



The PML-method for a scattering problem for a local perturbation of an open periodic waveguide

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Abstract

The perfectly matched layer method (PML method) is a truncation technique well known for the numerical treatment of wave scattering problems in unbounded domains. In this paper, we study the convergence of the PML method for the wave scattering from an open waveguide in $\mathbb{R}_+^2 = \{x \in \mathbb{R}^2 : x_2 > 0\}$, where the refractive index is assumed to be a local perturbation of a function which is periodic with respect to x_1 and equal to one above a finite height. The problem is challenging from the theoretical, and also from the numerical, point of view due to the existence of guided waves. A typical way to deal with this difficulty is to apply the limiting absorption principle. Based on the Floquet-Bloch transform and a curve deformation theory, the solution, derived from the limiting absorption principle, is rewritten as the line integral (with respect to the Floquet-Bloch parameter) of the solution of a system of quasi-periodic problems. By comparing the Dirichlet-to-Neumann maps on a straight line above the locally perturbed periodic layer, we finally show that the PML method converges exponentially with respect to the PML parameter. Finally, some numerical examples are shown to illustrate the theoretical results.

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1 Introduction

Let $k > 0$ be the wavenumber which is fixed throughout the paper and $n \in L^\infty(\mathbb{R}_+^2)$ be 2π -periodic with respect to x_1 and equals one for $x_2 > h_0$ for some $h_0 > 0$. By

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\mathbb{R}_+^2 we denote the half plane $\mathbb{R}_+^2 := \{x \in \mathbb{R}^2 : x_2 > 0\}$. Furthermore, let $q \in L^\infty(\mathbb{R}_+^2)$ and $f \in L^2(\mathbb{R}_+^2)$ have compact supports in $Q := (0, 2\pi) \times (0, h_0)$. Then we will solve the following equations

$$\Delta u + k^2(n + q)u = -f \text{ in } \mathbb{R}_+^2, \quad u = 0 \text{ for } x_2 = 0, \quad (1)$$

complemented by a suitable radiating condition stated below.

The solution of (1) is understood in the variational sense; that is,

$$\int_{\mathbb{R}_+^2} \left[\nabla u \cdot \nabla \bar{\psi} - k^2(n + q)u\bar{\psi} \right] dx = \int_Q f \bar{\psi} dx \quad (2)$$

for all $\psi \in H_0^1(\mathbb{R}_+^2)$ with compact support. By standard regularity theorems it is known that for $x_2 > h_0$ the solution u is a classical solution of the Helmholtz equation and thus analytic.

As mentioned above, a further condition is needed to assure uniqueness. Similar to [1], we will derive a radiation condition by the limiting absorption principle; that is, the solution u should be the limit (as $\varepsilon > 0$ tends to zero) of the solutions $u_\varepsilon \in H^1(\mathbb{R}_+^2)$ corresponding to wavenumbers $k + i\varepsilon$ instead of k .

The investigation of wave propagation problems in closed wave guides, i.e. where \mathbb{R}_+^2 is replaced by $\mathbb{R} \times (0, h_0)$ with some $h_0 > 0$ and (1) is complemented by some boundary condition at the line $x_2 = h_0$, has a long history. For a classical approach we refer to [2] and the references therein. A different approach based on a singular perturbation theory has been proposed in [3]. Both of the approaches are based on the Floquet-Bloch theory which transforms the problem set up in the unbounded domain $\mathbb{R} \times (0, h_0)$ to a family of problems set up in the bounded domain $(0, 2\pi) \times (0, h_0)$ (if 2π is the periodicity) with additional quasi-periodicity boundary conditions at the vertical boundaries. For closed semi-waveguides $(0, \infty) \times (0, h_0)$ the limiting absorption principle has been shown in [4]. The spectral decomposition of the propagating waves in closed periodic waveguides is investigated in [5, 6]. Numerical methods are also developed based on the limiting absorption principle. Since even for closed waveguides the domain $\mathbb{R} \times (0, h_0)$ is still unbounded one option is to approximate the Dirichlet-to-Neumann map on the periodicity boundaries by solving certain cell problems. A Riccati-equation based method was proposed for the first time in [7] and then applied to other cases in [8–10]. Also, a doubling recursive process was proposed in [11] and further investigated in [12–14].

Open waveguide problems are unbounded with respect to both of the directions x_1 and x_2 . The Floquet-Bloch transform transforms the problem in \mathbb{R}_+^2 to a family of quasi-periodic problems in $(0, 2\pi) \times (0, \infty)$ which is still unbounded. Since the solution is quasi-periodic with respect to x_1 it allows a Rayleigh expansion (i.e. Fourier expansion with respect to x_1) for $x_2 > h_0$. In contrast to the case of closed waveguide problems where the Floquet-Bloch transformed problems are singular at certain values of the Floquet-Bloch parameter (which we call quasi-momentums, see Definition 1 (b)) open waveguide problems are more complicated because of the additional existence of so-called cutoff values (also called the Rayleigh anomalies, see Definition 1 (a))

which appear in the Rayleigh expansion and destroy the analytic dependence of the solution on the Floquet-Bloch parameter. The existence of quasi-momentums leads to the existence of propagative or guided modes (in the sense of Definition 1 (b)) which are quasi-periodic solutions of (1) for $q = f = 0$ and, thus, do not decay as $x_1 \rightarrow \pm\infty$. The functional analytic approach using a singular perturbation theory as in [3] can also be applied to the case of open waveguides, see [1, 15–18].

For some related radiation problems as, for example, wave scattering by periodic surfaces of special types, guided waves do not exist, and the situation is simpler. For example, when the surface is a graph of a bounded function and the boundary condition is Dirichlet, see [19]. With the help of the Floquet-Bloch transform, these problems are again reduced to families of coupled quasi-periodic problems which are now regular for all Floquet-Bloch parameters, see [20, 21] for absorbing backgrounds and [22, 23] for non-absorbing cases.

The Floquet-Bloch transform is not only useful for theoretical investigations but also for the design of numerical solvers. In [24–27], the authors developed a series of (higher order) numerical methods to solve these problems based on the Floquet-Bloch transform. For more detailed explanations on the radiation conditions for this kind of problem see [28] and for the related boundary integral equation method see [29].

One of the most difficult tasks in simulating wave scattering from locally perturbed periodic layers comes from the domain which is unbounded in two dimensions. It is easier to deal with unboundedness in the x_1 direction due to the periodicity; for the x_2 direction, an efficient truncation method is necessary to reduce the problem to a closed waveguide as a precursor to discretisation by a finite element or other volume discretisation method. In [24–26], the exact but non-local transparent boundary condition was adopted, and in [27, 29] the PML method was applied. The PML method, which was proposed by J.-P. Berenger in 1994 in [30], is well known for its simplicity with respect to numerical implementation. However, as it is not exact, convergence as a function of the PML parameters has to be shown. For periodic surface scattering problems, exponential convergence for quasi-periodic problems has been proved in [31]. For general rough surface scattering problems, we refer to [32] where algebraic convergence has been shown. The authors in [32] raised the question whether or not exponential convergence on compact subsets could be expected. In [27], this question was positively answered for periodic structures and wavenumbers $2k \notin \mathbb{N}$. High-order algebraic convergence was proved for all positive wavenumbers in [33].

In this paper, we will apply the PML method with respect to the variable x_2 to approximate the open waveguide problem by a closed waveguide problem and study its convergence rate, following the technique introduced in [27]. Compared to a direct implementation of the (non-local) radiation condition proposed in [1], the PML method benefits from a local boundary condition, which is easily implemented in a finite element method. In a first step we will adopt the curve deformation technique (i.e., replace integration on a real interval by integration along a carefully designed complex curve) in the inverse Floquet-Bloch transform, developed in [34, 35] for closed waveguide problems, to handle the case of guided modes. As a side product, the radiation condition, proposed in [1], can easily be derived from this form of the inverse Floquet-Bloch transform. Compared to the representations that follow from the well-posedness results in [17, 36], the new formulation is easier to be implemented numerically.

For unperturbed periodic problems the family of Floquet-Bloch transformed problems are uncoupled with respect to the Floquet-Bloch parameter. For perturbed problems, however, they are coupled and have to be solved simultaneously. We show uniqueness and existence of this system.

Then, in a second step, we apply the PML method to truncate the problem into a closed waveguide problem and derive the system of (coupled) problems on a bounded domain. By comparing the quasi-periodic Dirichlet-to-Neumann maps for the open waveguide and the closed one arising from the PML approximation we finally prove the exponential convergence of the PML method.

The paper is organised as follows. In Sect. 2, we recall the definitions and properties of guided (or propagating) modes. In Sect. 3, the curve deformation technique for the inverse Floquet-Bloch transform is applied to reformulate the scattering problems, and this approach is extended to locally perturbed cases in Sect. 4. In Sect. 5, the convergence analysis of the PML method is studied. In the final Sect. 6 a numerical example is presented.

2 Propagating modes

First we recall some definitions. A function ϕ is α -quasi-periodic (for some $\alpha \in \mathbb{R}$) if $\phi(x_1 + 2\pi) = e^{2\pi i\alpha}\phi(x_1)$ for all x_1 . We define the layer $W_h := \mathbb{R} \times (0, h)$, the space $H^1_{\alpha,0}(W_h) := \{u \in H^1_{loc}(W_h) : u = 0 \text{ for } x_2 = 0, u(\cdot, x_2) \text{ is } \alpha\text{-quasi-periodic for all } x_2\}$ of quasi-periodic functions, and the corresponding local space $H^1_{\alpha,0,loc}(\mathbb{R}^2_+) = \{u : u|_{W_h} \in H^1_{\alpha,0}(W_h) \text{ for all } h > 0\}$.

Definition 1 (a) $\alpha \in \mathbb{R}$ is called a cut-off value if there exists $\ell \in \mathbb{Z}$ with $|\ell + \alpha| = k$.
 (b) $\alpha \in \mathbb{R}$ is called a quasi-momentum (or Floquet spectral value) if there exists a non-trivial $\phi \in H^1_{\alpha,0,loc}(\mathbb{R}^2_+)$ such that

$$\Delta\phi + k^2 n \phi = 0 \text{ in } \mathbb{R}^2_+ \tag{3}$$

satisfying the Rayleigh expansion

$$\phi(x) = \sum_{\ell \in \mathbb{Z}} \phi_\ell(h_0) e^{i(\ell+\alpha)x_1 + i\sqrt{k^2 - (\ell+\alpha)^2}(x_2 - h_0)} \text{ for } x_2 > h_0. \tag{4}$$

Here, $\phi_\ell(h_0) = \frac{1}{2\pi} \int_0^{2\pi} \phi(x_1, h_0) e^{-i(\ell+\alpha)x_1} dx_1$ are the Fourier coefficients of $\phi(\cdot, h_0) e^{-i\alpha x_1}$. The convergence is uniform for $x_2 \geq h_0 + \delta$ for all $\delta > 0$. The functions ϕ are called propagating (or guided) modes. The branch of the square root is taken such that the square root is holomorphic in $\mathbb{C} \setminus i\mathbb{R}_{\leq 0}$ and such that $\sqrt{z} > 0$ for $z > 0$.

If we decompose k into $k = \hat{\ell} + \kappa$ with $\hat{\ell} \in \mathbb{N} \cup \{0\}$ and $\kappa \in (-1/2, 1/2]$ we observe that the cut-off values are given by $\pm\kappa + \ell$ for any $\ell \in \mathbb{Z}$.

Since with α also $\alpha + \ell$ for every $\ell \in \mathbb{Z}$ is a quasi-momentum we can restrict ourselves to quasi-momentums in $(-1/2, 1/2]$.

We define the spaces of periodic functions with boundary conditions for $x_2 = 0$ by $H^1_{per,0}(Q) := \{\psi \in H^1(Q) : \psi = 0 \text{ for } x_2 = 0, \psi \text{ is } 2\pi - \text{periodic with respect to } x_1\}$ and, analogously, $H^1_{per,0}(Q^\infty)$ for $Q^\infty := (0, 2\pi) \times (0, \infty)$.

For the proof that there exists at most a finite number of quasi-momentums we need the following result.

Lemma 2 (a) (Part (a) in Theorem 3.1, [1]) Let $u \in H^1_{\alpha,0,loc}(\mathbb{R}^2_+)$ be a α -quasi-periodic solution of $\Delta u + k^2 nu = -f$ in \mathbb{R}^2_+ satisfying the Rayleigh expansion (4). Then $\tilde{u}(x) := e^{-i\alpha x_1} u(x)$ for $x \in Q$ is in $H^1_{per,0}(Q)$ and satisfies

$$\begin{aligned} & \int_Q \left[\nabla \tilde{u} \cdot \nabla \overline{\psi} - 2i\alpha \partial_1 \tilde{u} \overline{\psi} - (k^2 n - \alpha^2) \tilde{u} \overline{\psi} \right] dx \\ & - i \sum_{\ell \in \mathbb{Z}} \sqrt{k^2 - (\ell + \alpha)^2} \tilde{u}_\ell(h_0) \overline{\psi}_\ell(h_0) \\ & = \int_Q e^{-i\alpha x_1} f(x) \overline{\psi(x)} dx \quad \text{for all } \psi \in H^1_{per,0}(Q). \end{aligned} \tag{5}$$

- (b) (Part (b) in Theorem 3.1, [1]) If $\tilde{u} \in H^1_{per,0}(Q)$ solves (5) then $u(x) = e^{i\alpha x_1} \tilde{u}(x)$ for $x \in Q$ and its extension by the Rayleigh expansion (4) is in $H^1_{\alpha,0,loc}(\mathbb{R}^2_+)$ and satisfies (1).
- (c) The variational equation (5) can be written as $(I - K_{k,\alpha})\tilde{u} = r_\alpha$ in $H^1_{per,0}(Q)$ where $r_\alpha \in H^1_{per,0}(Q)$ and $K_{k,\alpha}$ is a compact operator from $H^1_{per,0}(Q)$ into itself. The operator depends continuously on $\alpha \in [-1/2, 1/2]$ and $k > 0$. Furthermore, for every $\hat{k} > 0$ and $\hat{\alpha} \in [-1/2, 1/2]$ which is not a cut-off value with respect to \hat{k} there exist neighborhoods $U, V \subset \mathbb{C}$ of \hat{k} and $\hat{\alpha}$, respectively, such that $K_{k,\alpha}$ depends analytically on $(k, \alpha) \in U \times V$. Finally, r_α depends analytically on $\alpha \in \mathbb{C}$.

