Sweeping preconditioners for the iterative solution of quasiperiodic Helmholtz transmission problems in layered media

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Abstract

We present a sweeping preconditioner for quasi-optimal Domain Decomposition Methods (DD) applied to Helmholtz transmission problems in periodic layered media. Quasi-optimal DD (QO DD) for Helmholtz equations rely on transmission operators that are approximations of Dirichlet-to-Neumann (DtN) operators. Employing shape perturbation series, we construct approximations of DtN operators corresponding to periodic domains, which we then use as transmission operators in a non-overlapping DD framework. The Robin-to-Robin (RtR) operators that are the building blocks of DD are expressed via robust boundary integral equation formulations. We use Nyström discretizations of quasiperiodic boundary integral operators to construct high-order approximations of RtR. Based on the premise that the quasi-optimal transmission operators should act like perfect transparent boundary conditions, we construct an approximate LU factorization of the tridiagonal QO Schwarz iteration matrix associated with periodic layered media, which is then used as a double sweep preconditioner. We present a variety of numerical results that showcase the effectiveness of the sweeping preconditioners applied to QO DD for the iterative solution of Helmholtz transmission problems in periodic layered media.

Keywords: Helmholtz transmission problems, domain decomposition methods, periodic layered media, sweeping preconditioners.

AMS subject classifications: 65N38, 35J05, 65T40,65F08

1 Introduction

The numerical simulation of interactions between electromagnetic, acoustic, and elastic waves with periodic layered media has numerous applications in the fields of optics, photonics, and geophysics [6]. Given the important technological applications of periodic layered media, the simulation of wave propagation in such environments has attracted significant attention [7, 18, 24, 26, 27]. Regardless of the type of discretization (finite elements, finite differences, boundary integral operators), iterative solvers are the preferred method of solution especially for high-frequency layered configurations that involve large numbers of layers which may contain inclusions. The iterative solution of high-frequency Helmholtz and Maxwell equations in complex media is a challenging computational problem [13], and one successful strategy to tackle this problem relies on sweeping preconditioners [11]. We present in this paper several preconditioners for a DD formulation of such problems in two dimensional periodic layered media.

DD are natural candidates for the solution of Helmholtz transmission problems in periodic layered media [24, 26, 27]. Local subdomain solutions (the subdomains may or may not coincide with the periodic layers) are linked iteratively via Robin type transmission conditions defined on inter-domain interfaces. Ideally, the transmission operators should act as transparent boundary conditions that allow information to flow out of each subdomain with very little information being reflected back. As such, for a given subdomain, optimal transmission operators on the subdomain interface consist of Dirichlet-to-Neumann (DtN) operators associated with the adjacent subdomain that shares the same interface. In practice, the transmission operators are constructed via various approximations of DtN operators that rely either on Fourier calculus [2, 12] or Perfectly Matched Layers [29, 31]; the ensuing DD are referred to as Quasi-Optimal DD (QO DD) or Optimized Schwarz Methods [13].

The main goal of this paper is the design of QO DD for the solution of Helmholtz transmission problems in periodic layered media separated by grating profiles (i.e. graphs of periodic functions). We present two strategies of subdomain partitions: (1) the subdomains coincide with the layer subdomains and the subdomain interfaces coincide with the grating profiles of material discontinuity of the layered medium; and (2) the subdomains consist of horizontal slabs whose flat boundaries do not intersect any of the grating profiles of material discontinuity. We note that the DD partition strategy (2) is only applicable to layered media configurations where the height of the layers is larger than the roughness of their interfaces. In each subdomain a local quasiperiodic Helmholtz equation with generalized Robin conditions must be solved (the wavenumber may be discontinuous in case (2)), and generalized Robin data on the subdomain boundaries are linked with those corresponding to the adjacent subdomain. The generalized Robin data corresponding to a given subdomain is defined in terms of transmission operators that are approximations of DtN operators corresponding to the adjacent subdomain. Such approximations of periodic DtN operators can be obtained via high-order shape perturbation series in case (1) [25]. Specifically, using as a small parameter the roughness/elevation height of the grating, the periodic DtN operators are expressed as a perturbation series whose terms can be computed recursively. The zeroth order terms of the perturbation series coincide with DtN of layered domains with flat interfaces, which can be written explicitly in terms of Fourier multipliers. In the case of the subdomain partition (2), since the subdomain interfaces are flat, the transmission operators are chosen to be the aforementioned Fourier multipliers. We establish that the ensuing QO DD corresponding to both subdomain partitions are equivalent to the original transmission problem, with the caveat that the roughness of the grating profiles must be small enough for the subdomain partition in case (2).

