau)}}{e^{4\pi\mu}-1}\right)(k^2q(\tau)+\mu^2-\alpha^2).$$

Then we obtain the integral equation

$$v(t)-\frac{1}{\mu}(Lv)(t)=1.$$

We observe that $|l(t,\tau)|\leqslant C$. By the Neumann series, we can show that

$$v(t)=\sum_{m=0}^{\infty}\left(\frac{1}{\mu}L\right)^m 1=1+\frac{1}{\mu}\int_0^{2\pi} l(t,\tau)\,\mathrm{d}\tau+O\left(\frac{1}{\mu^2}\right). \tag{4.16}$$

In the second case, if $v(0)=0$, then the integral equation becomes $v(t)-\frac{1}{\mu}(Lv)(t)=0$. Taking the norm of both sides of the equation $\mu v(t)=(Lv)(t)$, we find that $\mu\leqslant\|L\|\leqslant C$. This implies that there are only finitely many $\mu=\mu_{n,1}$ with $v(0)=0$ (cf. Lemma 3.5).

It remains to estimate the derivative $v'(t)$. We first compute $\partial_t \frac{1}{\mu}(Lv)(t)$ by

$$\begin{aligned}
\partial_t \frac{1}{\mu}(Lv)(t) &= \partial_t \frac{1}{\mu}\int_0^{2\pi} l(t,\tau)v(\tau)\,\mathrm{d}\tau \\
&= \partial_t \frac{1}{2\mu}\int_0^{t} (k^2 q(\tau)+\mu^2-\alpha^2)v(\tau)\,\mathrm{d}\tau \\
&\quad + \partial_t \frac{1}{2\mu}\int_t^{2\pi} e^{2\mu(t-\tau)}(k^2 q(\tau)+\mu^2-\alpha^2)v(\tau)\,\mathrm{d}\tau \\
&\quad + \partial_t \frac{1}{2\mu}\int_0^{2\pi} \frac{e^{2\mu(t-\tau)}-e^{2\mu(2\pi-\tau)}}{e^{4\pi\mu}-1}(k^2 q(\tau)+\mu^2-\alpha^2)v(\tau)\,\mathrm{d}\tau \\
&= \int_t^{2\pi} e^{2\mu(t-\tau)}(k^2 q(\tau)+\mu^2-\alpha^2)v(\tau)\,\mathrm{d}\tau \\
&\quad + \int_0^{2\pi} \frac{e^{2\mu(t-\tau)}}{e^{4\pi\mu}-1}(k^2 q(\tau)+\mu^2-\alpha^2)v(\tau)\,\mathrm{d}\tau.
\end{aligned}$$

It follows that

$$\begin{aligned}
\frac{\partial_t v(t)}{v(t)} = \frac{\partial_t \frac{1}{\mu}(Lv)(t)}{v(t)} &= \frac{1}{v(t)}\int_t^{2\pi} e^{2\mu(t-\tau)}(k^2 q(\tau)+\mu^2-\alpha^2)v(\tau)\,\mathrm{d}\tau \\
&\quad + \frac{1}{v(t)}\int_0^{2\pi} \frac{e^{2\mu(t-\tau)}}{e^{4\pi\mu}-1}(k^2 q(\tau)+\mu^2-\alpha^2)v(\tau)\,\mathrm{d}\tau.
\end{aligned}$$

Hence, for sufficiently large μ (cf. (4.16)),

$$\left\| \frac{\partial_t v(t)}{v(t)} \right\|_{L^\infty} \leqslant C.$$

Recalling the upward modes $u_n^+(x_2) = e^{-\mu_{n,1}x_2} v_{n,2}(x_2)$ for $\eta_n > 2$ defined in Definition 3.2, we need to estimate $v_{n,2}$ and $v_{n,2}'$. Similarly to the discussions in Step 2, we know that $\mu_{n,1}^2 - \alpha_n^2 = O(1)$ as n tends to infinity. Since $v_{n,2}$ is a periodic function, we have $v_{n,2}(0) = v_{n,2}(2\pi)$, $v_{n,2}'(0) = v_{n,2}'(2\pi)$. Thus we can apply the methods in Step 3 to estimate $v_{n,2}$ and $v_{n,2}'$. Hence we have that for sufficiently large n there exists a constant M such that

$$\left| \frac{v_{n,2}'(d)}{v_{n,2}(d)} \right| \leqslant \left\| \frac{v_{n,2}'(t)}{v_{n,2}(t)} \right\|_{L^\infty} \leqslant M.$$

□

Theorem 4.1. The DtN map $T^+ \colon H_{\hat\alpha}^{1/2}(\mathbb{R}) \to H_{\hat\alpha}^{-1/2}(\mathbb{R})$ is continuous, i.e., there exists a positive constant C such that

$$\|T^+ f\|_{H_{\hat\alpha}^{-1/2}(\mathbb{R})} \leqslant C \|f\|_{H_{\hat\alpha}^{1/2}(\mathbb{R})} \quad \text{for all } f \in H_{\hat\alpha}^{1/2}(\mathbb{R}). \tag{4.17}$$

Proof. For any $f \in H_{\hat\alpha}^{1/2}(\mathbb{R})$, we obtain that

$$\begin{aligned}
\|T^+ f\|^2_{H_{\hat\alpha}^{-1/2}(\mathbb{R})} &= \mathtt{p}\sum_{n\in\mathbb{Z}} (1+\alpha_n^2)^{-1/2} \left| \frac{u_n^{+\prime}(d)}{u_n^+(d)} \right|^2 |f_n|^2 \\
&= \mathtt{p}\sum_{n\in\mathbb{Z}} (1+\alpha_n^2)^{1/2} \left[(1+\alpha_n^2)^{-1/2} \left| \frac{u_n^{+\prime}(d)}{u_n^+(d)} \right| \right]^2 |f_n|^2.
\end{aligned}$$

By Lemma 3.4, it suffices to prove that (4.17) holds for T^+ with a summation running over all n with $\eta_n > 2$, i.e., with $|n|$ sufficiently large. If follows from $|\mu_{n,1}| = O(|n|)$ (cf. Lemma 3.5) and the boundedness of $\frac{v'_{n,2}(d)}{v_{n,2}(d)}$ (cf. Lemma 4.1) that

$$(1+\alpha_n^2)^{-1/2}\left|\frac{{u_n^+}'(d)}{u_n^+(d)}\right| = \frac{\left|-\mu_{n,1} + \frac{v'_{n,2}(d)}{v_{n,2}(d)}\right|}{(1+\alpha_n^2)^{1/2}} \leqslant C \text{ for all } \eta_n > 2.$$

Hence, we have that for any $f \in H^{1/2}_{\hat{\alpha}}(\mathbb{R})$ there exists a constant $C > 0$ such that

$$\|T^+ f\|_{H^{-1/2}_{\hat{\alpha}}(\mathbb{R})} \leqslant C\|f\|_{H^{1/2}_{\hat{\alpha}}(\mathbb{R})},$$

which completes the proof. □

Remark 4.2. Lemma 4.1 and Theorem 4.1 also hold for the downward DtN map T^-.

4.2 Variational formulation

To truncate the computational domain for the scattering problem to a bounded periodic cell (see Figure 2), we introduce the bounded domain

$$C := \{(x_1, x_2)^{\mathrm{T}} \in \mathbb{R}^2 : 0 < x_1 < \mathtt{p},\ b < x_2 < d\},$$

and the boundaries

$$\tilde{\Gamma}_d := \{(x_1, x_2)^{\mathrm{T}} \in \mathbb{R}^2 : 0 < x_1 < \mathtt{p},\ x_2 = d\},$$
$$\tilde{\Gamma}_b := \{(x_1, x_2)^{\mathrm{T}} \in \mathbb{R}^2 : 0 < x_1 < \mathtt{p},\ x_2 = b\}.$$

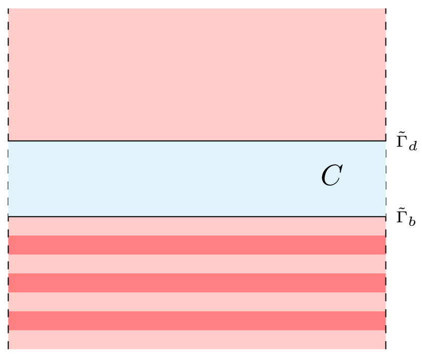

Figure 2: Illustration of a periodic cell $C := (0, \mathtt{p}) \times (b, d)$, which is covered by a homogeneous medium in $x_2 > d$ and sits above an inhomogeneous half plane $x_2 < b$.