Proof For the proof for the parts (a) and (b) we refer to [1]. For (c) we choose

$$(u, v)_* = \int_Q [\nabla u \cdot \nabla \overline{v} + u \overline{v}] dx + \sum_{\ell \in \mathbb{Z}} |\ell| u_\ell(h_0) \overline{v_\ell(h_0)} \tag{6}$$

as the inner product in $H^1_{per,0}(Q)$. The Theorem of Riesz implies the existence of $r \in H^1_{per,0}(Q)$ and an operator $K_{k,\alpha}$ from $H^1_{per,0}(Q)$ into itself that (5) can be written as $(I - K_{k,\alpha})\tilde{u} = r_\alpha$. The compact imbedding of $H^1_{per,0}(Q)$ in $L^2(Q)$ and the boundedness of $\sqrt{k^2 - (\ell + \alpha)^2} - |\ell|$ yield compactness of $K_{k,\alpha}$.

The fact that $\hat{\alpha}$ is not a cutoff value implies the existence of $c > 0$ with $|\hat{k}^2 - (\ell + \hat{\alpha})^2| \geq c$ for all $\ell \in \mathbb{Z}$. We show that there exists $c_1 > 0$ and $\delta > 0$ such that also $|\text{Re}[k^2 - (\ell + \alpha)^2]| \geq c_1$ for all $\ell \in \mathbb{Z}$ and all $k, \alpha \in \mathbb{C}$ with $|k - \hat{k}| < \delta$ and $|\alpha - \hat{\alpha}| < \delta$. We consider three cases:

- (i) $|\ell| \geq \hat{k} + 2$. Then $\operatorname{Re}[(\ell + \alpha)^2 - k^2] = (\ell + \operatorname{Re} \alpha)^2 - (\operatorname{Im} \alpha)^2 - (\operatorname{Re} k)^2 + (\operatorname{Im} k)^2 \geq (|\ell| - 1)^2 - (\operatorname{Re} k)^2 - (\operatorname{Im} \alpha)^2 \geq (\hat{k} + 1)^2 - (\operatorname{Re} k)^2 - (\operatorname{Im} \alpha)^2 \geq c_1$ for sufficiently small $|\operatorname{Re} k - \hat{k}|$ and $|\operatorname{Im} \alpha|$.
- (ii) $|\ell| \leq \hat{k} + 2$ and $\hat{k}^2 - (\ell + \hat{\alpha})^2 \geq c$. Then $\operatorname{Re}[k^2 - (\ell + \alpha)^2] = (\operatorname{Re} k)^2 - (\operatorname{Im} k)^2 - (\ell + \operatorname{Re} \alpha)^2 + (\operatorname{Im} \alpha)^2 \geq c + [(\operatorname{Re} k)^2 - \hat{k}^2] - (\operatorname{Im} k)^2 + [(\ell + \hat{\alpha})^2 - (\ell + \operatorname{Re} \alpha)^2] \geq c + [(\operatorname{Re} k)^2 - \hat{k}^2] - (\operatorname{Im} k)^2 - |\hat{\alpha} - \operatorname{Re} \alpha| \cdot 2(\hat{k} + 2)|\hat{\alpha} + \operatorname{Re} \alpha| \geq c_1$ for sufficiently small $|k - \hat{k}|$ and $|\hat{\alpha} - \alpha|$.
- (iii) $|\ell| \leq \hat{k} + 2$ and $(\ell + \hat{\alpha})^2 - \hat{k}^2 \geq c$. Then $\operatorname{Re}[(\ell + \alpha)^2 - k^2] = (\ell + \operatorname{Re} \alpha)^2 - (\operatorname{Im} \alpha)^2 - (\operatorname{Re} k)^2 + (\operatorname{Im} k)^2 \geq c + [\hat{k}^2 - (\operatorname{Re} k)^2] - (\operatorname{Im} \alpha)^2 + [(\ell + \operatorname{Re} \alpha)^2 - (\ell + \hat{\alpha})^2] \geq c + [\hat{k}^2 - (\operatorname{Re} k)^2] - (\operatorname{Im} \alpha)^2 - |\hat{\alpha} - \operatorname{Re} \alpha| \cdot 2(\hat{k} + 2)|\hat{\alpha} + \operatorname{Re} \alpha| \geq c_1$ for sufficiently small $|k - \hat{k}|$ and $|\hat{\alpha} - \alpha|$.

Recalling our choice of the branch of the square root function we observe that the square roots in (5) are holomorphic with respect to k and α and their derivatives with respect to k or α are bounded with respect to ℓ . Therefore, the operator $K_{k,\alpha}$ depends analytically on k and α in neighborhoods $U, V \subset \mathbb{C}$ of \hat{k} and $\hat{\alpha}$, respectively. \square

Under the following assumption it can easily be shown as in, e.g., [1] that every propagating mode ϕ corresponding to some quasi-momentum α is evanescent; that is, $\phi_\ell(\pm h_0) = 0$ for all $|\ell + \alpha| \leq k$; that is, there exist $c, \delta > 0$ with $|\phi(x)| \leq c e^{-\delta x^2}$ for all $x_2 > h_0$.

Assumption 3 Let $|\ell + \alpha| \neq k$ for all quasi-momentums α and all $\ell \in \mathbb{Z}$; that is, the cut-off values are not quasi-momentums.

Lemma 4 Under Assumption 3 there exists at most a finite number of quasi-momentums in $[-1/2, 1/2]$. Furthermore, if α is a quasi-momentum with mode ϕ then $-\alpha$ is a quasi-momentum with mode $\bar{\phi}$. Therefore, we can numerate the quasi-momentums in $[-1/2, 1/2]$ such they are given by $\{\hat{\alpha}_j : j \in J\}$ where $J \subset \mathbb{Z}$ is symmetric with respect to 0 and $\hat{\alpha}_{-j} = -\hat{\alpha}_j$ for $j \in J$. Furthermore, it is known that every eigenspace

$$\hat{X}_j = \{\phi \in H^1_{\hat{\alpha}_j, 0, loc}(\mathbb{R}^2_+) : \phi \text{ satisfies (3) and (4)}\} \tag{7}$$

is finite dimensional with some dimension $m_j > 0$.

Proof We recall that $\pm\kappa$ are the cut-off values in $[-1/2, 1/2]$. We can cover the set $[-1/2, 1/2] \setminus \{\kappa, -\kappa\}$ by at most three open sets $U_j \subset \mathbb{C}$ such that the operator $K_{k,\alpha}$ depends analytically on $\alpha \in \cup_j U_j$. Assume that there exists an infinite number of quasi-momentums in $[-1/2, 1/2]$. Then a subsequence converges to some $\alpha \in [-1/2, 1/2]$ and, without loss of generality, this subsequence lies in one of the U_j . By the analytic Fredholm theory (see, e.g. [37]) either every point of U_j is a quasi-momentum or the discrete set of quasi-momentums has no limits point in U_j ; that is, $\alpha \in [-1/2, 1/2] \cap \partial U_j$ which implies that α coincides with κ or $-\kappa$. In any case, by a perturbation argument, α is a quasi-momentum which contradics Assumption 3. \square

In [1] it is shown that a suitable basis of \hat{X}_j is given by the eigenfunctions $\{\hat{\phi}_{\ell,j} : \ell = 1, \dots, m_j\}$ of the following selfadjoint generalised eigenvalue problem

$$-2i \int_{Q^\infty} \bar{\psi} \partial_1 \hat{\phi}_{\ell,j} dx = \lambda_{\ell,j} 2k \int_{Q^\infty} n \hat{\phi}_{\ell,j} \bar{\psi} dx, \quad \psi \in \hat{X}_j, \tag{8a}$$

for $\ell = 1, \dots, m_j$ with normalization

$$2k \int_{Q^\infty} n \hat{\phi}_{\ell,j} \overline{\hat{\phi}_{\ell',j}} dx = \delta_{\ell,\ell'}. \tag{8b}$$

3 The limiting absorption solution for the unperturbed case

First we study the unperturbed problem with a wavenumber $k + i\varepsilon$ for some $k > 0$ and $\varepsilon > 0$. Then the Theorem of Lax-Milgram implies that the problem $\Delta u_\varepsilon + (k + i\varepsilon)^2 u_\varepsilon = -f$ has a unique solution $u_\varepsilon \in H^1(\mathbb{R}_+^2)$ with $u_\varepsilon = 0$ for $x_2 = 0$. We apply the (periodic) Floquet-Bloch transform to u_ε . Therefore,

$$\tilde{u}(x, \varepsilon, \alpha) = \sum_{\ell \in \mathbb{Z}} u_\varepsilon(x_1 + 2\pi\ell, x_2) e^{-i(x_1 + 2\pi\ell)\alpha}$$

is in $H^1_{per,0}(Q^\infty)$ and is the unique periodic (wrt x_1) solution of $\Delta \tilde{u}(\cdot, \varepsilon, \alpha) + 2i\alpha \partial_1 \tilde{u}(\cdot, \varepsilon, \alpha) + [(k + i\varepsilon)^2 - \alpha^2] \tilde{u}(\cdot, \varepsilon, \alpha) = -\tilde{f}(\cdot, \alpha)$ in Q^∞ with $\tilde{u}(\cdot, \varepsilon, \alpha) = 0$ for $x_2 = 0$. We note that the function \tilde{f} has the form $\tilde{f}(x, \alpha) = e^{-i\alpha x_1} f(x)$ because the support of f is in Q . By the analog of Lemma 2 (equation (5)) the function \tilde{u} satisfies

$$\begin{aligned} & \int_Q \left[\nabla \tilde{u} \cdot \nabla \bar{\psi} - 2i\alpha \partial_1 \tilde{u} \bar{\psi} - ((k + i\varepsilon)^2 n - \alpha^2) \tilde{u} \bar{\psi} \right] dx \\ & - i \sum_{\ell \in \mathbb{Z}} \sqrt{(k + i\varepsilon)^2 - (\ell + \alpha)^2} \tilde{u}_\ell(h_0) \overline{\psi_\ell(h_0)} \\ & = \int_Q f(x) e^{-i\alpha x_1} \overline{\psi(x)} dx \quad \text{for all } \psi \in H^1_{per,0}(Q). \end{aligned} \tag{9}$$

We write this in the form

$$(I - K_{\varepsilon,\alpha}) \tilde{u}(\varepsilon, \alpha) = R_\alpha f \quad \text{in } H^1_{per,0}(Q) \tag{10}$$

where

$$((I - K_{\varepsilon,\alpha})v, \psi)_* = \int_Q \left[\nabla v \cdot \nabla \bar{\psi} - 2i\alpha \partial_1 v \bar{\psi} - ((k + i\varepsilon)^2 n - \alpha^2) v \bar{\psi} \right] dx$$

$$-i \sum_{\ell \in \mathbb{Z}} \sqrt{(k+i\varepsilon)^2 - (\ell+\alpha)^2} v_\ell(h_0) \overline{\psi_\ell(h_0)}, \tag{11a}$$

$$(R_\alpha g, \psi)_* = \int_Q g(x) e^{-i\alpha x_1} \overline{\psi(x)} dx \tag{11b}$$

for all $v, \psi \in H^1_{per,0}(Q)$ and $g \in L^2(Q)$, where $(\cdot, \cdot)_*$ is given by (6).

It is the aim to apply the following abstract representation theorem. First, we introduce the (punctured) cylinder $B_\delta := \{(\varepsilon, \alpha) \in [0, \delta] \times \mathbb{C} : |\alpha| < \delta, \varepsilon + |\alpha| > 0\} \subset \mathbb{R} \times \mathbb{C}$, which is an extension from the results in Sect. 5 in [1].

Theorem 5 *Let $0 \in V \subset \mathbb{C}$ be an open set. Let $K(\varepsilon, \alpha) : H \rightarrow H$ be a family of compact operators from a (complex) Hilbert space H into itself and $r(\varepsilon, \alpha) \in H$ such that $(\varepsilon, \alpha) \mapsto K(\varepsilon, \alpha)$ and $(\varepsilon, \alpha) \mapsto r(\varepsilon, \alpha)$ are continuously differentiable on $[0, \varepsilon_0] \times \overline{V}$ for some $\varepsilon_0 > 0$.¹ Set $L(\varepsilon, \alpha) := I - K(\varepsilon, \alpha)$ and assume the following:*

- (i) *The null space $\mathcal{N} := \mathcal{N}(L(0, 0))$ is not trivial and the Riesz number of $L(0, 0)$ is one; that is, the algebraic and geometric multiplicities of the eigenvalue 1 of $K(0, 0)$ coincide. Let $P : H \rightarrow \mathcal{N} \subset H$ be the projection operator onto \mathcal{N} corresponding to the direct decomposition $H = \mathcal{N} \oplus \mathcal{R}(L(0, 0))$,*
- (ii) *$A := iP \frac{\partial}{\partial \varepsilon} L(0, 0)|_{\mathcal{N}} : \mathcal{N} \rightarrow \mathcal{N}$ is selfadjoint and positive definite and $B := -P \frac{\partial}{\partial \alpha} L(0, 0)|_{\mathcal{N}} : \mathcal{N} \rightarrow \mathcal{N}$ is selfadjoint and one-to-one.*

Let $\{\lambda_\ell, \phi_\ell : \ell = 1, \dots, m\}$ be an orthonormal eigensystem of the following generalized selfadjoint problem in the m -dimensional space \mathcal{N} :

$$-B\phi_\ell = \lambda_\ell A\phi_\ell \text{ in } \mathcal{N} \text{ with normalization } (A\phi_\ell, \phi_{\ell'})_H = \delta_{\ell, \ell'}. \tag{12}$$

We set $M := \{(\varepsilon, \alpha) \in \mathbb{R} \times \mathbb{C} : \sigma \operatorname{Im} \alpha \leq 0\}$ if all λ_ℓ have the same sign $\sigma \in \{+, -\}$, otherwise we set $M := \mathbb{R} \times \mathbb{R}$. Then there exists $\delta > 0$ such that:

- (a) *For $(\varepsilon, \alpha) \in M \cap B_\delta$ the equation $L(\varepsilon, \alpha)u(\varepsilon, \alpha) = r(\varepsilon, \alpha)$ has a unique solution $u(\varepsilon, \alpha) \in H$, and $u(\varepsilon, \alpha)$ has the form*

$$u(\varepsilon, \alpha) = u^b(\varepsilon, \alpha) - \sum_{\ell=1}^m \frac{r_\ell}{i\varepsilon - \lambda_\ell \alpha} \phi_\ell \text{ for } (\varepsilon, \alpha) \in M \cap B_\delta, \tag{13}$$

where $r_\ell = (Pr(0, 0), \phi_\ell)_H$ are the expansion coefficients of $A^{-1}Pr(0, 0)$ with respect to the inner product $(A \cdot, \cdot)_H$; that is, $Pr(0, 0) = \sum_{\ell=1}^m r_\ell A\phi_\ell$. Furthermore, $u^b(\varepsilon, \alpha)$ depends continuously on $(\varepsilon, \alpha) \in M \cap B_\delta$ and there exists $c > 0$ with $\|u^b(\varepsilon, \alpha)\|_H \leq c \|r\|_{C^1(\overline{B_\delta}; H)}$ for all $(\varepsilon, \alpha) \in M \cap B_\delta$.²

¹ That is, the partial derivatives with respect to the real variable ε and the complex variable α exist in $(0, \varepsilon_0)$ and V , respectively, and can be continued continuously into $[0, \varepsilon_0]$ and \overline{V} , respectively.

