SCIENCE CHINA
Mathematics

• ARTICLES • https://doi.org/10.1007/s11425-024-2491-6

Direct and inverse time-harmonic scattering by Dirichlet periodic curves with local perturbations

Guanghui Hu[1,*] & Andreas Kirsch[2]

[1]*School of Mathematical Sciences and LPMC, Nankai University, Tianjin* 300071*, China;*
[2]*Department of Mathematics, Karlsruhe Institute of Technology* (*KIT*)*, Karlsruhe* 76131*, Germany*

Email: ghhu@nankai.edu.cn, andreas.kirsch@kit.edu

Received February 19, 2024; accepted September 4, 2025; published online March 5, 2026

Abstract This is a continuation of Hu and Kirsch's previous work (2024) on well-posedness of time-harmonic scattering by locally perturbed periodic curves of Dirichlet kind. The scattering interface is supposed to be given by a non-self-intersecting Lipschitz curve. We study properties of Green's function and prove new well-posedness results for scattering of plane waves at a propagative number. In such a case, there exist guided waves to the unperturbed problem, which are also known as bound states in the continuum (BICs) in physics. In this paper, the uniqueness of the forward scattering follows from an orthogonal constraint condition enforced on the total field to the unperturbed scattering problem. This constraint condition, which is also valid under the Neumann boundary condition, is derived from the singular perturbation arguments and also from the approach of approximating a plane wave by point source waves. For the inverse problem of determining the defect, we prove several uniqueness results using a finite or infinite number of point sources and plane waves, depending on whether *a priori* information on the size and height of the defect is available.

Keywords Helmholtz equation, non-self-intersecting periodic curve, local perturbation, Dirichlet boundary condition, plane wave, uniqueness, inverse problem

MSC(2020) 35J05, 78M35, 78A46

Citation: Hu G H, Kirsch A. Direct and inverse time-harmonic scattering by Dirichlet periodic curves with local perturbations. Sci China Math, 2026, 69, https://doi.org/10.1007/s11425-024-2491-6

1 Introduction

This paper is concerned with the transverse electric (TE) polarization of time-harmonic electromagnetic scattering from perfectly conducting gratings with a localized defect. The first part deals with well-posedness of the mathematical model for plane wave incidences and properties of Green's function. In the second part, we study uniqueness of the inverse problems of determining the local perturbation from near/far-field data excited by plane and point source waves. Throughout this paper, the cross-section of the scattering surface is supposed to be a non-self-intersecting periodic curve with a local perturbation. In the TE polarization case, the grating diffraction problem can be modeled by the Dirichlet boundary value problem of the two-dimensional Helmholtz equation in the unbounded domain above the interface,

* Corresponding author

complemented with a proper radiation condition at infinity. We refer to [2, 37] for a comprehensive introduction to electromagnetic scattering theory for diffraction gratings.

In the absence of the defect, the wave field for a plane wave incidence is well-known to be quasiperiodic, due to the periodicity of the scattering interface and the quasi-periodicity of the incoming plane wave. The Rayleigh expansion radiation condition (which was originally proposed by Rayleigh [38] in 1907) has been widely used in the literature concerning the mathematical analysis and numerical approximation of wave scattering in periodic structures. With the Fredholm theory, it is also well known that the forward scattering model is well-posed for all incident frequencies excluding a discrete set with the only accumulating point at infinity. However, the Rayleigh expansion radiation condition does not always lead to uniqueness (although existence can always be justified via a variational argument), because of the existence of guided/Floquet wave modes to the homogeneous problem, which exponentially decay in the direction orthogonal to the periodicity direction [3, 16, 21, 24]. If the interface is given by the graph of some periodic function (a weaker condition was proposed in [4, 5]), uniqueness and existence can be proved (which implies the absence of guided waves) for the Dirichlet boundary value problem of the Helmholtz equation at an arbitrary frequency; see [12, 25]. Since an incoming point source is not quasi-periodic, the Rayleigh expansion condition is not valid any more. Instead, the upward propagation radiation condition [7] or the angular spectrum representation condition [4, 5] can be used for proving well-posedness within the framework of rough surface scattering problems, provided that the domain with a geometrical condition admits no guided waves. Since a locally perturbed periodic curve can be treated as a special rough curve, it was proved in [20] that Green's function to the perturbed scattering problem satisfies a half-plane Sommerfeld radiation condition and the scattered field generated by a plane wave and caused by the defect fulfills the same radiation condition, as long as guided modes can be excluded.

The mathematical analysis is more involved for locally perturbed scattering problems when guided waves exist in periodic structures. An open wave-guide radiation condition (which is equivalent to the closed wave-guide radiation condition [14] based on dispersion curves) was proposed in [31] for acoustic scattering by inhomogeneous periodic layers in a half-plane. Such a radiation condition was derived from the limiting absorption principle (LAP) and the Floquet-Bloch transform and was later extended to investigate well-posedness of wave scattering by layered periodic media in $\mathbb{R}^2$ and by periodic tubes in $\mathbb{R}^3$; see [15, 26–28, 31, 32]. This open wave guide radiation condition consists of a radiating part and a propagating (guided) part. It was recently shown in [28] that the radiating part satisfies a Sommerfeld-type radiation condition and, due to the existence of cut-off values, the radiating part decays as $|x_1|^{-1/2}$ in the periodicity direction. In Hu and Kirsch's previous work [19], the open wave guide radiation condition has been adopted to prove well-posedness of Dirichlet and Neumann boundary value problems of the Helmholtz equation in a locally perturbed periodic structure. By constructing a Dirichlet-to-Neumann operator on the boundary of a truncated domain, uniqueness and existence of time-harmonic scattering by incoming point source waves, plane waves and surface waves are established. This has generalized the results of [20] to scattering interfaces given by non-self-intersecting curves, for which the forward solutions may contain guided wave modes.

For an incident plane wave, the well-posedness results of [19] are based on the uniqueness assumption on the forward scattering model in periodic structures. This is equivalent to the statement that the quasi-periodicity of the incoming plane wave (i.e., $k \sin\theta$, where θ is the incident angle) is not a propagative number; see Definition 2.1(ii). Otherwise, solutions to the unperturbed scattering problem are not unique, and neither are those for the perturbed problem; see Section 4 for detailed discussions. In the first part of this paper, we propose an additional constraint condition on solutions of the unperturbed problem to ensure uniqueness. For this purpose, we adopt two different approaches to the Dirichlet boundary value problem: the limiting absorption principle by replacing k by $k+\mathrm{i}\epsilon$ (Subsection 4.1) and the approximation by point source waves (Subsection 4.2). It is shown in Theorems 4.4(i) and 4.8 that both methods yield the same constraint condition. The limiting absorption arguments for approximating wave-numbers have complemented the work of [29], where the LAP for approximating refractive indices, the continuity with respect to incident angles together with the method of approximating plane waves by point source waves were justified for scattering by layered periodic media. In the first part, we also justify some properties of Green's function to perturbed and unperturbed scattering problems; see Sections 3 and 4. In particular, the mixed reciprocity relation between point source and plane wave incidences will be verified in Theorem 4.10.

We remark that radiation conditions and numerical approximations with exact boundary conditions (DtN maps) were also considered in [13, 23] for wave propagating in a closed periodic wave-guide and in a photonic crystal containing a local perturbation. We refer to [35, 42] for numerical methods based on LAP and the Floquet-Bloch transform and to [40] using the boundary integral equation method in combination with perfectly matched absorbing layers.

The second part of this paper concerns inverse scattering problems of recovering the localized defect by assuming *a priori* knowledge of the unperturbed periodic structure. Using infinitely many point sources or plane waves at a fixed energy, we prove that the position and shape of the local defect can be uniquely determined by the corresponding near-field data measured on a line segment above the interface; see Subsection 5.1. As is seen in the proof of Theorem 5.5, the complexity of the solution structure gives rise to essential difficulties in justifying linear independence of the wave fields for different angles. If some *a priori* information on the defect is available, one can prove uniqueness with a finite number of incoming waves by adopting Colton and Slemann's idea of determining a bounded sound-soft obstacle [9]; see also [18] for the corresponding results in periodic structures with a fixed direction. A counterexample will be constructed to show that one incident plane wave is impossible to imply uniqueness in general. In Subsection 5.4, we discuss uniqueness results using far-field patterns of incoming point source waves over a finite or infinite number of observation directions.

In this paper, we choose the square root function to be holomorphic in the cutted plane $\mathbb{C} \setminus (\mathrm{i}\mathbb{R}_{\leqslant 0})$. In particular, $\sqrt{t} = \mathrm{i}\sqrt{|t|}$ for $t \in \mathbb{R}_{<0}$. The functions ϕ are called guided (or propagating or Floquet) modes. The Fourier transform is defined as

$$(\mathcal{F}\phi)(\omega) := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(s)\, \mathrm{e}^{-\mathrm{i}s\omega}\, ds, \quad \omega \in \mathbb{R},$$

which can be considered as a unitary operator from $L^2(\mathbb{R})$ onto itself. For a domain $\Omega \subset \mathbb{R}^2$, the weighted Sobolev space $H^1_\rho(\Omega)$ is defined by

$$H^1_\rho(\Omega) := \{u : (|1 + |x_1|^2)^{\rho/2} u \in H^1(\Omega)\}, \quad \rho \in \mathbb{R}.$$

2 Radiation conditions and well-posedness results

In this section, we describe the mathematical model for the TE polarization of time-harmonic electromagnetic scattering from a perfectly conducting periodic surface with local perturbations. We first recall some notations, define the open wave-guide radiation, and then present some well-posedness results from Hu and Kirsch's previous work [19].

Let $D \subset \mathbb{R}^2$ be a 2π-periodic domain with respect to the x_1-direction. The boundary $\Gamma := \partial D$ is supposed to be given by a non-self-intersecting Lipschitz curve which is bounded in the x_2-direction and 2π-periodic with respect to x_1. Let $\tilde{D}$ be a local perturbation of D in the way that $\Gamma \setminus \tilde{\Gamma}$ and $\tilde{\Gamma} \setminus \Gamma$ are bounded, where $\tilde{\Gamma} = \partial\tilde{D}$ is the perturbed boundary, which is also assumed to be a non-self-intersecting curve (see Figure 1). Suppose that $\tilde{D}$ is filled by a homogeneous and isotropic medium and that $\tilde{\Gamma}$ is a perfectly reflecting curve of Dirichlet kind. Let u^{in} be an incoming wave incident onto $\tilde{\Gamma}$. The scattered field u^{sc} can be governed by the boundary value problem of the Helmholtz equation

$$\Delta u^{sc} + k^2 u^{sc} = 0 \quad \text{in } \tilde{D}, \quad u^{sc} = -u^{in} \quad \text{on } \tilde{\Gamma},$$

complemented by some radiation condition in $\tilde{D}$ explained below. To specify this radiation condition, we need to introduce several definitions and make some assumptions.

For the forward scattering problem, we suppose without loss of generality (changing the period of the periodic structure if otherwise) that the perturbations $\Gamma \setminus \tilde{\Gamma}$ and $\tilde{\Gamma} \setminus \Gamma$ are contained in the disc

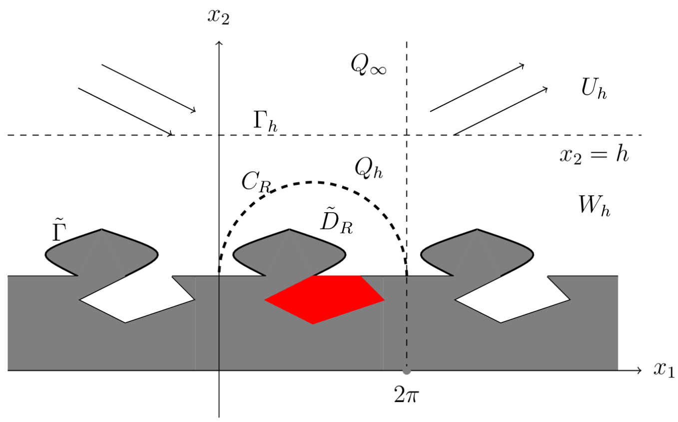

Figure 1 (Color online) Illustration of wave scattering from a perfectly reflecting periodic curve with a local perturbation in $(0, 2\pi)$. The red area denotes the perturbed domain. The scattering interface is supposed to be a non-self-intersecting curve

$\{x \in \mathbb{R}^2 : (x_1 - \pi)^2 + x_2^2 < \pi^2\}$. We fix $R, h_0 > \pi$ throughout this paper and use the following notations for $h > h_0$ (see Figure 1):

$$\begin{aligned}
&Q_h := \{x \in D : 0 < x_1 < 2\pi,\ x_2 < h\}, \quad Q_\infty := \{x \in D : 0 < x_1 < 2\pi\},\\
&\Gamma_h := (0, 2\pi) \times \{h\}, \quad W_h := \{x \in D : x_2 < h\}, \quad U_h := \{x \in D : x_2 > h\},\\
&C_R := \{x \in D : (x_1 - \pi)^2 + x_2^2 = R^2\}, \quad \Sigma_R := \{x \in D : (x_1 - \pi)^2 + x_2^2 > R^2\},\\
&D_R := \{x \in D : (x_1 - \pi)^2 + x_2^2 < R^2\}, \quad \tilde{D}_R := \{x \in \tilde{D} : (x_1 - \pi)^2 + x_2^2 < R^2\}.
\end{aligned}$$

We recall that a function $\phi \in L^2_{\rm loc}(\mathbb{R})$ is called α-quasi-periodic if $\phi(x_1 + 2\pi) = \mathrm{e}^{2\pi\alpha i}\phi(x_1)$ for all $x_1 \in \mathbb{R}$. Below, we introduce some function spaces[1)]

$$\begin{aligned}
&H^1_{\rm loc}(\tilde{D}) := \{u|_{\tilde{D}} : u \in H^1_{\rm loc}(\mathbb{R}^2)\},\\
&H^1_{{\rm loc},0}(\tilde{D}) := \{u \in H^1_{\rm loc}(\tilde{D}) : u = 0 \text{ on } \partial\tilde{D}\},\\
&H^1_*(\Sigma_R) := \left\{ u \in H^1_{\rm loc}(\Sigma_R) : \begin{array}{l} u|_{W_h \cap \Sigma_R} \in H^1(W_h \cap \Sigma_R) \text{ for all } h > h_0, \\ u = 0 \text{ on } \partial\Sigma_R \cap \partial D \end{array} \right\},\\
&H^1_{\alpha,{\rm loc}}(D) := \{u \in H^1_{\rm loc}(D) : u(\cdot, x_2) \text{ is } \alpha\text{-quasi-periodic}\},\\
&H^1_{\alpha,{\rm loc},0}(D) := \{u \in H^1_{\alpha,{\rm loc}}(D) : u = 0 \text{ on } \partial D\}.
\end{aligned}$$

Definition 2.1. (i) $\alpha \in [-1/2, 1/2]$ is called a *cut-off value* if there exists $\ell \in \mathbb{Z}$ such that $|\alpha + \ell| = k$.

(ii) $\alpha \in [-1/2, 1/2]$ is called a *propagative number* if there exists a non-trivial $\phi \in H^1_{\alpha,{\rm loc},0}(D)$ such that

$$\Delta\phi + k^2\phi = 0 \quad \text{in } D, \tag{2.1}$$

and ϕ satisfies the upward Rayleigh expansion

$$\phi(x) = \sum_{\ell\in\mathbb{Z}} \phi_\ell\, \mathrm{e}^{\mathrm{i}(\ell+\alpha)x_1}\, \mathrm{e}^{\mathrm{i}\sqrt{k^2-(\ell+\alpha)^2}(x_2-h_0)} \quad \text{for } x_2 > h_0 \tag{2.2}$$

for some $\phi_\ell \in \mathbb{C}$, where the convergence is uniform for $x_2 \geqslant h_0 + \varepsilon$ for every $\varepsilon > 0$.

Remark 2.2. The solutions to (2.1) and (2.2) are usually referred to as guided modes. It will be proved in Lemma 4.1(i) that the Rayleigh coefficient ϕ_l must vanish if $k^2 > (l + a)^2$. Hence, the non-trivial solution to the homogeneous problem must exponentially decay in the positive x_2-direction, if $|\alpha + l| \neq k$ for all $l \in \mathbb{Z}$. In physical literature (see, e.g., [1, 41]), the guided model $\phi(\cdot, \alpha, k)$ of (2.2) is called a BIC if $|\alpha| < k$.

1) The definitions hold also for D instead of $\tilde{D}$.

In Definition 2.1, we restrict the quasi-periodic parameter α to the interval $[-1/2, 1/2]$, because an α-quasi-periodic function must be also $(\alpha + j)$-quasi-periodic for any $j \in \mathbb{N}$. The possible existence of guided waves leads to essential difficulties in proving well-posedness of forward scattering problems under the Rayleigh expansion condition (2.2), because they are solutions to the homogeneous problem when $u^{in} = 0$. It is worthy mentioning that the set of propagative numbers must be empty, if the unperturbed domain D fulfills the following geometrical condition (see [4, 5]):

$$(x_1, x_2) \in D \Rightarrow (x_1, x_2 + s) \in D \quad \text{for all } s > 0. \tag{2.3}$$

In the special case where Γ is given by the graph of some function, uniqueness was verified in [12, 25] under different regularity assumptions enforced on Γ. Below, we discuss the existence of propagative numbers. Throughout this paper, we make the following assumptions.

Assumption 2.3. *Let $|\ell + \alpha| \neq k$ for every propagative number $\alpha \in [-1/2, 1/2]$ and every $\ell \in \mathbb{Z}$, i.e., no cut-off value is a propagative number.*

Note that this assumption can be automatically fulfilled if the geometrical condition (2.3) holds. Under Assumption 2.3, it can be shown (see, e.g., [32, Lemma 4.2(d)] for the case of a flat curve $\Gamma = \Gamma_0$ and an additional index of refraction) that at most a finite propagative number exists in the interval $[-1/2, 1/2]$. Furthermore, if α is a propagative number with mode ϕ, then $-\alpha$ is a propagative number with mode $\overline{\phi}$. Therefore, we can number the propagative numbers in $[-1/2, 1/2]$ such that they are given by $\{\hat{\alpha}_j : j \in J\}$, where $J \subset \mathbb{Z}$ is finite and symmetric with respect to 0 and $\hat{\alpha}_{-j} = -\hat{\alpha}_j$ for $j \in J$. Furthermore, it is known that (under Assumption 2.3) every mode ϕ is evanescent, i.e., it exponentially decays as x_2 tends to infinity in D, and it satisfies $|\phi(x)| \leqslant c\,\mathrm{e}^{-\delta|x_2|}$ for $x_2 \geqslant h_0$ and some $c, \delta > 0$, which are independent of x. The corresponding space

$$X_j := \{\phi \in H^1_{\hat{\alpha}_j, loc, 0}(D) : u \text{ satisfies (2.1) and (2.2) for } \alpha = \hat{\alpha}_j\} \tag{2.4}$$

of modes is finite-dimensional with some dimension $m_j > 0$. We refer to Lemma 4.1 for discussions on these properties in periodic Sobolev spaces.

On X_j, we define the sesquilinear form $B : X_j \times X_j \to \mathbb{C}$ by

$$B(\phi, \psi) := -2\mathrm{i} \int_{Q_\infty} \frac{\partial \phi}{\partial x_1} \overline{\psi}\, dx, \quad \phi, \psi \in X_j. \tag{2.5}$$

The sesquilinear form B coincides with the derivative of the variational formulation with respect to α and thus $B(\phi, \phi)$ physically represents the energy flux of the guided mode ϕ. Using integration by parts and the exponential decay of $\phi \in X_j$, we obtain $B(\phi, \psi) = \overline{B(\psi, \phi)}$ for all $\phi, \psi \in X_j$. This implies that B is Hermitian and that $B(\phi, \phi)$ is real-valued for all $\phi \in X_j$. Now we assume that B is non-degenerate on every X_j in the sense that the following assumption holds.

Assumption 2.4. *For every $j \in J$, $\psi \in X_j$ and $\psi \neq 0$, the linear form $B(\cdot, \psi) : X_j \to \mathbb{C}$ is non-trivial on X_j, i.e., there exists $\phi \in X_j$ with $B(\phi, \psi) \neq 0$.*

The Hermitian sesquilinear form B defines the cones $\{\psi \in X_j : B(\psi, \psi) \gtrless 0\}$ of propagating waves traveling to the right and left, respectively (see also [14, 26, 28, 32]). We construct a basis of X_j with elements in these cones by taking the inner product $(\cdot, \cdot)_{X_j}$ and consider the following eigenvalue problem in X_j for every fixed $j \in J$. Determine $\lambda_{\ell,j} \in \mathbb{R}$ and non-trivial $\hat{\phi}_{\ell,j} \in X_j$ with

$$B(\hat{\phi}_{\ell,j}, \psi) = -2\mathrm{i} \int_{Q_\infty} \frac{\partial \hat{\phi}_{\ell,j}}{\partial x_1} \overline{\psi}\, dx = \lambda_{\ell,j} \left(\hat{\phi}_{\ell,j}, \psi\right)_{X_j} \quad \text{for all } \psi \in X_j \tag{2.6}$$

and $\ell = 1, \ldots, m_j$. We normalize the basis such that $(\hat{\phi}_{\ell,j}, \hat{\phi}_{\ell',j})_{X_j} = \delta_{\ell,\ell'}$ for $\ell, \ell' = 1, \ldots, m_j$. Then $\lambda_{\ell,j} = B(\hat{\phi}_{\ell,j}, \hat{\phi}_{\ell,j})$ and Assumption 2.4 is equivalent to $\lambda_{\ell,j} \neq 0$ for all $\ell = 1, \ldots, m_j$ and $j \in J$. Physically, the assumption (2.4) is equivalent to the assumption that the group velocity of each guided mode is non-vanishing (see [28, Remark 1.4]).

Now we are able to formulate the open waveguide radiation condition for our Dirichlet boundary value problem (see [19]).

Definition 2.5. Let $\psi_+, \psi_- \in C^\infty(\mathbb{R})$ be any functions with $\psi_\pm(x_1) = 1$ for $\pm x_1 \geqslant \sigma$ (for some $\sigma > \max\{R, 2\pi\} + 1$) and $\psi_\pm(x_1) = 0$ for $\pm x_1 \leqslant \sigma - 1$.

A solution $u \in H^1_{\rm loc}(\Sigma_R)$ of the Helmholtz equation $(\Delta + k^2)u = 0$ satisfies the open waveguide radiation condition with respect to an inner product $(\cdot,\cdot)_{X_j}$ in X_j if u has in Σ_R a decomposition into $u = u_{\rm rad} + u_{\rm prop}$ which satisfies the following conditions.