We consider the downward DtN map T^- (cf. Definition 4.2) on $\tilde{\Gamma}_b$ and the standard upward DtN map T on $\tilde{\Gamma}_d$ (cf. (4.2)). Formulating the radiation conditions over $\tilde{\Gamma}_d$ and $\tilde{\Gamma}_b$ with the help of the DtN maps, we consider the boundary value problem

$$\begin{cases} \Delta u(x_1, x_2) + k^2 \tilde{q}(x_1, x_2) u(x_1, x_2) = 0 & (x_1, x_2)^{\mathrm{T}} \in C, \\ [Tu(\cdot, d)](x_1) \;=\; \left.\frac{\partial u(x_1,x_2)}{\partial x_2}\right|_{x_2=d} + 2i\beta e^{i\hat{\alpha}x_1 - i\beta d} & \text{on } \tilde{\Gamma}_d, \\ [T^- u(\cdot, b)](x_1) = -\left.\frac{\partial u(x_1,x_2)}{\partial x_2}\right|_{x_2=b} & \text{on } \tilde{\Gamma}_b. \end{cases}$$

Multiply both sides of the Helmholtz equation in C by the complex conjugate of $v \in H^1_{\hat{\alpha}}(C)$ and then integrate over C. Due to the Green's formula and the DtN maps, we obtain the variational formulation: Find $u \in H^1_{\hat{\alpha}}(C)$ such that

$$a(u, v) = F(v) \text{ for any } v \in H^1_{\hat{\alpha}}(C), \tag{4.18}$$

where

$$\begin{aligned} a(u, v) &:= \int_C \nabla u(x_1, x_2) \cdot \nabla \bar{v}(x_1, x_2) - k^2 \tilde{q}(x_1, x_2) u(x_1, x_2) \bar{v}(x_1, x_2) \,\mathrm{d}x_1 \,\mathrm{d}x_2 \qquad (4.19)\\ &\quad - \int_{\tilde{\Gamma}_d} T u \bar{v} \,\mathrm{d}s - \int_{\tilde{\Gamma}_b} T^- u \bar{v} \,\mathrm{d}s,\\ F(v) &:= \int_{\tilde{\Gamma}_d} -2i\beta e^{i\hat{\alpha}x_1 - i\beta d} \bar{v} \,\mathrm{d}s. \qquad (4.20) \end{aligned}$$

Theorem 4.2. The sesquilinear form $a(\cdot, \cdot) : H^1_{\hat{\alpha}}(C) \times H^1_{\hat{\alpha}}(C) \to \mathbb{C}$ defined in (4.19) is strongly elliptic over $H^1_{\hat{\alpha}}(C)$.

Proof. By the mapping properties of T^-, we can choose an $N \in \mathbb{N}$ such that, for any $|n| \geqslant N$ (cf. Lemma 4.1),

$$-\frac{{u_n^-}'(b)}{u_n^-(b)} = -\mu_{n,1} - \frac{v_{n,1}'(b)}{v_{n,1}(b)} < -\mu_{n,1} + O(M) < 0. \tag{4.21}$$

For any quasi-periodic function $f \in H^{1/2}_{\hat{\alpha}}(\mathbb{R})$, defining

$$T_1^- f = \sum_{|n|>N} -\frac{{u_n^-}'(b)}{u_n^-(b)} f_n e^{i\alpha_n x_1} \quad \text{and} \quad T_2^- f = \sum_{|n|\leqslant N} -\frac{{u_n^-}'(b)}{u_n^-(b)} f_n e^{i\alpha_n x_1}, \tag{4.22}$$

we have $T^- f = T_1^- f + T_2^- f$. Then we can decompose $a(u, v)$ into two parts such that

$$a(u, v) = B(u, v) - Q(u, v),$$

where

$$\begin{aligned} B(u, v) &= \int_C \nabla u \cdot \nabla \bar{v} + u\bar{v} \,\mathrm{d}x - \int_{\tilde{\Gamma}_d} T u \bar{v} \,\mathrm{d}s - \int_{\tilde{\Gamma}_b} T_1^- u \bar{v} \,\mathrm{d}s,\\ Q(u, v) &= \int_C \left(k^2 \tilde{q}(x_1, x_2) + 1\right) u(x_1, x_2) \bar{v}(x_1, x_2) \,\mathrm{d}x_1 \,\mathrm{d}x_2 + \int_{\tilde{\Gamma}_b} T_2^- u \bar{v} \,\mathrm{d}s. \end{aligned}$$

Taking $v = u$ in $B(u, v)$ gives

$$B(u, u) = \int_C |\nabla u|^2 + |u|^2 \,\mathrm{d}x - \int_{\tilde{\Gamma}_d} T u \bar{u} \,\mathrm{d}s + \mathtt{p} \sum_{|n|>N} \frac{{u_n^-}'(b)}{u_n^-(b)} |u_n|^2.$$

It follows from the definition of T that, for the Fourier expansion $u(x_1, d) = \sum_n u_n e^{i\alpha_n x_1}$,

$$\begin{aligned} -\operatorname{Re}\left(\int_{\tilde{\Gamma}_d} T u \bar{u} \,\mathrm{d}s\right) &= -\operatorname{Re}\left(\int_{\tilde{\Gamma}_d} \left(\sum_{n\in\mathbb{N}} i\beta_n u_n e^{i\alpha_n x_1}\right)\left(\sum_{n\in\mathbb{N}} \bar{u}_n e^{-i\alpha_n x_1}\right) \mathrm{d}s\right)\\ &= -\operatorname{Re}\left(\mathtt{p} \sum_{n\in\mathbb{N}} i\beta_n |u_n|^2\right)\\ &= \mathtt{p} \sum_{|\alpha_n|>k} |\beta_n| |u_n|^2\\ &\geqslant 0. \end{aligned}$$

By the inequality (4.21), we have that $\operatorname{Re} B(u,u) \geqslant \|u\|^2_{H^1_{\hat\alpha}(C)}$. Hence, $B(u,v)$ is coercive.

Next, we claim that $\operatorname{Re} Q(u,v)$ is a compact form. To see this, we note that the Riesz representation asserts the existence of two bounded linear operators $K_1\colon H^1_{\hat\alpha}(C) \to H^1_{\hat\alpha}(C)$ and $K_2\colon H^1_{\hat\alpha}(C) \to H^1_{\hat\alpha}(C)$ such that

$$\begin{aligned}(K_1 u, v)_{H^1_{\hat\alpha}(C)} &= \operatorname{Re} \int_C (k^2 \tilde q(x_1,x_2) + 1) u(x_1,x_2) \bar v(x_1,x_2)\, \mathrm{d}x_1\, \mathrm{d}x_2,\\ (K_2 u, v)_{H^1_{\hat\alpha}(C)} &= \operatorname{Re} \int_{\tilde\Gamma_b} T_2^- u \bar v \,\mathrm{d}s.\end{aligned}$$

Let $v = K_1 u$, we have that

$$\|K_1 u\|^2_{H^1_{\hat\alpha}(C)} \leqslant C \|u\|_{L^2(C)} \|K_1 u\|_{L^2(C)} \leqslant C \|u\|_{L^2(C)} \|K_1 u\|_{H^1_{\hat\alpha}(C)}. \tag{4.23}$$

Suppose that $\{u_n\}_{n=1}^{+\infty}$ is a bounded sequence in $H^1_{\hat\alpha}(C)$. Then by the Rellich-Kondrachov theorem, there exists a subsequnce $\{u_{n_i}\}_{i=1}^{+\infty}$ such that $\{u_{n_i}\}$ is (strongly) convergent in $L^2(C)$. By the estimate (4.23), $\{K_1 u_{n_i}\}$ is a Cauchy sequence in $H^1_{\hat\alpha}(C)$ and hence $\{K_1 u_{n_i}\}$ is convergent in $H^1_{\hat\alpha}(C)$. This implies that K_1 is compact. Since there are only finitely many terms in the summation of $T_2^- u$ (cf. (4.22))), it follows that K_2 is compact.