² Here, $\|r\|_{C^1(\overline{B_\delta}; H)} = \sup_{(\varepsilon, \delta) \in B_\delta} \|r(\varepsilon, \delta)\|_H + \sup_{(\varepsilon, \delta) \in B_\delta} \|\partial_\varepsilon r(\varepsilon, \delta)\|_H + \sup_{(\varepsilon, \delta) \in B_\delta} \|\partial_\alpha r(\varepsilon, \delta)\|_H$.

- (b) If all λ_ℓ have the same sign $\sigma \in \{+, -\}$ then $u^b(\varepsilon, \cdot)$ depends analytically³ on $\alpha \in \{\alpha \in \mathbb{C} : |\alpha| < \delta, \sigma \operatorname{Im} \alpha < 0\}$ for every $\varepsilon \in (0, \delta)$.
- (c) For $\varepsilon = 0$ the part $u^b(0, \cdot)$ depends analytically on $\alpha \in \{\alpha \in \mathbb{C} : |\alpha| < \delta\}$.

Proof We project the equation $u(\varepsilon, \alpha) - K(\varepsilon, \alpha)u(\varepsilon, \alpha) = r(\varepsilon, \alpha)$ onto \mathcal{N} and $\mathcal{R} := \mathcal{R}((L(0, 0))$. Decomposing $u(\varepsilon, \alpha)$ into $u(\varepsilon, \alpha) = u^N(\varepsilon, \alpha) + u^R(\varepsilon, \alpha)$ with $u^N(\varepsilon, \alpha) \in \mathcal{N}$ and $u^R(\varepsilon, \alpha) \in \mathcal{R}$ the equation is equivalent to the system

$$\begin{aligned} u^N(\varepsilon, \alpha) - PK(\varepsilon, \alpha)[u^N(\varepsilon, \alpha) + u^R(\varepsilon, \alpha)] &= Pr(\varepsilon, \alpha), \\ u^R(\varepsilon, \alpha) - QK(\varepsilon, \alpha)[u^N(\varepsilon, \alpha) + u^R(\varepsilon, \alpha)] &= Qr(\varepsilon, \alpha). \end{aligned}$$

The operator $[I - QK(0, 0)]|_{\mathcal{R}} : \mathcal{R} \rightarrow \mathcal{R}$ is invertible. Therefore, there exists $\delta_1 > 0$ such that $[I - QK(\varepsilon, \alpha)]|_{\mathcal{R}} : \mathcal{R} \rightarrow \mathcal{R}$ is invertible for all $(\varepsilon, \alpha) \in B_\delta$. Set $T(\varepsilon, \alpha) := [I - QK(\varepsilon, \alpha)]|_{\mathcal{R}}^{-1} : \mathcal{R} \rightarrow \mathcal{R}$. Then we solve the second equation for $u^R(\varepsilon, \alpha)$ and substitute it into the first equation which gives

$$\begin{aligned} u^N(\varepsilon, \alpha) - PK(\varepsilon, \alpha)[I + T(\varepsilon, \alpha)QK(\varepsilon, \alpha)]u^N(\varepsilon, \alpha) &= Pr(\varepsilon, \alpha) \\ &+ PK(\varepsilon, \alpha)T(\varepsilon, \alpha)Qr(\varepsilon, \alpha) \end{aligned}$$

in the finite dimensional space \mathcal{N} . We abbreviate this as $C(\varepsilon, \alpha)u^N(\varepsilon, \alpha) = g(\varepsilon, \alpha)$. We note that $C(0, 0) = 0$ and $g(0, 0) = Pr(0, 0)$ and $\partial_\varepsilon C(0, 0) = -P\partial_\varepsilon K(0, 0)|_{\mathcal{N}} = -iA$ and $\partial_\alpha C(0, 0) = -P\partial_\alpha K(0, 0)|_{\mathcal{N}} = -B$.

We compare the equation $C(\varepsilon, \alpha)u^N(\varepsilon, \alpha) = g(\varepsilon, \alpha)$ with the linearized equation

$$[i\varepsilon A + \alpha B]\tilde{u}(\varepsilon, \alpha) = -g(0, 0) = -Pr(0, 0) \text{ in } \mathcal{N}.$$

This equation is explicitly solved by

$$\tilde{u}(\varepsilon, \alpha) = -\sum_{\ell=1}^m \frac{r_\ell}{i\varepsilon - \lambda_\ell \alpha} \phi_\ell \text{ for all } (\varepsilon, \alpha) \in M \text{ where } Pr(0, 0) = \sum_{\ell=1}^m r_\ell A\phi_\ell.$$

Indeed, if $M = \mathbb{R} \times \mathbb{R}$ then $|i\varepsilon - \lambda_\ell \alpha|^2 = \varepsilon^2 + \lambda_\ell^2 \alpha^2 \geq \gamma(\varepsilon^2 + \alpha^2)$ for all $(\varepsilon, \alpha) \in M$ with $\gamma = \min\{1, \lambda_1^2, \dots, \lambda_m^2\}$. If all λ_ℓ have the same sign $\sigma \in \{+, -\}$ then $|i\varepsilon - \lambda_\ell \alpha|^2 = \varepsilon^2 + \lambda_\ell^2 |\alpha|^2 - 2\varepsilon \lambda_\ell \operatorname{Im} \alpha \geq \gamma(\varepsilon^2 + |\alpha|^2)$ for all $(\varepsilon, \alpha) \in \mathbb{R} \times \mathbb{C}$ with $\sigma \operatorname{Im} \alpha \leq 0$.

Next we show the existence of $c > 1$ such that

$$\frac{1}{c} \|v\|_H \leq \sqrt{\varepsilon^2 + |\alpha|^2} \|[i\varepsilon A + \alpha B]^{-1}v\|_H \leq c \|v\|_H \tag{14}$$

for all $v \in \mathcal{N}$ and $(\varepsilon, \alpha) \in M$. Indeed, let $u = [i\varepsilon A + \alpha B]^{-1}v$. Then, as before, $u = \sum_{\ell=1}^m \frac{v_\ell}{i\varepsilon - \lambda_\ell \alpha} \phi_\ell$ where v_ℓ are the coefficients in the expansion $A^{-1}v = \sum_{\ell=1}^m v_\ell \phi_\ell$.

³ Since the notions of a complex differentiable, a holomorphic, or an analytic function from a domain in \mathbb{C} into a Banach space coincide (see, e.g. [1]), we use the notion of analyticity in the following.

By the orthonormality of $\{\phi_\ell : \ell = 1, \dots, m\}$ with respect to $(Au, v)_H$ we have $(Au, u)_H = \sum_{\ell=1}^m \frac{|v_\ell|^2}{|i\varepsilon - \lambda_\ell \alpha|^2} \leq \frac{1}{\gamma(\varepsilon^2 + |\alpha|^2)} \sum_{\ell=1}^m |v_\ell|^2 = \frac{1}{\gamma(\varepsilon^2 + |\alpha|^2)} (v, A^{-1}v)_H$. Also, the norms $\sqrt{(Av, v)_H}$ and $\sqrt{(u, A^{-1}u)_H}$ are equivalent to $\|v\|_H$ and $\|u\|_H$, respectively, which proves (14).

In particular we have that $\|\tilde{u}(\varepsilon, \alpha)\|_H \leq \frac{c}{\sqrt{\varepsilon^2 + |\alpha|^2}}$. We set $S_{\varepsilon, \alpha} := [i\varepsilon A + \alpha B]^{-1}$ and note that $(\varepsilon, \alpha) \mapsto S_{\varepsilon, \alpha}$ is continuous on M and $\|S_{\varepsilon, \alpha}\| \leq \frac{c}{\sqrt{\varepsilon^2 + |\alpha|^2}}$ for all $(\varepsilon, \alpha) \in M$. If all λ_ℓ have the same sign then $S_{\varepsilon, \alpha}$ depends analytically on α .

Now we consider the difference $v = \tilde{u}(\varepsilon, \alpha) - u^N(\varepsilon, \alpha)$ and have

$$[i\varepsilon A + \alpha B]v(\varepsilon, \alpha) = g(\varepsilon, \alpha) - g(0, 0) + [C(\varepsilon, \alpha) + i\varepsilon A + \alpha B]v(\varepsilon, \alpha) - [C(\varepsilon, \alpha) + i\varepsilon A + \alpha B]\tilde{u}(\varepsilon, \alpha)$$

which we write in the form

$$(I - S_{\varepsilon, \alpha}[C(\varepsilon, \alpha) + i\varepsilon A + \alpha B])v(\varepsilon, \alpha) = S_{\varepsilon, \alpha}[g(\varepsilon, \alpha) - g(0, 0)] - S_{\varepsilon, \alpha}[C(\varepsilon, \alpha) + i\varepsilon A + \alpha B]\tilde{u}(\varepsilon, \alpha)$$

From $\|S_{\varepsilon, \alpha}\| \leq \frac{c}{\sqrt{\varepsilon^2 + |\alpha|^2}}$ and $\|C(\varepsilon, \alpha) + i\varepsilon A + \alpha B\| \leq c(\varepsilon^2 + |\alpha|^2)$ we note that the operator on the left hand side is a small perturbation of the identity. Therefore, this equation is uniquely solvable for all $(\varepsilon, \alpha) \in M \cap B_\delta$ for sufficiently small $\delta > 0$, and the solution v depends continuously on $(\varepsilon, \alpha) \in M \cap B_\delta$, and $\|v\|_H \leq c\|r\|_{C^1(\overline{B_\delta}, H)}$ for all $(\varepsilon, \alpha) \in M \cap B_\delta$ because $\|\tilde{u}(\varepsilon, \alpha)\|_H \leq \frac{c}{\sqrt{\varepsilon^2 + |\alpha|^2}}$ and $\|g(0, 0) - g(\varepsilon, \alpha)\|_H \leq c\sqrt{\varepsilon^2 + |\alpha|^2}$. This implies that $u^N := \tilde{u} - v$ satisfies $C(\varepsilon, \alpha)u^N(\varepsilon, \alpha) = g(\varepsilon, \alpha)$. Furthermore, in the case that all λ_ℓ have the same sign σ the function $v(\varepsilon, \cdot)$ is analytic in $\{\alpha \in \mathbb{C} : |\alpha| < \delta, \sigma \operatorname{Im} \alpha < 0\}$. If $\varepsilon = 0$ then $v(0, \alpha)$ is analytic and uniformly bounded in $\{\alpha \in \mathbb{C} : |\alpha| < \delta, \alpha \neq 0\}$. Finally, we have that

$$u^R(\varepsilon, \alpha) = T(\varepsilon, \alpha) Q K(\varepsilon, \alpha) u^N(\varepsilon, \alpha) + T(\varepsilon, \alpha) Q r(\varepsilon, \alpha) = T(\varepsilon, \alpha) Q (K(\varepsilon, \alpha) - K(0, 0)) u^N(\varepsilon, \alpha) + T(\varepsilon, \alpha) Q r(\varepsilon, \alpha)$$

because $QK(0, 0)u^N(\varepsilon, \alpha) = Qu^N(\varepsilon, \alpha) = 0$. This shows continuity and boundedness of $u^R(\varepsilon, \alpha)$ and ends the proof. □

Later we only need the following conclusions from the previous theorem.

Corollary 6 *Let the assumptions of part (b) of Theorem 5 hold. Then the following holds.*

- (a) $I - K(\varepsilon, \alpha)$ is an isomorphism from H onto itself for all $(\varepsilon, \alpha) \in M \cap B_\delta = \{(\varepsilon, \alpha) \in [0, \delta) \times \mathbb{C} : |\alpha| < \delta, \sigma \operatorname{Im} \alpha \leq 0, \varepsilon + |\alpha| > 0\}$, and the mapping $(\varepsilon, \alpha) \mapsto (I - K(\varepsilon, \alpha))^{-1}$ is continuous from $M \cap B_\delta$ into $\mathcal{L}(H, H)$.
- (b) For fixed $\varepsilon \in (0, \delta)$ and $r \in H$ the mapping $\alpha \mapsto (I - K(\varepsilon, \alpha))^{-1}r$ is analytic on $\{\alpha \in \mathbb{C} : |\alpha| < \delta, \sigma \operatorname{Im} \alpha < 0\}$.

We want to apply Theorem 5 and Corollary 6 to the equation (10) in a neighborhood $V \subset \mathbb{C}$ of some quasi-momentum $\hat{\alpha}_j$ for some $j \in J$ where V is chosen such that it does not contain a cut-off value. (This is possible by Assumption 3 and Lemma 2.) Therefore, we set $K(\varepsilon, \alpha) := K_{\varepsilon, \hat{\alpha}_j + \alpha}$ and $r(\varepsilon, \alpha) := R_{\hat{\alpha}_j + \alpha} f$ and have to check the assumptions of the previous theorem. The operator K and the right hand side r are continuously differentiable with respect to (ε, α) in a neighborhood of $(0, 0)$. It has been shown in [1] that the eigenvalue problem (12) is equivalent to the eigenvalue problem (8a), (8b) and that all the other assumptions of the theorem are satisfied under the following additional assumption.

Assumption 7 $\lambda_{\ell, j} \neq 0$ for all $\ell = 1, \dots, m_j$ and $j \in J$.

In [1] it has shown that the application of Theorem 5 allows us to take the limit $\varepsilon \rightarrow 0$. The following result has been shown.

Theorem 8 *The solution u_ε converges to some solution u of $\Delta u + k^2 nu = -f$ in $H^1(K)$ for every K of the form $K = (-R, R) \times (0, H)$. Furthermore, $u = 0$ for $x_2 = 0$, and u satisfies the radiation condition of Definition 9 below for $q = 0$ with*

$$\psi^\pm(x_1) = \frac{1}{2} \left[1 \pm \frac{2}{\pi} \int_0^{x_1/2} \frac{\sin t}{t} dt \right], \quad x_1 \in \mathbb{R}.$$

The coefficients $a_{\ell, j}$ in (16) are given by

$$a_{\ell, j} = \frac{2\pi i}{|\lambda_{\ell, j}|} \int_Q f(x) \overline{\hat{\phi}_{\ell, j}(x)} dx. \tag{15}$$

Definition 9 Let $\psi^\pm \in C^\infty(\mathbb{R})$ be any pair of functions with $\psi^\pm(x_1) = 1 + \mathcal{O}(1/|x_1|)$ as $\pm x_1 \rightarrow \infty$ and $\psi^\pm(x_1) = \mathcal{O}(1/|x_1|)$ as $\pm x_1 \rightarrow -\infty$.