(a) The propagating part $u_{\rm prop}$ has the form

$$u_{\rm prop}(x) = \sum_{j\in J}\Bigg[\psi_+(x_1)\sum_{\ell:\lambda_{\ell,j}>0} a_{\ell,j}\,\hat{\phi}_{\ell,j}(x) + \psi_-(x_1)\sum_{\ell:\lambda_{\ell,j}<0} a_{\ell,j}\,\hat{\phi}_{\ell,j}(x)\Bigg] \tag{2.7}$$

for $x \in \Sigma_R$ and some $a_{\ell,j} \in \mathbb{C}$. Here, for every $j \in J$, the scalars $\lambda_{\ell,j} \in \mathbb{R}$ and $\hat{\phi}_{\ell,j} \in \hat{X}_j$ for $\ell = 1, \ldots, m_j$ are given by the eigenvalues and corresponding eigenfunctions, respectively, of the self-adjoint eigenvalue problem (2.6).

(b) The radiating part $u_{\rm rad} \in H^1_*(\Sigma_R)$ satisfies the generalized angular spectrum radiation condition

$$\int_{-\infty}^{\infty}\left|\frac{\partial(\mathcal{F}u_{\rm rad})(\omega,x_2)}{\partial x_2} - {\rm i}\sqrt{k^2-\omega^2}\,(\mathcal{F}u_{\rm rad})(\omega,x_2)\right|^2 d\omega \to 0, \quad x_2 \to \infty. \tag{2.8}$$

The above radiation condition has been earlier studied in [15, 26–28, 31, 32] for layered periodic structures. It has been shown in [32] for the case of half-plane source problems with an inhomogeneous period layer that the radiation condition of Definition 2.5 for the inner product $(\phi,\psi)_{X_j} = 2k\int_{Q_\infty} n\,\phi\,\overline{\psi}\,dx$ is a consequence of the limiting absorption principle by replacing k with $k + {\rm i}\epsilon$ and $\epsilon > 0$. Here, the function n stands for the refractive index of the inhomogeneous layer.

Assumption 2.6 (Absence of bound states). *There are no bound states to the perturbed scattering problem, i.e., any solution $u \in H^1_0(\tilde{D})$ of $\Delta u + k^2 u = 0$ in $\tilde{D}$ must vanish identically.*

One can remove this assumption if the domain $\tilde{D}$ fulfils the condition (2.3). Note that with this geometrical condition on $\tilde{D}$, the unperturbed domain D should also meet the requirement (2.3) and thus the existence of propagating modes $\hat{\phi}_{\ell,j}$ is excluded [5].

In this paper, we make Assumptions 2.3, 2.4 and 2.6 without mentioning this any more. We consider the following two kinds of incoming waves:

(i) Point source waves: $u^{in}(x) := \Phi(x;y) = \frac{\rm i}{4}H_0^{(1)}(k|x-y|)$ with the source position $y \in \tilde{D}_R$.

(ii) Plane waves: $u^{in}(x) = {\rm e}^{{\rm i}kx\cdot\hat{\theta}}$, where $\hat{\theta} = (\sin\theta, -\cos\theta)$ is the incident direction with some incident angle $\theta \in (-\pi/2, \pi/2)$.

Before stating uniqueness and existence results, we recall the Sommerfeld radiation condition used in [20, 28].

Definition 2.7. A function $v \in C^\infty(U_{h_0}\cap\Sigma_R)$ satisfies the Sommerfeld radiation condition in $U_{h_0}\cap\Sigma_R$ if $v \in H^1_\rho(W_h\cap\Sigma_R)$ for all $h > h_0$ and all $\rho < 1$ and

$$\sup_{x\in C_a\cap U_h}|x|^{1/2}\left|\frac{\partial v(x)}{\partial r} - {\rm i}kv(x)\right| \to 0, \quad a \to \infty, \quad \sup_{x\in U_h}|x|^{1/2}|v(x)| < \infty \tag{2.9}$$

for all $h > h_0$ where $r = |x|$.

It was shown in Hu and Kirsch's previous paper [19] that the radiation condition for the radiating part of the open waveguide radiation condition of Definition 2.5 is equivalent to the above Sommerfeld radiation condition. We remark that the point source wave $\Phi(x;y)$ with $y \in D_R$ satisfies the Sommerfeld radiation condition of Definition 2.7 with the index $\rho < 0$, because $\Phi(x;y) \sim |x|^{-1/2}$ as $|x| \to \infty$ in $\mathbb{R}^2$. However, plane waves and quasi-periodic surface waves are not included. Such kinds of wave modes belong to $H^1_\rho(W_h\cap\Sigma_R)$ for all $h > h_0$ with the index $\rho < -1/2$. An integral form of the above Sommerfeld radiation condition is defined as follows.

Definition 2.8. Let a_j be a sequence in $\mathbb{R}$ such that $a_j \to \infty$ and suppose that $\tilde{D}_{a_j}$ are Lipschitz domains. A solution $v \in H^1_{\rm loc}(\Sigma_R)$ satisfies the Sommerfeld radiation condition in an integral form if

$$\left\|\frac{\partial v}{\partial r} - {\rm i}kv\right\|_{H^{-1/2}(C_{a_j})} \to 0, \quad j \to \infty,$$

where $r = |x|$.

Lemma 2.9. (i) *If v satisfies the Sommerfeld radiation condition of Definition* 2.7 *with the index $\rho \geqslant 0$, then v also fulfills the integral form of the radiation condition defined by Definition* 2.8.

(ii) *The condition* (b) *for the radiating part of u in Definition* 2.5 *is equivalent to the Sommerfeld radiation condition of Definition* 2.7.

Lemma 2.9 and the following well-posedness results for incident plane and point source waves were proved in Hu and Kirsch's previous paper [19].

Proposition 2.10 (Well-posedness for point source waves)**.** *Let $u^{in} := \Phi(\cdot\,; y)$ be an incoming point source wave with $y \in \tilde{D}_R$. Then the locally perturbed scattering problem admits a unique solution u such that $u - u^{in} \in H^1_{\rm loc}(\tilde{D})$ and u satisfies the open waveguide radiation condition of Definition* 2.5. *Furthermore, the radiating part $u_{\rm rad}$ of u satisfies the Sommerfeld radiation conditions of Definitions* 2.7 *and* 2.8.

If $\partial\tilde{D}$ is given by a Lipschitz graph (i.e., guided waves are excluded), the results of Proposition 2.10 were verified in [20] within a more general framework for rough surface scattering problems. We remark that, in such a case, the scattered field $u^{sc} := u - u^{in}$ does not satisfy the open waveguide radiation condition of Definition 2.5 and either the Sommerfeld radiation condition of Definition 2.7, because $u^{in} = \Phi(\cdot; y)$ does not belong to $H^1(\Sigma_R)$. In fact, u^{sc} fulfills the Sommerfeld radiation condition with the index $\rho < 0$.

Proposition 2.11 (Well-posedness for plane waves)**.** *Let $\alpha := k \sin\theta$ be not a propagative number* (*see Definition* 2.1(ii))*. Then the perturbed scattering problem for a plane wave incidence $u^{in}(x) = {\rm e}^{{\rm i}kx\cdot\hat{\theta}}$ admits a unique solution $u = u^{in} + u^{sc} \in H^1_{{\rm loc},0}(\tilde{D})$ such that the scattered part u^{sc} has a decomposition in the form $u^{sc} = u^{sc}_{\rm unpert} + u^{sc}_{\rm pert}$ in the region Σ_R, where $u^{sc}_{\rm unpert} \in H^1_{\alpha,{\rm loc}}(D)$ is the scattered field corresponding to the unperturbed problem that satisfies the upward Rayleigh expansion* (2.2) *with the quasi-periodic parameter $\alpha = k\sin\theta$. The part $u^{sc}_{\rm pert} \in H^1_{\rm loc}(\Sigma_R)$ fulfils the open waveguide radiation condition of Definition* 2.5 *and the radiating part of $u^{sc}_{\rm pert}$ satisfies the Sommerfeld radiation conditions of Definitions* 2.7 *and* 2.8.

We emphasize in Proposition 2.11 that, since $k\sin\theta$ is assumed to be no critical wavenumber (or equivalently, no BIC exists at the pair $(\alpha, k) \in \mathbb{R}^2$ with $\alpha = k\sin\theta$), the unperturbed scattered field $u^{sc}_{\rm unpert}$ is unique. In the subsequent Sections 3 and 4, we carry out further studies on forward scattering problems, including properties of Green's function to perturbed and unperturbed problems and well-posedness for a plane wave incidence at a critical wavenumber (i.e., when a BIC occurs). Theorems 3.1, 4.4 and 4.8 will be used later for investigating inverse problems in Section 5.

3 Properties of Green's function

Let $\Phi(x; y)$ be the fundamental solution of the Helmholtz equation. Green's function G for $\tilde{D}$ satisfies $G(\cdot\,; y) - \Phi(\cdot\,; y) \in H^2_{\rm loc}(\tilde{D})$ for all $y \in \tilde{D}$ and the open waveguide radiation condition, i.e., it has the decomposition in the form

$$G(\cdot\,; y) = G_{\rm rad}(\cdot\,; y) + G_{\rm prop}(\cdot\,; y) \quad \text{in } \tilde{D},$$

where $G_{\rm prop}(\cdot\,; y)$ is the propagating part. The radiating part $G_{\rm rad}(\cdot\,; y)$ includes the incoming wave and satisfies $G_{\rm rad}(\cdot\,; y) \in H^1(W_h \backslash \{B_\epsilon(y)\})$ for all $h > h_0$ and some $\epsilon > 0$ and also satisfies the Sommerfeld radiation condition. We prove the following properties of $G(x; y)$.

Theorem 3.1. (i) *Green's function to the perturbed scattering problem satisfies $G(x; y) = G(y; x)$ for all $x, y \in \tilde{D}$ and $x \neq y$.*

(ii) *In the unperturbed case* (*i.e., $\tilde{D} = D$*)*, the propagating part $G_{\rm prop}$ of G takes the explicit form*

$$G_{\rm prop}(x; y) = 2\pi{\rm i} \sum_{j\in J} \left[\psi_+(x_1) \sum_{\lambda_{\ell,j}>0} \frac{1}{\lambda_{\ell,j}} \hat{\phi}_{\ell,j}(x) \overline{\hat{\phi}_{\ell,j}(y)} - \psi_-(x_1) \sum_{\lambda_{\ell,j}<0} \frac{1}{\lambda_{\ell,j}} \hat{\phi}_{\ell,j}(x) \overline{\hat{\phi}_{\ell,j}(y)} \right] \tag{3.1}$$

for all $x, y \in D$ and $x \neq y$.

Remark 3.2. In the perturbed case, the propagating part of G can be decomposed into $G_{\rm prop} = G^{(0)}_{\rm prop} + G^{(1)}_{\rm prop}$, where $G^{(0)}_{\rm prop}$ represents the counterpart corresponding to Green's function of the unperturbed problem taking the form (3.1), while $G^{(1)}_{\rm prop}$ denotes the propagating part caused by the defect.

To prove Theorem 3.1, we need an auxiliary lemma. Below, we take $R > \pi$ as a variable and suppose that $D_R := \{x \in D : |x| < R\}$ is always a Lipschitz domain. Otherwise, we can slightly change the shape of the part C_R to achieve this. In the remaining part of this paper, we do not mention this any more.

Lemma 3.3. *Let*

$$
\begin{aligned}
u_{\rm prop}(x) &= \psi^+(x_1)\sum_{j\in J}\sum_{\lambda_{\ell,j}>0} a_{\ell,j}\,\hat\phi_{\ell,j}(x) + \psi^-(x_1)\sum_{j\in J}\sum_{\lambda_{\ell,j}<0} a_{\ell,j}\,\hat\phi_{\ell,j}(x),\\
v_{\rm prop}(x) &= \psi^+(x_1)\sum_{j\in J}\sum_{\lambda_{\ell,j}>0} b_{\ell,j}\,\hat\phi_{\ell,j}(x) + \psi^-(x_1)\sum_{j\in J}\sum_{\lambda_{\ell,j}<0} b_{\ell,j}\,\hat\phi_{\ell,j}(x)
\end{aligned}
$$

be the propagating parts of two solutions satisfying the open waveguide radiation condition. Then

$$
\int_{C_R}\left[v_{\rm prop}\,\frac{\partial u_{\rm prop}}{\partial\nu} - u_{\rm prop}\,\frac{\partial v_{\rm prop}}{\partial\nu}\right] ds \to 0 \quad \textit{as } R\to\infty.
$$

Remark 3.4. The path C_R can be replaced by ∂D_R because of the boundary condition on ∂D. Since $u_{\rm prop}, v_{\rm prop} \in H^1(D_R)$ and $\Delta u_{\rm prop}, \Delta v_{\rm prop} \in L^2(D_R)$, the integral over ∂D_R is understood in the dual form of $\langle H^{-1/2}(\partial D_R), H^{1/2}(\partial D_R)\rangle$. The integral over C_R is understood in the dual form of $\langle H^{-1/2}(C_R), H_0^{1/2}(C_R)\rangle$ (see, e.g., [36]).

Proof. We first recall Green's second formula for any bounded Lipschitz domain Ω. For $w, v \in H^1(\Omega)$ satisfying $\Delta w, \Delta v \in L^2(\Omega)$, we have

$$
\int_\Omega [w\,\Delta v - v\,\Delta w]\,dx = \int_{\partial\Omega}[w\,\partial_\nu v - v\,\partial_\nu w]\,ds,
$$

where the right-hand side is understood as the dual forms for $\partial_\nu v, \partial_\nu w \in H^{-1/2}(\partial\Omega)$ and $w, v \in H^{1/2}(\partial\Omega)$. Application of Green's formula to D_R yields

$$
\int_{C_R}\left[v_{\rm prop}\,\frac{\partial u_{\rm prop}}{\partial\nu} - u_{\rm prop}\,\frac{\partial v_{\rm prop}}{\partial\nu}\right] ds = \int_{D_R}[v_{\rm prop}\,(\Delta+k^2)u_{\rm prop} - u_{\rm prop}\,(\Delta+k^2)v_{\rm prop}]\,dx.
$$

From the forms of $u_{\rm prop}$ and $v_{\rm prop}$, we conclude that

$$
\Delta u_{\rm prop} + k^2 u_{\rm prop} = \sum_{j\in J}\sum_{\lambda_{\ell,j}>0} a_{\ell,j}\,(\Delta+k^2)[\psi^+\,\hat\phi_{\ell,j}] + \sum_{j\in J}\sum_{\lambda_{\ell,j}<0} a_{\ell,j}\,(\Delta+k^2)[\psi^-\,\hat\phi_{\ell,j}]
$$

and the same for $v_{\rm prop}$. Therefore, since $\psi^+(x_1)\psi^-(x_1) = 0$ for all $x_1 \in \mathbb{R}$,

$$
\begin{aligned}
&\int_{D_R} v_{\rm prop}\,(\Delta+k^2)u_{\rm prop}\,dx\\
&\quad= \sum_{j_1\in J}\sum_{\lambda_{\ell_1,j_1}>0} a_{\ell_1,j_1}\sum_{j_2\in J}\sum_{\lambda_{\ell_2,j_2}>0} b_{\ell_2,j_2}\int_{D_R^+}[\psi^+\,\hat\phi_{\ell_2,j_2}]\,(\Delta+k^2)[\psi^+\,\hat\phi_{\ell_1,j_1}]\,dx\\
&\qquad+ \sum_{j_1\in J}\sum_{\lambda_{\ell_1,j_1}<0} a_{\ell_1,j_1}\sum_{j_2\in J}\sum_{\lambda_{\ell_2,j_2}<0} b_{\ell_2,j_2}\int_{D_R^-}[\psi^-\,\hat\phi_{\ell_2,j_2}]\,(\Delta+k^2)[\psi^-\,\hat\phi_{\ell_1,j_1}]\,dx,
\end{aligned}
$$

where $D_R^+ = \{x \in D_R : \sigma - 1 < x_1 < \sigma\}$ and $D_R^- = \{x \in D_R : -\sigma < x_1 < -\sigma + 1\}$. Here, we suppose that both D_R^+ and D_R^- are Lipschitz domains by the choice of $\sigma > \max\{R, 2\pi\} + 1$. An analogous formula holds for $u_{\rm prop}$ and $v_{\rm prop}$ interchanged. Taking the difference and applying Green's theorem yields for the integral over D_R^+:

$$
\int_{D_R^+}[\psi^+\,\hat\phi_{\ell_2,j_2}]\,(\Delta+k^2)[\psi^+\,\hat\phi_{\ell_1,j_1}] - [\psi^+\,\hat\phi_{\ell_1,j_1}]\,(\Delta+k^2)[\psi^+\,\hat\phi_{\ell_2,j_2}]\,dx
$$

$$= \int_{\partial D_R^+} \psi^+ \left[\hat{\phi}_{\ell_2,j_2} \frac{\partial[\psi^+ \hat{\phi}_{\ell_1,j_1}]}{\partial\nu} - \hat{\phi}_{\ell_1,j_1} \frac{\partial[\psi^+ \hat{\phi}_{\ell_2,j_2}]}{\partial\nu}\right] ds$$
$$= \int_{S_R} \psi^+ \left[\hat{\phi}_{\ell_2,j_2} \frac{\partial[\psi^+ \hat{\phi}_{\ell_1,j_1}]}{\partial\nu} - \hat{\phi}_{\ell_1,j_1} \frac{\partial[\psi^+ \hat{\phi}_{\ell_2,j_2}]}{\partial\nu}\right] ds$$
$$+ \int_{\gamma_R} \left[\frac{\partial \hat{\phi}_{\ell_1,j_1}}{\partial x_1} \hat{\phi}_{\ell_2,j_2} - \frac{\partial \hat{\phi}_{\ell_2,j_2}}{\partial x_1} \hat{\phi}_{\ell_1,j_1}\right] ds,$$

where $S_R = \{x \in D : |x| = R,\ \sigma - 1 < x_1 < \sigma\}$ and $\gamma_R = \{x \in D : x_1 = \sigma,\ |x| < R\}$. We remark that, since $\hat{\phi}_{\ell,j}$ vanish on ∂D, the integral over γ_R is understood in the dual form of $\langle H^{-1/2}(\gamma_R), H_0^{1/2}(\gamma_R)\rangle$ (see, e.g., [36]). The integral over S_R tends to zero as $R \to \infty$ because of the exponential decay. The integral over γ_R tends to

$$\int_{x_1=\sigma} \left[\frac{\partial \hat{\phi}_{\ell_1,j_1}}{\partial x_1} \hat{\phi}_{\ell_2,j_2} - \frac{\partial \hat{\phi}_{\ell_2,j_2}}{\partial x_1} \hat{\phi}_{\ell_1,j_1}\right] ds = \int_{x_1=\sigma} \left[\frac{\partial \hat{\phi}_{\ell_1,j_1}}{\partial x_1} \overline{\hat{\phi}_{\ell_2,-j_2}} - \frac{\partial \overline{\hat{\phi}_{\ell_2,-j_2}}}{\partial x_1} \hat{\phi}_{\ell_1,j_1}\right] ds$$

because $\hat{\phi}_{\ell_2,-j_2} = \overline{\hat{\phi}_{\ell_2,j_2}}$. Now we conclude from $\lambda_{\ell_1,j_1} > 0$ and $-\lambda_{\ell_2,-j_2} = \lambda_{\ell_2,j_2} > 0$ that $j_1 \neq -j_2$. Note that $\ell_1 \in \{1, \dots, m_{j_1}\}$, $\ell_2 \in \{1, \dots, m_{j_2}\}$ and $m_{j_2} = m_{-j_2}$. Therefore, the integral vanishes by the proof of [28, Lemma 2.6]. □

Below, we carry out the proof of Theorem 3.1 by using Lemma 3.3. The symmetry of Green's function will be used in the proof of Theorem 5.4 for our inverse problems. Write $B(x,\delta) := \{z \in \mathbb{R}^2 : |z-x| < \delta\}$.

Proof of Theorem 3.1. (i) We fix $x, y \in \tilde{D}$ with $x \neq y$ and choose $\delta > 0$ such that $B(x,\delta) \cup B(y,\delta) \subset \tilde{D}$ and $\overline{B(x,\delta)} \cap \overline{B(y,\delta)} = \emptyset$. Then we choose $R > 0$ sufficiently large and set

$$D_{R,\delta} := \{z \in \tilde{D} : |z| < R,\ |z-x| > \delta,\ |z-y| > \delta\}.$$

Using $\Delta_z G(z;x) + k^2 G(z;x) = 0$ and $\Delta_z G(z;y) + k^2 G(z;y) = 0$ in $D_{R,\delta}$ and the application of Green's second formula in $D_{R,\delta}$ yields

$$0 = \int_{D_{R,\delta}} [G(z;x)\, \Delta_z G(z;y) - G(z;y)\, \Delta_z G(z;x)]\, dz$$
$$= \left(\int_{|z|=R} - \int_{|z-x|=\delta} - \int_{|z-y|=\delta}\right) \left[\frac{\partial G(z;y)}{\partial\nu(z)} G(z;x) - \frac{\partial G(z;x)}{\partial\nu(z)} G(z;y)\right] ds(z).$$

Here, we have used the vanishing of $G(\cdot\,;y)$ and $G(\cdot\,;x)$ on $\partial D_{R,\delta} \cap \tilde{\Gamma}$. Note that the normal direction at C_R is supposed to point into Σ_R and that at $\partial B(x,\delta)$ or $\partial B(y,\delta)$ to point into $D_{R,\delta}$. We consider first the integral over $\partial B(x,\delta)$. For $|z-x| \leqslant \delta$, the terms $G(\cdot\,;y)$ and $G(\cdot;x) - \Phi(\cdot;x)$ and their gradients are smooth. Therefore,

$$\int_{|z-x|=\delta} \left[\frac{\partial G(z;y)}{\partial\nu(z)} G(z;x) - \frac{\partial G(z;x)}{\partial\nu(z)} G(z;y)\right] ds(z)$$
$$= \int_{|z-x|=\delta} \left[\frac{\partial G(z;y)}{\partial\nu(z)} \Phi(z;x) - \frac{\partial \Phi(z;x)}{\partial\nu(z)} G(z;y)\right] ds(z) + \mathcal{O}(\delta)$$
$$= G(x;y) + \mathcal{O}(\delta),$$

where we applied Green's representation formula to $G(\cdot\,;y)$ in the disk $B(x,\delta)$. For $\delta \to 0$, we get

$$\int_{|z-x|=\delta} \left[\frac{\partial G(z;y)}{\partial\nu(z)} G(z;x) - \frac{\partial G(z;x)}{\partial\nu(z)} G(z;y)\right] ds(z) \to G(x;y).$$

The integral over $\partial B(y,\delta)$ is treated in the same way, just by interchanging the roles of x and y.