Hence, $\operatorname{Re} a(u,v)$ is the sum of a coercive form and a compact form, implying the strong ellipticity of the sesquilinear form $a(u,v)$ over $H^1_{\hat\alpha}(C)$. □

4.3 Well-posedness results

In this section we shall prove that our scattering problem admits a unique solution for all wavenumbers $k > 0$ except for a discrete set. The exceptional wavenumbers in this discrete set can accumulate only at infinity and are bounded below by a positive constant.

First, we study the unique solvability at small wavenumbers. Lemma 3.4 shows the asymptotic behavior of η_n as n tends to infinity at a fixed wavenumber k. Motivated by the arguments in the proof of Lemma 3.4, we derive the behavior of η_n for fixed n and k tending to 0. Some technical proofs will be presented in the Appendix.

Lemma 4.2. Suppose that $k > 0$ is sufficiently small. Then:

(i) $\eta_n > 2$ for all $n \neq 0$.

(ii) For $n = 0$, we have $|\eta_0| < 2$ if $q(x_2) > \sin^2\theta$ in $x_2 < b$.

The proof of the first assertion is given by Lemma C.1 in Appendix C and that of the second one in Appendix B. By Lemma 4.2, we can compute the coefficients in the downward DtN map T^- explicitly. Recall from (DRC) and (4.6) that $u_n^-(x_2) e^{i\alpha_n x_1}$ denotes the n-th downward wave mode. Using Definition 3.2 and Lemma 3.2 (a) and (c), we obtain for small wavenumbers that

$$-\frac{{u_n^-}'(b)}{u_n^-(b)} = \begin{cases} -\mu_{n,1} - \frac{v_{n,1}'(b)}{v_{n,1}(b)} & \text{for } n \neq 0,\\ i\theta_0 - \frac{v_{0,1}'(b)}{v_{0,1}(b)} & \text{for } n = 0.\end{cases} \tag{4.24}$$

where $\mu_{n,1} > 0$ if $n \neq 0$ and $\theta_0 \in (0, 1/2)$. Note that u_n^-, $v_{n,1}$, $\mu_{n,1}$ and θ_0 all depend on the wavenumber. Their asymptotic properties as $k \to +0$ are shown below.

Lemma 4.3. Suppose that $k > 0$ is sufficiently small.

(i) For $n \neq 0$, the term $\frac{v_{n,1}'(b)}{v_{n,1}(b)}$ is real-valued and

$$\left| \frac{v_{n,1}'(b)}{v_{n,1}(b)} \right| = O(k^2) \quad \text{as} \quad k \to +0.$$

(ii) For $n = 0$ and $q(x_2) > \sin^2\theta$ for $x_2 < b$. Then it holds that

$$\theta_0 = O(k), \quad \left|\frac{v'_{0,1}(b)}{v_{0,1}(b)}\right| = o(1) \quad \text{as} \quad k \to +0.$$

(iii) For $n \neq 0$, we have $\mu_{n,1} > |n| - \frac{1}{2\pi}\ln 2 > 0$ as $k \to +0$.

Proof. For the proof of the asymptotic results in (i), (ii) and (iii) we refer to Lemmas C.1, C.2 and C.3 in the Appendix C (Note that, for similarity reasons, we prove the results for the upper radiation condition instead of the analogous results for the lower radiation condition). It remains to prove that $\frac{v'_{n,1}(b)}{v_{n,1}(b)}$ is real-valued for $n \neq 0$ if $k > 0$ is sufficiently small. We retain the notation used in Section 3. Recall from Lemma 3.2 that $v_{n,1}$ is a linear combination of the fundamental solutions of (3.1), that is,

$$v_{n,1}(x_2) = e^{-\mu_{n,1}x_2}(c_1 w_{n,1}(x_2) + c_2 w_{n,2}(x_2)),$$

where $(c_1, c_2)^{\mathrm{T}}$ is an eigenvector associated to the eigenvalue $\lambda_{n,1}$ of the matrix W_n. Since $q(x_2)$ is real-valued, the fundamental solutions $w_{n,1}(x_2)$ and $w_{n,2}(x_2)$ are real-valued. Due to $\eta_n > 2$ (cf. Lemma 4.2), $\mu_{n,1}$ and $(c_1, c_2)^{\mathrm{T}}$ are also real-valued. Hence $v_{n,1}(x_2)$ is real-valued, which completes the proof. $\square$

Theorem 4.3 (Solvability at small wavenumbers)**.** Assume that, for any $b - 2\pi < x_2 \leqslant b$, we have $q(x_2) > \sin^2\theta$. Then the variational formulation (4.18) admits a unique solution $u \in H^1_{\hat{\alpha}}(C)$ for all $k \in (0, k_0)$ and all directions of incidence.

Proof. By Theorem 4.2 and the Fredholm alternative, it is sufficient to prove that the solution of the variational formulation (4.18) is unique if $k > 0$ is sufficiently small. Taking $v = u$ in the variational formulation (4.18) with $u^{\mathrm{in}} = 0$, we see

$$0 = a(u, u) = \int_C |\nabla u(x)|^2 - k^2\tilde{q}(x)|u(x)|^2 \,\mathrm{d}x - \int_{\tilde{\Gamma}_d} Tu\bar{u}\,\mathrm{d}s - \int_{\tilde{\Gamma}_b} T^-u\bar{u}\,\mathrm{d}s. \tag{4.25}$$

For $k \in (0, k_0)$ with $k_0 > 0$ sufficiently small, the upward and downward DtN maps T and T^- can be rephrased as

$$\int_{\tilde{\Gamma}_d} Tu\bar{u}\,\mathrm{d}s = \mathtt{p}ik\cos\theta|u_0(d)|^2 - \mathtt{p}\sum_{n\neq 0}|\beta_n||u_n(d)|^2,$$

$$\int_{\tilde{\Gamma}_b} T^-u\bar{u}\,\mathrm{d}s = \mathtt{p}\left(i\theta_0 - \frac{v'_{0,1}(b)}{v_{0,1}(b)}\right)|u_0(b)|^2 - \mathtt{p}\sum_{n\neq 0}\left(\mu_{n,1} + \frac{v'_{n,1}(b)}{v'_{n,1}(b)}\right)|u_n(b)|^2,$$

where $u_n(d)$ and $u_n(b)$ are the Fourier coefficients of $e^{-i\alpha x_1}u(x_1, x_2)$ on $\tilde{\Gamma}_d$ and $\tilde{\Gamma}_d$, respectively. The real and imaginary parts can be written as

$$\mathrm{Re}\int_{\tilde{\Gamma}_d} Tu\bar{u}\,\mathrm{d}s = -\mathtt{p}\sum_{n\neq 0}|\beta_n||u_n(d)|^2 < 0,$$

$$\mathrm{Im}\int_{\tilde{\Gamma}_d} Tu\bar{u}\,\mathrm{d}s = \mathtt{p}k\cos\theta|u_0(d)|^2 > 0,$$

$$\mathrm{Re}\int_{\tilde{\Gamma}_b} T^-u\bar{u}\,\mathrm{d}s = -\mathtt{p}\frac{v'_{0,1}(b)}{v_{0,1}(b)}|u_0(b)|^2 - \mathtt{p}\sum_{n\neq 0}\left(\mu_{n,1} + \frac{v'_{n,1}(b)}{v'_{n,1}(b)}\right)|u_n(b)|^2,$$

$$\mathrm{Im}\int_{\tilde{\Gamma}_b} T^-u\bar{u}\,\mathrm{d}s = \mathtt{p}\theta_0|u_0(b)|^2 > 0.$$