A solution u of $\Delta u + k^2 nu = -f$ in \mathbb{R}_+^2 satisfies the open waveguide radiation condition if u has a decomposition into $u = u_{rad} + u_{prop}$ where:

(i) The propagating part has the form

$$u_{prop}(x) = \psi^+(x_1) \sum_{j \in J} \sum_{\ell: \lambda_{\ell, j} > 0} a_{\ell, j} \hat{\phi}_{\ell, j}(x) + \psi^-(x_1) \sum_{j \in J} \sum_{\ell: \lambda_{\ell, j} < 0} a_{\ell, j} \hat{\phi}_{\ell, j}(x) \tag{16}$$

for some $a_{\ell, j} \in \mathbb{C}$ defined in equation (15).

(ii) The radiating part satisfies $u_{rad} \in H^1(W_H)$ for all $H > h_0$ and its Fourier transform $(\mathcal{F}u_{rad})(\omega, x_2)$ with respect to x_1 satisfies the generalized Sommerfeld radiation condition

$$\int_{-\infty}^{\infty} \left| \partial_2 (\mathcal{F}u_{rad})(\omega, x_2) - i\sqrt{k^2 - \omega^2} (\mathcal{F}u_{rad})(\omega, x_2) \right|^2 d\omega \longrightarrow 0, \quad x_2 \rightarrow \infty. \tag{17}$$

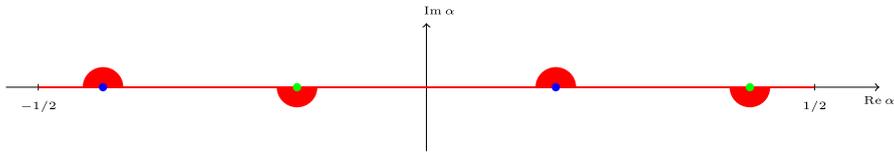


Fig. 1 The set \mathcal{A} (red), $\hat{\alpha}_j$ for $j \in J^+$ (green), $\hat{\alpha}_j$ for $j \in J^-$ (blue) (color figure online)

Here we define the Fourier transform as

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

We note that we can replace ψ^\pm by any pair of functions $\tilde{\psi}^\pm$ with $\tilde{\psi}^\pm(x_1) = 1$ for $\pm x_1 \geq T + 1$ (for some $T > 2\pi$) and $\tilde{\psi}^\pm(x_1) = 0$ for $\pm x_1 \leq T$. This is because the differences $(\psi^\pm - \tilde{\psi}^\pm)\hat{\phi}_{\ell,j}$ are in $H^1(W_H)$ for all H and decay exponentially as $x_2 \rightarrow \infty$ and thus can be subsumed into the radiating part. This representation give rise to the open waveguide radiation condition (Fig. 1).

In this paper we do not repeat the proof of Theorem 8 but use Corollary 6 in a different way. For the remaining part of the paper we make the following assumption.

Assumption 10 For every $j \in J$ all of the eigenvalues $\lambda_{1,j}, \dots, \lambda_{m_j,j}$ have the same sign $\sigma_j \in \{+, -\}$.

Then we group the quasi-momentum $\hat{\alpha}_j$ into right- and left going by defining $J^\pm := \{j \in J : \sigma_j = \pm\}$. Furthermore, we define the following sets

$$\mathcal{A}_j := \{\alpha \in \mathbb{C} : |\alpha - \hat{\alpha}_j| < \delta, \pm \text{Im } \alpha < 0\} \quad \text{for } j \in J^\pm \quad (\text{open half discs}),$$

$$\mathcal{A} := I \cup \bigcup_{j \in J} \overline{\mathcal{A}_j} \setminus \bigcup_{j \in J} (\hat{\alpha}_j - \delta, \hat{\alpha}_j + \delta),$$

$$\mathcal{M} := \{(\varepsilon, \alpha) \in [0, \delta] \times \mathcal{A} : \varepsilon + |\alpha - \hat{\alpha}_j| > 0 \text{ for all } j \in J\}.$$

Application of Corollary 6 to the equation (10) yields the following result .

Lemma 11 *Let Assumptions 3, 7, and 10 hold. Then there exists $\delta > 0$ such that the operators $I - K_{\varepsilon,\alpha}$, defined in (11a), are isomorphisms from $H^1_{per,0}(Q)$ onto itself for all $(\varepsilon, \alpha) \in \mathcal{M}$, and $(\varepsilon, \alpha) \mapsto (I - K_{\varepsilon,\alpha})^{-1}$ is continuous on \mathcal{M} . If $\mathcal{K} \subset \mathcal{M}$ is compact then $\|(I - K_{\varepsilon,\alpha})^{-1}\|$ is uniformly bounded with respect to $(\varepsilon, \alpha) \in \mathcal{K}$. Furthermore, for every $\varepsilon \in (0, \delta)$ the unique solution $\tilde{u}(\varepsilon, \alpha)$ of (10) depends analytically on $\alpha \in \bigcup_{j \in J} \mathcal{A}_j$.*

Formulated in terms of the variational problem (5) we have the following. For every $f \in L^2(Q)$ and $(\varepsilon, \alpha) \in \mathcal{M}$ there exist a unique solution $\tilde{u}(\cdot, \varepsilon, \alpha) \in H^1_{per,0}(Q)$ of (5) which depends continuously on $(\varepsilon, \alpha) \in \mathcal{M}$; that is, $\tilde{u} \in C(\mathcal{M}, H^1_{per,0}(Q))$. For every compact set $\mathcal{K} \subset \mathcal{M}$ there exists $c > 0$ with $\|\tilde{u}(\cdot, \varepsilon, \alpha)\|_{H^1(Q)} \leq c\|f\|_{L^2(Q)}$ for

all $(\varepsilon, \alpha) \in \mathcal{K}$. Finally, for every $\varepsilon \in (0, \delta)$ the solution $\tilde{u}(\cdot, \varepsilon, \alpha)$ depends analytically on $\alpha \in \bigcup_{j \in J} \mathcal{A}_j$.

We recall that the original field u_ε is given by the inverse Floquet-Bloch transform; that is,

$$u_\varepsilon(x_1 + 2\pi p, x_2) = \int_{-1/2}^{1/2} \tilde{u}(x, \varepsilon, \alpha) e^{i\alpha x_1} e^{2\pi p\alpha i} d\alpha, \quad x \in Q, \quad p \in \mathbb{Z}.$$

Therefore, if $\tilde{u}(x, \varepsilon, \alpha)$ is analytic in, say, $\{\alpha \in \mathbb{C} : |\alpha - \hat{\alpha}_j| < \delta, \text{Im } \alpha < 0\}$ then we can modify the path of integration in this integral from the segment $(\hat{\alpha}_j - \delta/2, \hat{\alpha}_j + \delta/2)$ to $\Gamma_j^- := \{\alpha \in \mathbb{C} : |\alpha - \hat{\alpha}_j| = \delta/2, \text{Im } \alpha < 0\}$. With the analogous change for $j \in J^-$ we define the global path

$$\Gamma = I \cup \bigcup_{j \in J^+} \Gamma_j^- \cup \bigcup_{j \in J^-} \Gamma_j^+ \quad \text{where now}$$

$$I := [-1/2, 1/2] \setminus \bigcup_{j \in J} (\hat{\alpha}_j - \delta/2, \hat{\alpha}_j + \delta/2)$$

which connects $-1/2$ with $+1/2$. Application of the previous lemma yields the following form of the Limiting Absorption Principle.

Theorem 12 *Let Assumptions 3, 7, and 10 hold. There exists $\delta > 0$ such that for all $f \in L^2(Q)$ and $\varepsilon \in (0, \delta)$, there is a unique solution $u_\varepsilon \in H_0^1(\mathbb{R}_+^2)$ of (1) for $q = 0$ and wavenumber $k + i\varepsilon$, given by*

$$u_\varepsilon(x_1 + 2\pi p, x_2) = \int_{\Gamma} \tilde{u}(x, \varepsilon, \alpha) e^{i\alpha x_1} e^{2\pi p\alpha i} d\alpha, \quad x \in Q, \quad p \in \mathbb{Z},$$

where $\tilde{u}(\cdot, \varepsilon, \alpha) \in H_{per,0}^1(Q)$ satisfies (5) for all $\alpha \in \Gamma$. Furthermore, u_ε converges to some solution $u \in H^1((-R, R) \times (0, h_0))$ of (1) for $q = 0$, for any $R > 0$. The function u has the representation as

$$u(x_1 + 2\pi p, x_2) = \int_{\Gamma} \tilde{u}(x, 0, \alpha) e^{i\alpha x_1} e^{2\pi p\alpha i} d\alpha, \quad x \in Q, \quad p \in \mathbb{Z},$$

where $\tilde{u}(\cdot, 0, \alpha) \in H_{per,0}^1(Q)$ is the solution of (5) for $\alpha \in \Gamma$ and $\varepsilon = 0$.

Proof This comes directly from the continuous dependence of $\tilde{u}(\cdot, \varepsilon, \alpha)$ on $(\varepsilon, \alpha) \in [0, \delta) \times \Gamma \subset \mathcal{M}$. □

Remark Since for all $\alpha \in \Gamma$, $I - K_{0,\alpha}$ is an isomorphism, the uniqueness of (9)-(10) holds.

4 The perturbed case

In this section, we move on to the case that n is locally perturbed by a function q , i.e., to studying the solution to $\Delta u + k^2(n + q)u = -f$. According to [17], the radiation condition given by Definition 9 guarantees the unique solvability of this problem. Now we will focus on the new formulation in terms of complex contour integrals.

We recall the definition of the path Γ , observe that $\Gamma \subset \mathcal{A}$, and define the operator P from $C(\mathcal{A}, H^1_{per,0}(Q))$ into $L^2(Q)$ by

$$(Pg)(x) = \int_{\Gamma} g(x, \beta) e^{i\beta x_1} d\beta, \quad x \in Q, \quad g \in C(\mathcal{A}, H^1_{per,0}(Q)).$$

Then it is easily seen that P is compact. Indeed, let $g_j \in C(\mathcal{A}, H^1_{per,0}(Q))$ be bounded; that is, $\sup_{\beta \in \mathcal{A}} \|g_j(\cdot, \beta)\|_{H^1(Q)} \leq c$ for all $j \in \mathbb{N}$. Then $\|Pg_j\|_{H^1(Q)} \leq c_1 \int_{\Gamma} \|g_j(\cdot, \beta)\|_{H^1(Q)} d\beta \leq c_2$ for all j . The compactness of $H^1_{per,0}(Q)$ in $L^2(Q)$ yields compactness of P .

We consider now the local perturbation of the periodic case; that is, we look at (1) for arbitrary $q \in L^2(Q)$. We rewrite the equation for $k + i\varepsilon$ instead of k as

$$\Delta u_\varepsilon + (k + i\varepsilon)^2 n u_\varepsilon = -f - (k + i\varepsilon)^2 q u_\varepsilon \quad \text{in } \mathbb{R}^2_+.$$

The (periodic) Floquet-Bloch transformed equation has the form

$$\begin{aligned} &\Delta \tilde{u}_\varepsilon(\cdot, \alpha) + 2i\alpha \partial_1 \tilde{u}_\varepsilon(\cdot, \alpha) + [(k + i\varepsilon)^2 n - \alpha^2] \tilde{u}_\varepsilon(\cdot, \alpha) \\ &= -f e^{-i\alpha x_1} - (k + i\varepsilon)^2 q u_\varepsilon e^{-i\alpha x_1} \\ &= -f e^{-i\alpha x_1} - (k + i\varepsilon)^2 q e^{-i\alpha x_1} \int_{-1/2}^{1/2} \tilde{u}_\varepsilon(\cdot, \beta) e^{i\beta x_1} d\beta \quad \text{in } Q^\infty \end{aligned} \tag{18}$$

for $\alpha \in [-1/2, 1/2]$ and in variational form (compare with (9))

$$\begin{aligned} &\int_Q \left[\nabla \tilde{u}_\varepsilon(\cdot, \alpha) \cdot \nabla \bar{\psi} - 2i\alpha \partial_1 \tilde{u}_\varepsilon(\cdot, \alpha) \bar{\psi} - [(k + i\varepsilon)^2 n - \alpha^2] \tilde{u}_\varepsilon(\cdot, \alpha) \bar{\psi} \right] dx \\ &- i \sum_{\ell \in \mathbb{Z}} \sqrt{(k + i\varepsilon)^2 - (\ell + \alpha)^2} \tilde{u}_{\varepsilon,\ell}(h_0, \alpha) \overline{\psi_\ell(h_0)} \\ &= \int_Q f e^{-i\alpha x_1} \bar{\psi} dx + (k + i\varepsilon)^2 \int_Q q e^{-i\alpha x_1} \bar{\psi} \int_{-1/2}^{1/2} \tilde{u}_\varepsilon(\cdot, \beta) e^{i\beta x_1} d\beta dx \end{aligned} \tag{19}$$

for all $\psi \in H^1_{per,0}(Q)$. As in (9) we write this as

$$(I - K_{\varepsilon,\alpha})\tilde{u}_\varepsilon(\cdot, \alpha) = R_\alpha f + (k + i\varepsilon)^2 R_\alpha \left(q \int_{-1/2}^{1/2} \tilde{u}_\varepsilon(\cdot, \beta) e^{i\beta x_1} d\beta \right).$$

Now we observe that the operators $K_{\varepsilon,\alpha}$ depend smoothly on $\alpha \in \mathcal{A}$. Considering the right hand side as a source and modifying the path of integration is the motivation to study (for fixed $\varepsilon > 0$) the equation

$$(I - K_{\varepsilon,\alpha})v_\varepsilon(\cdot, \alpha) = R_\alpha f + (k + i\varepsilon)^2 R_\alpha(q P v_\varepsilon) \text{ in } H^1_{per,0}(Q) \quad (20)$$

for $\alpha \in \Gamma$ where we recall the definitions of $K_{\varepsilon,\alpha} : H^1_{per,0}(Q) \rightarrow H^1_{per,0}(Q)$ and $R_\alpha : L^2(Q) \rightarrow H^1_{per,0}(Q)$ from (11a), (11b). The corresponding variational formulation is (19) with $\int_{-1/2}^{1/2} v_\varepsilon(\cdot, \beta) e^{i\beta x_1} d\beta$ replaced by $P v_\varepsilon$; that is,

$$\begin{aligned} & \int_Q \left[\nabla v_\varepsilon(\cdot, \alpha) \cdot \nabla \bar{\psi} - 2i\alpha \partial_1 v_\varepsilon(\cdot, \alpha) \bar{\psi} - [(k + i\varepsilon)^2 n - \alpha^2] v_\varepsilon(\cdot, \alpha) \bar{\psi} \right] dx \\ & - i \sum_{\ell \in \mathbb{Z}} \sqrt{(k + i\varepsilon)^2 - (\ell + \alpha)^2} v_{\varepsilon,\ell}(h_0, \alpha) \overline{\psi_\ell(h_0)} \\ & = \int_Q f e^{-i\alpha x_1} \bar{\psi} dx + (k + i\varepsilon)^2 \int_Q q e^{-i\alpha x_1} \bar{\psi} \int_\Gamma v_\varepsilon(\cdot, \beta) e^{i\beta x_1} d\beta dx \quad (21) \end{aligned}$$

for all $\psi \in H^1_{per,0}(Q)$ and $\alpha \in \Gamma$.