It remains to show that the integral over $C_R := \{z \in D : |z| = R\}$ tends to zero as R tends to infinity. Substituting the decomposition $G(\cdot\,;y) = G_{\mathrm{rad}}(\cdot\,;y) + G_{\mathrm{prop}}(\cdot\,;y)$ into the integral yields that

$$\int_{C_R} \left[\frac{\partial G(z;y)}{\partial\nu(z)} G(z;x) - \frac{\partial G(z;x)}{\partial\nu(z)} G(z;y)\right] ds(z)$$

consists of four integrals. The integral

$$\int_{C_R}\left[\frac{\partial G_{\rm prop}(z;y)}{\partial\nu(z)}\,G_{\rm prop}(z;x)-\frac{\partial G_{\rm prop}(z;x)}{\partial\nu(z)}\,G_{\rm prop}(z;y)\right]ds(z)$$

tends to zero by the previous lemma. For the other parts, we note that the integral over $C_R\cap W_h$ tends to zero as $R\to\infty$, because, for example,

$$\begin{aligned}&\left|\int_{C_R\cap W_h}\frac{\partial G_{\rm rad}(z;y)}{\partial\nu(z)}\,G_{\rm prop}(z;x)\,ds(z)\right|\\&\quad\leqslant c\left\|\frac{\partial G_{\rm rad}(\cdot\,;y)}{\partial\nu}\right\|_{H^{-1/2}(C_R\cap W_h)}\|G_{\rm prop}(\cdot,x)\|_{H^{1/2}(C_R\cap W_h)}\\&\quad\leqslant c'\,\|G_{\rm rad}(\cdot\,;y)\|_{H^1(V_R)}\,\|G_{\rm prop}(\cdot,x)\|_{H^1(V_R)},\end{aligned}$$

where $V_R:=\{z\in D\cap W_h:||z|-R|<1/2\}$, $\|G_{\rm rad}(\cdot\,;y)\|_{H^1(U_R)}$ tends to zero and $\|G_{\rm prop}(\cdot,x)\|_{H^1(V_R)}$ is bounded.

Hence it remains to consider the integral over $C_{R,h}:=\{z\in C_R:z_2>h\}$. Here, we use the Sommerfeld radiation condition for $G_{\rm rad}(\cdot,x)$ and $G_{\rm rad}(\cdot\,;y)$ which yields that

$$\int_{C_{R,h}}\left[\frac{\partial G_{\rm rad}(z;y)}{\partial\nu(z)}\,G_{\rm rad}(z;x)-\frac{\partial G_{\rm rad}(z;x)}{\partial\nu(z)}\,G_{\rm rad}(z;y)\right]ds(z)$$

tends to zero. Using the estimates

$$|G_{\rm rad}(z;x)|+|\nabla_z G_{\rm rad}(z;x)|\leqslant\frac{c}{\sqrt{|z|}},\quad |G_{\rm prop}(z;x)|+|\nabla_z G_{\rm prop}(z;x)|\leqslant c\,{\rm e}^{-\sigma z_2}$$

for some $c>0$ and the same for y replacing x, we obtain

$$\begin{aligned}&\int_{C_{R,h}}\left|\frac{\partial G_{\rm prop}(z;y)}{\partial\nu(z)}\,G_{\rm rad}(z;x)-\frac{\partial G_{\rm rad}(z;x)}{\partial\nu(z)}\,G_{\rm prop}(z;y)\right|ds(z)\\&\quad+\int_{C_{R,h}}\left|\frac{\partial G_{\rm rad}(z;y)}{\partial\nu(z)}\,G_{\rm prop}(z;x)-\frac{\partial G_{\rm prop}(z;x)}{\partial\nu(z)}\,G_{\rm rad}(z;y)\right|ds(z)\\&\quad\leqslant c\,\frac{R}{\sqrt{R}}\int_0^\pi {\rm e}^{-R\sigma\sin t}\,dt.\end{aligned}\tag{3.2}$$

Using $\sin t\geqslant\frac{2}{\pi}t$ on $[0,\pi/2]$, one deduces that the right-hand side of (3.2) tends to zero as $R\to\infty$, because

$$\int_0^\pi {\rm e}^{-R\sigma\sin t}\,dt=2\int_0^{\pi/2}{\rm e}^{-R\sigma\sin t}\,dt\leqslant 2\int_0^{\pi/2}{\rm e}^{-2R\sigma t/\pi}\,dt=\frac{\pi}{R\sigma}(1-{\rm e}^{-R\sigma}).$$

(ii) For fixed $y\in D$, we choose $\epsilon>0$ less than the distance between y and Γ. Introduce a cut-off function $\chi\in C_0^\infty(\mathbb{R}^2)$ with $\chi(x)=1$ for $|x-y|<\epsilon/2$ and $\chi(x)=0$ for $|x-y|\geqslant\epsilon$. Then $v:=G(\cdot\,;y)-\chi\,\Phi(\cdot\,;y)\in H^1_{\rm loc}(D)$ coincides with $G(\cdot\,;y)$ for $|x-y|\geqslant\epsilon$ and satisfies $\Delta v+k^2v=-g_y$ in D and $v=0$ on Γ, where

$$g_y:=\Delta\chi\,\Phi(\cdot\,;y)+2\nabla\chi\cdot\nabla\Phi(\cdot\,;y)\in L^2(D)$$

has compact support. If σ in the definition of the radiation condition is chosen to be larger than $|y_1|+\epsilon$ then by [19, Theorem 3.5],

$$G_{\rm prop}(x;y)=v_{\rm prop}(x)=\sum_{j\in J}\left[\psi_+(x_1)\sum_{\lambda_{\ell,j}>0}\hat\phi_{\ell,j}(x)\,a_{\ell,j}(y)+\psi_-(x_1)\sum_{\lambda_{\ell,j}<0}\hat\phi_{\ell,j}(x)\,a_{\ell,j}(y)\right]$$

for $|x_1|\geqslant\sigma$, where the coefficients $a_{\ell,j}(y)$ are given by

$$a_{\ell,j}(y)=\frac{2\pi{\rm i}}{|\lambda_{\ell,j}|}\int_{\epsilon/2<|x-y|<\epsilon}g_y(x)\,\overline{\hat\phi}_{\ell,j}(x)\,dx.$$

To calculate $a_{\ell,j}(y)$, we rewrite g_y as $g_y(x) = (\Delta + k^2)(\chi(x)\Phi(x;y))$ for $x \neq y$. Consequently, the application of Green's formula yields

$$\begin{aligned}
a_{\ell,j}(y) &= \frac{2\pi\mathrm{i}}{|\lambda_{\ell,j}|} \int_{\epsilon/2<|x-y|<\epsilon} g_y(x)\, \overline{\hat{\phi}_{\ell,j}(x)}\, dx \\
&= \frac{2\pi\mathrm{i}}{|\lambda_{\ell,j}|} \int_{|x-y|=\epsilon/2} \left[\frac{\partial \overline{\hat{\phi}_{\ell,j}(x)}}{\partial \nu(x)}\, \Phi(x;y) - \frac{\partial \Phi(x;y)}{\partial \nu(x)}\, \overline{\hat{\phi}_{\ell,j}(x)} \right] ds(x) \\
&= \frac{2\pi\mathrm{i}}{|\lambda_{\ell,j}|}\, \overline{\hat{\phi}_{\ell,j}(y)},
\end{aligned} \tag{3.3}$$

where we have used the facts that $\chi(x) = 1$ on $|x-y| = \epsilon/2$ and $\chi(x) = 0$ on $|x-y| = \epsilon$. □

From the proof of Theorem 3.1, we conclude the following corollary.

Corollary 3.5. *Let $u \in H^1_{\mathrm{loc},0}(\tilde{D})$ be an open wave-guide radiating solution to the Helmholtz equation $(\Delta + k^2)u = 0$ in Σ_R, where $\tilde{D}_R$ is supposed to be a Lipschitz domain. We have the representation*

$$u(x) = \int_{C_R} \left[\frac{\partial u(z)}{\partial \nu(z)}\, G(z;x) - \frac{\partial G(z;x)}{\partial \nu(z)}\, u(z) \right] ds(z), \quad x \in \Sigma_R. \tag{3.4}$$

Proof. We fix $x \in \Sigma_R$ and choose $R' > R$ such that $x \in \tilde{D}_{R'}$ where $\tilde{D}_{R'}$ is a Lipschitz domain. Application of Green's representation formula yields

$$u(x) = \left(\int_{C_R} - \int_{C_{R'}} \right) \left[\frac{\partial u(z)}{\partial \nu(z)}\, G(z;x) - \frac{\partial G(z;x)}{\partial \nu(z)}\, u(z) \right] ds(z), \quad x \in \Sigma_R. \tag{3.5}$$

By the proof of Theorem 3.1, the integral over $C_{R'}$ tends to zero as R' tends to infinity, which together with (3.5) finishes the proof of (3.4). □

4 Scattering of plane waves at a propagative number

As shown in Proposition 2.11, uniqueness and existence of a weak solution for an incoming plane wave are guaranteed under the open waveguide radiation condition, provided that $k \sin\theta$ is not a propagative number. If $k \sin\theta = \hat{\alpha}_j$ is a propagative number , there still exists an $\hat{\alpha}_j$-quasi-periodic solution $u_0 \in H^1_{\mathrm{loc}}(D)$ of the unperturbed problem (see Lemma 4.1(i) below). However, uniqueness fails and the general solution takes the form

$$u = u_0 + \sum_{\ell=1}^{m_j} c_\ell\, \hat{\phi}_{\ell,j} \quad \text{in } D, \tag{4.1}$$

where $\hat{\phi}_{\ell,j} \in X_j$ (see (2.4) and (2.6)) and $c_\ell \in \mathbb{C}$ are arbitrary. A general solution to the locally perturbed scattering problem is described in [19, Corollary 4.10] when $k \sin\theta$ is a propagative number. The purpose of this section is to propose an additional constraint on solutions of the unperturbed problem to fix the coefficients c_ℓ in (4.1), so that the forward problem is always uniquely solvable. We employ two methods: the limiting absorption principle for approximating the wave-number with a positive imaginary part in Subsection 4.1 and the method of approximating the plane wave by point source waves in Subsection 4.2.

4.1 The limiting absorption principle and singular perturbation arguments

We first consider the scattering problem in a periodic domain D without defects. Let $u^{in}(x) = \mathrm{e}^{\mathrm{i}k(x_1 \sin\theta - x_2 \cos\theta)}$ with $\theta \in (-\pi/2, \pi/2)$ be the incident plane wave. Set

$$\alpha := k \sin\theta \quad \text{and} \quad \beta_n := \sqrt{k^2 - (n+\alpha)^2}, \quad n \in \mathbb{N},$$

where the square root is chosen such that $\operatorname{Im} \sqrt{t} \geqslant 0$ for $t \leqslant 0$. Obviously, $u^{in}(x) = \mathrm{e}^{\mathrm{i}\alpha x_1 - \mathrm{i}\beta_0 x_2}$. Since the wave-number $k > 0$ is fixed, we omit the dependence on k for simplicity. We look for an α-quasi-periodic total field $u \in H^1_{\alpha,0}(Q_h) := \{u \in H^1_\alpha(Q_h) : u = 0 \text{ on } \partial Q_h \cap \Gamma\}$ for all $h > h_0$ such that $u^{sc} = u - u^{in}$ satisfies the upward α-quasiperiodic Rayleigh expansion (2.2).

Introduce the α-quasi-periodic and periodic, respectively, Sobolev spaces on Γ_h with $h > h_0$ by

$$H^{1/2}_\alpha(\Gamma_h) := \{f \in H^{1/2}(\Gamma_h) : \mathrm{e}^{-\mathrm{i}\alpha x_1} f(x_1, h) \text{ is } 2\pi\text{-periodic in } x_1\},$$
$$H^{1/2}_{per}(\Gamma_h) := \{f \in H^{1/2}(\Gamma_h) : f(x_1, h) \text{ is } 2\pi\text{-periodic in } x_1\}.$$

Define the periodic and quasi-periodic, respectively, Dirichlet-to-Neumann maps on the artificial boundary Γ_h by

$$(T_k f)(x_1, h) := \sum_{n\in\mathbb{Z}} \mathrm{i}\beta_n\, f_n\, \mathrm{e}^{\mathrm{i}nx_1}, \quad f(x_1, h) = \sum_{n\in\mathbb{Z}} f_n\, \mathrm{e}^{\mathrm{i}nx_1} \in H^{1/2}_{\mathrm{per}}(\Gamma_h), \tag{4.2}$$

$$(\tilde{T}_k \tilde{f})(x_1, h) := \sum_{n\in\mathbb{Z}} \mathrm{i}\beta_n\, \tilde{f}_n\, \mathrm{e}^{\mathrm{i}(n+\alpha)x_1}, \quad \tilde{f}(x_1, h) = \sum_{n\in\mathbb{Z}} \tilde{f}_n \mathrm{e}^{\mathrm{i}(n+\alpha)x_1} \in H^{1/2}_\alpha(\Gamma_h). \tag{4.3}$$

It is well known that $T_k : H^{1/2}_{\mathrm{per}}(\Gamma_h) \to H^{-1/2}_{\mathrm{per}}(\Gamma_h)$ and $\tilde{T}_k : H^{1/2}_\alpha(\Gamma_h) \to H^{-1/2}_\alpha(\Gamma_h)$ are bounded linear operators. The following variational formulation for $u \in H^1_{\alpha,0}(Q_h)$ can be easily derived:

$$\tilde{a}_k(u, \phi) = -2\mathrm{i}k\cos\theta\, \mathrm{e}^{-\mathrm{i}kh\cos\theta} \int_{\Gamma_h} \mathrm{e}^{\mathrm{i}\alpha x_1}\, \overline{\phi}\, ds \quad \text{for all } \phi \in H^1_{\alpha,0}(Q_h), \tag{4.4}$$

where

$$\tilde{a}_k(u, \phi) := \int_{Q_h} [\nabla u \cdot \overline{\nabla\phi} - k^2 u\, \overline{\phi}]\, dx - \int_{\Gamma_h} \tilde{T}_k u\, \overline{\phi}\, ds, \quad u, \phi \in H^1_{\alpha,0}(Q_h).$$

Defining $v := \mathrm{e}^{-\mathrm{i}\alpha x_1} u \in H^1_{\mathrm{per},0}(Q_h) := \{v \in H^1_{\mathrm{per}}(Q_h), v = 0 \text{ on } \Gamma \cap \partial Q_h\}$ and $\psi := \mathrm{e}^{-\mathrm{i}\alpha x_1}\phi$ for $\phi \in H^1_{\alpha,0}(Q_h)$, we get the periodic form

$$a_k(v, \psi) = -2\mathrm{i}k\cos\theta\, \mathrm{e}^{-\mathrm{i}kh\cos\theta} \int_0^{2\pi} \overline{\psi(x_1, h)}\, dx_1 \quad \text{for all } \psi \in H^1_{\mathrm{per},0}(Q_h), \tag{4.5}$$

where now

$$a_k(v, \psi) := \int_{Q_h} \left[\nabla v \cdot \overline{\nabla\psi} - 2\mathrm{i}\alpha \frac{\partial v}{\partial x_1}\, \overline{\psi} - (k^2 - \alpha^2)\, v\, \overline{\psi}\right] dx - \int_{\Gamma_h} T_k v\, \overline{\psi}\, ds$$

for $v, \psi \in H^1_{\mathrm{per},0}(Q_h)$. We equip $H^1_{\mathrm{per},0}(Q_h)$ with the inner product

$$\langle v, \psi\rangle := \int_{Q_h} \nabla v \cdot \nabla\overline{\psi}\, dx + 2\pi \sum_{n\in\mathbb{Z}} (1 + n^2)^{1/2} v_n\, \overline{\psi}_n, \quad \psi, v \in H^1_{\mathrm{per},0}(Q_h), \tag{4.6}$$

where ψ_n and v_n denote the Fourier coefficients of $\psi(x_1, h)$ and $v(x_1, h)$, respectively. By the representation theorem of Riesz, there exist $f^{(k)} \in H^1_{\mathrm{per},0}(Q_h)$ and a linear bounded operator L_k from $H^1_{\mathrm{per},0}(Q_h)$ into itself with

$$\langle f^{(k)}, \psi\rangle = -2\mathrm{i}k\cos\theta\, \mathrm{e}^{-\mathrm{i}kh\cos\theta} \int_0^{2\pi} \overline{\psi(x_1, h)}\, dx_1, \tag{4.7}$$

$$\langle L_k v, \psi\rangle = a_k(v, \psi) = \int_{Q_h} \left[\nabla v \cdot \nabla\overline{\psi} - 2\mathrm{i}k\sin\theta \frac{\partial v}{\partial x_1}\, \overline{\psi} - k^2\cos^2\theta\, v\, \overline{\psi}\right] dx - 2\pi \sum_{n\in\mathbb{N}} \mathrm{i}\beta_n v_n \overline{\psi}_n \tag{4.8}$$

for all $\psi, v \in H^1_{\mathrm{per},0}(Q_h)$. Then the operator equation (4.5) can be rewritten as

$$L_k v = f^{(k)} \quad \text{in } H^1_{\mathrm{per},0}(Q_h). \tag{4.9}$$

One can show that the operator $K_k := I - L_k$, given by

$$\langle K_k\, v, \psi\rangle := \int_{Q_h} \left[2\mathrm{i}k\sin\theta \frac{\partial v}{\partial x_1}\, \overline{\psi} + k^2\cos^2\theta\, v\, \overline{\psi}\right] dx \ + 2\pi \sum_{n\in\mathbb{Z}} (\sqrt{1 + n^2} + \mathrm{i}\beta_n) v_n \overline{\psi}_n$$

for all $\psi, v \in H^1_{\text{per},0}(Q_h)$, is compact as an operator from $H^1_{\text{per},0}(Q_h)$ into itself. In fact, the first integral can be reformulated as

$$\int_{Q_h} \left[2\mathrm{i}k\sin\theta\,\frac{\partial v}{\partial x_1}\,\overline{\psi} + k^2\cos^2\theta\, v\,\overline{\psi}\right] dx = \int_{Q_h} \left[-2\mathrm{i}k\sin\theta\, v\,\frac{\partial\overline{\psi}}{\partial x_1} + k^2\cos^2\theta\, v\,\overline{\psi}\right] dx,$$

which is a compact form due to the compact embedding of $H^1_{\text{per},0}(Q_h) \to L^2(Q_h)$. The summation in the definition of K_k is also compact, because of the boundedness of the sequence $n \mapsto \sqrt{1+n^2} + \mathrm{i}\beta_n$ for $n \in \mathbb{Z}$.

Below, we collect some properties of the operator L_k.

Lemma 4.1. *Suppose that $\alpha + n \neq \pm k$ for any $n \in \mathbb{Z}$, i.e., α is not a cut-off value.*

(i) *For $k > 0$, the equation (4.9) admits at least one solution $v \in H^1_{\text{per},0}(Q_h)$. The null space $\mathcal{N} := \mathcal{N}(L_k) = \mathcal{N}(L_k^*)$ is finite-dimensional and consists of surface wave modes only, i.e.,*

$$v(x) = \sum_{n\in\mathbb{Z}:|n+\alpha|>k} v_n\, \mathrm{e}^{\mathrm{i}nx_1 - |\beta_n|(x_2-h)}, \quad x_2 > h. \tag{4.10}$$

(ii) *The Riesz number of L_k is one, i.e., $\mathcal{N}(L_k) = \mathcal{N}(L_k^2)$. Moreover, it holds that the orthogonal decomposition $H^1_{\text{per},0}(Q_h) = \mathcal{N}(L_k) \oplus \mathcal{R}(L_k)$. Here, $\mathcal{R}(L_k)$ denotes the range of the operator L_k.*

(iii) *If $\operatorname{Im} k > 0$, there is a unique solution to (4.9) in $H^1_{\text{per},0}(Q_h)$ for any $h > h_0$.*

Proof. (i) The form of $v \in \mathcal{N}$ given by (4.10) can be derived by setting $\phi = u = v\mathrm{e}^{\mathrm{i}\alpha x_1}$ in the homogeneous form of (4.4), taking the imaginary part and using the definition of $\tilde{T}_k$. The adjoint operator L_k^* of L_k is defined by

$$\begin{aligned}\langle L_k^* v, \psi\rangle &= \langle v, L_k\psi\rangle = \overline{\langle L_k\psi, v\rangle} = \overline{a_k(\psi, v)} \\ &= \int_{Q_h} [\nabla u\cdot\overline{\nabla\phi} - k^2 u\overline{\phi}]\, dx + \sum_{n\in\mathbb{Z}} \mathrm{i}\overline{\beta_n}\, u_n\, \overline{\phi}_n\end{aligned}$$

for all $v, \psi \in H^1_{\text{per},0}(Q_h)$, where $u = \mathrm{e}^{\mathrm{i}\alpha x_1} v$ and $\phi = \mathrm{e}^{\mathrm{i}\alpha x_1}\psi$. From this, we conclude that $\mathcal{N}(L_k) = \mathcal{N}(L_k^*)$. The existence of $v \in H^1_{\text{per},0}(Q_h)$ follows from the fact that $\langle f^{(k)}, \psi\rangle = 0$ for all $\psi \in \mathcal{N}$ and the Fredholm alternative. The space $\mathcal{N}$ is finite-dimensional, because K_k is compact.

(ii) It is obvious that $\mathcal{N}(L_k) \subset \mathcal{N}(L_k^2)$. To prove the reverse direction, we assume $L_k^2 w = 0$ for some $w \in H^1_{\text{per},0}(Q_h)$ and set $v = L_k w \in \mathcal{R}(L_k)$. Since $v \in \mathcal{N}(L_k) = \mathcal{N}(L_k^*)$, we obtain

$$\|v\|^2 = \langle v, v\rangle = \langle v, L_k w\rangle = \langle L_k^* v, w\rangle = 0,$$

which proves $\mathcal{N}(L_k^2) \subset \mathcal{N}(L_k)$ and thus the coincidence $\mathcal{N}(L_k^2) = \mathcal{N}(L_k)$. This also implies $\mathcal{N} \cap \mathcal{R} = \emptyset$ and hence $H^1_{\text{per},0}(Q_h) = \mathcal{N} \oplus \mathcal{R}$. The orthogonality between $\mathcal{N}$ and $\mathcal{R}$ follows from the relation $\mathcal{N}(L_k) = \mathcal{N}(L_k^*)$.

(iii) We apply the uniqueness result of [6] to the proof of the third assertion. By the Fredholm alternative, it suffices to prove uniqueness. Let $k \in \mathbb{C}$ with $\operatorname{Im} k > 0$ and set $\alpha = k\sin\theta \in \mathbb{C}$. Assuming $L_k v = 0$ for some $v \in H^1_{\text{per},0}(Q_h)$, we need to prove $v \equiv 0$. It then follows that $a_k(v, \psi) = 0$ for all $\psi \in H^1_{\text{per},0}(Q_h)$, which implies that v satisfies the elliptic equation $(\Delta + 2\mathrm{i}\alpha\partial_1 + k^2 - \alpha^2)v = 0$ in D, and the Dirichlet boundary condition $v = 0$ on Γ together with the periodic expansion $v = \sum_{n\in\mathbb{Z}} v_n \mathrm{e}^{\mathrm{i}nx_1 + \mathrm{i}\beta_n x_2}$ in $x_2 > h$.