Taking the real part of (4.25) and using the asymptotic behavior of $\mu_{n,1}$ and Lemma 4.3 (ii), we arrive at

$$
\begin{aligned}
0 &= \operatorname{Re}[a(u,u)] \\
&= \|\nabla u\|^2_{L^2(C)} - k^2\int_C \operatorname{Re}\tilde q(x)|u(x)|^2\,\mathrm{d}x - \operatorname{Re}\int_{\tilde\Gamma_d} Tu\bar u\,\mathrm{d}s - \operatorname{Re}\int_{\tilde\Gamma_b} T^- u\bar u\,\mathrm{d}s \\
&\geqslant \|\nabla u\|^2_{L^2(C)} - C_0k^2\|u\|^2_{L^2(C)} + \frac{\mathtt{p}}{C_0}\sum_{n\neq 0}|n||u_n(b)|^2 + \frac{\mathtt{p}}{C_0}|u_0(b)|^2 - \frac{2\pi}{C_0}|u_0(b)|^2 + o(1)|u_0(b)|^2 \\
&\geqslant C_1\|u\|^2_{H^1(C)} - \frac{\mathtt{p}}{C_0}|u_0(b)|^2,
\end{aligned}
\tag{4.26}
$$

where the constants $C_0, C_1 > 0$ do not depend on the direction of incidence. Taking the imaginary part of (4.25) and letting k tend to zero give that

$$
\begin{aligned}
0 &= \operatorname{Im}[a(u,u)] \\
&= -k^2\int_C \operatorname{Im}\tilde q(x)|u(x)|^2\,\mathrm{d}x - \operatorname{Im}\int_{\tilde\Gamma_d} Tu\bar u\,\mathrm{d}s - \operatorname{Im}\int_{\tilde\Gamma_b} T^- u\bar u\,\mathrm{d}s \\
&\geqslant -\mathtt{p}k\cos\theta|u_0(d)|^2 - \mathtt{p}\theta_0|u_0(b)|^2.
\end{aligned}
\tag{4.27}
$$

Since $\cos\theta$ and θ_0 are positive, we have that $|u_0(d)| = |u_0(b)| = 0$. Combining this and (4.26) implies that $\|u\|_{H^1(C)} = 0$, which completes the uniqueness proof for small wavenumbers. □

Theorem 4.4. Fix the angle of incidence $\theta \in (-\pi/2, \pi/2)$. Then the variational problem (4.18) has a unique solution for all wavenumbers $k > 0$ not contained in a discrete subset of the positive reals. The only possible accumulating point of this discrete set is infinity.

Proof. Without loss of generality we may assume that, for any $b - 2\pi < x_2 \leqslant b$, we have $q(x_2) > \sin^2\theta$. Otherwise we could replace q by $q_C := C^2 q$ and k by $k_C := k/C$ with a big constant $C > 0$. Then our assumption is fulfilled with q_C and k_C, and the resulting theorem for q_C and k_C implies the theorem for q and k.

We shall carry out the proof by applying the analytic Fredholm theory [3, Theorem 8.26] to our wavenumber-dependent variational formulation. For this purpose we need to transfer the dependence of the α-quasiperodic Sobolev space on k to an equivalent variational formulation, for which the underlying function space is independent of the wavenumber. Setting $\hat a(u,v) := a(\hat u, \hat v)$ for $u, v \in H^1_{per}(C)$ with $\hat u := e^{-i\hat\alpha x_1}u$ as well as $\hat v := e^{-i\hat\alpha x_1}v$, we obtain a new sesquilinear form $\hat a(\cdot,\cdot)$ defined on $H^1_{per}(C)$:

$$
\begin{aligned}
\hat a(u,v) = &\int_C \nabla u(x)\cdot\nabla\bar v(x) - i\hat\alpha\frac{\partial u(x)}{\partial x_1}\bar v(x) + i\hat\alpha u(x)\frac{\partial \bar v(x)}{\partial x_1} - (k^2\tilde q(x) - \hat\alpha^2)u(x)\bar v(x)\,\mathrm{d}x \\
&- \int_{\tilde\Gamma_d}\hat T u\bar v\,\mathrm{d}s - \int_{\tilde\Gamma_b}\hat T^- u\bar v\,\mathrm{d}s.
\end{aligned}
\tag{4.28}
$$

Here the operators $\hat T$ and $\hat T^-$ are periodic DtN maps defined over the space $H^{1/2}_{per}(\tilde\Gamma_d)$ and $H^{1/2}_{per}(\tilde\Gamma_b)$, respectively. Using the decomposition of T^- in (4.22), we can rewrite $\hat a(u,v)$ as $\hat a_1(u,v) - \hat a_2(u,v)$, where

$$
\begin{aligned}
\hat a_1(u,v) &:= \int_C \nabla u\cdot\nabla\bar v + u\bar v\,\mathrm{d}x - \int_{\tilde\Gamma_d}\hat T u\bar v\,\mathrm{d}s - \int_{\tilde\Gamma_b}\hat T_1^- u\bar v\,\mathrm{d}s, \\
\hat a_2(u,v) &:= \int_C i\hat\alpha\frac{\partial u(x)}{\partial x_1}\bar v(x) - i\hat\alpha u(x)\frac{\partial\bar v(x)}{\partial x_1} + (k^2\tilde q(x) - \hat\alpha^2 + 1)u(x)\bar v(x)\,\mathrm{d}x + \int_{\tilde\Gamma_b}\hat T_2^- u\bar v\,\mathrm{d}s.
\end{aligned}
$$

By the Riesz representation theorem, the sesquilinear forms $\hat{a}_1(\cdot,\cdot)$ and $\hat{a}_2(\cdot,\cdot)$ give rise to the wavenumber-dependent operators $A(k)$ and $K(k)$, respectively, where $A(k)$ is a bounded invertible operator on $H^1_{per}(C)$ and $K(k) : H^1_{per}(C) \to H^1_{per}(C)$ is compact (cf. the proof of Theorem 4.2 and [17, Section 4]). It follows from [10, Lemma 6] and the analytic dependence of the wave modes on k that both, $A(k)$ and $K(k)$, are analytic operators with respect to the wavenumber k. Combining the uniqueness result (cf. Theorem 4.3) and the argument in [2, Theorem 2.1], we can show that $(A(k) - K(k))^{-1}$ exists for all k except those in a discrete set. By the analytic Fredholm theory, the only possible accumulating point of this discrete set is at infinity. This concludes the proof. □

Appendices

A Floquet theory

This appendix is mainly based on [6, Chapter 1] and [15, Chapter 9]. Consider the general second-order ODE

$$a_0(x)y''(x) + a_1(x)y'(x) + a_2(x)y(x) = 0, \tag{A.1}$$

where the coefficients $a_0(x)$, $a_1(x)$ and $a_2(x)$ are complex-valued, piecewise continuous and periodic with the period p.

Theorem A.1. There are a non-zero constant ρ and a non-trival solution $\psi(x)$ of (A.1) such that

$$\psi(x + p) = \rho\psi(x). \tag{A.2}$$

Proof. Let $\phi_1(x)$ and $\phi_2(x)$ be the linearly independent solutions of (A.1) which satisfy the initial conditions

$$\begin{aligned} \phi_1(0) = 1,\ \phi_1'(0) = 0; \\ \phi_2(0) = 0,\ \phi_2'(0) = 1. \end{aligned} \tag{A.3}$$

Since $\phi_1(x + p)$ and $\phi_2(x + p)$ are also linearly independent solution of (A.1), there are constants $A_{ij} (1 \leqslant i, j \leqslant 2)$ such that

$$\begin{aligned} \phi_1(x + p) = A_{11}\phi_1(x) + A_{12}\phi_2(x), \\ \phi_2(x + p) = A_{21}\phi_1(x) + A_{22}\phi_2(x), \end{aligned} \tag{A.4}$$

where the matrix $A = (A_{ij})$ is non-singular. Every solution $\psi(x)$ of (A.1) has the form

$$\psi(x) = c_1\phi_1(x) + c_2\phi_2(x), \tag{A.5}$$

where c_1 and c_2 are constant. By (A.4), we have that (A.2) holds if

$$\begin{aligned} (A_{11} - \rho)c_1 + A_{21}c_2 = 0, \\ A_{12}c_1 + (A_{22} - \rho)c_2 = 0. \end{aligned}$$

The function ψ of (A.5) is non-trival if c_1 and c_2 are not both zero. Hence, a non-trival ψ exists if and only if

$$\det \begin{pmatrix} A_{11} - \rho & A_{21} \\ A_{12} & A_{22} - \rho \end{pmatrix} = 0,$$

i.e.,

$$\rho^2 - (A_{11} + A_{22})\rho + \det A = 0. \tag{A.6}$$

This is a quadratic equation for ρ. Since A is non-singular, (A.6) has at least one non-trival solution. This completes the proof. □

An alternative form of (A.6) can be obtained as follows. It follows from (A.3) and (A.4) that

$$A_{11} = \phi_1(p),\ A_{12} = \phi_1'(p),\ A_{21} = \phi_2(p),\ A_{22} = \phi_2'(p).$$

Hence using Liouville's formula for the Wronskian

$$W(\phi_1, \phi_2)(x) := \det \begin{pmatrix} \phi_1(x) & \phi_2(x) \\ \phi_1'(x) & \phi_2'(x) \end{pmatrix}$$

[16, Lemma 3.11] and the fact that $W(\phi_1, \phi_2)(0) = 1$, we get

$$\det A = W(\phi_1, \phi_2)(p) = e^{\left(-\int_0^p \frac{a_1(x)}{a_0(x)}\,\mathrm{d}x\right)}.$$

Thus (A.6) can be rewritten as

$$\begin{aligned} &\rho^2 - \eta\rho + e^{\left(-\int_0^p \frac{a_1(x)}{a_0(x)}\,\mathrm{d}x\right)} = 0, \\ &\eta = \phi_1(p) + \phi_2'(p). \end{aligned} \tag{A.7}$$

In particular, all of the zeros ϱ of (A.7) or equivalently of (A.6) are different from zero.