The exchange of Robin data amongst the subdomains in DD is realized via quasiperiodic Robin-to-Robin (RtR) operators that map incoming to outgoing subdomain Robin data. Following the methodology introduced in [26], we express quasiperiodic RtR operators in terms of robust boundary integral equation formulations. The discretization of the RtR maps is realized by extending the high-order Nyström method, based on trigonometric interpolation and windowing quasiperiodic Green functions [26], to the case of DtN transmission operators. Since the terms in the shape deformation series expansions of DtN operators are expressed in terms of Fourier multipliers [25], the discretization of the QO transmission operators is straightforward within the framework of trigonometric interpolation. Using Nyström discretization RtR matrices, we discretize the QO DD formulation for layered transmission problems in the form of a block tridiagonal matrix which we invert using Krylov subspace iterative methods. However, the numbers of iterations required for the solution of QO DD linear systems grows with the number of layers, especially for high frequency/high-contrast configurations. In order to alleviate this situation, we construct a double sweep preconditioner based on an approximate LU factorization of the block tridiagonal QO DD/Schwarz iteration matrix that uses similar ideas to those introduced in [29]. The key insight in our construction of the LU factorization is related to the observation that if the transmission operators were to behave as perfect transparent boundary conditions, certain blocks in the QO DD matrix can be approximated by zero [29]. This approximation renders the LU factorization particularly simple as it bypasses altogether the need for inversions of block matrices. We mention that it is possible to formulate the Optimized Schwartz method using different, quite efficient, methods such as source transfers or polarized traces [28, 31] that lead to superior iterative behavior. Their implementation in the present context is the subject of ongoing investigation.

We present a variety of numerical results that highlight the benefits of QO DD formulations for the solution of transmission problems in periodic layered media, as well as the effectiveness of the sweeping preconditioners in the presence of large numbers of layers at high frequencies. With regards to the latter regime, we find that the sweeping preconditioners used in conjunction with QO DD and slab subdomain partitions are particularly effective. We mention that the quasi-optimal transmission operators based on Fourier square-root principal symbol approximations of DtN operators have been already used in several contributions [2, 16, 29]; we simply extend the square root Fourier calculus to the periodic setting and incorporate it within the high-order shape deformation expansions technology introduced in [25]. Furthermore, the construction of the sweeping preconditioners that we employ in this paper was originally introduced in [29] and further elaborated upon in [13]. The main contributions of this paper are (a) the integration of these two important ideas within a high-order Nyström discretization of robust quasiperiodic boundary integral equation formulations of RtR maps, as well as (b) the analysis of the quasiperiodic QO DD. The generalization of the DD with slab subdomain partitioning is currently under investigation; this would entail careful treatment of cross points (i.e. points on the subdomain boundaries where the wavenumbers are discontinuous), which we plan to pursue along the lines of the contribution [16].