We claim that $\operatorname{Im}\beta_n > 0$ for all $n \in \mathbb{Z}$, if $\operatorname{Im} k > 0$. Recall that the square root function $z \mapsto \sqrt{z}$ was chosen to be holomorphic in the region $\{z \in \mathbb{C} : z \notin \mathrm{i}\mathbb{R}_{\leqslant 0}\}$. In particular, we have $\operatorname{Im}\sqrt{z} > 0$ for all $z \in C := \{z \in \mathbb{C} : \operatorname{Re} z < 0 \text{ or } \operatorname{Im} z > 0\}$. It is easily seen that $k^2 - (n + k\sin\theta)^2 \in C$ for all $k \in \mathbb{C}$ with $\operatorname{Im} k > 0$ and $\operatorname{Re} k > 0$ and all $n \in \mathbb{Z}$ provided that $|\sin\theta| < 1$. Indeed, if n is such that $|n + \operatorname{Re} k\sin\theta| \leqslant \operatorname{Re} k$, then

$$\begin{aligned}\operatorname{Im}[k^2 - (n + k\sin\theta)^2] &= 2\operatorname{Im} k\,[\operatorname{Re} k - (n + \operatorname{Re} k\sin\theta)\sin\theta] \\ &\geqslant 2\operatorname{Im} k\operatorname{Re} k\,(1 - |\sin\theta|) > 0.\end{aligned}$$

If n is such that $|n + \operatorname{Re} k \sin\theta| > \operatorname{Re} k$, then

$$\begin{aligned}\operatorname{Re}[k^2 - (n + k\sin\theta)^2] &= (\operatorname{Re} k)^2 - (\operatorname{Im} k)^2 - (n + \operatorname{Re} k \sin\theta)^2 + (\operatorname{Im} k)^2 \sin^2\theta \\ &= (\operatorname{Re} k)^2 - (n + \operatorname{Re} k \sin\theta)^2 - (\operatorname{Im} k)^2 \cos^2\theta < 0.\end{aligned}$$

This proves $\operatorname{Im}\beta_n > 0$ for all $n \in \mathbb{Z}$.

Setting $u^s = v\, e^{i\alpha x_1}$, we deduce that u^s fulfills the homogeneous boundary value problem of the Helmholtz equation

$$\Delta u^s + k^2 u^s = 0 \quad \text{in } D, \quad u^s = 0 \quad \text{on } \partial D,$$

and the quasi-periodic Rayleigh expansion condition (2.2) in $x_2 > h$. Since $\operatorname{Im}\beta_n > 0$, the function u^s decays exponentially to zero as $x_2 \to \infty$ in D. By elliptic boundary regularity in Lipschitz domains with the zero boundary condition, we have $u^s \in C^{0,\gamma}(\overline{Q_h})$ for any $h > h_0$, where the Hölder exponent $\gamma > 0$ depends on the Lipschitz constant of Γ; we refer to [17, Chapter 4, Theorem 4.3] for the proof valid for C^1-smooth boundaries, which is also applicable to Lipschitz curves in $\mathbb{R}^2$. The boundary behavior of the Dirichlet boundary value problem of elliptic equations in a non-smooth domain can be further found in [33, Chapter 7]. Hence, this together with the interior regularity gives $u^s \in C^2(D) \cap C(\overline{D})$ and u^s must be bounded in the infinite strip $Q_\infty := \{x \in D : 0 < x_1 < 2\pi\}$. On the other hand, the α-quasi-periodicity of u^s gives

$$u^s(x_1 + 2n\pi, x_2) = e^{i2\pi nk\sin\theta} u^s(x_1, x_2) \quad \text{for all } x \in D.$$

This in combination with the boundedness of $\|u\|\|_{L^\infty(Q_\infty)}$ yields the growth condition

$$|u^s(x)| \leqslant C\, e^{\operatorname{Im} k\, |\sin\theta|\, |x|}, \quad x \in D$$

for some $C > 0$. Now, applying [6, Theorem 3.1], we get $u^s \equiv 0$ in D and thus $v = 0$ in $H^1_{\mathrm{per},0}(Q_h)$ for all $h > h_0$. □

Now we suppose that $k \sin\theta = \hat{\alpha}_j$ for some $j \in J$ is a propagative number , which implies $\mathcal{N} \neq \emptyset$. Replacing k by $k + i\epsilon$ with $\epsilon > 0$, we consider the perturbed operator equation

$$L(\epsilon)\, v_\epsilon = f(\epsilon) \quad \text{in } H^1_{\mathrm{per},0}(Q_h)$$

with $L(\epsilon) = L_{k+i\epsilon}$ and $f(\epsilon) = f^{(k+i\epsilon)}$. We want to study the convergence and limit of $v(\epsilon)$ as $\epsilon \to 0^+$ by applying the following singular perturbation result from [29, Theorem 2.7 and Remark 2.8].

Lemma 4.2. *Let $I = (0, \epsilon_0)$ for some small $\epsilon_0 > 0$. Let $K(\epsilon)$ be compact operators from some Hilbert space X into itself and $f(\epsilon) \in \mathcal{R}(L(\epsilon))$ for all $\epsilon \in [0, \epsilon_0)$, where $L(\epsilon) := I - K(\epsilon)$. Furthermore, let $L(\epsilon)$ be one-to-one (thus invertible) for all $\epsilon \in I$ and let $L(0) = I - K(0)$ have Riesz number one. Let $P : X \to \mathcal{N} := N(L(0))$ be the projection onto the nullspace of $L(0)$ along the direct decomposition $X = \mathcal{N} \oplus \mathcal{R}$, where $\mathcal{R} = \mathcal{R}(L(0))$. Finally, let $f(\epsilon)$ and $K(\epsilon)$ be continuously differentiable functions in $\epsilon \in [0, \epsilon_0)$ and let $PL'(0)|_{\mathcal{N}}$ be an isomorphism from $\mathcal{N}$ onto itself, where $L'(0)$ denotes the one-sided derivative of $L(\epsilon)$ at $\epsilon = 0^+$.*

Then the mapping $\epsilon \mapsto v(\epsilon) := [L(\epsilon)]^{-1} f(\epsilon)$ has a continuous extension to $[0, \epsilon_0)$ into X. The limit $v(0) = \lim_{\epsilon \to 0^+} v(\epsilon)$ is the unique solution of the system

$$L(0)\, v(0) = f(0), \quad [PL'(0)]\, v(0) = Pf'(0), \tag{4.11}$$

where $f'(0)$ denotes the right-hand derivative of $f(\epsilon)$ at $\epsilon = 0$. Moreover, there exist $\delta \in (0, \epsilon_0)$ and $c > 0$ such that

$$\|v(\epsilon_1)\|_X \leqslant c\Big[\sup_{\epsilon \in [0,\delta]} \|f(\epsilon)\|_X + \sup_{\epsilon \in [0,\delta]} \|f'(\epsilon)\|_X\Big] \quad \textit{for all } \epsilon_1 \in [0, \delta].$$

The original version of Lemma 4.2 can be found in [8, Theorem 1.32, Subsection 1.4]. A more direct proof is presented in [29] with the characterization of the equation (4.11) of the limiting solution. To apply Lemma 4.2 to the operator equation (4.9), we set $X = H^1_{\mathrm{per},0}(Q_h)$ and denote by $P : H^1_{\mathrm{per},0}(Q_h) \to \mathcal{N}$

the projection operator. For $\psi \in H^1_{\mathrm{per},0}(Q_h)$, it follows from the definitions of $f^{(k)}$ and L_k that (e.g., (4.7) and (4.8))

$$
\begin{aligned}
\langle f(\epsilon), \psi \rangle &= -2\mathrm{i}(k+\mathrm{i}\epsilon)\cos\theta\, \mathrm{e}^{-\mathrm{i}(k+\mathrm{i}\epsilon)h\cos\theta} \int_0^{2\pi} \overline{\psi(x_1,h)}\, dx_1, \\
\langle L(\epsilon)v, \psi \rangle &= \int_{Q_h} \left[\nabla v \cdot \nabla \overline{\psi} - 2\mathrm{i}(k+\mathrm{i}\epsilon)\sin\theta \frac{\partial v}{\partial x_1}\, \overline{\psi} - (k+\mathrm{i}\epsilon)^2 \cos^2\theta v \overline{\psi} \right] dx \\
&\quad - 2\pi \sum_{n\in\mathbb{Z}} \mathrm{i}\sqrt{(k+\mathrm{i}\epsilon)^2 - [n + (k+\mathrm{i}\epsilon)\sin\theta]^2}\, v_n\, \overline{\psi_n},
\end{aligned}
\tag{4.12}
$$

where $v(x_1,h) = \sum_{n\in\mathbb{Z}} v_n \mathrm{e}^{\mathrm{i}nx_1} \in X$ and $\psi(x_1,h) = \sum_{n\in\mathbb{Z}} \psi_n \mathrm{e}^{\mathrm{i}nx_1} \in X$. From the above expressions, we observe that f and L are differentiable with respect to ϵ in a neighborhood of 0 provided that $k\sin\theta$ is not a cut-off value. By Lemmas 4.1(iii), $L(\epsilon)$ is invertible and thus $f(\epsilon) \in \mathcal{R}(L(\epsilon))$ for all $\epsilon > 0$. On the other hand, we have $f(0) \in \mathcal{R}$, because by (i) and (ii) in Lemma 4.1, $f(0)$ is orthogonal to $\mathcal{N}$ and X admits the orthogonal decomposition $X = \mathcal{N} \oplus \mathcal{R}$.

Since the null space $\mathcal{N}$ consists of evanescent wave modes only and $(I-P)h$ is orthogonal to $\mathcal{N}$ for any $h \in H^1_{\mathrm{per},0}(Q_h)$, it holds that

$$
\begin{aligned}
\langle Pf(0), \psi \rangle &= \langle f(0), \psi \rangle = -2\mathrm{i}k\cos\theta\, \mathrm{e}^{-\mathrm{i}kh\cos\theta} \int_0^{2\pi} \overline{\psi(x_1,h)}\, dx_1 = 0, \\
\langle Pf'(0), \psi \rangle &= \langle f'(0), \psi \rangle = 2\cos\theta(1 - \mathrm{i}kh\cos\theta)\, \mathrm{e}^{-\mathrm{i}kh\cos\theta} \int_0^{2\pi} \overline{\psi(x_1,h)}\, dx_1 = 0
\end{aligned}
$$

for all $\psi \in \mathcal{N}$. This implies that $f(0), f'(0) \in \mathcal{R}$ and $Pf(0) = Pf'(0) = 0$. On the other hand, simple calculations show for $v, \psi \in \mathcal{N}$ that

$$
\begin{aligned}
\langle PL'(0)v, \psi \rangle &= \langle L'(0)v, \psi \rangle \\
&= \int_{Q_h} \left[2\sin\theta \frac{\partial v}{\partial x_1}\, \overline{\psi} - 2\mathrm{i}k\cos^2\theta v \overline{\psi} \right] dx + 2\mathrm{i}\pi \sum_{n\in\mathbb{Z}: |n+\alpha|>k} \frac{(n+\alpha)\sin\theta - k}{\sqrt{(n+\alpha)^2 - k^2}}\, v_n\, \overline{\psi}_n.
\end{aligned}
\tag{4.13}
$$

It remains to justify the one-to-one property of the mapping $PL'(0)|_{\mathcal{N}}$ from $\mathcal{N}$ onto itself, which is given by the lemma below.

Lemma 4.3. *$PL'(0)$ is one-to-one on $\mathcal{N}$.*

Proof. First, we show that

$$
\langle PL'(0)v, \psi \rangle = 2 \int_{Q_\infty} \left[\sin\theta \frac{\partial v}{\partial x_1}\, \overline{\psi} - \mathrm{i}k\cos^2\theta\, v\, \overline{\psi} \right] dx
\tag{4.14}
$$

for all $v, \psi \in \mathcal{N}$, where v and ψ are extended into $Q_\infty \setminus Q_h$ by

$$
\begin{aligned}
v(x) &= \sum_{n\in\mathbb{Z}: |n+\alpha|>k} v_n\, \mathrm{e}^{-\sqrt{(n+\alpha)^2-k^2}(x_2-h) + \mathrm{i}nx_1}, \quad x_2 > h, \\
\psi(x) &= \sum_{n\in\mathbb{Z}: |n+\alpha|>k} \psi_n\, \mathrm{e}^{-\sqrt{(n+\alpha)^2-k^2}(x_2-h) + \mathrm{i}nx_1}, \quad x_2 > h.
\end{aligned}
$$

Indeed, we compute

$$
\begin{aligned}
& 2 \int_{Q_\infty \setminus Q_h} \left[\sin\theta \frac{\partial v}{\partial x_1}\, \overline{\psi} - \mathrm{i}k\cos^2\theta\, v\, \overline{\psi} \right] dx \\
&= 4\pi\mathrm{i} \int_h^\infty \sum_{n\in\mathbb{Z}:\, |n+\alpha|>k} v_n\, \overline{\psi_n}\, (\sin\theta\, n - k\cos^2\theta)\, \mathrm{e}^{-2\sqrt{(n+\alpha)^2-k^2}(x_2-h)} dx_2 \\
&= 2\pi\mathrm{i} \sum_{n\in\mathbb{Z}:\, |n+\alpha|>k} v_n\, \overline{\psi_n}\, \frac{\sin\theta\, n - k\cos^2\theta}{\sqrt{(n+\alpha)^2 - k^2}}
\end{aligned}
$$

$$= 2\pi \mathrm{i} \sum_{n\in\mathbb{Z}:\,|n+\alpha|>k} v_n\, \overline{\psi_n}\, \frac{(n+\alpha)\sin\theta - k}{\sqrt{(n+\alpha)^2-k^2}}.$$

This in combination with (4.13) yields (4.14).

Assume now that $\langle PL'(0)v,\cdot\rangle$ vanishes identically on $\mathcal{N}$ for some $v\in\mathcal{N}$. Then $\langle PL'(0)v,v\rangle = 0$ and thus

$$\sin\theta \int_{Q_\infty} \frac{\partial v}{\partial x_1}\,\overline{v}\,dx = \mathrm{i}k\cos^2\theta \int_{Q_\infty} |v|^2 dx. \tag{4.15}$$

We substitute $v(x) = \mathrm{e}^{-\mathrm{i}k\sin\theta x_1} u(x)$ again and have

$$\sin\theta \int_{Q_\infty} \left[-\mathrm{i}k\sin\theta\,|u|^2 + \frac{\partial u}{\partial x_1}\,\overline{u}\right] dx = \mathrm{i}k\cos^2\theta \int_{Q_\infty} |u|^2 dx,$$

i.e.,

$$\sin\theta\,\mathrm{Im} \int_{Q_\infty} \frac{\partial u}{\partial x_1}\,\overline{u}\,dx = k \int_{Q_\infty} |u|^2 dx.$$

Now we use the fact that u is also an eigenfunction and thus

$$\int_{Q_\infty} [|\nabla u|^2 - k^2|u|^2]\,dx = 0.$$

Hence,

$$\|\nabla u\|^2_{L^2(Q_\infty)} = k^2\|u\|^2_{L^2(Q_\infty)}\| = k\left|\sin\theta\,\mathrm{Im}\int_{Q_\infty} \frac{\partial u}{\partial x_1}\,\overline{u}\,dx\right|.$$

Supposing that ∇u does not vanish identically, we can estimate using $|\sin\theta| < 1$ that

$$\|\nabla u\|^2_{L^2(Q_\infty)} < k\|u\|_{L^2(Q_\infty)}\|\partial_1 u\|_{L^2(Q_\infty)} = \|\nabla u\|_{L^2(Q_\infty)}\|\partial_1 u\|_{L^2(Q_\infty)},$$

i.e., $\|\nabla u\|_{L^2(Q_\infty)} < \|\partial_1 u\|_{L^2(Q_\infty)}$, which is impossible. This implies that ∇u vanishes identically. Therefore, u is constant and thus zero by the boundary condition. □

Now, applying Lemma 4.2, we conclude that the unique solution $v(\epsilon)$ to (4.9) converges to v in X and the limiting function v fulfils the equations

$$L_k v = f^{(k)} \quad \text{and} \quad PL'(0)v = 0.$$

The second equation provides an additional constraint on $v\in X$ (see (4.14)), i.e.,

$$0 = \int_{Q_\infty} \left[\sin\theta \frac{\partial v}{\partial x_1}\,\overline{\psi}\,dx - \mathrm{i}k\cos^2\theta v\,\overline{\psi}\right] dx \quad \text{for all } \psi\in\mathcal{N}. \tag{4.16}$$

Setting $u = \mathrm{e}^{\mathrm{i}k\sin\theta x_1} v$ and $\phi = \mathrm{e}^{\mathrm{i}k\sin\theta x_1}\psi$, we return to quasi-periodic settings to get

$$\sin\theta \int_{Q_\infty} \frac{\partial u}{\partial x_1}\,\overline{\phi}\,dx = \mathrm{i}k \int_{Q_\infty} u\,\overline{\phi}\,dx$$

i.e.,

$$\int_{Q_\infty} \left(\sin\theta \frac{\partial u}{\partial x_1} - \mathrm{i}ku\right)\overline{\phi}\,dx = 0 \quad \text{for all } \phi\in X_j, \tag{4.17}$$

where $X_j \subset H^1_{\alpha,0}(Q_h)$ for all $h > R$ denotes the eigenspace (2.4) corresponding to the propagative number $\hat{\alpha}_j = k\sin\theta$. If we make the ansatz (4.18) for u:

$$u = u_0 + \sum_{\ell=1}^{m_j} c_\ell\,\hat{\phi}_{\ell,j} \quad \text{in } D, \quad c_\ell\in\mathbb{C}, \tag{4.18}$$

where $u_0 \in H^1_{\alpha,0}(Q_h)$ for all $h > h_0$ is a particular solution (for example, given by Lemma 4.1(i)), then it follows from (4.17) that

$$\sum_{l=1}^{m_j}\left[\sin\theta\int_{Q_\infty}\frac{\partial\hat{\phi}_{\ell,j}}{\partial x_1}\,\overline{\phi}\,dx - \mathrm{i}k\int_{Q_\infty}\hat{\phi}_{\ell,j}\,\overline{\phi}\,dx\right]c_l = \int_{Q_\infty}\left(\sin\theta\frac{\partial u_0}{\partial x_1} - \mathrm{i}ku_0\right)\overline{\phi}\,dx$$

for all $\phi \in X_j$. Therefore, the coefficients c_ℓ should fulfill the finite-dimensional algebraic system $(A-B)\,\mathcal{C} = Y$ with

$$\mathcal{C} = (c_1, c_2, \ldots, c_{m_j})^\top \in \mathbb{C}^{m_j\times 1}, \quad A = \mathrm{diag}(a_{\ell,\ell}) \in \mathbb{C}^{m_j\times m_j},$$
$$B = (b_{\ell,\ell'})_{\ell,\ell'=1}^{m_j} \in \mathbb{C}^{m_j\times m_j}, \quad Y = (y_1, y_2, \ldots, y_{m_j})^\top \in \mathbb{C}^{m_j\times 1}$$

given by

$$\begin{aligned} y_\ell &:= \int_{Q_\infty}\left(\sin\theta\frac{\partial u_0}{\partial x_1} - \mathrm{i}ku_0\right)\overline{\phi_{l,j}}\,dx, \\ b_{\ell,\ell'} &:= \mathrm{i}k\int_{Q_\infty}\hat{\phi}_{\ell',j}\,\overline{\hat{\phi}_{\ell,j}}\,dx, \\ a_{\ell,\ell} &:= \mathrm{i}/2\ \sin\theta\,\lambda_{\ell,j} \end{aligned}$$

for $\ell, \ell' = 1, 2, \ldots, m_j$. Note that in deriving the entries of A, we have used the normalizations (see (2.6))

$$\int_{Q_\infty}\frac{\partial\hat{\phi}_{\ell,j}}{\partial x_1}\,\overline{\hat{\phi}_{\ell',j}}\,dx = \mathrm{i}\ \frac{\lambda_{\ell,j}}{2}\ \delta_{\ell,\ell'}.$$

The well-posedness of scattering from unperturbed and perturbed periodic curves of Dirichlet kind is summarized as follows.

Theorem 4.4. *Let $k > 0$ be fixed and $\theta \in (-\pi/2, \pi/2)$ be an arbitrary angle. Set $\alpha = k\sin\theta$ and suppose that $\alpha + n \neq \pm k$ for any $n \in \mathbb{Z}$ (i.e., α is not a cut-off value).*

(i) *In the unperturbed case, there exists a unique solution $u_{\text{unpert}} \in H^1_{\alpha,\text{loc},0}(D)$ such that $u^{sc}_{\text{unpert}} := u_{\text{unpert}} - u^{in}$ satisfies the upward α-quasiperiodic Rayleigh expansion* (2.2) *as well as the constraint condition*

$$\int_{Q_\infty}\left(\alpha\frac{\partial u_{\text{unpert}}}{\partial x_1} - \mathrm{i}k^2 u_{\text{unpert}}\right)\overline{\hat{\phi}_{\ell,j}}\,dx = 0 \tag{4.19}$$

for all $\ell = 1, 2, \ldots, m_j$, if $\alpha = k\sin\theta = \alpha_j$ for some $j \in \{1, 2, \ldots, J\}$ is a propagative number.

(ii) *For locally perturbed periodic curves, there exists a unique solution $u \in H^1_{\alpha,\text{loc},0}(\tilde{D})$ such that $u = u^{in} + u^{sc}_{\text{unpert}} + u^{sc}_{\text{pert}}$ in Σ_R, where u^{sc}_{unpert} is given by the assertion* (i) *and $u^{sc}_{\text{pert}} \in H^1_{\text{loc}}(\Sigma_R)$ fulfills the open waveguide radiation condition of Definition* 2.5 *and the radiating part of u^{sc}_{pert} satisfies the Sommerfeld radiation conditions of Definitions* 2.7 *and* 2.8.

Proof. (i) By Lemma 4.1(i), existence of $u_{\text{unpert}} \in H_{\alpha,\text{loc},0}(D)$ follows from the Fredholm alternative and uniqueness holds if α is not a propagative number. Now suppose that $\alpha = \hat{\alpha}_j$ for some $j \in J$. Multiplying the identity (4.17) by k gives the constraint condition (4.19). Assume that there are two solutions $u^{(1)}_{\text{unpert}}$ and $u^{(2)}_{\text{unpert}}$ and set $w = u^{(1)}_{\text{unpert}} - u^{(2)}_{\text{unpert}}$. It then follows from the limiting absorption argument that the periodic function $v = \mathrm{e}^{-\mathrm{i}\alpha x_1}w \in \mathcal{N}$ fulfills the relation (4.16), i.e., $\langle PK'(0)v, \psi\rangle = 0$ for all $\psi \in \mathcal{N}$. Applying Lemma 4.3 yields $v = 0$ and thus $w = v\mathrm{e}^{\mathrm{i}\alpha x_1} = 0$.