Theorem A.1 leads to the existence of two linearly independent solutions of (A.1) having the special form given in Theorem A.2 below.

Theorem A.2. There are linearly independent solutions $\psi_1(x)$ and $\psi_2(x)$ of (A.1) such that either

(1) (A.7) has two distinct roots or only one root ρ with $\mathrm{rank}(A^{\mathrm{T}} - \rho I) = 0$.

$$\psi_1(x) = e^{m_1 x} v_1(x),\ \psi_2(x) = e^{m_2 x} v_2(x),$$

where m_1, m_2 are constant, not necessarily distinct, and v_1, v_2 are periodic functions with period p, or

(2) (A.7) has only one root ρ with $\mathrm{rank}(A^{\mathrm{T}} - \rho I) = 1$.

$$\psi_1(x) = e^{mx} v_1(x),\ \psi_2(x) = e^{mx}(x v_1(x) + v_2(x)),$$

where m is constant, and v_1, v_2 are periodic with period p.

Proof. Consider two cases as follows.

(1) Suppose that (A.6) has distinct solutions ρ_1 and ρ_2. Then by the proof of Theorem A.1, there are non-trival solutions ψ_1 and ψ_2 of (A.1) such that

$$\psi_k(x + p) = \rho_k \psi_k(x),\ k = 1, 2. \tag{A.8}$$

It is easy to show that ψ_1 and ψ_2 are linearly independent. Since ρ_1 and ρ_2 are non-zero, we can define m_1 and m_2 so that

$$e^{pm_k} = \rho_k,\ k = 1, 2. \tag{A.9}$$

We can construct a new function $v_k(x)$,

$$v_k(x) = e^{-m_k x}\psi_k(x). \tag{A.10}$$

By (A.8) and (A.9),

$$v_k(x + p) = e^{-m_k(x+p)}\rho_k \psi_k(x) = v_k(x).$$

Thus,

$$\psi_k(x) = e^{m_k x} v_k(x),$$

where $v_k(x)$, $k = 1, 2$ are periodic functions.

(2) Suppose that (A.6) has a repeated solution ρ. We define m so that

$$e^{pm} = \rho.$$

By Theorem A.1, there is a non-trival solution Ψ_1 of (A.1) such that

$$\Psi_1(x+p) = \rho\Psi_1(x). \tag{A.11}$$

Let Ψ_2 be any solution of (A.1) which is linearly independent of Ψ_1. Since Ψ_2 also satisfies (A.1), there are constants d_1 and d_2 such that

$$\Psi_2(x+p) = d_1\Psi_1(x) + d_2\Psi_2(x) \tag{A.12}$$

Next we calculate d_2. With the help of (A.11) and (A.12), we obtain

$$W(\Psi_1, \Psi_2)(x+p) = \rho d_2 W(\Psi_1, \Psi_2)(x).$$

Hence by Liouville's formula for the Wronskian,

$$\rho d_2 = e^{-\int_x^{x+p} \frac{a_1(t)}{a_0(t)}\,\mathrm{d}t} = e^{-\int_0^{p} \frac{a_1(t)}{a_0(t)}\,\mathrm{d}t},$$

since the integrand has period p. Futhermore the right-hand side in the above equation is equal to ρ^2 since ρ is the repeated solution of (A.7). Hence $d_2 = \rho$. From (A.12) we now have

$$\Psi_2(x+p) = d_1\Psi_1(x) + \rho\Psi_2(x). \tag{A.13}$$

Now, there are two possibilities to consider:

Possibility 1: $d_1 = 0$

In this case (A.13) implies

$$\Psi_2(x+p) = \rho\Psi_2(x).$$

This together with (A.11) indicates that we have the same situation as in (A.8) but with $\rho_1 = \rho_2 = \rho$. In other words, $(A^{\mathrm{T}} - \rho I)\mathbf{x} = 0$ has two linearly independent solutions, i.e., $\mathrm{rank}(A^{\mathrm{T}} - \rho I) = 0$. Consequently, this case is covered by part (1) of the theorem.

Possibility 2: $d_1 \neq 0$

In this case we define

$$\begin{aligned} v_1(x) &:= e^{-mx}\Psi_1(x), \\ v_2(x) &:= e^{-mx}\Psi_2(x) - \left(\frac{d_1}{p\rho}\right) x v_1(x). \end{aligned}$$

Then due to (A.11) and (A.13) v_1 and v_2 have period p. In this case, $(A^{\mathrm{T}} - \rho I)\mathbf{x} = 0$ has only one non-trival solution, i.e., $\mathrm{rank}(A^{\mathrm{T}} - \rho I) = 1$. Therefore, since

$$\begin{aligned} \Psi_1(x) &= e^{mx} v_1(x), \\ \Psi_2(x) &= e^{mx}\left(\left(\frac{d_1}{p\rho}\right) x v_1(x) + v_2(x)\right), \end{aligned}$$

part (2) is covered with $\psi_1(x) := \Psi_1(x)$ and $\psi_2(x) := (p\rho/d_1)\Psi_2(x)$.

$\square$

B Proof of Lemma 4.2 (ii)

In this section, we mainly follow [6, Section 2.1 and 2.2]. For simplicity, we omit the proofs presented in this reference paper. Here we consider the second-order equation

$$(p(x)y'(x))' + (\lambda s(x) - q(x))y(x) = 0, \tag{B.1}$$

where λ is a real parameter. The coefficient functions $p(x)$, $s(x)$ and $q(x)$ are real-valued and periodic with period p. Furthermore, we assume the existence of a constant $s > 0$ such that $s(x) \geqslant s$.

To show the dependence of the solutions on λ, we denote the fundamental solutions of (B.1) by $\phi_1(x, \lambda)$ and $\phi_2(x, \lambda)$. Then corresponding to (A.7), we define

$$\eta(\lambda) := \phi_1(p, \lambda) + \phi_2'(p, \lambda).$$

Whether λ is real or complex, $\phi_1(x, \lambda)$ and $\phi_2(x, \lambda)$ and their derivatives are analytic functions of λ for fixed x, see [5, Section 1.7]. Hence, $\eta(\lambda)$ is an analytic function of λ.

Now we introduce two eigenvalue problems associated to (B.1) on the interval $[0, p]$, where λ is regarded as a parameter. These two problems will be used in the investigation of $\eta(\lambda)$.

The periodic eigenvalue problem: Consider (B.1) in $[0, p]$ and periodic boundary conditions:

$$\begin{aligned} &(p(x)y'(x))' + (\lambda s(x) - q(x))y(x) = 0 \text{ in } [0, p], \\ &y(0) = y(p), \ y'(0) = y'(p). \end{aligned} \tag{B.2}$$

It is a self-adjoint problem and has a countable set of eigenvalues λ. We shall denote the eigenfunctions throughout by $\psi_n(x)$ and the eigenvalues by λ_n $(n = 0, 1, \ldots)$, where

$$\lambda_0 \leqslant \lambda_1 \leqslant \lambda_2 \leqslant \cdots, \text{ and } \lambda_n \to \infty \text{ as } n \to \infty.$$

The $\psi_n(x)$ can be chosen to be real-valued and to form an orthonormal basis over $[0, p]$ with weight function $s(x)$. Thus

$$\int_0^p \psi_m(x)\psi_n(x)s(x)\,\mathrm{d}x = \begin{cases} 1 & (m = n), \\ 0 & (m \neq n). \end{cases}$$

The semi-periodic eigenvalue problem: Consider (B.1) in $[0, p]$ and semi-periodic boundary conditions:

$$\begin{aligned} &(p(x)y'(x))' + (\lambda s(x) - q(x))y(x) = 0 \text{ in } [0, p], \\ &y(0) = -y(p), \ y'(0) = -y'(p). \end{aligned} \tag{B.3}$$

It is also a self-adjoint problem and we shall denote the eigenfunctions by $\xi_n(x)$ and the eigenvalues λ by μ_n $(n = 0, 1, \cdots)$, where

$$\mu_0 \leqslant \mu_1 \leqslant \mu_2 \leqslant \cdots, \text{ and } \mu_n \to \infty \text{ as } n \to \infty.$$

Now we use the existence of the eigenvalues λ_n and μ_n in the eigenvalue problems (B.2) and (B.3) to study the behavior of $\eta(\lambda)$. We refer to Figure 3 for a rough idea of the function $\eta(\lambda)$.