The paper is organized as follows: in Section 2 we present the formulation of Helmholtz transmission problems in periodic layered media. In Section 3 we present QO DD formulations of the periodic Helmholtz transmission problem. We continue in Section 4 with the construction of quasi-optimal transmission operators based on high-order shape perturbation series. We show in Section 5 a means to express the QO DD RtR operators in terms of robust quasiperiodic boundary integral equation formulations, which, in turn, enable us to analyze the equivalence between the QO DD formulations and the original Helmholtz transmission problems. Finally, we conclude in Section 6 with the construction of the sweeping preconditioner and a presentation of a variety of numerical results that illustrate the effectiveness of these preconditioners in the context considered in this paper.

2 Scalar transmission problems

We consider the problem of two dimensional quasiperiodic scattering by penetrable homogeneous periodic layers. We assume that the layers are given by $\Omega_j = \{(x_1, x_2) \in \mathbb{R}^2 : \overline{F_j} + F_j(x_1) \leq x_2 \leq \overline{F_{j-1}} + F_{j-1}(x_1)\}$ for $1 \leq j \leq N$ and $\Omega_0 = \{(x_1, x_2) \in \mathbb{R}^2 : \overline{F_0} + F_0(x_1) \leq x_2\}$ and $\Omega_{N+1} = \{(x_1, x_2) \in \mathbb{R}^2 : x_2 \leq \overline{F_N} + F_N(x_1)\}$. All the functions F_j are periodic with principal period d, that is $F_j(x_1 + d) = F_j(x_1)$ for all $0 \leq j \leq N$, and $\overline{F_j} \in \mathbb{R}, 0 \leq j \leq N$. We assume that the medium occupying the layer Ω_j is homogeneous and its permittivity is ϵ_j; the wavenumber k_j in the layer Ω_j is given by $k_j = \omega\sqrt{\epsilon_j}$. We assume that a plane wave $u^{inc}(\mathbf{x}) = \exp(i(\alpha x_1 - \beta x_2))$, where $\alpha^2 + \beta^2 = k_0^2$, impinges on the layered structure, and we are interested in looking for α

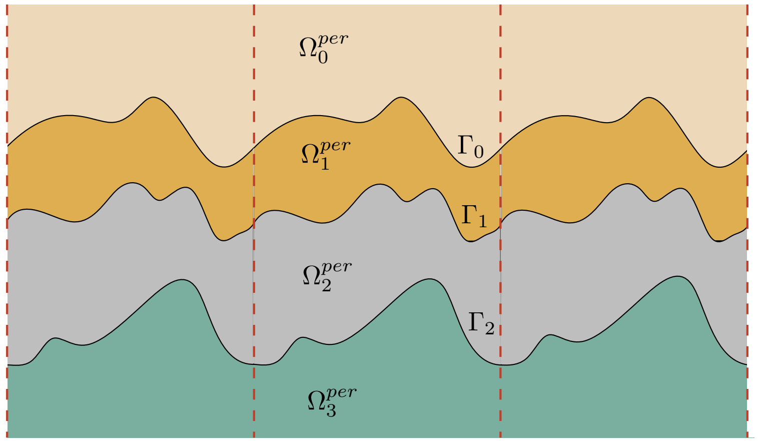

Figure 1: Typical periodic layer structure with $N = 2$.

quasiperiodic fields u_j that satisfy the following system of equations:

$$\begin{aligned}
\Delta u_j + k_j^2 u_j &= 0, && \text{in} \quad \Omega_j^{per} := \{(x_1, x_2) \in \Omega_j : 0 \le x_1 \le d\},\\
u_j + \delta_0^j u^{inc} &= u_{j+1}, && \text{on} \quad \Gamma_j = \{(x_1, x_2) : 0 \le x_1 \le d,\ x_2 = \overline{F_j} + F_j(x_1)\},\\
\gamma_j(\partial_{\nu_j} u_j + \delta_0^j \partial_{\nu_j} u^{inc}) &= -\gamma_{j+1}\partial_{\nu_{j+1}} u_{j+1}, && \text{on} \quad \Gamma_j.
\end{aligned} \tag{2.1}$$