(ii) Once the unperturbed scattering problem is uniquely solvable, the uniqueness and existence of u^{sc}_{pert} can be justified in the same way as in [19, Theorem 4.7]. □

As a corollary of Theorem 4.4(i), we obtain well-posedness of the following quasi-periodic boundary value problem:

$$\Delta v + k^2 v = 0 \quad \text{in } D, \quad v = -g \quad \text{on } \Gamma, \tag{4.20}$$

where $g = w|_\Gamma \in H^{1/2}_\alpha(\Gamma)$ with the function w of the form

$$w(x) = \sum_{n\in\mathbb{Z}:\, |\alpha_n|<k} c_n\, e^{i(\alpha+n)x_1 - i\beta_n x_2}, \quad c_n \in \mathbb{C}, \quad x \in Q_\infty.$$

Corollary 4.5. *Let $\alpha \in \mathbb{R}$ be arbitrary. The quasi-periodic boundary value problem* (4.20) *always admits a unique solution $v \in H^1_\alpha(Q_h)$ for all $h > h_0$, which fulfills the Rayleigh expansion condition* (2.2)*. In the case where $\alpha = \hat{\alpha}_j$ is a critical wavenumber, the unique solution v is additionally required to satisfy the orthogonal relation*

$$\int_{Q_\infty} \left(\alpha \frac{\partial(v+w)}{\partial x_1} - ik^2(v+w)\right)\overline{\hat{\phi}_{\ell,j}}\, dx = 0$$

for all $\ell = 1, 2, \ldots, m_j$.

Remark 4.6. It remains unclear to us whether the boundary value problem (4.20) with a general $g \in H^{1/2}_\alpha(\Gamma)$ is well-posed. For example, g is the restriction to Γ of the incoming surface wave $e^{i\alpha_n x_1 - i\beta_n x_2}$ with $|\alpha_n| > k$. In such a case, the function $f^{(k)}$ on the right-hand side of the variational formulation (4.9), which can be expressed as

$$\langle f^{(k)}, \psi\rangle := -2i\beta_n\, e^{-i\beta_n h} \int_0^{2\pi} \overline{\psi(x_1, h)} e^{inx_1}\, dx_1 \quad \text{for all } \psi \in X$$

does not belong to the range of $L^{(k)}$. In fact, $f^{(k)}$ is not orthogonal to the null space $\mathcal{N}$ of $L^{(k)}$. However, if Γ is given by a Lipschitz graph, it is well known that the boundary value problem (4.20) admits a unique solution satisfying the α-quasiperiodic upward Rayleigh expansion condition.

Remark 4.7. For plane waves, the approach of using the limiting absorption principle presented in this subsection also applies to the Neumann boundary condition as well as transmission conditions for penetrable gratings.

4.2 Methods of approximation by point sources

In this section, we provide another proof of Theorem 4.4 by approximating a plane wave with point source waves. We prove that, when the location of the source tends to infinity, the total fields excited by point sources converge to the total field of a plane wave and the limiting solution fulfills the same orthogonal constraint condition (4.19) at a critical wavenumber.

We first consider the unperturbed scattering problem.

Theorem 4.8. *Let Assumptions* 2.3 *and* 2.4 *hold and write $\hat{\theta} = (\sin\theta, -\cos\theta)^\top \in \mathbb{R}^2$ with a fixed $\theta \in (-\pi/2, \pi/2)$. Assume that*

(i) *$\alpha := k\sin\theta$ is not a cut-off value in the sense of Definition* 2.1(i);

(ii) *the function $v(\cdot;\hat{\theta}) \in H^1_{\alpha,\mathrm{loc},0}(D)$ given by Theorem* 4.4(i) *is the unique solution to the unperturbed scattering problem corresponding to the plane wave $u^{in}(x;\hat{\theta}) = e^{ikx\cdot\hat{\theta}}$.*

Let $G_t = G(\cdot; z_t)$ with $z_t := -t\hat{\theta} = (-t\sin\theta, t\cos\theta)$ be the unique total field of the unperturbed scattering problem of the point source at z_t for $t\cos\theta > 2h_0$ (*see Proposition* 2.10)*. Then we have the convergence*

$$\frac{1}{\gamma}\lim_{t\to\infty}[\sqrt{t}e^{-ikt}G_t(x)] = v(x;\hat{\theta}) \quad \text{in } H^1(Q_h), \quad \gamma := \frac{e^{i\pi/4}}{\sqrt{8k\pi}} \tag{4.21}$$

for any $h > h_0$.

Remark 4.9. The limiting function in (4.21) relies essentially on the form of the unique solution $v(\cdot;\hat{\theta})$ to the unperturbed scattering problem, if $k\sin\hat{\theta}$ happens to be a critical wavenumber. In this paper, v is derived from the LAP for approximating wave-numbers. However, the analytical continuation arguments with respect to α or the LAP for approximating the refractive index in a slab lead to a limiting solution satisfying constraint conditions different from (4.19); see [29]. If $k\sin\hat{\theta}$ is not a critical wavenumber, the limiting solutions obtained from these different approximation arguments are identical.

Proof. We carry out the proof following the lines in the proof of [29, Theorem 5.2] for inhomogeneous periodic layers. The proof will be divided into four steps.

Step 1. Reduction to the convergence proof for part of the radiating part.

As done in the proof of Theorem 3.1(ii), for each z_t we choose a t-dependent cut-off function $\chi_t \in C_0^\infty(\mathbb{R}^2)$ with $\chi_t(x) = 1$ for $|x - z_t| < \epsilon/2$ and $\chi_t(x) = 0$ for $|x - z_t| \geqslant \epsilon$, where $\epsilon > 0$ is fixed. Then $w_t := G_t - \chi_t\, \Phi(\cdot; z_t) \in H^1_{\mathrm{loc}}(D)$ coincides with G_t for $|x - z_t| \geqslant \epsilon$ and satisfies $\Delta w_t + k^2 w_t = -f_t$ in D and $w_t = 0$ on Γ, where

$$f_t := \Delta\chi_t\, \Phi(\cdot, z_t) + 2\nabla\chi_t \cdot \nabla_x \Phi(\cdot, z_t) = (\Delta + k^2)[(\chi_t - 1)\Phi(\cdot, z_t)] \in L^2(D)$$

has compact support. Let $w_{t,\mathrm{rad}}$ and $w_{t,\mathrm{prop}}$ be the radiating and propagating parts of w_t, respectively. The radiating part $w_{t,\mathrm{rad}}$ satisfies the inhomogeneous Helmholtz equation

$$(\Delta + k^2) w_{t,\mathrm{rad}} = -f_t - g_t \quad \text{in } D, \quad w_{t,\mathrm{rad}} = 0 \quad \text{on } \Gamma, \tag{4.22}$$

where

$$g_t := (\Delta + k^2) w_{t,\mathrm{prop}} = \sum_{j\in J} \sum_{l=1}^{m_j} a_{l,j}(t)\, \varphi_{l,j}$$

and

$$\varphi_{\ell,j}(x) = \begin{cases} 2\,\psi_+'(x_1)\, \dfrac{\partial \hat{\phi}_{\ell,j}(x)}{\partial x_1} + \psi_+''(x_1)\, \hat{\phi}_{\ell,j}(x), & \text{if } \lambda_{\ell,j} > 0, \\ 2\,\psi_-'(x_1)\, \dfrac{\partial \hat{\phi}_{\ell,j}(x)}{\partial x_1} + \psi_-''(x_1)\, \hat{\phi}_{\ell,j}(x), & \text{if } \lambda_{\ell,j} < 0. \end{cases} \tag{4.23}$$

Note that g_t is supported in the x_1-direction and exponentially decays in the x_2-direction and that the well-posedness of $w_{t,\mathrm{rad}}$ is a consequence of [19, Theorem 4.5]. The coefficients $a_{l,j}(t) \in \mathbb{C}$ of the propagating part $w_{t,\mathrm{prop}}$ have been computed explicitly in Theorem 3.1(ii), given by (see (3.3))

$$a_{l,j}(t) = \frac{2\pi \mathrm{i}}{|\lambda_{\ell,j}|}\, \overline{\hat{\phi}_{\ell,j}(z_t)} \quad \text{for all } j \in J, \quad l = 1, 2, \ldots, m_j.$$

This implies that

$$|a_{l,j}(t)| \leqslant c\mathrm{e}^{-\delta t}, \quad \|g_t\|_{L^\infty(D)} \leqslant c\mathrm{e}^{-\delta t} \quad \text{for all } t \geqslant 2h_0/\cos\theta, \tag{4.24}$$

with some $c > 0$ independent of t. The same estimate holds for the propagating part (see (2.7)):

$$\|w_{t,\mathrm{prop}}\|_{L^\infty(D)} \leqslant C \sum_{j\in J} \sum_{l=1}^{m_j} |a_{l,j}(t)| \leqslant C\mathrm{e}^{-\delta t} \quad \text{for all } t \geqslant 2h_0/\cos\theta. \tag{4.25}$$

The form of w_t leads to a decomposition of G_t as follows:

$$G_t = w_t + \chi_t \Phi(\cdot\,; z_t) = w_{t,\mathrm{rad}} + w_{t,\mathrm{prop}} + \chi_t \Phi(\cdot\,; z_t).$$

Hence, the radiating part $G_{t,\mathrm{rad}}$ of G_t equals $w_{t,\mathrm{rad}} + \chi_t\Phi(\cdot\,; z_t)$, while the propagating part $G_{t,\mathrm{prop}}$ coincides with $w_{t,\mathrm{prop}}$. By (4.25) and the definition of χ_t,

$$\sqrt{t}\mathrm{e}^{-\mathrm{i}kt} \|w_{t,\mathrm{prop}}(\cdot) + \chi_t\Phi(\cdot\,; z_t)\|_{H^1(Q_h)} \to 0 \quad \text{as } t \to \infty$$

for any fixed $h > h_0$. Therefore, it remains to consider the convergence of $w_{t,\mathrm{rad}}$ as $t \to \infty$.

Step 2. Floquet-Bloch transform $w_{t,\mathrm{rad}}$ to a family of quasi-periodic problems.

For $g \in C_0^\infty(\mathbb{R})$, the Floquet-Bloch transform F is defined by

$$(Fg)(x_1, \alpha) := \sum_{n\in\mathbb{Z}} g(x_1 + 2\pi n)\, \mathrm{e}^{-\mathrm{i}2\pi n\alpha}, \quad x_1 \in \mathbb{R}, \quad \alpha \in [-1/2, 1/2].$$

The transform F extends to a unitary operator from $L^2(\mathbb{R})$ to $L^2((-1/2,1/2)\times(0,2\pi))$. If g depends on two variables x_1 and x_2, then the symbol F means the Floquet-Bloch transform with respect to x_1. The inverse Floquet-Bloch transform is defined by $g=\int_{-1/2}^{1/2}(Fg)(\cdot,\alpha)d\alpha$. Taking the Floquet-Bloch transform on both sides of the equation (4.22) yields

$$(\Delta+k^2)w_{t,\alpha}=-(Ff_t)(\cdot,\alpha)-(Fg_t)(\cdot,\alpha)\quad\text{in } Q_\infty,\quad w_{t,\alpha}=0\quad\text{on }\Gamma,\tag{4.26}$$

where $w_{t,\alpha}=(Fw_{t,\mathrm{rad}})(\cdot,\alpha)\in L^2((-1/2,1/2),H^1_{\alpha,0}(Q_\infty))$ (see [34]). Here, $H^1_{\alpha,0}(Q_\infty)$ is defined as the restriction of $H^1_{\alpha,\mathrm{loc},0}(D)$ to Q^∞. The above equation is understood in the variational sense that

$$\int_{Q_\infty}[\nabla w_{t,\alpha}\cdot\overline{\nabla\psi}-k^2w_{t,\alpha}\overline{\psi}]\,dx=\int_{Q_\infty}[(Ff_t)(x,\alpha)+(Fg_t)(x,\alpha)]\overline{\psi}\,dx\tag{4.27}$$

for all $\psi\in H^1_{\alpha,0}(Q_\infty)$. We know from Theorem 3.1(ii) and [19, Theorem 3.5] that for each $t>2h_0/\cos\theta$, this variational formulation is solvable for all $\alpha\in\mathbb{R}$ under the generalized Rayleigh expansion condition (2.8) of $w_{t,\alpha}$, due to the orthogonality of the right-hand side of (4.26) with the null space X_α by the choice of $a_{l,j}(t)$. Let $v_{t,\alpha}\in H^1_\alpha(U_{h_0})$ be the unique solution of the equation

$$(\Delta+k^2)v_{t,\alpha}=-(Ff_t)(\cdot,\alpha)-(Fg_t)(\cdot,\alpha)\quad\text{in } U_{h_0},\quad v_{t,\alpha}=0\quad\text{on }\Gamma_{h_0},$$

together with the generalized Rayleigh expansion condition (2.8) in $x_2>h_0$. It is easy to observe that

$$\int_{U_{h_0}}[\nabla(w_{t,\alpha}-v_{t,\alpha})\cdot\overline{\nabla\psi}-k^2(w_{t,\alpha}-v_{t,\alpha})\overline{\psi}]\,dx=\int_{\Gamma_{h_0}}(\tilde{T}_kw_{t,\alpha})\,\overline{\psi}\,ds\tag{4.28}$$

for all $\psi\in H^1_{\alpha,0}(Q_\infty)$, where $\tilde{T}_k$ denotes the α-quasiperiodic Dirichlet-to-Neumann map defined by (4.3). Simple calculations using (4.27) and (4.28) show that the variational equation for $w_{t,\alpha}$ can be equivalently written as

$$\begin{aligned}(\mathbb{L}_\alpha w_{t,\alpha},\psi)_{H^1(Q_{h_0})}&:=\int_{Q_{h_0}}[\nabla w_{t,\alpha}\cdot\overline{\nabla\psi}-k^2w_{t,\alpha}\overline{\psi}]\,dx-\int_{\Gamma_{h_0}}\tilde{T}_kw_{t,\alpha}\overline{\psi}\,ds\\&=\int_{Q_{h_0}}(Fg_t)(x,\alpha)\overline{\psi}\,dx+\int_{\Gamma_{h_0}}\frac{\partial v_{t,\alpha}}{\partial\nu}\overline{\psi}\,ds\end{aligned}\tag{4.29}$$

for all $\psi\in H^1_{\alpha,0}(Q_{h_0})$, which is defined as the restriction of $H^1_{\alpha,0}(Q_\infty)$ to Q_{h_0}. Note that by the choice of the cut-off function χ_t with $t\cos\theta>2h_0$, the function f_t and thus Ff_t vanish in Q_{h_0}. Moreover, we recall from [29, Lemma 5.3] that the normal derivative $\partial_\nu v_{t,\alpha}(x_1,h_0)$ can be computed explicitly as

$$\begin{aligned}\frac{\partial v_{t,\alpha}(x_1,h_0)}{\partial x_2}&=\frac{1}{2\pi}\sum_{l\in\mathbb{Z}}\mathrm{e}^{\mathrm{i}\sqrt{k^2-(l+\alpha)^2}(t\cos\theta-h_0)}\,\mathrm{e}^{\mathrm{i}(l+\alpha)(x_1+t\sin\theta)}\\&\quad+\frac{1}{\sqrt{2\pi}}\sum_{l\in\mathbb{Z}}\int_{h_0}^\infty(Fg_t)_l(y_2,\alpha)\mathrm{e}^{\mathrm{i}\sqrt{k^2-(l+\alpha)^2}(y_2-h_0)}\,dy_2\,\mathrm{e}^{\mathrm{i}(l+\alpha)x_1},\end{aligned}$$

where $(Fg_t)_l(y_2,\alpha)$ are the Fourier coefficients of $(Fg_t)_l(\cdot,y_2,\alpha)$, defined by

$$(Fg_t)_l(y_2,\alpha)=\frac{1}{\sqrt{2\pi}}\int_0^{2\pi}(Fg_t)_l(y_1,y_2,\alpha)\mathrm{e}^{-\mathrm{i}(l+\alpha)y_1}dy_1.$$

Hence, we get a family of quasi-periodic operator equations

$$\mathbb{L}_\alpha w_{t,\alpha}=r_{t,\alpha}\quad\text{in } H^1_{\alpha,0}(Q_{h_0}),$$

where $r_{t,\alpha}\in H^1_{\alpha,0}(Q_{h_0})$ is defined by

$$(r_{t,\alpha},\psi)_{H^1(Q_{h_0})}:=\int_{Q_{h_0}}(Fg_t)(x,\alpha)\overline{\psi}\,dx+\frac{1}{\sqrt{2\pi}}\sum_{l\in\mathbb{Z}}\mathrm{e}^{\mathrm{i}\sqrt{k^2-(l+\alpha)^2}(t\cos\theta-h_0)+\mathrm{i}(l+\alpha)t\sin\theta}\,\overline{\psi_l(h_0)}$$

$$+\sum_{l\in\mathbb{Z}}\overline{\psi_l(h_0)}\int_{h_0}^{\infty}(Fg_t)_l(y_2,\alpha)\mathrm{e}^{\mathrm{i}\sqrt{k^2-(l+\alpha)^2}(y_2-h_0)}\,dy_2.$$

By the definition of g_t, F and the estimate of $a_{l,j}(t)$ (see (4.24)), it follows that

$$|(Fg_t)(x,\alpha)|+|\partial_\alpha(Fg_t)(x,\alpha)|\leqslant c\,\mathrm{e}^{-\delta(t+|x_2|)}\quad \text{in } x_2>h_0 \tag{4.30}$$

for all $t>0$ and $\alpha\in[-1/2,1/2]$.

Step 3. Prove the convergence of the dominant part of G_t as t tends to infinity.

Let $k=\hat{l}+\kappa$ with $\hat{l}\in\mathbb{Z}$ and $\kappa\in(-1/2,1/2]$. Then $\pm\kappa$ are cut-off values, and they can decompose the interval $[-1/2,1/2]$ into at most three open intervals $I_1\cup I_2\cup I_3$ such that their interiors are disjoint. Note that some of these intervals can degenerate into points, and the cut-off values are contained in the boundary points of I_m, $m=1,2,3$. Write $k\sin\theta=\tilde{l}+\tilde{\alpha}$ with $\tilde{l}\in\mathbb{Z}$ and $\tilde{\alpha}\in(-1/2,1/2]$. Since $k\sin\theta$ is not a cut-off value, we suppose without loss of generality that $\tilde{\alpha}\in I_{\tilde{m}}$ is an interior point for some $\tilde{m}\in\{1,2,3\}$. Next, we find a subset $\mathcal{L}\subset\{-\tilde{l},\ldots,\tilde{l}\}\subset\mathbb{Z}$ such that

$$|\alpha+l|<k\quad\text{for all }\alpha\in I_{\tilde{m}},\quad l\in\mathcal{L},$$
$$|\alpha+l|>k\quad\text{for all }\alpha\in I_{\tilde{m}},\quad l\in\mathbb{Z}\backslash\mathcal{L}.$$

To find the dominant part of G_t, we decompose the Floquet-Bloch transform of the fundamental solution $\Phi_t(x)=\Phi(x;z_t)$ with $t\cos\theta>2h_0$ and $x\in Q_{h_0}$ into

$$\Phi_{t,\alpha}(x)=(F\Phi_t)(x,\alpha)=\frac{\mathrm{i}}{4\pi}\sum_{l\in\mathbb{Z}}\frac{\mathrm{e}^{\mathrm{i}(\alpha+l)(x_1+t\sin\theta)+\mathrm{i}\sqrt{k^2-(l+\alpha)^2}(t\cos\theta-x_2)}}{\sqrt{k^2-(l+\alpha)^2}}=\Phi_{t,\alpha}^{(1)}+\Phi_{t,\alpha}^{(2)},$$

where $\Phi_{t,\alpha}^{(2)}:=\Phi_{t,\alpha}-\Phi_{t,\alpha}^{(1)}$ with

$$\Phi_{t,\alpha}^{(1)}(x):=\frac{\mathrm{i}}{4\pi}\sum_{l\in\mathcal{L}}\frac{\mathrm{e}^{\mathrm{i}t[(\alpha+l)\sin\theta+\sqrt{k^2-(l+\alpha)^2}\cos\theta]}}{\sqrt{k^2-(l+\alpha)^2}}\,v_{l,\alpha}^{in}(x),\quad v_{l,\alpha}^{in}(x):=\mathrm{e}^{\mathrm{i}((\alpha+l)x_1-\sqrt{k^2-(l+\alpha)^2}x_2)}.$$

Note that the Floquet-Bloch transform of $\Phi(x;y)$ is nothing else but the quasi-periodic fundamental solution to the Helmholtz equation. For $l\in\mathcal{L}$, $v_{l,\alpha}^{in}$ is an incident plane wave with the unit direction $(\alpha+l,-\sqrt{k^2-(l+\alpha)^2})/k$. We denote by $v_{l,\alpha}$ the unique α-quasiperiodic total field generated by $v_{l,\alpha}^{in}$ (see Theorem 4.4(i)). In particular, $v_{\tilde{l},\tilde{\alpha}}=v(\cdot;\hat{\theta})$ when $l=\tilde{l}$ and $\alpha=\tilde{\alpha}$. We remark that $v_{l,\alpha}$ is required to satisfy the orthogonal condition (4.19), if α is a critical wavenumber. By linear superposition, the total field excited by $\Phi_{t,\alpha}^{(1)}$, which we denote by $w_{t,\alpha}^{(1)}$, can be represented as

$$w_{t,\alpha}^{(1)}(x)=\frac{\mathrm{i}}{4\pi}\sum_{l\in\mathcal{L}\backslash\{\tilde{l}\}}\frac{\mathrm{e}^{\mathrm{i}t[(\alpha+l)\sin\theta+\sqrt{k^2-(l+\alpha)^2}\cos\theta]}}{\sqrt{k^2-(l+\alpha)^2}}\,v_{l,\alpha}(x)+W_{t,\alpha}(x),$$
$$W_{t,\alpha}(x):=\frac{\mathrm{i}}{4\pi}\frac{\mathrm{e}^{\mathrm{i}t[(\alpha+\tilde{l})\sin\theta+\sqrt{k^2-(\tilde{l}+\alpha)^2}\cos\theta]}}{\sqrt{k^2-(\tilde{l}+\alpha)^2}}\,v_{\tilde{l},\alpha}(x).$$

It was proved in [29] that the inverse Floquet-Bloch transform of $w_{t,\alpha}^{(1)}$ (more precisely, $W_{t,\alpha}$) constitutes the dominant part of G_t as $t\to\infty$. In fact, using stationary arguments, one deduces that (see, e.g., [29, Section 5])

$$\int_{I_{\tilde{m}}}W_{t,\alpha}(x)\,d\alpha=\gamma\frac{\mathrm{e}^{\mathrm{i}tk}}{\sqrt{t}}v(x;\hat{\theta})+o(t^{-1/2}),$$

and using partial integration yields (see Appendix A.2)

$$\int_{I_{\tilde{m}}}[w_{t,\alpha}^{(1)}(x)-W_{t,\alpha}(x)]\,d\alpha=O(t^{-1}),\quad \int_{[-1/2,1/2]\backslash I_{\tilde{m}}}w_{t,\alpha}^{(1)}(x)\,d\alpha=O(t^{-1}), \tag{4.31}$$

as $t \to \infty$. This proves

$$\lim_{t\to\infty}\left[\sqrt{t}\mathrm{e}^{-\mathrm{i}kt}\int_{-1/2}^{1/2} w_{t,\alpha}^{(1)}(x)\,d\alpha\right] = v(x;\hat{\theta}) \quad \text{in } H^1(Q_h), \quad h > h_0.$$

Step 4. Show the decay of the remaining part.