Theorem B.1. (1) The numbers λ_n and μ_n occur in the order

$$\lambda_0 < \mu_0 \leqslant \mu_1 < \lambda_1 \leqslant \lambda_2 < \mu_2 \leqslant \mu_3 < \lambda_3 \leqslant \lambda_4 < \cdots.$$

(2) $\eta(\lambda)$ decreases from 2 to -2 in the intervals $[\lambda_{2m}, \mu_{2m}]$.

(3) $\eta(\lambda)$ increases from -2 to 2 in the intervals $[\mu_{2m+1}, \lambda_{2m+1}]$.

(4) $\eta(\lambda) > 2$ in the intervals $(-\infty, \lambda_0)$ and $(\lambda_{2m+1}, \lambda_{2m+2})$.

(5) $\eta(\lambda) < -2$ in the intervals (μ_{2m}, μ_{2m+1}).

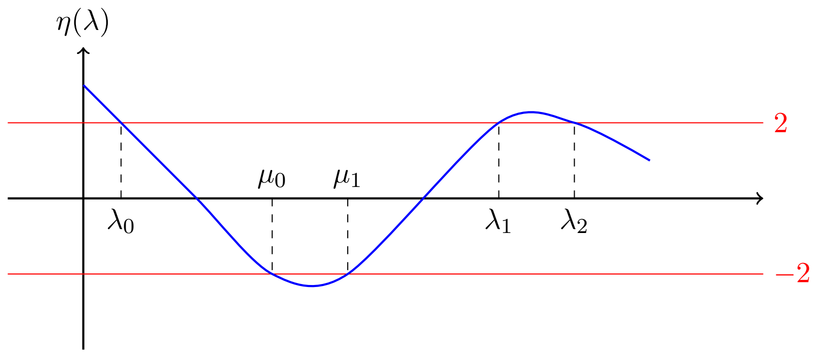

Figure 3: An illustration of dependence of η on λ.

Proof of Lemma 4.2 (ii).
For $n = 0$, the ordinary differential equation (3.1) takes the form

$$u_0''(x_2) + k^2(q(x_2) - \sin^2\theta)u_0(x_2) = 0. \tag{B.4}$$

Then we consider the periodic eigenvalue problem

$$\begin{aligned} &u_0''(x_2) + \lambda(q(x_2) - \sin^2\theta)u_0(x_2) = 0 \text{ in } (0, 2\pi), \\ &u_0(0) = u_0(2\pi),\ u_0'(0) = u_0'(2\pi). \end{aligned} \tag{B.5}$$

Integrating by parts and using $q(x_2) > \sin^2\theta$, one can show that the periodic eigenvalue problem (B.5) has nonnegative eigenvalues. Furthermore, $\lambda = 0$ is the first eigenvalue of (B.5). Applying Theorem B.1 with $\lambda = k^2$, it follows that the constant η_0 associated to (B.4) (i.e., η_n defined by (3.5) with $n = 0$) must lie in $(-2, 2)$ if $k > 0$ is sufficiently small.

C Asymptotic behavior of $\frac{v_{n,1}'(d)}{v_{n,1}(d)}$ for $k \to +0$

Lemma C.1. If the positive wavenumber k is sufficiently small and if $n \neq 0$, then

$$\eta_n > 2, \quad \mu_{n,1} > |n| - \frac{1}{2\pi}\ln 2 > 0 \quad \text{if} \quad n \neq 0.$$

Proof. With the same method as in the proof of Lemma 3.4, we can estimate η_n by constructing subsolutions and supersolutions for ODEs. Consequently,

$$\begin{aligned} \eta_n &= w_{n,1}(2\pi) + w_{n,2}'(2\pi) \\ &\geqslant \frac{1}{2}e^{2\pi\beta_n^+} + \frac{1}{2}e^{-2\pi\beta_n^+} + \frac{1}{2}e^{2\pi\beta_n^+} + \frac{1}{2}e^{-2\pi\beta_n^+} \\ &> 2. \end{aligned}$$

Furthermore, $\eta_n \to e^{2\pi|n|} + e^{-2\pi|n|}$ as $k \to +0$. From

$$\lambda_{n,j}^2 - \eta_n\lambda_{n,j} + 1 = 0, \quad j = 1, 2,$$

we know $\lambda_{n,1} > \frac{1}{2}(e^{2\pi|n|} + e^{-2\pi|n|}) > 1$ and $0 < \lambda_{n,2} < 1$ as $k \to +0$. Then it follows that

$$e^{2\pi\mu_{n,1}} = \lambda_{n,1} > \frac{1}{2}(e^{2\pi|n|} + e^{-2\pi|n|}) > \frac{1}{2}e^{2\pi|n|}$$

as $k \to +0$. Hence, one obtains $\mu_{n,1} > |n| - \frac{1}{2\pi}\ln 2 > 0$ for any $n \neq 0$ as $k \to +0$. □

In what follows, for simplicity of notation, we drop the subscript n in α_n, u_n and $\mu_{n,j}$, $\lambda_{n,j}$ for simplicity.

Lemma C.2. For fixed $n \neq 0$, the term $\left|\frac{v'_{n,1}(d)}{v_{n,1}(d)}\right| = O(k^2)$ as $k \to +0$.

Proof. By using arguments similar to the proof of Lemma 4.1, we investigate the asymptotic behavior of $\frac{v'_{n,1}(d)}{v_{n,1}(d)}$ as $k \to +0$ for fixed $n \neq 0$. The proof consists of three steps.

Step 1: Fundamental solutions. We look for solutions to the differential equation $u''(t) + (k^2 q(t) - \alpha^2)u(t) = 0$ in the form $u(t) = \psi(t)\varphi(t)$. Here the ψ are the solutions of $u''(t) - \alpha^2 u(t) = 0$ with initial conditions (4.7) or (4.8). Clearly, we find that $\varphi(t)$ should satisfy the equation

$$\varphi(t) = 1 - k^2 \int_0^t \Big[q(\sigma)V^2(\sigma)(\tilde{H}(t) - \tilde{H}(\sigma))\Big]\varphi(\sigma)\,\mathrm{d}\sigma \tag{C.1}$$

where

$$\tilde{H}(t) := \frac{1}{\alpha}\begin{cases}\tanh(\alpha t) & \text{with condition (4.7)},\\ \coth(\alpha t) & \text{with condition (4.8)},\end{cases}$$

and

$$V(t) := \begin{cases}\cosh(\alpha t) & \text{with condition (4.7)},\\ \sinh(\alpha t) & \text{with condition (4.8)}.\end{cases}$$

We can reformulate (C.1) as the operator equation

$$\varphi(t) + k^2 K\varphi(t) = 1,\ \ j = 1, 2, \tag{C.2}$$

where $(K\varphi)(t) = \int_0^t k(t,\sigma)\varphi(\sigma)\,\mathrm{d}\sigma$ and $k(t,\sigma) = q(\sigma)V^2(\sigma)(\tilde{H}(t) - \tilde{H}(\sigma))$. We note that the kernels $k(t,\sigma)$ are of different form under the different initial conditions (4.7) and (4.8). With the estimates of $k(t,\sigma)$, we have that

$$\|k^2 K\| \leqslant \frac{Ck^2}{\alpha} = C\frac{k^2}{k\sin\theta + n} = O(k).$$

Since sufficiently small k guarantees that $\|k^2K\| < 1$, by a Neumann series argument, $(I + k^2K)^{-1}$ exists and

$$\varphi(t) = 1 - k^2(K1)(t) + O(k^2). \tag{C.3}$$

We also need to estimate $\varphi'(t)$. By (C.2) and (C.3) we have that

$$\begin{aligned}\varphi(t) &= 1 - k^2(K1)(t) + k^4K(K1)(t) + \cdots,\\ \varphi'(t) &= -[\partial_t k^2 K]\{1 + O(k^2)\}.\end{aligned}$$

It remains to estimate $\|\partial_t k^2 K\|$. From the definition of K,

$$\partial_t[k^2(K\varphi)(t)] = k^2\int_0^t \frac{V^2(\sigma)}{V^2(t)}q(\sigma)\varphi(\sigma)\,\mathrm{d}\sigma.$$

This implies that $\|\partial_t k^2 K\| \leqslant Ck^2$.