Lemma 13 *Let Assumptions 3, 7 and 10 hold. Then there exists $\delta > 0$ such that for all $f \in L^2(Q)$ and $\varepsilon \in (0, \delta)$ there exist a unique solution $v_\varepsilon \in C(\Gamma, H^1_{per,0}(Q))$ of (20) and (21). The function $(\varepsilon, \alpha) \mapsto v_\varepsilon(\cdot, \alpha)$ can be extended to $v \in C(\mathcal{M}, H^1_{per,0}(Q))$ and $v(\cdot, \varepsilon, \alpha)$ depends analytically on $\alpha \in \bigcup_{j \in J} \mathcal{A}_j$ for every $\varepsilon \in (0, \delta)$.*

Furthermore, $v(\cdot, \varepsilon, \alpha) \in H^1_{per,0}(Q)$ is the unique solution of (18) for all $(\varepsilon, \alpha) \in \mathcal{M}$.

Proof First we introduce the operator $T : L^2(Q) \rightarrow C(\Gamma, H^1_{per,0}(Q))$ as $Tg = w_g$ where $w_g \in C(\Gamma, H^1_{per,0}(Q))$ is the unique solution of

$$(I - K_{\varepsilon,\alpha})w_g(\cdot, \alpha) = R_\alpha g \text{ in } H^1_{per,0}(Q) \text{ for all } \alpha \in \Gamma.$$

The existence and boundedness of T is assured by Lemma 11. Then we can write (20) as the fixpoint equation

$$v = T(f + (k + i\varepsilon)^2 q P v) = T f + (k + i\varepsilon)^2 T(q P v) \text{ in } C(\Gamma, H^1_{per,0}(Q))$$

which is of Fredholm type because of the compactness of P . Therefore, it suffices to prove uniqueness. Let $v \in C(\Gamma, H^1_{per,0}(Q))$ be a solution corresponding to $f = 0$. Define $w(\cdot, \alpha) \in H^1_{per,0}(Q)$ as the unique solution of

$$(I - K_{\varepsilon,\alpha})w(\cdot, \alpha) = (k + i\varepsilon)^2 R_\alpha(q P v) \text{ in } H^1_{per,0}(Q) \text{ for all } \alpha \in \mathcal{A}.$$

Then $w \in C(\mathcal{A}, H^1_{per,0}(Q))$, again by Lemma 11. Furthermore, $(I - K_{\varepsilon,\alpha})(v(\cdot, \alpha) - w(\cdot, \alpha)) = 0$ for all $\alpha \in \Gamma$ which implies that $v(\cdot, \alpha) = w(\cdot, \alpha)$ for all $\alpha \in \Gamma$. Therefore, $Pv = Pw$ which shows that w satisfies

$$(I - K_{\varepsilon,\alpha})w(\cdot, \alpha) = (k + i\varepsilon)^2 R_\alpha(q P w) \text{ in } H^1_{per,0}(Q) \text{ for all } \alpha \in \mathcal{A}. \tag{22}$$

Since w depends analytically on $\alpha \in \bigcup_{j \in J} \mathcal{A}_j$ we can change the path of integration and have

$$(Pw)(x) = \int_{-1/2}^{1/2} w(x, \beta) e^{i\beta x_1} d\beta, \quad x \in Q.$$

Therefore, (22) implies that $w(\cdot, \alpha)$ satisfies (19) for $f = 0$ and all $\alpha \in [-1/2, 1/2]$. Standard arguments (setting $\psi = w$ and taking the imaginary part) yields that $w(\cdot, \alpha)$ vanishes for all $\alpha \in [-1/2, 1/2]$. Therefore, $Pw = 0$ and $w(\cdot, \alpha)$ satisfies $(I - K_{\varepsilon,\alpha})w(\cdot, \alpha) = 0$ for all $\alpha \in \mathcal{A}$ which implies again that $w(\cdot, \alpha)$ vanishes in Q for all $\alpha \in \mathcal{A}$.

So far, we kept $\varepsilon > 0$ fixed. However, the extension $w = w(\cdot, \varepsilon, \alpha)$ of $v = v_\varepsilon(\cdot, \alpha)$ is in $C(\mathcal{M}, H^1_{per,0}(Q))$ which ends the proof. \square

Since $(\varepsilon, \alpha) \mapsto v(\cdot, \varepsilon, \alpha)$ is continuous on $[0, \delta) \times \Gamma$ we can let ε tend to zero in (21). We have therefore shown the Limiting Absorption Principle in the following form.

Theorem 14 *Let Assumptions 3, 7 and 10. Then there exists $\delta > 0$ such that for all $f \in L^2(Q)$ and $\varepsilon \in (0, \delta)$ there exist a unique solution $u_\varepsilon \in H^1_0(\mathbb{R}^2_+)$ of (1) for k replaced by $k + i\varepsilon$, and u_ε has the form*

$$u_\varepsilon(x_1, x_2) = \int_\Gamma v_\varepsilon(x, \alpha) e^{i\alpha x_1} d\alpha, \quad x \in W_{h_0},$$

where $v_\varepsilon(\cdot, \alpha) \in H^1_{per,0}(Q)$ satisfies (21) for all $\alpha \in \Gamma$. Furthermore, u_ε converges to some solution $u \in H^1_{loc,0}(W_{h_0})$ of (1). The convergence is in $H^1(K)$ for every $K = (-R, R) \times (0, h_0)$. The function u has the representation as

$$u(x_1, x_2) = \int_\Gamma v_0(x, \alpha) e^{i\alpha x_1} d\alpha, \quad x \in W_{h_0}, \tag{23}$$

where $v_0(\cdot, \alpha) \in H^1_{per,0}(Q)$ is the solution of (21) for $\alpha \in \Gamma$ and $\varepsilon = 0$; that is,

$$(I - K_{0,\alpha})v_0(\alpha) = R_\alpha f + k^2 R_\alpha(q P v_0) \text{ in } H^1_{per,0}(Q), \alpha \in \Gamma, \tag{24}$$

or, in variational form,

$$\begin{aligned} & \int_Q \left[\nabla v_0(\cdot, \alpha) \cdot \nabla \bar{\psi} - 2i\alpha \partial_1 v_0(\cdot, \alpha) \bar{\psi} - [k^2 n - \alpha^2] v_0(\cdot, \alpha) \bar{\psi} \right] dx \\ & - i \sum_{\ell \in \mathbb{Z}} \sqrt{k^2 - (\ell + \alpha)^2} v_{0,\ell}(h_0, \alpha) \overline{\psi_\ell(h_0)} \\ & = \int_Q f e^{-i\alpha x_1} \bar{\psi} dx + k^2 \int_Q q e^{-i\alpha x_1} \bar{\psi} \int_\Gamma v_0(\cdot, \beta) e^{i\beta x_1} d\beta dx \end{aligned} \tag{25}$$

for all $\psi \in H^1_{per,0}(Q)$ and $\alpha \in \Gamma$. v_0 is continuous with respect to α and thus $v_0 \in C(\Gamma, H^1_{per,0}(Q))$.

Remark 1 (25) is the variational formulation of the following coupled system of boundary value problems (formulated only for $\varepsilon = 0$) for $v_0(\cdot, \alpha) \in H^1_{per,0}(Q)$:

$$\begin{aligned} \Delta v_0(\cdot, \alpha) + 2i\alpha \partial_1 v_0(\cdot, \alpha) + [k^2 n - \alpha^2] v_0(\cdot, \alpha) \\ = -f e^{-i\alpha x_1} - k^2 q e^{-i\alpha x_1} \int_\Gamma v_0(\cdot, \beta) e^{i\beta x_1} d\beta \text{ in } Q, \end{aligned} \tag{26a}$$

$$v_0(\cdot, \alpha) = 0 \text{ for } x_2 = 0, \tag{26b}$$

$$\partial_2 v_{0,\ell}(h_0, \alpha) = i\sqrt{k^2 - (\ell + \alpha)^2} v_{0,\ell}(h_0, \alpha), \tag{26c}$$

for all $\alpha \in \Gamma$.

Theorem 15 Let Assumptions 3, 7 and 10 hold. Let $v_0 \in C(\Gamma, H^1_{per,0}(Q))$ be a solution of the system (25). Then the corresponding field u , defined in (23), has an extension into \mathbb{R}^2_+ which satisfies (1) and the radiation condition of Definition 9.

Proof From (24) we conclude that $(I - K_{0,\alpha})v_0(\alpha) = g_\alpha$ in $H^1_{per,0}(Q)$ for all $\alpha \in \Gamma$ with $g_\alpha := R_\alpha f + k^2 R_\alpha(q P v_0(\alpha))$. By Lemma 11 $\alpha \mapsto v_0(\alpha)$ is continuous in \mathcal{A} and can be extended analytically into $\cup_{j \in J} \mathcal{A}_j$. We consider the parts Γ_j^\pm of the integration curve in (23). Let, for example, $j \in J^+$. Then $v_0(x, \alpha)e^{i\alpha x_1}$ has the representation (cf Theorem 5)

$$v_0(x, \alpha) e^{i\alpha x_1} = v^b(x, 0, \alpha) e^{i\alpha x_1} + \frac{1}{\alpha - \hat{\alpha}_j} \sum_{\ell=1}^{m_j} \frac{r_{\ell,j}}{\lambda_{\ell,j}} \hat{\phi}_{\ell,j}(x) e^{i(\alpha - \hat{\alpha}_j)x_1}, \quad x \in Q, \tag{27}$$

for $0 < |\alpha - \hat{\alpha}_j| < \delta$. The part v^b is analytic in $\{\alpha \in \mathbb{C} : |\alpha - \hat{\alpha}_j| < \delta\}$ and v_0 analytic in $\{\alpha \in \mathbb{C} : 0 < |\alpha - \hat{\alpha}_j| < \delta\}$. Now we extend $v_0(\cdot, \alpha)$ into $Q^\infty \setminus Q$ by

$$v_0(x, \alpha) = \sum_{\ell \in \mathbb{Z}} v_{0,\ell} e^{i\sqrt{k^2 - (\ell + \alpha)^2}(x_2 - h_0)} e^{i\ell x_1}, \quad x_2 > h_0,$$

for all $\alpha \in I \cup \{\alpha \in \mathbb{C} : 0 < |\alpha - \hat{\alpha}_j| < \delta/2\}$ where $v_{0,\ell} = v_{0,\ell}(h_0, \alpha)$ are the Fourier coefficients of $v_0(\cdot, \alpha)$ on $(0, 2\pi) \times \{h_0\}$. We note that for $|\ell| \geq k + 1$ we have that $\text{Re}[k^2 - (\ell + \alpha)^2] = k^2 - (\ell + \text{Re } \alpha)^2 + (\text{Im } \alpha)^2 < 0$ for sufficiently small $\delta > 0$. Therefore, $\text{Im } \sqrt{k^2 - (\ell + \alpha)^2} > 0$, and the series $\sum_{|\ell| \geq k+1} v_{0,\ell} e^{i\sqrt{k^2 - (\ell + \alpha)^2}(x_2 - h_0)} e^{i\ell x_1}$ decays exponentially as $x_2 \rightarrow \infty$. The finite sum $\sum_{|\ell| < k+1} v_{0,\ell} e^{i\sqrt{k^2 - (\ell + \alpha)^2}(x_2 - h_0)} e^{i\ell x_1}$ can grow exponentially.

Since the functions $\hat{\phi}_{\ell,j}$ are already solutions of the Helmholtz equation in all of \mathbb{R}_+^2 we can take (27) as the definition of $v^b(x, 0, \alpha)$ for $x_2 > h_0$ and $0 < |\alpha - \hat{\alpha}_j| < \delta$. Then v^b is still analytic in $\{\alpha \in \mathbb{C} : 0 < |\alpha - \hat{\alpha}_j| < \delta\}$. Therefore,

$$\begin{aligned} \int_{\Gamma_j^-} v_0(x, \alpha) e^{i\alpha x_1} d\alpha &= \int_{\Gamma_j^-} u^b(x, 0, \alpha) e^{i\alpha x_1} d\alpha + \int_{\Gamma_j^-} \frac{1}{\alpha - \hat{\alpha}_j} e^{i(\alpha - \hat{\alpha}_j)x_1} d\alpha \sum_{\ell=1}^{m_j} \frac{r_{\ell,j}}{\lambda_{\ell,j}} \hat{\phi}_{\ell,j}(x) \\ &= \int_{\hat{\alpha}_j - \delta/2}^{\hat{\alpha}_j + \delta/2} u^b(x, 0, \alpha) e^{i\alpha x_1} d\alpha + \int_{C^-} \frac{1}{\alpha} e^{i\alpha x_1} d\alpha \sum_{\ell=1}^{m_j} \frac{r_{\ell,j}}{\lambda_{\ell,j}} \hat{\phi}_{\ell,j}(x) \end{aligned}$$

for $x \in Q^\infty$ where $C^- := \{\alpha \in \mathbb{C} : |\alpha| = \delta/2, \text{Im } \alpha < 0\}$. We compute

$$\begin{aligned} \int_{C^-} \frac{1}{\alpha} e^{i\alpha x_1} d\alpha &= \int_{C^-} \frac{d\alpha}{\alpha} + \int_{C^-} \frac{\cos(\alpha x_1) - 1}{\alpha} d\alpha + i \int_{C^-} \frac{\sin(\alpha x_1)}{\alpha} d\alpha \\ &= \pi i + \int_{-\delta/2}^{\delta/2} \frac{\cos(\alpha x_1) - 1}{\alpha} d\alpha + i \int_{-\delta/2}^{\delta/2} \frac{\sin(\alpha x_1)}{\alpha} d\alpha \end{aligned}$$

because the integrands of the second and third integrals are holomorphic. The second integral vanishes because the integrand is an odd function. Substituting $t = \alpha x_1$ in the third integral yields

$$\int_{C^-} \frac{d\alpha}{\alpha} = \pi i + 2i \int_0^{\delta x_1/2} \frac{\sin t}{t} dt.$$

Integration for $j \in J^-$; that is, integration over Γ_j^+ is done analogously. Furthermore, integration over the half circles with centers $\pm \kappa$ are reduced to the integrals over the

segments $(\pm\kappa - \delta/2, \pm\kappa + \delta/2)$. Therefore,

$$\begin{aligned}
 u(x) &= \int_{\Gamma} v_0(x, \alpha) e^{i\alpha x_1} d\alpha \\
 &= \int_I v_0(x, \alpha) e^{i\alpha x_1} d\alpha + \sum_{j \in J^+} \int_{\Gamma_j^-} v_0(x, \alpha) e^{i\alpha x_1} d\alpha + \sum_{j \in J^-} \int_{\Gamma_j^+} v_0(x, \alpha) e^{i\alpha x_1} d\alpha \\
 &= \int_I v_0(x, \alpha) e^{i\alpha x_1} d\alpha + \sum_{j \in J} \int_{\hat{\alpha}_j - \delta/2}^{\hat{\alpha}_j + \delta/2} v^b(x, 0, \alpha) e^{i\alpha x_1} d\alpha \\
 &\quad + 2\pi i \left[\frac{1}{2} + \frac{1}{\pi} \int_0^{\delta x_1/2} \frac{\sin t}{t} dt \right] \sum_{j \in J^+} \sum_{\ell=1}^{m_j} \frac{r_{\ell,j}}{\lambda_{\ell,j}} \hat{\phi}_{\ell,j}(x) \\
 &\quad - 2\pi i \left[\frac{1}{2} - \frac{1}{\pi} \int_0^{\delta x_1/2} \frac{\sin t}{t} dt \right] \sum_{j \in J^-} \sum_{\ell=1}^{m_j} \frac{r_{\ell,j}}{\lambda_{\ell,j}} \hat{\phi}_{\ell,j}(x), \quad x \in \mathbb{R}_+^2.
 \end{aligned}$$

With $\psi^\pm(x_1) = \frac{1}{2} \pm \frac{1}{\pi} \int_0^{\delta x_1/2} \frac{\sin t}{t} dt$ we have shown the decomposition of u into a radiating part u_{rad} and the propagating part u_{prop} of the form (16). We have to show part (ii) of the radiation condition of Definition 9.