To prove (4.21), we only need to show for $w_{t,\alpha}^{(2)} := w_{t,\alpha} - w_{t,\alpha}^{(1)}$ that

$$\lim_{t\to\infty}\left[\sqrt{t}\mathrm{e}^{-\mathrm{i}kt}\int_{-1/2}^{1/2} w_{t,\alpha}^{(2)}(x)\,d\alpha\right] = 0 \quad \text{in } H^1(Q_h), \quad h > h_0. \tag{4.32}$$

Recalling the variational formulation for the total field $w_{t,\alpha}^{(1)}$ (see (4.29) for the definition of $\mathbb{L}_\alpha$), i.e.,

$$(\mathbb{L}_\alpha w_{t,\alpha}^{(1)}, \psi)_{H^1(Q_{h_0})} := \frac{1}{\sqrt{2\pi}}\sum_{l\in\mathcal{L}} \mathrm{e}^{\mathrm{i}\sqrt{k^2-(l+\alpha)^2}(t\cos\theta - h_0)+\mathrm{i}(l+\alpha)t\sin\theta}\,\overline{\psi_l(h_0)}$$

for all $\psi \in H^1_{\alpha,0}(Q_{h_0})$, we find that $w_{t,\alpha}^{(2)}$ are solutions of $\mathbb{L}_\alpha w_{t,\alpha}^{(2)} = \sum_{j=1}^3 r_{t,\alpha}^{(j)}$, where

$$\begin{aligned}
(r_{t,\alpha}^{(1)}, \psi)_{H^1(Q_{h_0})} &:= \int_{Q_{h_0}} (Fg_t)(x,\alpha)\overline{\psi}\,dx,\\
(r_{t,\alpha}^{(2)}, \psi)_{H^1(Q_{h_0})} &:= \frac{1}{\sqrt{2\pi}}\sum_{l\notin\mathcal{L}} \mathrm{e}^{-\sqrt{(l+\alpha)^2-k^2}(t\cos\theta-h_0)+\mathrm{i}(l+\alpha)t\sin\theta}\,\overline{\psi_l(h_0)},\\
(r_{t,\alpha}^{(3)}, \psi)_{H^1(Q_{h_0})} &:= \sum_{l\in\mathbb{Z}} \overline{\psi_l(h_0)}\int_{h_0}^{\infty} (Fg_t)_l(y_2,\alpha)\mathrm{e}^{\mathrm{i}\sqrt{k^2-(l+\alpha)^2}(y_2-h_0)}\,dy_2.
\end{aligned}$$

Since every cut-off value is assumed to be no critical wavenumber, one may divide the interval $[-1/2, 1/2]$ into the union $\Lambda_1 \cup \Lambda_2$ of two types of closed sub-intervals with non-intersecting interiors, where Λ_1 does not contain any critical wavenumber and Λ_1 contains no cut-values. In Λ_1, one can deduce from the decaying of Fg_t (see (4.30)) and partial integration that (see [29] for the details)

$$\int_{\Lambda_1} \|w_{t,\alpha}^{(2)}\|_{H^1(Q_{h_0})}\,d\alpha \leqslant c\left(\sum_{l\notin\mathcal{L}}\int_{\Lambda_1} \mathrm{e}^{-t\sqrt{(l+\alpha)^2-k^2}\cos\theta}d\alpha\right)^{1/2} \leqslant c\,t^{-1}.$$

Since $r_{t,\alpha}^{(j)}$ are differentiable with respect to $\alpha \in \Lambda_2$ for $j = 1, 2, 3$, the integral over Λ_2 can be estimated by applying Lemma 4.2 to get (see also [29])

$$\int_{\Lambda_2} \|w_{t,\alpha}^{(2)}\|_{H^1(Q_{h_0})}\,d\alpha \leqslant c\,t\mathrm{e}^{-\delta t} \quad \text{for all } t\cos\theta \geqslant 2h_0.$$

Combining the previous two estimates yields (4.32) and thus finishes the proof of Theorem 4.8. □

Now we study the limit of Green's function to the locally perturbed scattering problem when the source position tends to infinity.

Theorem 4.10. *Let Assumptions* 2.3, 2.4 *and* 2.6 *hold and write* $\hat{\theta} = (\sin\theta, -\cos\theta)^\top \in \mathbb{R}^2$ *with* $\theta \in (-\pi/2, \pi/2)$. *Assume that* $\alpha := k\sin\theta$ *is not a cut-off value in the sense of Definition* 2.1(i). *Let* $u_t = u(\cdot; z_t)$ *with* $z_t := -t\hat{\theta}$ *be the unique total field of the perturbed scattering problem of the point source at* z_t *for* $t\cos\theta > 2h_0$ (*see Proposition* 2.10), *which satisfies the open waveguide radiation condition of Definition* 2.5. *Then we have the convergence*

$$\frac{1}{\gamma}\lim_{t\to\infty}[\sqrt{t}\mathrm{e}^{-\mathrm{i}kt}u_t(x)] = w(x;\hat{\theta}) \quad \text{in } H^1(\tilde{D}_R), \quad \gamma := \frac{\mathrm{e}^{\mathrm{i}\pi/4}}{\sqrt{8k\pi}} \tag{4.33}$$

for any $R > \pi$, *where* $w \in H^1_{\mathrm{loc},0}(\tilde{D})$ *with the decomposition* $w = u^{in} + u^{sc}_{\mathrm{unpert}} + u^{sc}_{\mathrm{pert}}$ *in* Σ_R *denotes the unique solution to the perturbed scattering problem corresponding to the plane wave* $u^{in}(x;\hat{\theta}) = \mathrm{e}^{\mathrm{i}kx\cdot\hat{\theta}}$ *specified in Theorem* 4.4(ii).

Remark 4.11. In the absence of the defect, u_t coincides with Green's function G_t to the scattering problem in perfectly periodic structures, and $w = u^{in} + u^{sc}_{\rm pert}$ coincides with the limiting function v specified in Theorem 4.8.

Proof. By the proof of Proposition 2.10 (see [19]), the total field u_t can be decomposed into $u_t = G_t + u^{sc}_{t,\rm pert}$ in Σ_R, where G_t is Green's function to the unperturbed scattering problem and $u^{sc}_{t,\rm pert}$ corresponding to the defect satisfies the open waveguide radiation condition. It follows from Theorem 4.8 that

$$\frac{1}{\gamma}\lim_{t\to\infty}[\sqrt{t}\mathrm{e}^{-\mathrm{i}kt}\, G_t] = u^{in} + u^{sc}_{\rm unpert} =: w^{in} \quad \text{in } H^1(Q_h) \tag{4.34}$$

for all $h > h_0$. To prove the convergence (4.33), we define

$$v_t := 1/\gamma\sqrt{t}\mathrm{e}^{-\mathrm{i}kt}u_t - w \quad \text{in } \tilde{D},$$

which can be considered as the total field corresponding to $v^{in}_t := 1/\gamma\sqrt{t}\mathrm{e}^{-\mathrm{i}kt}G_t - w^{in}$. It is obvious that $v_t - v^{in}_t$ fulfills the open waveguide radiation condition.

Choose $R > \pi$ such that there is no bound state to the Helmholtz equation over the domain Σ_R and that k^2 is not the Dirichlet eigenvalue of the negative Laplacian operator over $\tilde{D}_R$. We suppose without loss of generality that the domain $\tilde{D}_R$ is Lipschitz. Otherwise, one can slightly change the shape of C_R to get a Lipschitz domain. On the artificial curve C_R, one may construct the Dirichlet-to-Neumann operator Λ that is equivalent to the open waveguide radiation condition. The operator $\Lambda : H^{1/2}_0(C_R) \to H^{-1/2}(C_R)$ has been proved to be bounded and $-\Lambda$ can be decomposed into the sum of a coercive operator and a compact operator; see [19, Lemma 3.9]. With the aid of this DtN operator, one deduces the following boundary value problem for $v_t \in \{u \in H^1(\tilde{D}_R) : u = 0 \text{ on } \partial\tilde{D}_R \cap \tilde{\Gamma}\}$:

$$(\text{BVP}) : \begin{cases} (\Delta + k^2)v_t = 0 & \text{in } \tilde{D}_R, \\ \partial_\nu v_t = \Lambda\, v_t + (\partial_\nu v^{in}_t - \Lambda v^{in}_t) & \text{on } C_R, \end{cases}$$

where ν denotes the normal direction at C_R pointing into Σ_R. The well-posedness of the above boundary value problem follows from mapping properties of the DtN operator together with the assumption that there is no bound state over $\tilde{D}$ (see [19, Theorem 2.9(ii)]). Hence, using (4.34) and the boundedness of Λ, we arrive at

$$\|v_t\|_{H^1(\tilde{D}_R)} \leqslant c\,\|\partial_\nu v^{in}_t - \Lambda v^{in}_t\|_{H^{-1/2}(C_R)} \leqslant c\,\|v^{in}_t\|_{H^1(D_R)} \to 0,$$

as $t \to \infty$, which proves (4.34). □

5 Uniqueness results to inverse scattering

This section is concerned with uniqueness in determining the shape and location of the defect $\tilde{\Gamma}\backslash\Gamma$ from near/far-field data incited by plane or point source waves at a fixed wavenumber. We suppose that the unperturbed grating profile $\Gamma = \partial D$ is *a priori* known with the period 2π. Although we only discuss a localized defect appearing on the scattering interface, the uniqueness results of this section carry over to a perturbation caused by a bounded Dirichlet obstacle embedded inside D.

5.1 Uniqueness with infinitely many point source waves

Let $G(x;y)$ $(x \neq y)$ be the total field (Green's function) to the perturbed scattering problem with $u^{in} = \Phi(x;y)$; see Proposition 2.10.

Theorem 5.1. *Let $\tilde{\Gamma}$ be a local perturbation of the periodic curve Γ and suppose that* $\max\{x_2 : x \in \Gamma \cup \tilde{\Gamma}\} < h$ *for some $h \in \mathbb{R}$. Then $\tilde{\Gamma}$ can be uniquely determined by the near-field measurement data $\{G(x_1, h; y_j) : x_1 \in (a, b), y_j \in U_h, j = 1, 2, \ldots\}$, incited by infinitely many point source waves.*

Proof. Suppose that there are two local perturbations $\tilde{\Gamma}_1$ and $\tilde{\Gamma}_2$ which both lie below the line $x_2 = h$. Denote by $G_\ell(x; y_j)$ ($\ell = 1, 2$) the total fields corresponding to $\tilde{\Gamma}_\ell$ and the incoming source wave $\Phi(x; y_j)$, and let $\tilde{D}_j$ be the domain above $\tilde{\Gamma}_j$. Assuming

$$G_1(x_1, h; y_j) = G_2(x_1, h; y_j) \quad \text{for all } x_1 \in (a, b), \quad j \in \mathbb{N}, \tag{5.1}$$

we need to prove $\tilde{\Gamma}_1 = \tilde{\Gamma}_2$. By the analyticity of $G_\ell(\cdot; y_j)$ on $x_2 = h$, we deduce from (5.1) that $G_1(x; y_j) = G_2(x; y_j)$ on $x_2 = h$ for all $j \in \mathbb{N}$. With the open waveguide radiation condition of Definition 2.5, there exists a unique solution to the Dirichlet boundary value problem of the Helmholtz equation in the upper half-plane $x_2 > h$; we refer to Lemma 5.2 and Remark 5.3 below for the proof. Hence, for fixed $j \in \mathbb{N}$, the functions $G_1(\cdot; y_j)$ and $G_2(\cdot; y_j)$ must coincide in $x_2 > h$ and by unique continuation also coincide in $\Omega \backslash \{y_j\}$, where Ω denotes the unbounded component of $\tilde{D}_1 \cap \tilde{D}_2$. Consequently, the total fields G_ℓ ($\ell = 1, 2$) vanish on $\partial\Omega$.

If $\tilde{\Gamma}_1 \neq \tilde{\Gamma}_2$, we derive a contradiction as follows. Switching the notation if necessary, we can assume that (see Figure 2)

$$D^* = [(\tilde{D}_1 \cup \tilde{D}_2) \setminus \Omega\,] \cap \tilde{D}_1 \neq \emptyset.$$

It is obvious that $\partial D^* \subset \tilde{\Gamma}_1 \cup (\tilde{\Gamma}_2 \cap \partial\Omega)$. Noting that $y_j \notin D^*$ and $G_1 = G_2 = 0$ on $\tilde{\Gamma}_2 \cap \partial\Omega$, we obtain

$$(\Delta + k^2) G_1(x; y_j) = 0 \quad \text{in } D^*, \quad G_1(\cdot; y_j) = 0 \quad \text{on } \partial D^*$$

for all $j \in \mathbb{N}$. This implies that there exist infinitely many Dirichlet eigenfunctions $G_1(\,\cdot\,; y_j)$ for the negative Laplacian operator over the bounded domain D^* with the eigenvalue k^2. Now, it suffices to show the linear independence of $G_1(\,\cdot\,; y_j)$, which together with the finite-dimensional Dirichlet eigenspace (irrespective of boundary regularities) could lead to a contradiction. Assume that

$$\sum_{j=1}^{M} \lambda_j\, G_1(x; y_j) = 0, \quad x \in D^*$$

for some constants $\lambda_j \in \mathbb{C}$, where $y_j \in U_h$ for $j = 1, 2, \ldots, M$ are distinct point sources. Since $D^* \subset \tilde{D}_1$, applying the unique continuation yields

$$\sum_{j=1}^{J} \lambda_j\, G_1(x; y_j) = 0 \quad \text{for all } x \in \tilde{D}_1 \backslash \{y_j\}_{j=1}^{M}. \tag{5.2}$$

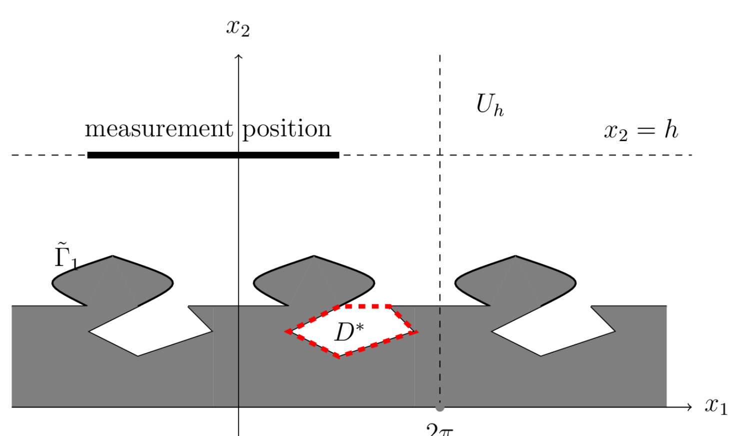

Figure 2 (Color online) Illustration of the gap domain $D^* \subset \tilde{D}_1 \backslash \overline{\tilde{D}_2}$ between two local perturbations. Here, $\tilde{\Gamma}_1 = \Gamma$ is identical with the unperturbed grating curve

Now, letting $x \to y_j$ in (5.2) and using the boundedness of $G_1(y_j; y_\ell)$ for $\ell \neq j$, we obtain $\lambda_j = 0$. The arbitrariness of $j = 1, 2, \ldots, J$ implies that the total fields corresponding to different point sources are indeed linearly independent. This finishes the proof of $\tilde{\Gamma}_1 = \tilde{\Gamma}_2$. □

In the proof of Theorem 5.1, we need the following uniqueness result to the homogeneous Dirichlet boundary value problem of the Helmholtz equation in the half plane $x_2 > h$. Let $\sigma > 0$ be the parameter of the cut-off function given in Definition 2.5.

Lemma 5.2. *Let $u \in H^1_{\mathrm{loc}}(U_h)$ be a solution of the Helmholtz equation $\Delta u + k^2 u = 0$ in U_h such that $u = 0$ on $x_2 = h$. Furthermore, let u be of the form $u = u_{\mathrm{rad}} + u_{\mathrm{prop}}$ where $u_{\mathrm{rad}} \in H^1(U_h \setminus U_H)$ for all $H > h$ satisfies the generalized angular spectrum radiation condition* (2.8) *and $u_{\mathrm{prop}} = \sum_{j\in J} u_j$ where $u_j = \sum_{\ell=1}^{m_j} a^{\pm}_{\ell,j} \hat{\phi}_{\ell,j}$ for $\pm x_1 \geqslant \sigma$. Then u vanishes in U_h.*

Proof. Let $I \subset \mathbb{R}$ be any bounded interval. Set $I_n = \{t + 2\pi n : t \in I\}$ for $n \in \mathbb{Z}$. Then, for sufficiently large $n > 0$,

$$\sum_{j\in J} \mathrm{e}^{2\pi n\alpha_j \mathrm{i}} \int_I u_j(x_1, h)\, dx_1 = \sum_{j\in J} \int_I u_j(x_1 + 2\pi n, h)\, dx_1 = \int_{I_n} u_{\mathrm{prop}}(x_1, h)\, dx_1 = -\int_{I_n} u_{\mathrm{rad}}(x_1, h)\, dx_1 \to 0$$

as $n \to \infty$. Here, we have used the quasiperiodicity of $\hat{\phi}_{l,j}$ and the definition of u_{prop}. Set $b_j := \int_I u_j(x_1, h)\, dx_1$ for abbreviation. Then $\sum_{j\in J} b_j\, \mathrm{e}^{2\pi n\alpha_j \mathrm{i}}$ tends to zero as $n \to \infty$. By induction with respect to $|J|$ (number of elements), one proves that all b_j vanish. Indeed, this is obviously true for $|J| = 1$. Let it hold for $|J| = p$ and let $\hat{J} = J \cup \{\alpha_\ell\}$ with $|J| = p$ and $\alpha_\ell \notin \{\alpha_j : j \in J\}$ and

$$\sum_{j\in J} b_j\, \mathrm{e}^{2\pi n\alpha_j \mathrm{i}} + b_\ell\, \mathrm{e}^{2\pi n\alpha_\ell \mathrm{i}} \to 0, \quad n \to \infty. \tag{5.3}$$

Multiplication of this formula by $\mathrm{e}^{2\pi\alpha_\ell \mathrm{i}}$ yields the first of the following formula:

$$\sum_{j\in J} b_j\, \mathrm{e}^{2\pi n\alpha_j \mathrm{i}}\, \mathrm{e}^{2\pi\alpha_\ell \mathrm{i}} + b_\ell\, \mathrm{e}^{2\pi(n+1)\alpha_\ell \mathrm{i}} \to 0, \quad n \to \infty,$$
$$\sum_{j\in J} b_j\, \mathrm{e}^{2\pi(n+1)\alpha_j \mathrm{i}} + b_\ell\, \mathrm{e}^{2\pi(n+1)\alpha_\ell \mathrm{i}} \to 0, \quad n \to \infty.$$

Note that the second one is (5.3) for $n + 1$ instead of n. Subtraction of the previous two relations yields

$$\sum_{j\in J} b_j\, \mathrm{e}^{2\pi n\alpha_j \mathrm{i}}\, [\mathrm{e}^{2\pi\alpha_\ell \mathrm{i}} - \mathrm{e}^{2\pi\alpha_j \mathrm{i}}] \to 0, \quad n \to \infty.$$

Now we apply the assumption of induction to $\tilde{b}_j = [\mathrm{e}^{2\pi\alpha_\ell \mathrm{i}} - \mathrm{e}^{2\pi\alpha_j \mathrm{i}}] b_j$ which gives $b_j = 0$ for all $j \in J$ and thus also $b_\ell = 0$.

Therefore, $\int_I u_j(x_1, h)\, dx_1 = 0$ for all $j \in J$ and all intervals I. This proves that u_{prop} vanishes for $x_1 > \sigma$. The same argument for $n \to -\infty$ yields that u_{prop} vanishes for $x_1 < -\sigma$. Therefore, u itself satisfies the generalized angular spectrum radiation condition and vanishes for $x_2 = h$. This yields $u = 0$ by arguing the same as in the proof of the last assertion of [28, Appendix, Lemma 7.1]. □

Remark 5.3. If u vanishes on a locally perturbed periodic curve $\tilde{\Gamma}$ instead of the straight line $x_2 = h$, it follows from [19, Theorem 2.8] that we still have $u_{\mathrm{prop}} = 0$. However, $u = u_{\mathrm{rad}} \in H^1_0(\tilde{D})$ becomes a bound state over the domain $\tilde{D}$; see [19, Theorem 2.9]. The above lemma presents a simple proof for the vanishing of the propagating part when $\tilde{\Gamma} = \partial\tilde{D}$ is a straight line.

The proof of Theorem 5.1 does not carry over to the Neumann boundary condition, because the property of a finite-dimensional eigenspace in the Neumann case requires boundary smoothness assumptions which usually cannot be fulfilled. Below, we present another proof relying on the blowing up argument of [22, 30], which applies to the Neumann and impedance boundary conditions, provided that the well-posedness of forward scattering problems can be justified.