Step 2: Characteristic exponents. Using the fundamental solutions in Step 1, the definition (3.5), and $k \to 0$, we have that

$$\eta = \frac{1}{2}(e^{2\pi\alpha_n} + e^{-2\pi\alpha_n})(1 - O(k)) + \frac{1}{2}(e^{2\pi\alpha_n} + e^{-2\pi\alpha_n})(1 - O(k))$$
$$+ \frac{1}{2}(e^{2\pi\alpha_n} - e^{-2\pi\alpha_n})O(k^2),$$

which implies $\lim_{k\to+0} \eta = e^{2\pi n} + e^{-2\pi n}$ for $|n| \neq 0$. Then by (3.4),

$$\begin{aligned}\lim_{k\to+0} \lambda_1 &= \lim_{k\to+0} \left[\frac{\eta}{2} + \sqrt{\frac{\eta^2}{4} - 1}\right] \\ &= \frac{1}{2}(e^{2\pi n} + e^{-2\pi n}) + \sqrt{\frac{e^{4\pi n} + 2 + e^{-4\pi n}}{4} - 1} \\ &= e^{2\pi n}.\end{aligned}$$

It follows from the Definition 3.1 that

$$\begin{aligned}\lim_{k\to+0} \mu_1 &= \lim_{k\to+0} \frac{1}{2\pi} \ln \lambda_1 = \lim_{k\to+0} \alpha, \\ \lim_{k\to+0} \mu_2 &= -\lim_{k\to+0} \mu_1 = -\lim_{k\to+0} \alpha.\end{aligned}$$

Furthermore, we know for $|n| \neq 0$ that

$$\lim_{k\to+0} [\mu_1 - \alpha] = 0, \quad \lim_{k\to+0} [\mu_2 + \alpha] = 0. \tag{C.4}$$

Step 3: Asymptotics of Hill's equation. According to the downward modes in case (a) of Definition 3.2, we assume that $u = e^{\mu t} v(t)$, where $v(0) = v(2\pi)$ and $v'(0) = v'(2\pi)$. Substituting the product presentation of u into $u''(t) + (k^2 q(t) - \alpha^2)u(t) = 0$, we have that

$$e^{\mu t}(v''(t) + 2\mu v'(t) + (k^2 q(t) + \mu^2 - \alpha^2)v(t)) = 0.$$

Then $(e^{2\mu t} v'(t))' = -e^{2\mu t}(k^2 q(t) + \mu^2 - \alpha^2)v(t)$. Hence

$$e^{2\mu t} v'(t) = v'(0) - \int_0^t e^{2\mu\tau}(k^2 q(\tau) + \mu^2 - \alpha^2)v(\tau)\, \mathrm{d}\tau.$$

By straightforward computation, we get the two identities

$$e^{4\pi\mu} e^{2\mu t} v'(t) = e^{4\pi\mu} v'(0) - e^{4\pi\mu} \int_0^t e^{2\mu\tau}(k^2 q(\tau) + \mu^2 - \alpha^2)v(\tau)\, \mathrm{d}\tau \tag{C.5}$$

and

$$e^{2\mu t} v'(t) = e^{4\pi\mu} v'(0) + \int_t^{2\pi} e^{2\mu\tau}(k^2 q(\tau) + \mu^2 - \alpha^2)v(\tau)\, \mathrm{d}\tau. \tag{C.6}$$

Subtracting (C.5) from (C.6) gives

$$\begin{aligned}v'(t) = &\frac{1}{1 - e^{4\pi\mu}} \int_t^{2\pi} e^{2\mu(\tau - t)}(k^2 q(\tau) + \mu^2 - \alpha^2)v(\tau)\, \mathrm{d}\tau \\ &+ \frac{e^{4\pi\mu}}{1 - e^{4\pi\mu}} \int_0^t e^{2\mu(\tau - t)}(k^2 q(\tau) + \mu^2 - \alpha^2)v(\tau)\, \mathrm{d}\tau.\end{aligned}$$

There are two cases to consider. We first suppose that $v(0) \neq 0$. Without loss of generality, let $v(0) = 1$. Then

$$\begin{aligned}
v(t) &= 1 + \int_0^t v'(\sigma)\,\mathrm{d}\sigma \\
&= 1 + \frac{1}{1-e^{4\pi\mu}} \int_0^t \int_\sigma^{2\pi} e^{2\mu(\tau-\sigma)}(k^2 q(\tau) + \mu^2 - \alpha^2) v(\tau)\,\mathrm{d}\tau\,\mathrm{d}\sigma \\
&\quad + \frac{e^{4\pi\mu}}{1-e^{4\pi\mu}} \int_0^t \int_0^\sigma e^{2\mu(\tau-\sigma)}(k^2 q(\tau) + \mu^2 - \alpha^2) v(\tau)\,\mathrm{d}\tau\,\mathrm{d}\sigma \\
&= 1 + \frac{1}{1-e^{4\pi\mu}} \int_0^{2\pi} \int_0^{\min(t,\tau)} e^{2\mu(\tau-\sigma)}\,\mathrm{d}\sigma (k^2 q(\tau) + \mu^2 - \alpha^2) v(\tau)\,\mathrm{d}\tau \\
&\quad + \frac{e^{4\pi\mu}}{1-e^{4\pi\mu}} \int_0^t \int_\tau^t e^{2\mu(\tau-\sigma)}\,\mathrm{d}\sigma (k^2 q(\tau) + \mu^2 - \alpha^2) v(\tau)\,\mathrm{d}\tau \\
&= 1 + \frac{1}{1-e^{4\pi\mu}} \int_0^{2\pi} \frac{1}{2\mu}(e^{2\mu\tau} - e^{2\mu\max(\tau-t,0)})(k^2 q(\tau) + \mu^2 - \alpha^2) v(\tau)\,\mathrm{d}\tau \\
&\quad + \frac{e^{4\pi\mu}}{1-e^{4\pi\mu}} \int_0^t \frac{1}{2\mu}(1 - e^{2\mu(\tau-t)})(k^2 q(\tau) + \mu^2 - \alpha^2) v(\tau)\,\mathrm{d}\tau \\
&= 1 + \frac{1}{1-e^{4\pi\mu}} \int_0^{2\pi} \frac{1}{2\mu}(e^{2\mu\tau} - e^{2\mu\max(\tau-t,0)})(k^2 q(\tau) + \mu^2 - \alpha^2) v(\tau)\,\mathrm{d}\tau \\
&\quad + \frac{e^{4\pi\mu}}{1-e^{4\pi\mu}} \int_0^{2\pi} \frac{1}{2\mu}(e^{2\mu\max(\tau-t,0)} - e^{2\mu(\tau-t)})(k^2 q(\tau) + \mu^2 - \alpha^2) v(\tau)\,\mathrm{d}\tau \\
&= 1 + \int_0^{2\pi} \frac{1}{2\mu}\Big(\frac{e^{2\mu\tau} - e^{4\pi\mu}e^{2\mu(\tau-t)}}{1-e^{4\pi\mu}} - e^{2\mu\max(\tau-t,0)}\Big)(k^2 q(\tau) + \mu^2 - \alpha^2) v(\tau)\,\mathrm{d}\tau.
\end{aligned}$$

We define an integral operator L by

$$(Lv)(t) := \int_0^{2\pi} l(t,\tau) v(\tau)\,\mathrm{d}\tau,$$

where

$$l(t,\tau) = \frac{1}{2}\left(\frac{e^{2\mu\tau} - e^{2\mu(2\pi-t+\tau)}}{1-e^{4\pi\mu}} - e^{2\mu\max(\tau-t,0)}\right)(k^2 q(\tau) + \mu^2 - \alpha^2).$$

Then we obtain the operator equation

$$v(t) - \frac{1}{\mu}(Lv)(t) = 1.$$

We observe that $|l(t,\tau)| \leqslant Ck^2$. By the Neumann series, we can show that

$$v(t) = \sum_{m=0}^{\infty}\left(\frac{1}{\mu}L\right)^m = 1 + \frac{1}{\mu}\int_0^{2\pi} l(t,\tau)\,\mathrm{d}\tau + O(k^4).$$

In the second case, if $v(d) = 0$, then the operator equation becomes $v(t) - \frac{1}{\mu}(Lv)(t) = 0$. Taking the norm of both sides of the equation $\mu v(t) = (Lv)(t)$, we find that $\mu \leqslant \|L\| \leqslant Ck^2$. Sufficiently small k guarantees that this case can not happen.