We set

$$v_{rad}(\cdot, \alpha) = \begin{cases} v_0(\cdot, \alpha), & \alpha \in I, \\ v^b(\cdot, 0, \alpha), & \alpha \in \bigcup_{j \in J} (\hat{\alpha}_j - \delta/2, \hat{\alpha}_j + \delta/2), \\ 0, & \text{else.} \end{cases} \tag{28}$$

Then $v_{rad} \in L^2((-1/2, 1/2), H^1_{per,0}(Q^H))$ for all $H > h_0$ where $Q^H = (0, 2\pi) \times (0, H)$ and $u_{rad}(x) = \int_{-1/2}^{1/2} v_{rad}(x, \alpha) e^{i\alpha x_1} d\alpha$. We conclude that $u_{rad} \in H^1(W_H)$ for all $H < h_0$ by the well known properties of the Floquet-Bloch transform. It remains to show the generalized angular spectral radiation condition (17). First we note that, with $\omega = \ell + \alpha$ where $\ell \in \mathbb{Z}$ and $\alpha \in (-1/2, 1/2]$,

$$\begin{aligned}
 (\mathcal{F}u_{rad})(\omega, x_2) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} u_{rad}(x_1, x_2) e^{-i\omega x_1} dx_1 \\
 &= \frac{1}{\sqrt{2\pi}} \sum_{m \in \mathbb{Z}} \int_0^{2\pi} u_{rad}(x_1 + 2\pi m, x_2) e^{-i(\ell+\alpha)(x_1+2\pi m)} dx_1 \\
 &= \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} v_{rad}(x_1, x_2, \alpha) e^{-i\ell x_1} dx_1 = v_{rad,\ell}(x_2, \alpha)
 \end{aligned}$$

which are the Fourier coefficients of $x_1 \mapsto v_{rad}(x, \alpha)$. Therefore,

$$\begin{aligned} & \int_{-\infty}^{\infty} \left| \partial_2(\mathcal{F}u_{rad})(\omega, x_2) - i\sqrt{k^2 - \omega^2} (\mathcal{F}u_{rad})(\omega, x_2) \right|^2 d\omega \\ &= \sum_{\ell \in \mathbb{Z}} \int_{-1/2}^{1/2} \left| \partial_2(\mathcal{F}u_{rad})(\ell + \alpha, x_2) - i\sqrt{k^2 - (\ell + \alpha)^2} (\mathcal{F}u_{rad})(\ell + \alpha, x_2) \right|^2 d\alpha \\ &= \sum_{\ell \in \mathbb{Z}} \int_{-1/2}^{1/2} \left| \partial_2 v_{rad,\ell}(x_2, \alpha) - i\sqrt{k^2 - (\ell + \alpha)^2} v_{rad,\ell}(x_2, \alpha) \right|^2 d\alpha. \end{aligned}$$

From the definition (28) of v_{rad} we observe that $\partial_2 v_{rad,\ell}(x_2, \alpha) - i\sqrt{k^2 - (\ell + \alpha)^2} v_{rad,\ell}(x_2, \alpha) = \partial_2 v_{0,\ell}(x_2, \alpha) - i\sqrt{k^2 - (\ell + \alpha)^2} v_{0,\ell}(x_2, \alpha) = 0$ for $\alpha \in I$ and $x_2 > h_0$. For $|\alpha - \hat{\alpha}_j| < \delta/2$ with $j \in J^+$ we change the path of integration into C_j^\mp and have from (27) that

$$\begin{aligned} & \sum_{\ell \in \mathbb{Z}} \int_{C_j^\mp} \left| \partial_2 v_\ell^b(x_2, 0, \alpha) - i\sqrt{k^2 - (\ell + \alpha)^2} v_\ell^b(x_2, 0, \alpha) \right|^2 d\alpha \\ & \leq c \sum_{\ell \in \mathbb{Z}} \sum_{\ell'=1}^{m_j} \left[\left| \partial_2 \hat{\phi}_{\ell',j,\ell}(x_2) \right|^2 + |\ell|^2 \left| \hat{\phi}_{\ell',j,\ell}(x_2) \right|^2 \right] \\ & \leq c \sum_{\ell'=1}^{m_j} \int_0^{2\pi} \left[\left| \partial_2 \hat{\phi}_{\ell',j}(x_1, x_2) \right|^2 + \left| \partial_1 \hat{\phi}_{\ell',j}(x_1, x_2) \right|^2 \right] dx_1 \end{aligned}$$

where $\hat{\phi}_{\ell',j,\ell}(x_2) = \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} \hat{\phi}_{\ell',j}(x_1, x_2) e^{-i(\ell + \hat{\alpha}_j)x_1} dx_1$ are the Fourier coefficients of $\hat{\phi}_{\ell',j}(x_1, x_2) e^{-i\hat{\alpha}_j x_1}$. The exponential decay of $\hat{\phi}_{\ell',j}$ and its derivatives yields that this expression tends to zero as $x_2 \rightarrow \infty$. □

Theorem 16 *In addition to Assumptions 3, 7 and 10 we assume that there are no trapped modes of the perturbed problem, i.e. there are no non-trivial solutions $u \in H_0^1(\mathbb{R}_+^2)$ of (1) for $f = 0$. Then, for every $f \in L^2(Q)$ there exists a unique solution $v_0 \in C(\Gamma, H_{per,0}^1(Q))$ of (24) and (25). The mapping $f \mapsto v_0$ is bounded.*

Proof As in the proof of Lemma 13 we introduce the operator $T_0 : L^2(Q) \rightarrow C(\Gamma, H_{per,0}^1(Q))$ by $T_0 g = w_g$ where $w_g \in C(\Gamma, H_{per,0}^1(Q))$ is the unique solution of

$$(I - K_{0,\alpha})w_g(\cdot, \alpha) = R_\alpha g \quad \text{in } H_{per,0}^1(Q) \text{ for all } \alpha \in \Gamma.$$

The existence and boundedness of T_0 is again assured by Lemma 11. Then we write (24) as the fixpoint equation

$$v_0 = T_0(f + k^2qPv_0) = T_0f + k^2T_0(qPv_0) \text{ in } C(\Gamma, H^1_{per,0}(Q))$$

which is again of Fredholm type because of the compactness of P . Therefore, it suffices to prove uniqueness. Let $v_0 \in C(\Gamma, H^1_{per,0}(Q))$ be a solution corresponding to $f = 0$. Define u by (23) in W_{h_0} . Then u satisfies $\Delta u + k^2nu = -k^2qu$ and the open waveguide radiation condition of Definition 9. A well known uniqueness result of Furuya ([36]) yields that u vanishes identically. This implies that $Pv_0 = u$ vanishes and thus $v_0 = 0$ by the injectivity of $I - K_{0,\alpha}$. □

5 The PML-method

Before we go deep into the PML method, we have to furthermore modify the contour Γ (see [27]) in neighborhoods of the cut-off values because the square root function in the definition (11a) of the operator $K_{0,\alpha}$ does not depend analytically on α . Let $k = \hat{\ell} + \kappa$ with $\hat{\ell} \in \mathbb{Z}_{\geq 0}$ and $\kappa \in (-1/2, 1/2]$. We make the additional assumption.

Assumption 17 Assume that the wavenumber $k > 0$ satisfies $2k \notin \mathbb{N}$.

With Assumption 17, $0 < |\kappa| < 1/2$ thus cut-off values are given by $\pm\kappa$. We show how to modify the path Γ of integration in the neighborhoods of $\pm\kappa$. Recall that $\sqrt{k^2 - (\ell + \alpha)^2} = \sqrt{\hat{\ell} + \kappa - \ell - \alpha} \sqrt{\hat{\ell} + \kappa + \ell + \alpha}$ We decompose

$$\begin{aligned} \sum_{\ell \in \mathbb{Z}} \sqrt{k^2 - (\ell + \alpha)^2} v_\ell(h_0) \overline{\psi_\ell(h_0)} &= \sum_{\ell \neq \pm \hat{\ell}} \sqrt{k^2 - (\ell + \alpha)^2} v_\ell(h_0) \overline{\psi_\ell(h_0)} \\ &+ \sqrt{\kappa - \alpha} \sqrt{2\hat{\ell} + \kappa + \alpha} v_{\hat{\ell}}(h_0) \overline{\psi_{\hat{\ell}}(h_0)} + \sqrt{\kappa + \alpha} \sqrt{2\hat{\ell} + \kappa - \alpha} v_{-\hat{\ell}}(h_0) \overline{\psi_{-\hat{\ell}}(h_0)}. \end{aligned}$$

Since $\sqrt{\kappa - \alpha} \sqrt{2\hat{\ell} + \kappa + \alpha}$ is holomorphic in $\{\alpha \in \mathbb{C} : |\alpha - \kappa| < \delta, \text{Im } \alpha < 0\}$ for sufficiently small $\delta > 0$ we modify Γ and replace $(\kappa - \delta/2, \kappa + \delta/2)$ by the half circle $\{\alpha \in \mathbb{C} : |\alpha - \kappa| = \delta/2, \text{Im } \alpha < 0\}$ in the definition of Γ . Analogously, we replace $(-\kappa - \delta/2, -\kappa + \delta/2)$ by the half circle $\{\alpha \in \mathbb{C} : |\alpha + \kappa| = \delta/2, \text{Im } \alpha > 0\}$. In the same way we replace the set \mathcal{A} by $\mathcal{A} \cup \{\alpha \in \mathbb{C} : |\alpha - \kappa| < \delta, \text{Im } \alpha < 0\} \cup \{\alpha \in \mathbb{C} : |\alpha + \kappa| < \delta, \text{Im } \alpha > 0\}$.

We define the PML-operator as in [27] by choosing a complex-valued function $\hat{s} \in C^1[0, h_0 + \tau]$ for some $\tau > 0$ (thickness of the PML-layer) such that $\hat{s}(x_2) = 0$ for $x_2 \leq h_0$ and $\text{Re } \hat{s}(x_2) > 0$ and $\text{Im } \hat{s}(x_2) > 0$ for $x_2 \in [h_0, h_0 + \tau]$. With such a function \hat{s} and parameter $\rho > 0$ we define the function s_ρ by $s_\rho(x_2) = 1 + \rho\hat{s}(x_2)$ for $x_2 \in [0, h_0 + \tau]$. In the following we choose the particular function

$$s_\rho(x_2) = 1 + \rho e^{i\pi/4} \left(\frac{x_2 - h_0}{\tau} \right)^m \text{ for } x_2 \in [h_0, h_0 + \tau], \quad s_\rho(x_2) = 1 \text{ for } x_2 \leq h_0,$$

where $m \geq 1$ is some integer and $\rho > 0$ is the PML-parameter which is assumed to be large. With this function s_ρ we define the operator Δ_ρ by

$$\Delta_\rho u = \frac{\partial^2 u}{\partial x_1^2} + \frac{1}{s_\rho} \frac{\partial u}{\partial x_2} \left(\frac{1}{s_\rho} \frac{\partial}{\partial x_2} \right),$$

and look at the boundary value problem to determine $u = u_\rho \in H_{loc}^1(W_{h_0+\tau})$ with

$$\Delta_\rho u + k^2(n + q)u = -f \text{ in } W_{h_0+\tau}, \quad u = 0 \text{ for } x \in \partial W_{h_0+\tau}. \tag{29}$$