Theorem 5.4. *Under the assumption of Theorem* 5.1*, the locally perturbed defect* $\tilde{\Gamma}$ *can be uniquely determined by the near-field measurement data*

$$\{G(x_1, h; y_1, h) : x_1 \in (a, b), y_1 \in (c, d)\}.$$

Here, $(a, b), (c, d) \subset \mathbb{R}$ *are finite intervals without intersections.*

Proof. We keep the notations in the proof of Theorem 5.1 to obtain

$$G_1(x; y_1, h) = G_2(x; y_1, h) \quad \text{for all } x \in \Omega, \quad y_1 \in (c, d). \tag{5.4}$$

Using the symmetry of $G_\ell(x; y)$ (see Theorem 3.1), we deduce from (5.4) and the unique continuation that

$$G_1^{sc}(x; y) = G_2^{sc}(x; y) \quad \text{for all } x, y \in \Omega, \quad x \neq y. \tag{5.5}$$

If $\tilde{\Gamma}_1 \neq \tilde{\Gamma}_2$, without loss of generality, we can choose a point y^* and a sub-boundary $\mathcal{S}$ of $\tilde{\Gamma}_1$ such that $y^* \in \mathcal{S} \subset (\partial\Omega \cap \tilde{\Gamma}_1) \cap \tilde{D}_2$ and

$$y^{(m)} := y^* + \nu(y^*)/m \in \Omega \cap \tilde{D}_2$$

for all $m \geqslant M$ with some $M \in \mathbb{N}$, where $\nu(y^*) \in \mathbb{S} := \{x \in \mathbb{R}^2 : |x| = 1\}$ denotes the unit normal direction at $y^* \in \tilde{\Gamma}_1$ pointing into $\tilde{D}_1$. Since y^* is bounded away from $\tilde{\Gamma}_2$, well-posdness of the forward scattering problem for $\tilde{\Gamma}_2$ implies that

$$\lim_{m\to\infty} \|G_2^{sc}(x; y^{(m)})\|_{H^{1/2}(\mathcal{S})} = \|G_2^{sc}(x; y^*)\|_{H^{1/2}(\mathcal{S})} < \infty. \tag{5.6}$$

On the other hand, it follows from the Dirichlet boundary condition $G_1^{sc}(x; y^*) = -\Phi(x; y^*)$ on $\mathcal{S}$ that

$$\lim_{m\to\infty} \|G_1^{sc}(x; y^{(m)})\|_{H^{1/2}(\mathcal{S})} = \|\Phi(x; y^*)\|_{H^{1/2}(\mathcal{S})} = \infty, \tag{5.7}$$

due to the singular behaviour $\Phi(x; y^*) = O(\ln|x - y^*|)$ as $|x - y^*| \to 0$. The previous two relations (5.6) and (5.7) obviously contradict the identity (5.5). This contradiction proves that $\tilde{\Gamma}_1 = \tilde{\Gamma}_2$. □

5.2 Uniqueness with infinitely many plane waves

Let u^{in} be a plane wave with a fixed wavenumber $k > 0$. To specify the dependence on the incident angle $\theta \in (-\pi/2, \pi/2)$, we rewrite the unique total field $u \in H^1_{\mathrm{loc},\alpha,0}(\tilde{D})$ to the perturbed scattering problem as (e.g., Theorem 4.4(ii))

$$u(x; \theta) = u_{\mathrm{unpert}}(x; \theta) + u^{sc}_{\mathrm{pert}}(x; \theta) \quad \text{in } \Sigma_R, \tag{5.8}$$

where $u_{\mathrm{unpert}}(x; \theta) = u^{in}(x; \theta) + u^{sc}_{\mathrm{unpert}}(x; \theta) \in H^1_{\alpha,\mathrm{loc},0}(D)$ is the total field to the unperturbed scattering problem, and $u^{sc}_{\mathrm{pert}}(x; \theta) \in H^1_{\mathrm{loc}}(\Sigma_R)$ is caused by the local defect which fulfils the open waveguide radiation condition of Definition 2.5. Note that, if $k \sin\theta = \hat{\alpha}_j + n$ for some $n \in \mathbb{Z}$ and some critical wavenumber $\hat{\alpha}_j$ $(j \in J)$, the unperturbed total field u_{unpert} is supposed to fulfil the additional constraint of Theorems 4.4 and 4.8.

Theorem 5.5. *Let* $\tilde{\Gamma}$ *be a local perturbation of the periodic curve* Γ *and suppose that* $\max\{x_2 : x \in \Gamma \cup \tilde{\Gamma}\} < h$ *for some* $h \in \mathbb{R}$*. Then* $\tilde{\Gamma}$ *can be uniquely determined by the near-field measurement data* $\{u(x_1, h; \theta_m) : x_1 \in (a, b), m = 1, 2, \ldots\}$*, incited by infinitely many plane waves with distinct incident angles* $\theta_m \in (-\pi/2, \pi/2)$*.*

Proof. We carry out the proof in the same way as in the proof of Theorem 5.1. It suffices to prove the linear independence of the total fields caused by different directions.

Set $\alpha(n) := k \sin\theta_n$ for $n = 1, \ldots, N$. We recall that the total field u_n corresponding to the incident angle θ_n has the decomposition into $u_n = u_n^{in} + u^{sc}_{n,\mathrm{unpert}} + u^{sc}_{n,\mathrm{pert}}$, where $u_n^{in}(x) = \mathrm{e}^{\mathrm{i}\alpha(n)x_1 - \mathrm{i}\sqrt{k^2 - \alpha(n)^2}x_2}$,

$u^{sc}_{n,\text{pert}}$ satisfies the open waveguide radiation condition and $u^{sc}_{n,\text{unpert}}$ is $\alpha(n)$-quasi-periodic, i.e., it has a Rayleigh expansion in the form

$$u^{sc}_{n,\text{unpert}}(x) = \sum_{\ell\in\mathbb{Z}} u_{\ell,n}\, \mathrm{e}^{\mathrm{i}\sqrt{k^2-(\ell+\alpha(n))^2}x_2}\, \mathrm{e}^{\mathrm{i}(\ell+\alpha(n))x_1}, \quad x_2 \geqslant h.$$

Let now $\sum_{n=1}^N \lambda_n u_n = 0$ in $\tilde{D}$. For fixed $m \in \{1,\dots,N\}$, $R > 0$ and $x_2 > h$, we have

$$\begin{aligned}
0 &= \frac{1}{2R}\sum_{n=1}^N \lambda_n \int_{-R}^R u_n(x)\, \mathrm{e}^{-\mathrm{i}\alpha(m)x_1}\, dx_1\\
&= \sum_{n=1}^N \lambda_n\, \mathrm{e}^{-\mathrm{i}\sqrt{k^2-\alpha(n)^2}x_2}\, \frac{1}{2R}\int_{-R}^R \mathrm{e}^{\mathrm{i}(\alpha(n)-\alpha(m))x_1}\, dx_1\\
&\quad + \sum_{n=1}^N \sum_{\ell\in\mathbb{Z}} \lambda_n\, u_{\ell,n}\, \mathrm{e}^{\mathrm{i}\sqrt{k^2-(\ell+\alpha(n))^2}x_2}\, \frac{1}{2R}\int_{-R}^R \mathrm{e}^{\mathrm{i}(\ell+\alpha(n)-\alpha(m))x_1}\, dx_1\\
&\quad + \frac{1}{2R}\int_{-R}^R u^{sc}_{n,\text{pert}}(x)\, \mathrm{e}^{-\mathrm{i}\alpha(m)x_1}\, dx_1.
\end{aligned} \tag{5.9}$$

We first estimate the first and second terms on the right-hand side of the above relation. It is obvious that there exists $\delta > 0$ such that

$$\min\{|\ell+\alpha(n)-\alpha(m)| : n,m \in \{1,\dots,N\},\ \ell\in\mathbb{Z},\ \ell+\alpha(n)-\alpha(m) \neq 0\} > \delta.$$

In the particular case where $\ell = 0$, we have

$$|\alpha(n)-\alpha(m)| > \delta \quad \text{for all } n \neq m, \quad n,m = 1,2,\dots,N,$$

because $\alpha(n) \neq \alpha(m)$ for $n \neq m$. We explicitly compute the first and second integrals as follows:

$$\begin{aligned}
&\sum_{n=1}^N \lambda_n\, \mathrm{e}^{-\mathrm{i}\sqrt{k^2-\alpha(n)^2}x_2}\, \frac{1}{2R}\int_{-R}^R \mathrm{e}^{\mathrm{i}(\alpha(n)-\alpha(m))x_1}\, dx_1\\
&\quad = \lambda_m\, \mathrm{e}^{-\mathrm{i}\sqrt{k^2-\alpha(m)^2}x_2} + \sum_{n\neq m, n=1}^N \lambda_n\, \mathrm{e}^{-\mathrm{i}\sqrt{k^2-\alpha(n)^2}x_2}\, \frac{1}{R}\, \frac{\sin[\alpha(n)-\alpha(m)R]}{\alpha(n)-\alpha(m)}\\
&\quad = \lambda_m\, \mathrm{e}^{-\mathrm{i}\sqrt{k^2-\alpha(m)^2}x_2} + \mathcal{O}(1/R)
\end{aligned}$$

and

$$\begin{aligned}
&\sum_{n=1}^N \sum_{\ell\in\mathbb{Z}} \lambda_n\, u_{\ell,n}\, \mathrm{e}^{\mathrm{i}\sqrt{k^2-(\ell+\alpha(n))^2}x_2}\, \frac{1}{2R}\int_{-R}^R \mathrm{e}^{\mathrm{i}(\ell+\alpha(n)-\alpha(m))x_1}\, dx_1\\
&\quad = \sum_{n=1}^N \sum_{\ell\in\mathbb{Z}} \lambda_n\, u_{\ell,n}\, \mathrm{e}^{\mathrm{i}\sqrt{k^2-(\ell+\alpha(n))^2}x_2}\, \frac{\sin[(\ell+\alpha(n)-\alpha(m))R]}{(\ell+\alpha(n)-\alpha(m))R}\\
&\quad = \mathrm{e}^{\mathrm{i}\sqrt{k^2-\alpha(m)^2}x_2} \sum_{n,\ell:\ell+\alpha(n)=\alpha(m)} \lambda_n\, u_{\ell,n} + \mathcal{O}(1/R).
\end{aligned}$$

Next, we estimate the third term of (5.9). By the definition of the open waveguide radiation condition, we can decompose $u^{sc}_{n,\text{pert}}$ into the sum $u^{sc}_{n,\text{pert}} = u^{sc,\text{prop}}_{n,\text{pert}} + u^{sc,\text{rad}}_{n,\text{pert}}$ in $\tilde{D}$, where the radiating part $u^{sc,\text{rad}}_{n,\text{pert}} \in H^1(W_h)$, and the propagating part $u^{sc,\text{prop}}_{n,\text{pert}}$ is of the form (2.7). The term involving $u^{sc,\text{rad}}_{n,\text{pert}}$ converges to zero as $R \to \infty$, because

$$\frac{1}{2R}\left|\int_{-R}^R u^{sc,\text{rad}}_{n,\text{pert}}(x_1,x_2)\, \mathrm{e}^{-\mathrm{i}\alpha(m)x_1}\, dx_1\right| \leqslant \frac{1}{2R}\int_{-R}^R |u^{sc,\text{rad}}_{n,\text{pert}}(x_1,x_2)|\, dx_1$$

$$\leqslant \frac{1}{\sqrt{2R}} \|u^{sc,\mathrm{rad}}_{n,\mathrm{pert}}(\cdot, x_2)\|_{L^2(\mathbb{R})}$$

for all $x_2 \geqslant h$. To estimate the propagating part, we observe that for $x_2 > h$, it has the form

$$\begin{aligned} u^{sc,\mathrm{prop}}_{n,\mathrm{pert}}(x) = \psi^+(x_1) \sum_{j\in J} \sum_{\ell:|\ell+\hat\alpha_j|>k} c^+_{\ell,j,n}\, \mathrm{e}^{-\sqrt{(\ell+\hat\alpha_j)^2-k^2}x_2}\, \mathrm{e}^{\mathrm{i}(\ell+\hat\alpha_j)x_1} \\ + \psi^-(x_1) \sum_{j\in J} \sum_{\ell:|\ell+\hat\alpha_j|>k} c^-_{\ell,j,n}\, \mathrm{e}^{-\sqrt{(\ell+\hat\alpha_j)^2-k^2}x_2}\, \mathrm{e}^{\mathrm{i}(\ell+\hat\alpha_j)x_1} \end{aligned}$$

for some coefficients $c^{\pm}_{\ell,j,n}$. Therefore,

$$\begin{aligned} &\frac{1}{2R}\int_{-R}^{R} u^{sc,\mathrm{prop}}_{n,\mathrm{pert}}(x_1,x_2)\, \mathrm{e}^{-\mathrm{i}\alpha(m)x_1}\, dx_1 \\ &= \sum_{j\in J} \sum_{\ell:|\ell+\hat\alpha_j|>k} c^+_{\ell,j,n}\, \mathrm{e}^{-\sqrt{(\ell+\hat\alpha_j)^2-k^2}x_2}\, \frac{1}{2R}\int_{-R}^{R} \psi^+(x_1)\, \mathrm{e}^{\mathrm{i}(\ell+\hat\alpha_j-\alpha(m))x_1}\, dx_1 \\ &\quad + \sum_{j\in J} \sum_{\ell:|\ell+\hat\alpha_j|>k} c^-_{\ell,j,n}\, \mathrm{e}^{-\sqrt{(\ell+\hat\alpha_j)^2-k^2}x_2}\, \frac{1}{2R}\int_{-R}^{R} \psi^-(x_1)\, \mathrm{e}^{\mathrm{i}(\ell+\hat\alpha_j-\alpha(m))x_1}\, dx_1 \end{aligned}$$

and

$$\begin{aligned} &\frac{1}{2R}\int_{-R}^{R} \psi^+(x_1)\, \mathrm{e}^{\mathrm{i}(\ell+\hat\alpha_j-\alpha(m))x_1}\, dx_1 \\ &= \frac{1}{2R}\int_{\sigma-1}^{\sigma} \psi^+(x_1)\, \mathrm{e}^{\mathrm{i}(\ell+\hat\alpha_j-\alpha(m))x_1}\, dx_1 + \frac{1}{2R}\int_{\sigma}^{R} \mathrm{e}^{\mathrm{i}(\ell+\hat\alpha_j-\alpha(m))x_1}\, dx_1 \end{aligned}$$

converges to zero as R tends to infinity uniformly with respect to ℓ by the same arguments as in the part (i) since $|\ell+\hat\alpha_j| > k > |\alpha(m)|$. The same argument applies to the term involving $\psi^-(x_1)$. Letting R tend to infinity in (5.9), we conclude that

$$\lambda_m\, \mathrm{e}^{-\mathrm{i}\sqrt{k^2-\alpha(m)^2}x_2} + \mathrm{e}^{\mathrm{i}\sqrt{k^2-\alpha(m)^2}x_2} \left[\sum_{n,\ell:\ell+\alpha(n)=\alpha(m)} \lambda_n\, u_{\ell,n} \right] = 0.$$

The linear independence of the exponential terms yields that $\lambda_m = 0$. This ends the proof of the linear independence of the total fields with different directions.

Finally, repeating the lines in the proof of Theorem 5.1 with $G_1(x;y_j) = u_1(x;\theta_m)$, we can prove the uniqueness by the same contradiction argument. □

In Appendix A, we provide another proof of the linear independence of the total fields $\{u(x;\theta_n)\}_{n=1}^N$ for any $N \in \mathbb{N}$.

5.3 Uniqueness with a finite number of plane waves

In Theorems 5.1 and 5.5, there is no requirement on the location, width and height of the defect. If some *a priori* information on the defect is available, we can prove uniqueness with a finite number of incoming waves by adopting Colton and Slemann's idea of determining a bounded sound-soft obstacle [9].

Theorem 5.6. *Let $k > 0$ be fixed and let $\tilde\Gamma$ be a local perturbation of the periodic curve Γ. Suppose that* $\max\{x_2 : x \in \Gamma \cup \tilde\Gamma\} < h$ *for some $h \in \mathbb{R}$ and that both $\Gamma\backslash\tilde\Gamma$ and $\tilde\Gamma\backslash\Gamma$ are contained in the rectangular domain $D_0 = (0,2\pi)\times(0,h)$. Let $N \geqslant hk^2/2$ be an integer. Then $\tilde\Gamma$ can be uniquely determined by the near-field measurement data $\{u(x_1,h;\theta_n) : x_1 \in (a,b), n = 1,2,\ldots,N+1\}$, where $\theta_n \in (-\pi/2,\pi/2)$ are distinct angles.*

Proof. Suppose that there are two local perturbations $\tilde\Gamma_1$ and $\tilde\Gamma_2$ lying below the line $x_2 = h$, which produce identical near-field data for each incident direction θ_m. Denote by $u_\ell(x;\theta_m)$ $(\ell = 1,2)$ the unique total field incited by the incoming plane wave $u^{in}(x;\theta_m) = e^{ik(x_1\sin\theta_m - x_2\cos\theta_m)}$ incident onto $\tilde{\Gamma}_\ell$. We proceed as in the proof of Theorem 5.1 to obtain

$$(\Delta + k^2)u_1(x;\theta_n) = 0 \quad \text{in } D^*, \quad u_1(\cdot;\theta_n) = 0 \quad \text{on } \partial D^*$$

for all $n = 1, 2, \dots, N, N+1$, where $D^* \subset D_0$ is a bounded domain. This implies that there exist $N+1$ Dirichlet eigenfunctions $u_1(\cdot;\theta_n) \in H_0^1(D^*)$ for the negative Laplacian operator over the bounded domain D^* with the eigenvalue k^2. Recalling the linear independence of $u_1(\cdot;\theta_n)$ (see the proof of Theorem 5.5), we conclude that the dimension of the Dirichlet eigenspace over D^* associated with k^2 must be greater than or equal to $N+1$. Below, we prove that this dimension cannot exceed N, which leads to a contradiction.

Denote by λ_j ($j \in \mathbb{N}$) the Dirichlet eigenvalues of D^*, which are arranged according to increasing magnitude and taken with respective to multiplicity. Let the multiplicity of k^2 be $m^* \in \mathbb{N}$ and suppose that k^2 is the m-th ($m \geqslant m^*$) eigenvalue such that

$$\lambda_{m+1} > k^2 = \lambda_m = \lambda_{m-1} = \cdots = \lambda_{m-m^*-1} > \lambda_{m-m^*-2} \geqslant \lambda_{m-m^*-3} \geqslant \cdots > \lambda_1 > 0.$$

Analogously, let $0 < \mu_1 \leqslant \mu_2 \leqslant \cdots \leqslant \mu_m$ be the first m eigenvalues of D_0. By the strong monotonicity property of the Dirichlet eigenvalues with respect to the domain, it holds that $\mu_m < \lambda_m = k^2$ due to the fact that $D^* \subset D_0$. This further implies that m^* is less than or equal to $(D_0, k^2)^\sharp \in \mathbb{N}$, which is defined as the sum of the multiplicities of the Dirichlet eigenvalues for D_0 that are less than k^2. On the other hand, if k^2 is a Dirichlet eigenvalue of the rectangular domain D_0, it is easy to derive, using the method of separating variables, the associated eigenfunctions

$$v_{l,j}(x_1, x_2) = \sin\left(\frac{l}{2}x_1\right) \sin\left(\frac{j\pi}{h}x_2\right),$$

where $l, j \in \mathbb{N}$ satisfy the relation

$$k^2 = \frac{l^2}{4} + \frac{j^2\pi^2}{h^2}. \tag{5.10}$$

Therefore, $(D_0, k^2)^\sharp$ coincides with the number of grid points $(l, j) \in \mathbb{N} \times \mathbb{N}$ lying in the positive orthant of the ellipse

$$\left(\frac{x_1}{2k}\right)^2 + \left(\frac{x_2}{hk/\pi}\right)^2 \leqslant 1.$$

Hence, $(D_0, k^2)^\sharp$ can be bounded by $hk^2/2$, one fourth of the area of the above ellipse. By the choice of N, we have $(D_0, k^2)^\sharp \leqslant N$. This contradicts the fact that there are $N+1$ linearly independent functions $u_1(x;\theta_m) \in H_0^1(D^*)$ for $m = 1, 2, \dots, N+1$. □

As a direct consequence of the proof of Theorem 5.6, we can obtain a uniqueness result with one plane wave with a fixed direction and frequency.

Corollary 5.7. *Let $k > 0$ be fixed and let $\tilde{\Gamma}$ be a local perturbation of the periodic curve Γ. Suppose that* $\max\{x_2 : x \in \Gamma \cup \tilde{\Gamma}\} < h$ *for some $h \in \mathbb{R}$ and that both $\Gamma\backslash\tilde{\Gamma}$ and $\tilde{\Gamma}\backslash\Gamma$ are contained in the rectangular domain $D_0 = (0, 2\pi) \times (0, h)$. If $k < \sqrt{1/4 + \pi^2/h^2}$, then $\tilde{\Gamma}$ can be uniquely determined by single near-field measurement data $\{u(x_1, h; \theta) : x_1 \in (a, b)\}$, where $\theta \in (-\pi/2, \pi/2)$ is arbitrary.*

Proof. From the proof of Theorem 5.6, we conclude that k^2 must be greater than or equal to the first Dirichlet eigenvalue μ_1 of the negative Laplacian operator over the domain D_0. In view of (5.10), one obtains $\mu_1 = \sqrt{1/4 + \pi^2/h^2} \leqslant k^2$, which is a contradiction to the condition that $k < \sqrt{1/4 + \pi^2/h^2}$. Hence, $u(x;\theta)$ cannot be a Dirichlet eigenfunction over any subdomain of D_0. This proves the desired uniqueness result by applying the same contradiction arguments of Theorem 5.6. □

Below, we present a counterexample to show that, if $k \geqslant \sqrt{1/4+\pi^2/h^2}$, it is in general impossible to uniquely determine the defect using a single plane wave when the Rayleigh frequency occurs. Such an example is motivated by the classification of unidentifiable polygonal gratings with one acoustic or elastic plane wave [10, 11]. Let the incident angle be $\theta = 0$ and set $k = 2$, leading to $u^{in}(x;\theta) = \mathrm{e}^{-\mathrm{i}2x_2}$. Define the piecewise linear function (see Figure 3)

$$x_2 = f(x_1) = \begin{cases} x_1, & \text{if } x_1 \in (0, \pi/2), \\ -x_1 + \pi, & \text{if } x_1 \in (\pi/2, \pi). \end{cases}$$

Let Γ be the π-periodic extensions of $\{x_2 = f(x_1) : x_1 \in (0,\pi)\}$ in the x_1-direction, and let $\tilde{\Gamma}$ be the local perturbation of Γ in $(0, 2\pi)$ shown as in Figure 3, where the dashed line segments denote the defect and D^* denotes the gap domain between D and $\tilde{D}$. In this case, we have

$$k > \sqrt{1/4+\pi^2/h^2}$$

for all $h > \pi$. Since Γ is the graph of a piecewise linear function, there exists a unique scattered field $u^{sc}_{\mathrm{unpert}} \in H^1_{\mathrm{loc},\alpha}(D)$ to the unperturbed scattering problem, taking the explicit form

$$u^{sc}_{\mathrm{unpert}}(x) = \mathrm{e}^{\mathrm{i}2x_2} - \mathrm{e}^{\mathrm{i}2x_1} - \mathrm{e}^{-\mathrm{i}2x_1}, \quad x \in D.$$

Note that the Rayleigh frequency occurs, since $k = 2$ and $\alpha = 0$ (i.e., $k = \alpha + n$ with $n = 2$). Moreover, the guide modes (surface waves) are excluded for the unperturbed scattering problem. Hence, the unique total field to the unperturbed problem can be expressed as

$$u_{\mathrm{unpert}} = u^{in} + u^{sc}_{\mathrm{unpert}} = 2(\cos 2x_2 - \cos 2x_1) = 4\sin(x_1 + x_2)\,\sin(x_1 - x_2), \quad x \in D.$$

Observing that $\tilde{\Gamma}$ is also the graph of a piecewise linear function, by [20] there exists a unique total field $u_{\mathrm{pert}} \in H^1_{\mathrm{loc},0}(\tilde{D})$ of the form $u_{\mathrm{pert}} = u_{\mathrm{unpert}} + u^{sc}_{\mathrm{pert}}$ in Σ_R, where $u^{sc}_{\mathrm{pert}} \in H^1_{\mathrm{loc}}(\tilde{D})$ consists of the radiating part only satisfying the Sommerfeld radiation conditions of Definitions 2.7 and 2.8. On the other hand, since the defect lies on the straight lines

$$x_2 = x_1, \quad x_2 = -x_1 + 2\pi, \quad x_1 \in \mathbb{R},$$

we conclude that u_{unperp} also vanishes on $\tilde{\Gamma}$. By uniqueness, this implies that $u^{sc}_{\mathrm{perp}} \equiv 0$ in $\tilde{D}$ and thus $u_{\mathrm{perp}} = u_{\mathrm{unperp}}$. In other words, the presence of the local defect does not produce any perturbation to u_{unperp}. We remark that u_{unpert} is a real-valued Dirichlet eigenfunction of the negative Laplacian operator over the rectangular domain D^*. Therefore, it is impossible to determine the perturbed boundary $\tilde{\Gamma}\backslash\Gamma$ from the near-field measurement data of u_{perp} on $x_2 = h$ for all $h > \pi$.