It remains to estimate the derivative $v'(t)$. We first compute $\partial_t \frac{1}{\mu}(Lv)(t)$.

$$\begin{aligned}\partial_t \frac{1}{\mu}(Lv)(t) = &\ \partial_t \frac{1}{2\mu} \int_0^{2\pi} \frac{e^{2\mu\tau} - e^{2\mu(2\pi - t + \tau)}}{1 - e^{4\pi\mu}} (k^2 q(\tau) + \mu^2 - \alpha^2) v(\tau)\,\mathrm{d}\tau \\ &- \partial_t \frac{1}{2\mu} \int_0^t (k^2 q(\tau) + \mu^2 - \alpha^2) v(\tau)\,\mathrm{d}\tau \\ &- \partial_t \frac{1}{2\mu} \int_t^{2\pi} e^{2\mu(\tau - t)} (k^2 q(\tau) + \mu^2 - \alpha^2) v(\tau)\,\mathrm{d}\tau \\ = &\int_0^{2\pi} \frac{e^{2\mu(2\pi - t + \tau)}}{1 - e^{4\pi\mu}} (k^2 q(\tau) + \mu^2 - \alpha^2) v(\tau)\,\mathrm{d}\tau \\ &+ \int_t^{2\pi} e^{2\mu(\tau - t)} (k^2 q(\tau) + \mu^2 - \alpha^2) v(\tau)\,\mathrm{d}\tau.\end{aligned}$$

It follows that

$$\begin{aligned}\frac{\partial_t v(t)}{v(t)} = \frac{\partial_t \frac{1}{\mu}(Lv)(t)}{v(t)} = &\frac{1}{v(t)} \int_0^{2\pi} \frac{e^{2\mu(2\pi - t + \tau)}}{1 - e^{4\pi\mu}} (k^2 q(\tau) + \mu^2 - \alpha^2) v(\tau)\,\mathrm{d}\tau \\ &+ \frac{1}{v(t)} \int_t^{2\pi} e^{2\mu(\tau - t)} (k^2 q(\tau) + \mu^2 - \alpha^2) v(\tau)\,\mathrm{d}\tau.\end{aligned}$$

Hence

$$\left\| \frac{\partial_t v(t)}{v(t)} \right\|_{L^\infty} \leqslant Ck^2.$$

We can use the argument in Step 3 to estimate $v_{n,1}(d)$ and $v'_{n,1}(d)$. We have that

$$\left| \frac{v'_{n,1}(d)}{v_{n,1}(d)} \right| \leqslant \left\| \frac{v'_{n,1}(t)}{v_{n,1}(t)} \right\|_{L^\infty} \leqslant Ck^2.$$

Hence $\left|\frac{v'_{n,1}(d)}{v_{n,1}(d)}\right|$ tends to 0 as $k \to +0$ for fixed $n \neq 0$. ☐

Now we study the asymptotic behavior for $n = 0$.

Lemma C.3. It holds that $\theta_0 = O(k)$ and $\left|\frac{v'_{0,1}(d)}{v_{0,1}(d)}\right| = o(1)$ as $k \to +0$.

Proof. (i) It follows from Lemma 4.2 that

$$\lambda_1 = \frac{\eta_0 + \sqrt{\eta_0^2 - 4}}{2},\ \lambda_2 = \frac{\eta_0 - \sqrt{\eta_0^2 - 4}}{2}.$$

are mutually conjugate. From Theorem B.1 and the analyticity of $\eta_0(k)$, we know that $\eta_0 \to 2$ as $k \to +0$ and $\theta_0 \sim k$ where $e^{i2\pi\theta_0} = \lambda_1$.

(ii) For notational convenience we write $v = v_{0,1}$ to drop the dependence on the subscripts. We shall present a sketch of the proof, following the argument in Step 3 of Lemma C.2.

According to the downward modes in case (c) in Definition 3.2, we assume that $u = e^{-i\theta_0 t} v(t)$, where $v(0) = v(2\pi)$ and $v'(0) = v'(2\pi)$. Substituting the product presentation of u into $u''(t) + k^2(q(t) - \sin^2\theta) u(t) = 0$, we have that

$$v''(t) - 2i\theta_0 v'(t) + (k^2(q(t) - \sin^2\theta) - \theta_0^2) v(t) = 0.$$

Then $(e^{-2i\theta_0 t} v'(t))' = -e^{2i\theta_0 t}(k^2(q(t) - \sin^2\theta) - \theta_0^2) v(t)$. Hence

$$e^{-2i\theta_0 t} v'(t) = v'(0) - \int_0^t e^{-2i\theta_0 \tau} (k^2(q(\tau) - \sin^2\theta) - \theta_0^2) v(\tau)\,\mathrm{d}\tau.$$

By straightforward computation, we get

$$
\begin{aligned}
v'(t) = & \frac{1}{1-e^{-4\pi i\theta_0}} \int_t^{2\pi} e^{-2i\theta_0(\tau-t)}(k^2(q(\tau)-\sin^2\theta)-\theta_0^2)v(\tau)\,\mathrm{d}\tau \\
& + \frac{e^{-4\pi i\theta_0}}{1-e^{-4\pi i\theta_0}} \int_0^{t} e^{-2i\theta_0(\tau-t)}(k^2(q(\tau)-\sin^2\theta)-\theta_0^2)v(\tau)\,\mathrm{d}\tau.
\end{aligned}
$$

Then we have

$$
\begin{aligned}
v(t) &= 1 + \int_0^t v'(\sigma)\,\mathrm{d}\sigma \\
&= 1 + \frac{1}{2i\theta_0}\int_0^{2\pi} \left(e^{2i\theta_0 \min(t-\tau,0)} + \frac{e^{2i\theta_0(t-\tau)} - e^{2i\theta_0(2\pi-\tau)}}{e^{4\pi i\theta_0}-1} \right) (k^2(q(\tau)-\sin^2\theta)-\theta_0^2)v(\tau)\,\mathrm{d}\tau.
\end{aligned}
$$

We define the integral operator L by

$$
(Lv)(t) \coloneqq \int_0^{2\pi} l(t,\tau)v(\tau)\,\mathrm{d}\tau,
$$

where

$$
l(t,\tau) = \frac{1}{2i}\left(e^{2i\theta_0 \min(t-\tau,0)} + \frac{e^{2i\theta_0(t-\tau)} - e^{2i\theta_0(2\pi-\tau)}}{e^{4\pi i\theta_0}-1} \right) (k^2(q(t)-\sin^2\theta)-\theta_0^2).
$$

Then we obtain the operator equation

$$
v(t) - \frac{1}{\theta_0}(Lv)(t) = 1.
$$

We observe that $|l(t,\tau)| \leqslant Ck^2$. By a Neumann series argument, we have that

$$
v(t) = \sum_{m=0}^{\infty} \left(\frac{1}{\theta_0}L\right)^m = 1 + \frac{1}{\theta_0}\int_0^{2\pi} l(t,\tau)\,\mathrm{d}\tau + O(k^2).
$$

By arguments similar to Step 3 of the proof of Lemma C.2, We can estimate $v'(t)$ and obtain that $\left|\frac{v_{0,1}'(d)}{v_{0,1}(d)}\right|$ tends to 0 as $k \to +0$. $\square$

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