Therefore, instead of (26a)–(26c) we consider

$$\begin{aligned} &\Delta_\rho v(\cdot, \alpha, \rho) + 2i\alpha \partial_1 v(\cdot, \alpha, \rho) + [k^2 n - \alpha^2] v(\cdot, \alpha, \rho) \\ &= -f e^{-i\alpha x_1} - k^2 q e^{-i\alpha x_1} \int_\Gamma v(\cdot, \beta, \rho) e^{i\beta x_1} d\beta \text{ in } (0, 2\pi) \times (0, h_0 + \tau), \end{aligned} \tag{30a}$$

$$v(\cdot, \alpha, \rho) = 0 \text{ for } x_2 = 0 \text{ or } x_2 = h_0 + \tau, \tag{30b}$$

for all $\alpha \in \Gamma$. To compare it with the exact solution we transform this problem to a problem on Q with the help of the Dirichlet to Neumann map. It is well known that the Dirichlet to Neumann map $\Lambda_\alpha : H_{per}^{1/2}(\gamma) \rightarrow H_{per}^{-1/2}(\gamma)$ for the original problem (where $\gamma = (0, 2\pi) \times \{h_0\}$), defined as

$$(\Lambda_\alpha \phi)(x_1, h_0) = i \sum_{\ell \in \mathbb{Z}} \sqrt{k^2 - (\ell + \alpha)^2} \phi_\ell(h_0) e^{i\ell x_1}, \tag{31}$$

is replaced by

$$(\Lambda_{\alpha, \rho} \phi)(x_1, h_0) = i \sum_{\ell \in \mathbb{Z}} \sqrt{k^2 - (\ell + \alpha)^2} \coth(-i\sqrt{k^2 - (\ell + \alpha)^2} \sigma_\rho) \phi_\ell(h_0) e^{i\ell x_1}, \tag{32}$$

where $\sigma_\rho = \int_{h_0}^{h_0+\tau} s_\rho(t) dt = \tau + \rho\chi$ with $\chi = (1 + i) \frac{\tau}{m+1}$. Therefore, (30a), (30b) is equivalent to (compare with (26a)–(26c))

$$\begin{aligned} &\Delta v(\cdot, \alpha, \rho) + 2i\alpha \partial_1 v(\cdot, \alpha, \rho) + [k^2 n - \alpha^2] v(\cdot, \alpha, \rho) \\ &= -f e^{-i\alpha x_1} - k^2 q e^{-i\alpha x_1} \int_\Gamma v(\cdot, \beta, \rho) e^{i\beta x_1} d\beta \text{ in } Q, \end{aligned} \tag{33a}$$

$$v(\cdot, \alpha, \rho) = 0 \text{ for } x_2 = 0, \tag{33b}$$

$$\partial_2 v_\ell(h_0, \alpha, \rho) = i\sqrt{k^2 - (\ell + \alpha)^2} \coth(-i\sqrt{k^2 - (\ell + \alpha)^2} \sigma_\rho) v_\ell(h_0, \alpha, \rho), \tag{33c}$$

for all $\alpha \in \Gamma$. Its variational form is given by

$$\begin{aligned} & \int_Q \left[\nabla v(\cdot, \alpha, \rho) \cdot \nabla \bar{\psi} - 2i\alpha \partial_1 v(\cdot, \alpha, \rho) \bar{\psi} - [k^2 n - \alpha^2] v(\cdot, \alpha, \rho) \bar{\psi} \right] dx \\ & - \langle \Lambda_{\alpha, \rho} v(\cdot, \alpha, \rho), \psi \rangle \\ & = \int_Q f e^{-i\alpha x_1} \bar{\psi} dx + k^2 \int_Q q e^{-i\alpha x_1} \bar{\psi} \int_{\Gamma} v(\cdot, \beta, \rho) e^{i\beta x_1} d\beta dx \end{aligned} \tag{34}$$

for all $\psi \in H^1_{per,0}(Q)$ and $\alpha \in \Gamma$. First we show

Lemma 18 *There exist $c > 0$ and $\mu > 0$ with*

$$\| \Lambda_{\alpha, \rho} - \Lambda_{\alpha} \|_{H^{1/2}(\gamma) \rightarrow H^{-1/2}(\gamma)} \leq c e^{-\mu \rho} \text{ for all } \rho \geq 0 \text{ and } \alpha \in \Gamma. \tag{35}$$

Proof We observe that the difference $\Lambda_{\alpha, \rho} - \Lambda_{\alpha}$ contains

$$\begin{aligned} & \sqrt{k^2 - (\ell + \alpha)^2} \left[\coth(-i\sqrt{k^2 - (\ell + \alpha)^2} \sigma_{\rho}) - 1 \right] \\ & = \frac{2\sqrt{k^2 - (\ell + \alpha)^2}}{e^{-2i\sqrt{k^2 - (\ell + \alpha)^2} \sigma_{\rho}} - 1} = \frac{2\sqrt{k^2 - (\ell + \alpha)^2}}{e^{-2i\sqrt{k^2 - (\ell + \alpha)^2}(\tau + \rho\chi)} - 1}. \end{aligned}$$

We set $\omega := \ell + \alpha = \omega_1 + i\omega_2$ with $\omega_j \in \mathbb{R}$ for abbreviation and $t(\omega) = 2\sqrt{k^2 - \omega^2} = t_1(\omega) + it_2(\omega)$ (with $t_j(\omega) \in \mathbb{R}$) and note that, by the choice of Γ , there exists $c_1 > 0$ with $|\omega| - k \geq c_1$ for all $\omega := \ell + \alpha, \ell \in \mathbb{Z}, \alpha \in \Gamma$. Then, with $\chi_1 = \text{Re } \chi = \frac{\tau}{m+1}$,

$$\begin{aligned} \frac{2\sqrt{k^2 - (\ell + \alpha)^2}}{e^{-2i\sqrt{k^2 - (\ell + \alpha)^2}(\tau + \rho\chi)} - 1} & = \frac{t(\omega)}{e^{-it(\omega)(\tau + \rho\chi)}} \\ & = \frac{t(\omega)}{e^{-i(t_1\tau + t_1\rho\chi_1 - t_2\rho\chi_1)} e^{\rho\chi_1(t_1 + t_2) + t_2\tau} - 1} \end{aligned}$$

and thus

$$\left| \frac{2\sqrt{k^2 - (\ell + \alpha)^2}}{e^{-2i\sqrt{k^2 - (\ell + \alpha)^2}(\tau + \rho\chi)} - 1} \right| \leq \frac{|t(\omega)|}{e^{\rho\chi_1(t_1 + t_2) + t_2\tau} - 1}$$

provided $t_1 + t_2 > 0$. We consider two cases:

- (a) $|\omega| \geq k + c_1$. Then $\omega_1^2 + \omega_2^2 \geq k^2 + c_1^2$ and thus $t_1^2 - t_2^2 = \text{Re}(t^2) = 4 \text{Re}(k^2 - \omega^2) = 4[k^2 - \omega_1^2 + \omega_2^2] \leq 4\omega_2^2 - 4c_1^2 \leq -3c_1^2 =: -c_2$ provided δ (in the definition of Γ) is small enough. Therefore, $t_2 > 0$ (by the choice of the square root function) and $|t_1| \leq t_2 - c_3$ where $c_3 > 0$ is independent of ω . Therefore,

$$\frac{|t(\omega)|}{e^{\rho\chi_1(t_1 + t_2) + t_2\tau} - 1} \leq \frac{|t(\omega)|}{e^{\rho\chi_1(t_2 - (t_2 - c_3))} - 1} = \frac{|t(\omega)|}{e^{\rho\chi_1 c_3} - 1} \leq c e^{-\rho\chi_1 c_3/2}.$$

(b) $|\omega| \leq k + c_1$. Then $\omega_1^2 + \omega_2^2 \leq k^2 - c_1^2$ and thus $t_1^2 - t_2^2 = \operatorname{Re}(t^2) = 4 \operatorname{Re}(k^2 - \omega^2) = 4[k^2 - \omega_1^2 + \omega_2^2] \geq 4\omega_2^2 + 4c_1^2 \geq 4c_1^2 =: c_4$. Therefore, $t_1 > 0$ (again by the choice of the square root function) and $|t_2| \leq t_1 - c_5$ where $c_5 > 0$ is independent of ω . Therefore,

$$\frac{|t(\omega)|}{e^{\rho\chi_1(t_1+t_2)+t_2\tau} - 1} \leq \frac{|t(\omega)|}{e^{\rho\chi_1(t_1-(t_1-c_5))+t_2\tau} - 1} = \frac{|t(\omega)|}{e^{\rho\chi_1 c_5+t_2\tau} - 1} \leq c e^{-\rho\chi_1 c_5/2}$$

because $t_2 = t_2(\omega)$ is bounded in this case.

□

Comparing the forms (25) and (34) and using the previous estimate a perturbation arguments in [27] yields the following result.

Theorem 19 *Let all the assumptions in Theorem 16 and Assumption 17 hold. There exists $\rho_0 > 0$ such that (34) has a unique solution $v(\cdot, \cdot, \rho) \in C(\Gamma, H_{per}^1(Q))$ for all $\rho \geq \rho_0$. Furthermore, there exist $c, \mu > 0$ with*

$$\max_{\alpha \in \Gamma} \|v(\cdot, \alpha, \rho) - v_0(\cdot, \alpha)\|_{H^1(Q)} \leq c e^{-\mu\rho}, \quad \rho \geq \rho_0. \tag{36}$$

As a corollary we transform this result into the fields u . Let

$$u(x_1, x_2) = \int_{\Gamma} v_0(x, \alpha) e^{i\alpha x_1} d\alpha, \quad u(x_1, x_2, \rho) = \int_{\Gamma} v(x, \alpha, \rho) e^{i\alpha x_1} d\alpha$$

for $x \in W_{h_0}$. Then we have

Corollary 20 *Let all the assumptions in Theorem 16 and Assumption 17 hold. There exists $\rho_0 > 0$ such that for all $R > 0$ there exist $c = c(R)$ and $\mu = \mu(R) > 0$ such that*

$$\|u(\cdot, \rho) - u\|_{H^1(Q_R)} \leq c e^{-\mu\rho}, \quad \rho \geq \rho_0. \tag{37}$$

Here, $Q_R = (-R, R) \times (0, h_0)$.

6 Numerical implementation

6.1 A hybrid spectral-FD-method

We use a hybrid spectral-FD method for the approximation of the PML problem (30a), (30b); that is, we expand $v(\cdot, \alpha)$ into the form

$$v(x_1, x_2; \alpha) = \sum_{\ell=-\infty}^{\infty} v_{\ell}(x_2, \alpha) e^{i\ell x_1}.$$

We expand $n(x_1, x_2) = \sum_{m=-\infty}^{\infty} n_m(x_2) e^{imx_1}$ and $f(x_1, x_2)e^{-i\alpha x_1} = \sum_{\ell=-\infty}^{\infty} f_{\ell}(x_2, \alpha) e^{i\ell x_1}$ and $q(x_1, x_2)e^{-i(\alpha-\beta)x_1} = \sum_{m=-\infty}^{\infty} q_m(x_2, \alpha - \beta) e^{imx_1}$ we observe that $v_{\ell}(x_2, \alpha)$ satisfies the following coupled system of ordinary differential equations

$$\begin{aligned} & a(x_2) v_{\ell}''(x_2, \alpha) + b(x_2) v_{\ell}'(x_2, \alpha) - (\ell + \alpha)^2 v_{\ell}(x_2, \alpha) \\ & + k^2 \sum_{m=-\infty}^{\infty} v_m(x_2, \alpha) n_{\ell-m}(x_2) \\ & = f_{\ell}(x_2, \alpha) - k^2 \sum_{m=-\infty}^{\infty} \int_{\Gamma} v_m(x_2, \beta) q_{\ell-m}(x_2, \alpha - \beta) d\beta, \quad x_2 \in (0, h_0 + \tau), \end{aligned}$$

and $v_{\ell}(0, \alpha) = v_{\ell}(h_0 + \tau, \alpha) = 0$ for all $\ell \in \mathbb{Z}$ and $\alpha \in \Gamma$. Here we have set $a = \frac{1}{s^2}$ and $b = \frac{1}{s} (\frac{1}{s})'$.

We restrict ℓ to $\ell \in \{-L, \dots, L\}$ for some $L \in \mathbb{N}$, truncate the series to $\sum_{m=-L}^L$, and approximate the integral by a quadrature rule $\int_{\Gamma} g(\beta) d\beta \approx \sum_{\mu=0}^M w_{\mu} g(\gamma_{\mu})$ for some $\gamma_{\mu} \in \Gamma$ and weights w_{μ} . Setting $\alpha = \gamma_v$ and $v_{\ell}(x_2, \gamma_v) = v_{\ell,v}(x_2)$ the system now reduces to

$$\begin{aligned} & a(x_2) v_{\ell,v}''(x_2) + b(x_2) v_{\ell,v}'(x_2) - (\ell + \gamma_v)^2 v_{\ell,v}(x_2) + k^2 \sum_{m=-L}^L v_{m,v}(x_2) n_{\ell-m}(x_2) \\ & = f_{\ell}(x_2, \gamma_v) - k^2 \sum_{m=-L}^L \sum_{\mu=0}^M w_{\mu} v_{m,\mu}(x_2) q_{\ell-m}(x_2, \gamma_v - \gamma_{\mu}), \quad x_2 \in (0, h_0 + \tau), \end{aligned}$$

and $v_{\ell,v}(0) = v_{\ell,v}(h_0 + \tau) = 0$ for all $\ell = -L, \dots, L$ and $v = 0, \dots, M$.

This coupled system of boundary value problems for ordinary differential equations is approximately solved by a finite difference method: Let $n_y \in \mathbb{N}$ and $h_y = (h_0 + \tau)/n_y$. Then $v_{\ell,v,j} \approx v_{\ell}(jh_y, \gamma_v)$ is determined by

$$\begin{aligned} & \frac{a(jh_y)}{h_y^2} [v_{\ell,v,j+1} + v_{\ell,v,j-1} - 2v_{\ell,v,j}] + \frac{b(jh_y)}{2h_y} [v_{\ell,v,j+1} - v_{\ell,v,j-1}] \\ & + k^2 \sum_{m=-L}^L v_{m,v,j} n_{\ell-m}(jh_y) - (\gamma_v + \ell)^2 v_{\ell,v,j} \\ & = -f_{\ell}(jh_y, \gamma_v) - k^2 \sum_{\mu=0}^M w_{\mu} \sum_{m=-L}^L q_{\ell-m}(jh_y, \gamma_v - \gamma_{\mu}) v_{m,\mu,j} \quad (38) \end{aligned}$$

for $\ell = -L, \dots, L$ and $j = 1, \dots, n_y - 1$ and $v = 0, \dots, M$.

If n and the perturbation q are separable; that is, of the forms $n(x) = n^{(1)}(x_1)n^{(2)}(x_2)$ and $q(x) = q^{(1)}(x_1)q^{(2)}(x_2)$, respectively, then the sum on the left hand side is, for fixed v and j , just a matrix-vector multiplication of $P := (n_{\ell-m}^{(1)})_{\ell,m=1}^L$

with $(v_{m,v,j})_{m=1}^L$. Furthermore, we set

$$Q_{(\ell,v),(m,\mu)} = q_{\ell-m}^{(1)}(\gamma_v - \gamma_\mu) w_\mu \quad \text{and} \quad v_{(m,\mu)} := v_{m,j,\mu}$$

for fixed j . Re-arranging the pairs (ℓ, v) and (m, μ) into one index each the double sum on the right hand side is just a matrix–vector multiplication. The matrices P and Q can be computed beforehand.

Remark 2 Usually, the PML method is used to replace the non-local boundary condition $\partial_2 u = \Lambda_\alpha u$ with the Dirichlet-to-Neumann map Λ_α on $(0, 2\pi) \times \{h_0 + \tau\}$ by local conditions in the PML-layer $(0, 2\pi) \times (h_0, h_0 + \tau)$. For the spectral method – which is already non-local with respect to x_1 – the condition $\partial_2 u = \Lambda_\alpha u$ is local and given by

$$\partial_{x_2} v_m(h_0 + \tau, \alpha) = i\sqrt{k^2 - (m + \alpha)^2} v_m(h_0 + \tau, \alpha).$$

Therefore, we set $a \equiv 1$ and $b \equiv 0$ in (38) and discretize the Rayleigh condition as

$$\frac{1}{2h_y} [v_{\ell,v,n_y} - v_{\ell,v,n_y-2}] = \sqrt{k^2 - (\ell + \gamma_v)^2} v_{\ell,v,n_y-1}.$$

We express v_{ℓ,v,n_y} by v_{ℓ,v,n_y-1} and v_{ℓ,v,n_y-2} and substitute this into equation (38) for $j = n_y - 1$. This yields again a system of $n_y - 1$ unknowns $v_{\ell,v,j}$, $j = 1, \dots, n_y - 1$.