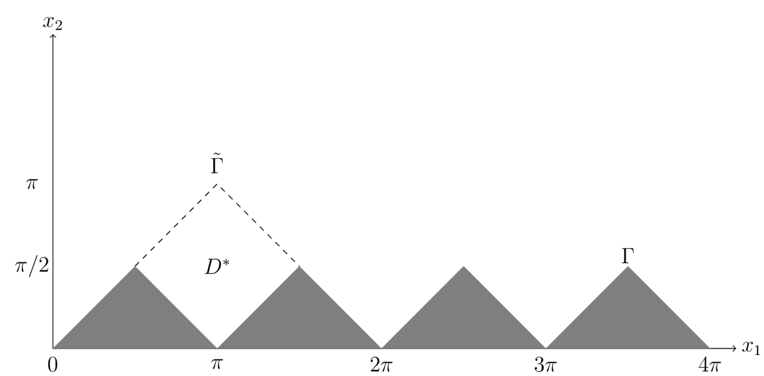

Figure 3 Illustration of Γ and its local perturbation $\tilde{\Gamma}$ which generate identical wave fields with $\theta = 0$ and $k = 2$. Here, $D^* = D\backslash\overline{\tilde{D}}$ represents the difference domain between D and $\tilde{D}$

5.4 Uniqueness using far-field data of point source waves

The symmetry of Green's function (see Theorem 3.1) together with Theorem 4.10 yields

$$\begin{aligned} u^{\infty}(-\hat{\theta}; x) &:= \lim_{t\to\infty} [\sqrt{t}\mathrm{e}^{-\mathrm{i}kt} u(z_t; x)] \\ &= \lim_{t\to\infty} [\sqrt{t}\mathrm{e}^{-\mathrm{i}kt} u(x; z_t)] \\ &= \gamma\, w(x; \hat{\theta}) \end{aligned} \tag{5.11}$$

in $H^1(\tilde{D}_R)$ for any $R > \pi$ with $\gamma := \frac{\mathrm{e}^{\mathrm{i}\pi/4}}{\sqrt{8k\pi}}$. Here, $z_t = t\hat{\theta}$ and $w(x;\hat{\theta})$ denotes the total field excited by the plane wave $u^{in}(x;\theta) = \mathrm{e}^{\mathrm{i}kx\cdot\hat{\theta}}$ (see Theorem 4.10). This means that the far-field data at the observation direction $-\hat{\theta}$ generated by the point source wave emitting from $x \in \tilde{D}$ is identical with the value of the total field at x of the plane wave $\mathrm{e}^{\mathrm{i}kx\cdot\hat{\theta}}$ multiplied by the constant γ. This is exactly the mixed reciprocity relation between point source and plane wave incidences in a perturbed periodic structure. Using this relation, we can prove uniqueness in determining the defect from the far-field patterns of one or many point source waves.

Theorem 5.8. *Let $\tilde{\Gamma}$ be a local perturbation of the periodic curve Γ and suppose that* $\max\{x_2 : x \in \Gamma \cup \tilde{\Gamma}\} < h$ *for some $h \in \mathbb{R}$. Then $\tilde{\Gamma}$ can be uniquely determined by the far-field measurement data* $\{u^{\infty}(-\hat{\theta}_m; x) : m = 1, 2, \ldots, x = (x_1, h), x_1 \in (a, b)\}$ *incited by infinitely many point waves lying on the line segment* $\{(x_1, h) : x_1 \in (a, b)\}$. *The same uniqueness result holds if we replace $u^{\infty}(-\hat{\theta}; x)$ by $u^{\infty}_{\mathrm{perp}}(-\hat{\theta}; x)$, the far-field pattern of the radiating part of the scattered field $u^{sc}_{\mathrm{perp}}(t\hat{\theta}; x)$ as $t \to \infty$.*

Proof. The first assertion follows directly from the mixed reciprocity relation (5.11) and the uniqueness result of Theorem 5.5. To prove the second assertion, we recall from Proposition 2.10 a decomposition of $u(x; z_t)$ into

$$u(x; z_t) = u^{in}(x; z_t) + u^{sc}_{\mathrm{unperp}}(x; z_t) + u^{sc}_{\mathrm{perp}}(x; z_t) \quad \text{in } \Sigma_R, \tag{5.12}$$

where $u^{sc}_{\mathrm{unperp}}(x; z_t)$ denotes the scattered field to the unperturbed scattering problem and $u^{sc}_{\mathrm{perp}}(x; z_t)$ denotes the part caused by the defect. Note that both $u^{sc}_{\mathrm{unperp}}(x; z_t)$ and $u^{sc}_{\mathrm{perp}}(x; z_t)$ fulfil the open waveguide radiation condition. Since the propagating part of $u^{sc}_{\mathrm{unperp}}(x; z_t)$ (resp. $u^{sc}_{\mathrm{perp}}(x; z_t)$) decays exponentially as $t \to \infty$, one deduces from (5.12) the corresponding decomposition of the far-field pattern:

$$u^{\infty}(\hat{\theta}; x) = \mathrm{e}^{\mathrm{i}k\hat{\theta}\cdot x} + u^{\infty}_{\mathrm{unperp}}(\hat{\theta}; x) + u^{\infty}_{\mathrm{perp}}(\hat{\theta}; x),$$

where $u^{\infty}_{\mathrm{unperp}}(\hat{\theta}; x)$ represents the far-field pattern of the radiating part of the scattered field $u^{sc}_{\mathrm{unperp}}(t\hat{\theta}; x)$ as $t \to \infty$. Since the unperturbed structure Γ is *a priori* given, the far-field pattern $u^{\infty}_{\mathrm{unperp}}(\hat{\theta}; x)$ is uniquely determined by $\mathrm{e}^{\mathrm{i}k\hat{\theta}\cdot x}$ and Γ. Hence, the knowledge of $u^{\infty}_{\mathrm{perp}}(\hat{\theta}; x)$ is equivalent to knowing $u^{\infty}(\hat{\theta}; x)$ for any fixed $\hat{\theta} \in \mathbb{S}$ and $x \in \tilde{D}$. This proves the second assertion of Theorem 5.8. □

If *a priori* information on the height and size of the defect is available, one can also determine the defect by taking the far-field measurement data at a finite number of observation directions excited by infinitely many point source waves.

Corollary 5.9. *Let the conditions of Theorem* 5.6 *hold. Then $\tilde{\Gamma}$ can be uniquely determined by the far-field data $u^{\infty}(\hat{\theta}_n; x_1, h)$ (or $u^{\infty}_{\mathrm{perp}}(\hat{\theta}_n; x_1, h)$) for all $x_1 \in (a, b)$, $n = 1, 2, \ldots, N + 1$, where $\hat{\theta}_n \in \mathbb{S}_+ := \{(x_1, x_2) \in \mathbb{S} : x_2 > 0\}$ are distinct observation directions. Moreover, the far-field data at a single observation direction (i.e., $N = 0$) are sufficient under the additional conditions of Corollary* 5.7.

Remark 5.10. The uniqueness with far-field patterns of plane wave incidences is unclear to us, due to the lack of the one-to-one correspondence between the far-field pattern and near-field data.

Acknowledgements The first author greatly acknowledges the hospitality of the Institute for Applied and Numerical Mathematics, Karlsruhe Institute of Technology as well as the Alexander von Humboldt-Stiftung. The second author was supported by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) (Grant Nos. Project-ID 258734477 and SFB 1173).

References

1 Abdrabou A, Lu Y Y. Indirect link between resonant and guided modes on uniform and periodic slabs. Phys Rev A, 2019, 99: 063818

2 Bao G, Li P. Maxwell's Equations in Periodic Structures. Applied Mathematical Sciences, vol. 208. Singapore: Springer; Beijing: Science Press, 2022

3 Bonnet-Bendhia A S, Starling F. Guided waves by electromagnetic gratings and non-uniqueness examples for the diffraction problem. Math Methods Appl Sci, 1994, 17: 305–338

4 Chandler-Wilde S N, Elschner J. Variational approach in weighted Sobolev spaces to scattering by unbounded rough surfaces. SIAM J Math Anal, 2010, 42: 2554–2580

5 Chandler-Wilde S N, Monk P. Existence, uniqueness, and variational methods for scattering by unbounded rough surfaces. SIAM J Math Anal, 2005, 37: 598–618

6 Chandler-Wilde S N, Ross C R. Uniqueness results for direct and inverse scattering by infinite surfaces in a lossy medium. Inverse Problems, 1995, 11: 1063–1067

7 Chandler-Wilde S N, Zhang B. A uniqueness result for scattering by infinite rough surfaces. SIAM J Appl Math, 1998, 58: 1774–1790

8 Colton D, Kress R. Integral Equation Methods in Scattering Theory. Classics in Applied Mathematics, vol. 72. Philadelphia: SIAM, 2013

9 Colton D, Sleeman B D. Uniqueness theorems for the inverse problem of acoustic scattering. IMA J Appl Math, 1983, 31: 253–259

10 Elschner J, Hu G. Global uniqueness in determining polygonal periodic structures with a minimal number of incident plane waves. Inverse Problems, 2010, 26: 115002

11 Elschner J, Hu G. Inverse scattering of elastic waves by periodic structures: Uniqueness under the third or fourth kind boundary conditions. Methods Appl Anal, 2011, 18: 215–244

12 Elschner J, Yamamoto M. An inverse problem in periodic diffractive optics: Reconstruction of Lipschitz grating profiles. Appl Anal, 2002, 81: 1307–1328

13 Fliss S, Joly P. Exact boundary conditions for time-harmonic wave propagation in locally perturbed periodic media. Appl Numer Math, 2009, 59: 2155–2178

14 Fliss S, Joly P. Solutions of the time-harmonic wave equation in periodic waveguides: Asymptotic behaviour and radiation condition. Arch Ration Mech Anal, 2016, 219: 349–386

15 Furuya T. Scattering by the local perturbation of an open periodic waveguide in the half plane. J Math Anal Appl, 2020, 489: 124149

16 Gotlib V Y. Solutions of the Helmholtz equation, concentrated near a plane periodic boundary. J Math Sci, 2000, 102: 4188–4194

17 Grigorian A. Analysis of Elliptic Differential Equations. A Lectrure Note in 2016, https://www.math.uni-bielefeld.de/∼grigor/elelect.pdf

18 Hettlich F, Kirsch A. Schiffer's theorem in inverse scattering theory for periodic structures. Inverse Problems, 1997, 13: 351–361

19 Hu G, Kirsch A. Time-harmonic scattering by locally perturbed periodic structures with Dirichlet and Neumann boundary conditions. arXiv:2402.11230, 2024

20 Hu G, Lu W, Rathsfeld A. Time-harmonic acoustic scattering from locally perturbed periodic curves. SIAM J Appl Math, 2021, 81: 2569–2595

21 Hu G, Rathsfeld A. Scattering of time-harmonic electromagnetic plane waves by perfectly conducting diffraction gratings. IMA J Appl Math, 2015, 80: 508–532

22 Isakov V. On uniqueness in the invese transmission scattering problem. Comm Partial Differential Equations, 1990, 15: 1565–1586

23 Joly P, Li J R, Fliss S. Exact boundary conditions for periodic waveguides containing a local perturbation. Commun Comput Phys, 2006, 1: 945–973

24 Kamotski I V, Nazarov S A. The augmented scattering matrix and exponentially decaying solutions of an elliptic problem in a cylindrical domain. J Math Sci, 2002, 111: 3657–3666

25 Kirsch A. Diffraction by periodic structures. In: Proceedings of the Lapland Conference on Inverse Problems. Berlin: Springer, 1993: 87–102

26 Kirsch A. Scattering by a periodic tube in $\mathbb{R}^3$: Part I. The limiting absorption principle. Inverse Problems, 2019, 35: 104004

27 Kirsch A. Scattering by a periodic tube in $\mathbb{R}^3$: Part II. A radiation condition. Inverse Problems, 2019, 35: 104005

28 Kirsch A. A scattering problem for a local perturbation of an open periodic waveguide. Math Methods Appl Sci, 2022, 45: 5737–5773

29 Kirsch A. On the scattering of a plane wave by a perturbed open periodic waveguide. Math Methods Appl Sci, 2023, 46: 10698–10718

30 Kirsch A, Kress R. Uniqueness in inverse obstacle scattering (acoustics). Inverse Problems, 1993, 9: 285–299
31 Kirsch A, Lechleiter A. A radiation condition arising from the limiting absorption principle for a closed full- or half-waveguide problem. Math Methods Appl Sci, 2018, 41: 3955–3975
32 Kirsch A, Lechleiter A. The limiting absorption principle and a radiation condition for the scattering by a periodic layer. SIAM J Math Anal, 2018, 50: 2536–2565
33 Krylov N V. Lectures on Elliptic and Parabolic Equations in Hölder Spaces. Providence: Amer Math Soc, 1996
34 Lechleiter A. The Floquet-Bloch transform and scattering from locally perturbed periodic surfaces. J Math Anal Appl, 2017, 446: 605–627
35 Lechleiter A, Zhang R. A convergent numerical scheme for scattering of aperiodic waves from periodic surfaces based on the Floquet-Bloch transform. SIAM J Numer Anal, 2017, 55: 713–736
36 Mclean W. Strongly Elliptic Systems and Boundary Integral Equations. Cambridge: Cambridge Univ Press, 2010
37 Petit R. Electromagnetic Theory of Gratings. Berlin: Springer, 1980
38 Rayleigh L. On the dynamical theory of gratings. Proc R Soc Lond A, 1907, 79: 399–416
39 Xu X, Hu G, Zhang B, et al. Uniqueness in inverse diffraction grating problems with infinitely many plane waves at a fixed frequency. SIAM J Appl Math, 2023, 83: 302–326
40 Yu X, Hu G, Lu W, et al. PML and high-accuracy boundary integral equation solver for wave scattering by a locally defected periodic surface. SIAM J Numer Anal, 2022, 60: 2592–2625
41 Yuan L, Lu Y Y. Bound states in the continuum on periodic structures surrounded by strong resonances. Phys Rev A, 2018, 97: 043828
42 Zhang R. Numerical methods for scattering problems in periodic waveguides. Numer Math, 2021, 148: 959–996

Appendix A

Appendix A.1 An alternative proof of the linear independence of total fields with different directions

Here, we present another proof by adopting the arguments of [39, Lemma 2.2]. Let $u(x;\theta_m)$ with $\theta_m \in (-\pi/2,\pi/2)$ be the uniquely determined total field of the perturbed scattering problem; see Theorems 4.4 and 4.8. Suppose that $\sum_{m=1}^M c_m u(x;\theta_m)=0$ for all $x\in\tilde{D}$, where $c_m\in\mathbb{C}$, $m=1,2,\dots,M$ with some $M\in\mathbb{N}$. By (5.8),

$$\sum_{m=1}^M c_m u_{\mathrm{unpert}}(x;\theta_m)+\sum_{m=1}^M c_m u^{sc}_{\mathrm{pert}}(x;\theta_m)=0 \quad \text{for all } x\in U_h, \quad h>h_0.$$

In view of the definition of the open waveguide radiation condition, u^{sc}_{unpert} can be decomposed into two parts, i.e.,

$$u^{sc}_{\mathrm{unpert}}(x;\theta_m)=u^{\mathrm{rad}}_{\mathrm{unpert}}(x;\theta_m)+u^{\mathrm{prop}}_{\mathrm{unpert}}(x;\theta_m) \quad \text{in } \Sigma_R, \tag{A.1}$$

where the radiating part $u^{\mathrm{rad}}_{\mathrm{unpert}}(x;\theta_m)$ decays as $|x|^{-1/2}$ in U_h as $|x|\to\infty$, whereas the propagating part $u^{\mathrm{prop}}_{\mathrm{unpert}}(x;\theta_m)$ exponentially decays as $x_2\to\infty$. This leads to

$$\lim_{H\to\infty}\frac{1}{H}\left|\int_H^{2H} u^{sc}_{\mathrm{pert}}(x;\theta_m)\mathrm{e}^{\mathrm{i}k\cos\theta_n x_2}\,dx_2\right| \leqslant \lim_{H\to\infty}\frac{1}{H}\int_H^{2H}|u^{sc}_{\mathrm{pert}}(x;\theta_m)|\,dx_2=0$$

for all $n,m=1,2,\dots,M$ and uniformly in all $x\in[0,2\pi]$. Now, multiplying $\mathrm{e}^{\mathrm{i}k\cos\theta_n x_2}$ with some $n\in\{1,2,\dots,M\}$ to both sides of (A.1), integrating over $(H,2H)$ with respect to x_2 and taking the limit as $H\to\infty$, we have

$$\lim_{H\to\infty}\frac{1}{H}\left|\int_H^{2H}\sum_{m=1}^M c_m\,u_{\mathrm{unpert}}(x;\theta_m)\mathrm{e}^{\mathrm{i}k\cos\theta_n x_2}\,dx_2\right|=0 \quad \text{for all } x_1\in(0,2\pi).$$

Since the unperturbed total field $u_{\mathrm{unpert}}(x;\theta_m)$ is $k\sin\theta_m$-quasiperiodic, the above relation also holds for all $x_1\in\mathbb{R}$. Therefore,

$$\lim_{H\to\infty}\frac{1}{H}\left|\int_H^{2H}\sum_{m=1}^M c_m(\mathrm{e}^{\mathrm{i}k\sin\theta_m x_1}+u^{sc}_{\mathrm{unpert}}(x;\theta_m))\mathrm{e}^{\mathrm{i}k\cos\theta_n x_2}\,dx_2\right|=0, \quad x_1\in\mathbb{R}.$$

By the proof of [39, Lemma 2.2], the previous relation implies $c_n = 0$. Using the arbitrariness of $1 \leqslant n \leqslant M$, one obtains $c_m = 0$ for all $m = 1, 2, \ldots, M$. This proves that $\{u(x;\theta_m)\}_{m=1}^M$ must be linearly independent for all $M \in \mathbb{N}$.

Appendix A.2 Proof of the asymptotics in (4.31)

We suppose that $I_{\tilde{m}} = (a, b) \subset [-1/2, 1/2]$, where the two ending points a and b may be the cut-off values of k. For any $l \in \mathcal{L}\backslash\{\tilde{l}\}$, it holds that $k > |l + \alpha|$. Set $f(\alpha) := (l + \alpha)\sin\theta + \sqrt{k^2 - (l + \alpha)^2}\cos\theta$ for $\alpha \in (a, b)$. It is easy to see that

$$f'(\alpha) = \sin\theta - \frac{l + \alpha}{\sqrt{k^2 - (l + \alpha)^2}}\cos\theta \neq 0 \quad \text{for all } l \in \mathcal{L}\backslash\{\tilde{l}\}, \quad \alpha \in (a, b)$$

and

$$g(\alpha) := \sqrt{k^2 - (l + \alpha)^2}\, f'(\alpha) = \sqrt{k^2 - (l + \alpha)^2}\sin\theta - (l + \alpha)\cos\theta$$

keeps a positive distance from zero for all $l \in \mathcal{L}\backslash\{\tilde{l}\}$ and $\alpha \in [a, b]$. Here and below, the prime always denotes the derivative with respect to α. Direct calculations show that

$$\begin{aligned}\int_a^b \frac{\mathrm{e}^{\mathrm{i}tf(\alpha)}\, v_{l,\alpha}}{\sqrt{k^2 - (l + \alpha)^2}}\, d\alpha &= \frac{-\mathrm{i}}{t}\int_a^b \frac{v_{l,\alpha}}{g(\alpha)}\, d\,\mathrm{e}^{\mathrm{i}tf(\alpha)} \\ &= \frac{-\mathrm{i}}{t}\left[\frac{\mathrm{e}^{\mathrm{i}tf(\alpha)}\, v_{l,\alpha}}{g(\alpha)}\bigg|_a^b - \int_a^b \left(\frac{v'_{l,\alpha}}{g(\alpha)} - v_{l,\alpha}\frac{g'(\alpha)}{g^2(\alpha)}\right)\mathrm{e}^{\mathrm{i}tf(\alpha)}\, d\alpha\right]. \end{aligned} \tag{A.2}$$

We note that $g(\alpha)$ does not vanish at the boundary points a and b for $l \neq \tilde{l}$ and that

$$\int_a^b |g'(\alpha)| d\alpha = \int_a^b \left|\frac{l + \alpha}{\sqrt{k^2 - (l + \alpha)^2}}\sin\theta + \cos\theta\right| d\alpha < \infty,$$

because g' has integrable singularities at the possible cut-off values on a or b. On the other hand, $v_{l,\alpha} \in H^1_{\alpha,\mathrm{loc},0}(D)$ can be chosen to depend continuously on $\alpha \in [-1/2, 1/2]$ (see [19, Theorem 3.3]) and $v_{l,\alpha} \in W^{1,1}([-1/2, 1/2]; H^1(Q_{h_0}))$ has only square-root singularities at cut-off values, which can be verified following the same arguments as in the proof of [28, Theorem 4.3] for inhomogeneous layers. Hence, the right-hand side of (A.2) decays as $O(t^{-1})$ as t tends to infinity. This together with the arbitrariness of $l \in \mathcal{L}\backslash\{\tilde{l}\}$ proves the first relation in (4.31). The second one can be verified analogously by noting that $f'(\alpha) \neq 0$ for all $l \in \mathcal{L}$ and $\alpha \in [-1/2, 1/2]\backslash(a, b)$.