Remark 3 Normally, the PML method is combined with the finite element method due to the convenience from local boundary conditions. The truncation by the Dirichlet-to-Neumann map Λ_α , which is a non-local boundary condition, is extremely complicated when implemented by the finite element method. However, in this section we use the hybrid spectral-FD-method instead of the finite element method due to its high convergence rate. Using this method, we can clearly see the convergence rate in Fig. 4, as is proved in Corollary 20, without extra pollution from the computational errors like in [27]. But we would like to draw to the reader’s attention that the spectral-FD-method is only convenient when n and q are separable. Thus as a universal tool for general n and q , the finite element method is more powerful and the advantage of the PML method becomes clear.

6.2 A particular example

We consider a simple example of the scattering of a mode corresponding to a constant refractive index $n > 1$ in the layer $\mathbb{R} \times (0, 1)$ by a local perturbation q . The propagating modes ϕ^\pm are assumed to be quasi-periodic solutions of $\Delta\phi + k^2 n\phi = 0$ in $\mathbb{R} \times (0, 1)$, $\Delta\phi + k^2\phi = 0$ for $x_2 > 1$, satisfy homogeneous boundary conditions for $x_2 = 0$ and the Rayleigh expansion for $x_2 > 1$ and continuity conditions for ϕ and $\partial_2\phi$ for $x_2 = 1$. They are of the form

$$\phi^\pm(x) = e^{\pm i\omega x_1} \begin{cases} \sin \sqrt{nk^2 - \omega^2} e^{-\sqrt{\omega^2 - k^2}(x_2-1)}, & x_2 > 1, \\ \sin(\sqrt{nk^2 - \omega^2} x_2), & 0 < x_2 < 1. \end{cases}$$

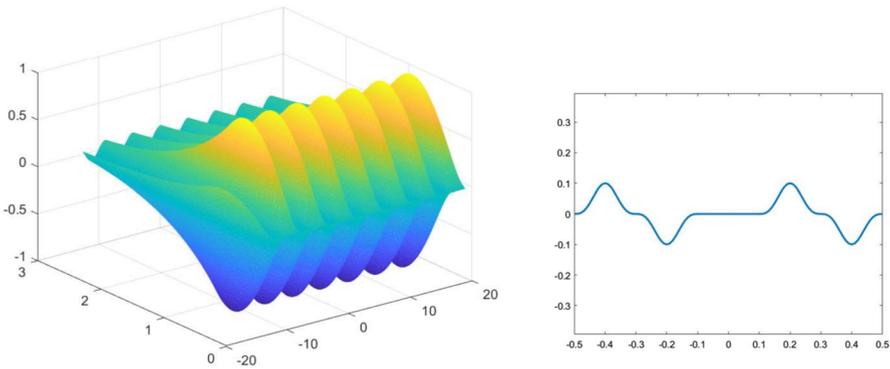


Fig. 2 The real part of the mode ϕ^+ (left) and the curve Γ (right)

Here, $\omega \in (k, \sqrt{nk})$ is a quasi-momentum if k, n , and ω satisfy the equation

$$\sqrt{\omega^2 - k^2} \sin(\sqrt{nk^2 - \omega^2}) + \sqrt{nk^2 - \omega^2} \cos(\sqrt{nk^2 - \omega^2}) = 0.$$

We choose the wavenumber $k > 0$ and frequency $\omega > k$ arbitrarily and determine the constant n such that $\sqrt{k^2n - \omega^2} \cot \sqrt{k^2n - \omega^2} = -\sqrt{\omega^2 - k^2}$. Therefore, we first determine $z \in (\pi/2, \pi)$ such that $z \cot z = -\sqrt{\omega^2 - k^2}$ and then determine n from $z = \sqrt{k^2n - \omega^2}$; that is, $n = \frac{z^2 + \omega^2}{k^2}$. We consider the particular example $k = 0.8$ and $\omega = 1.4$. Then $n \approx 9.8$. We observe that $\hat{\alpha} = 0.4$ and $\kappa = -0.2$ for this example. ϕ^+ is right-going, ϕ^- is left-going. The real part of ϕ^+ is shown in Fig. 2 (left).

We choose $h_0 = 2.5$ and the curve Γ a bit different than in the paper. The half circle $\{z \in \mathbb{C} : |z - a| = \delta, \pm \text{Im } z < 0\}$ for $a \in \mathbb{R}$ is replaced by the curve $\{t \mp i\tilde{\gamma}(t) \in \mathbb{C} : t \in (a - \delta, a + \delta)\}$ where

$$\tilde{\gamma}(t) = \varepsilon \sin^n \left[\frac{\pi}{2} \left(\frac{t - a}{\delta} + 1 \right) \right], \quad a - \delta < t < a + \delta.$$

For our example we take $n = 3$ and $\varepsilon = \delta = 0.1$. This leads to a global parameterization $\alpha = \gamma(t), t \in (0, T)$, of Γ . For the numerical integration of T -periodic functions on Γ we use the trapezoidal rule; that is, $\int_{\Gamma} g(\alpha) d\alpha \approx \sum_{\mu=0}^M w_{\mu} g(\gamma_{\mu})$ with $\gamma_{\mu} = \gamma(\mu T/M)$ for $\mu = 0, \dots, M$ and $w_{\mu} = \frac{T}{M} \gamma'(\mu T/M)$ for $\mu = 1, \dots, M - 1$ and $w_0 = w_M = \frac{T}{2M} \gamma'(0) = \frac{T}{2M}$.

The curve Γ is shown in Fig. 2 (right).

We consider the scattering of the mode ϕ^+ by a local perturbation $q = q(x)$. The total field $u^{tot} = u + \phi^+$ as the sum of the incident field $u^{inc} = \phi^+$, and the scattered field u satisfies $\Delta u^{tot} + k^2(n + q)u^{tot} = 0$. Therefore, the scattered field u satisfies $\Delta u + k^2(n + q)u = -k^2q\phi^+$ and the radiation condition of Definition 9. In this case the source is given by $f = k^2q\phi^+$. Writing the previous equation as

$$\Delta u + k^2nu = -k^2q\phi^+ - k^2qu$$

we can – under a smallness assumption on k^2q – iterate this fixpoint equation for u . The first iteration is the Born approximation u^B , defined as the solution of $\Delta u^B + k^2 n u^B = -k^2 q \phi^+$. As a particular example for the perturbation q we choose $q(x_1, x_2) = q_0 \sin^2(2\omega x_1)$ for $(x_1, x_2) \in (0, \pi/\omega) \times (0.2, 0.7)$ and zero else. Here, $q_0 > 0$ is a parameter. This perturbation has the property that

$$\begin{aligned} \int_Q f(x) \overline{\phi^-(x)} dx &= k^2 \int_Q q(x) \phi^+(x) \overline{\phi^-(x)} dx \\ &= k^2 q_0 \int_0^{\pi/\omega} \sin^2(2\omega x_1) e^{2i\omega x_1} dx_1 \int_{0.2}^{0.7} \sin^2(zx_2) dx_2 = 0 \quad \text{and} \\ \int_Q f(x) \overline{\phi^+(x)} dx &= k^2 \int_Q q(x) |\phi^+(x)|^2 dx > 0. \end{aligned} \tag{39}$$

From (15) we observe that the Born approximation u^B has a right-going mode but no left-going mode.

We choose the parameter $q_0 = n/2$; that is, the perturbation is (in the ∞ -norm) of order 50%. For constant n we rewrite the iterative scheme of (38) as

$$\begin{aligned} \frac{a(jh_y)}{h_y^2} [v_{\ell,v,j+1}^{(t+1)} + v_{\ell,v,j-1}^{(t+1)} - 2v_{\ell,v,j}^{(t+1)}] &+ \frac{b(jh_y)}{2h_y} [v_{\ell,v,j+1}^{(t+1)} - v_{\ell,v,j-1}^{(t+1)}] \\ &+ [k^2 n - (\gamma_v + \ell)^2] v_{\ell,v,j}^{(t+1)} \\ &= -f_\ell(jh_y, \gamma_v) - k^2 \sum_{\mu=0}^M w_\mu \sum_{m=-L}^L q_{\ell-m}(jh_y, \gamma_v - \gamma_\mu) v_{m,\mu,j}^{(t)} \end{aligned} \tag{40}$$

for $\ell = -L, \dots, L$ and $j = 1, \dots, n_y - 1$ and $v = 0, \dots, M$, and $t = 0, 1, \dots$. Setting $v_{m,\mu,j}^{(0)} = 0$ we obtain $v_{m,\mu,j}^{(1)}$ as the Born approximation. The field $u^{(t)}$ is then computed as the integral

$$\begin{aligned} u^{(t)}(x_1, x_2) &= \sum_{\ell=-L}^L \int_\Gamma v_\ell^{(t)}(x_2, \alpha) e^{i(\ell+\alpha)x_1} d\alpha \\ &\approx \sum_{\ell=-L}^L \sum_{\mu=0}^M v_\ell^{(t)}(x_2, \gamma_\mu) w_\mu e^{i(\ell+\gamma_\mu)x_1}. \end{aligned}$$

As a comparison with the PML-method for different parameters ρ we first use the Dirichlet-to-Neumann map as a boundary condition at $x_2 = h_0 + \tau$ as explained in Remark 2. We computed the relative error $e_t := \|u^{(t+1)} - u^{(t)}\|_\infty / \|u^{(t+1)}\|_\infty$ on

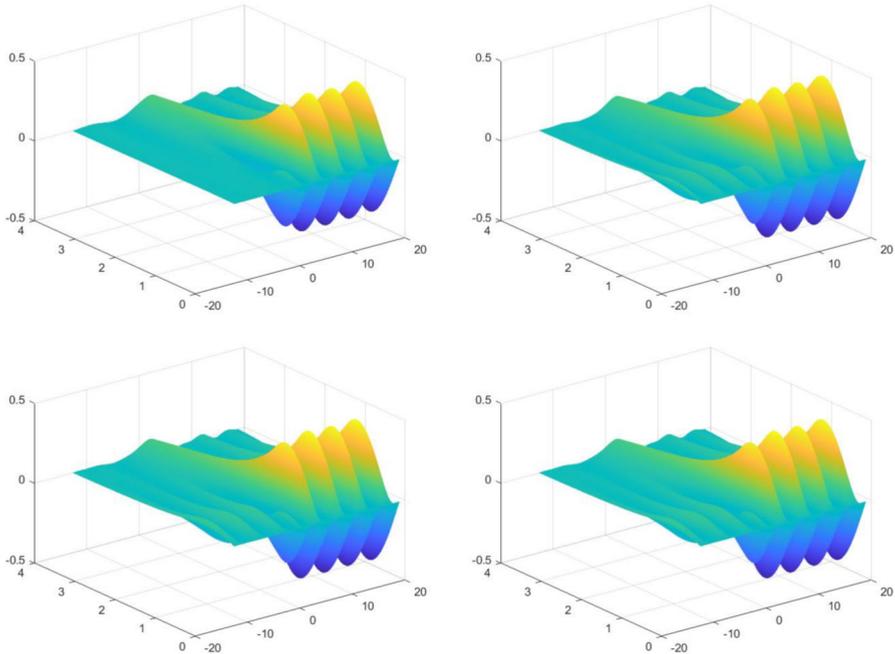


Fig. 3 Real parts of $u^{(1)}$ (i.e. Born), $u^{(2)}$, $u^{(5)}$, and $u^{(9)}$

$(-4\pi, 6\pi) \times (0, 4)$ between consecutive iterates for $t = 1, \dots, 8$ as

t :	1	2	3	4	5	6	7	8
e_t :	0.2276	0.0674	0.0205	0.0048	0.0017	0.0005	0.0001	0.0000

and show the iterations (real parts) $u^{(1)}$ (i.e. Born), $u^{(2)}$, $u^{(5)}$, and $u^{(9)}$ on $(-4\pi, 6\pi) \times (0, 4)$ for the Dirichlet-to-Neumann map in Fig. 3.

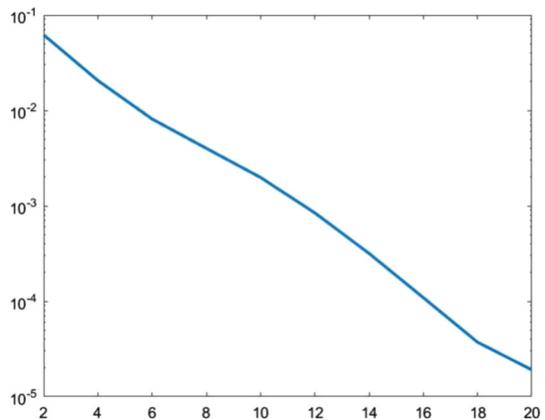
We clearly observe that the Born approximation; that is, the first iteration, has no left going mode because f is orthogonal to ϕ^- , see (39). The further iterations produce right hand sides which are not orthogonal to ϕ^- anymore and, therefore, left going modes of small amplitudes appear.

Next, we implemented the PML-method of (40) to show the dependence of the result with respect to the parameter ρ . We iterated this system and compared the 4th iteration of the PML-method for parameter $\rho = 2, 4, 6, \dots, 20$ with the 4th iteration of the system with Dirichlet-to-Neumann boundary condition. The (semi-logarithmic) plot of the relative errors

$$\max\{|u^{(4)PML}(x) - u^{(4)D2N}(x)| : x \in [-4\pi, 6\pi] \times [0, 0.9 * 2.5]\} / \|u^{(4)D2N}\|_\infty$$

of the 4th iterations is shown in Fig. 4. One clearly observes the exponential decay.

Fig. 4 Error as a function of ρ between the 4th iterates of the PML-method and the D2N-boundary condition



Finally, we summarize the settings of the parameters in our simulations:

k (wavenumber):	0.8
ω (quasi-momentum):	1.4
n (refractive index, determined from k and ω):	≈ 9.8
h_0 (height of domain without PML-layer):	2.5
τ (height of PML-layer):	1.5
s_ρ (PML-function):	$1 + \rho e^{i\pi/4}(x_2 - h_0)^3/\tau^3$
n_y (number of discretization points in $(0, h_0 + \tau)$):	512
L (summation bound for spectral representation):	7
M (number of discretization/integration points on Γ):	101

We observed that the results do not depend crucially on the values of n_y , L , or M , or the parameters of s_ρ .

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