where δ_0^j is the Kronecker delta symbol. Here ν_j denote the unit normals to the boundary $\partial\Omega_j$ pointing to the exterior of the subdomain Ω_j (i.e. for the domain Ω_0 we define $n_0(x_1) = (F_0'(x_1), -1)^\top$ and $\nu_0 = n_0/|n_0|$ on Γ_0, for the domains $\Omega_j,\ 1 \le j \le N$ we define $n_j(x_1) = (-F_{j-1}'(x_1), 1)^\top$ and $\nu_j = n_j/|n_j|$ on Γ_{j-1} as well as $n_j(x_1) = (F_j'(x_1), -1)^\top$ and $\nu_j = n_j/|n_j|$ on Γ_j, and finally, for the domain Ω_{N+1}, $n_{N+1}(x_1) = (-F_N'(x_1), 1)^\top$ and $\nu_{N+1} = n_{N+1}/|n_{N+1}|$ on Γ_N). We note that with this convention on unit normals we have that $\nu_j = -\nu_{j+1}$ as well as $n_j = -n_{j+1}$ on Γ_j. We also assume that u_0 and u_{N+1} in equations (2.1) are radiative in Ω_0 and Ω_{N+1} respectively. The latter requirement amounts to expressing the solutions u_0 and u_{N+1} in terms of Rayleigh series

$$u_0(x_1, x_2) = \sum_{r\in\mathbb{Z}} B_r^+ e^{i\alpha_r x_1 + i\beta_{0,r} x_2}, \quad x_2 > \overline{F_0} + \max F_0, \tag{2.2}$$

and

$$u_{N+1}(x_1, x_2) = \sum_{r\in\mathbb{Z}} B_r^- e^{i\alpha_r x_1 - i\beta_{N+1,r} x_2}, \quad x_2 < \overline{F_N} + \min F_N, \tag{2.3}$$

where $\alpha_r = \alpha + \frac{2\pi}{d} r$, $\beta_{0,r} = (k_0^2 - \alpha_r^2)^{1/2}$, and $\beta_{N+1,r} = (k_{N+1}^2 - \alpha_r^2)^{1/2}$. The branches of the square roots in the definition of $\beta_{0,r}$ and $\beta_{N+1,r}$ are chosen in such a way that $\sqrt{1} = 1$, and the branch cut coincides with the negative imaginary axis. We assume that the wavenumbers k_j and the quantities γ_j in the subdomains Ω_j are positive real numbers. In electromagnetic applications, $\gamma_j = 1$ or $\gamma_j = \epsilon_j^{-1}$ depending whether the incident radiation is transverse electric (TE) or transverse magnetic (TM). For the sake of simplicity, we consider in this contribution the case $\gamma_j = 1$; extensions to general positive γ_j are straightforward.

3 Domain decomposition approach

The transmission problem (2.1) can be formulated via boundary integral equations (BIEs) [1, 7] or via non-overlapping DD [24, 26]. Upon discretization, both the BIE and DD amount to solving block tridiagonal linear systems. In the case of large numbers of layers, the ensuing (large) linear systems are solved via direct methods [7, 26] that rely on Schur complements. As such, the applicability of direct solvers for the numerical solution of the transmission problem (2.1) is limited by the size of the Schur complements. Iterative solvers, on the other hand, do not suffer from the aforementioned size limitations, yet are challenged by the presence of significant multiple scattering, especially in high-contrast multi-layer configurations at high frequencies. In the high-frequency regime, relevant to technological applications, efficient preconditioners are needed in order to alleviate multiple scattering. The main scope of this contribution is to present such a preconditioner (referred to as the sweeping preconditioner [11, 29, 31]) in the context of DD formulation of quasiperiodic transmission problems.

The main idea of DD is to divide the computational domain into subdomains, and to match quasiperiodic subdomain solutions of Helmholtz equations via Robin type transmission conditions on the subdomain interfaces. We consider in what follows two strategies of partitioning the computational domain into non-overlapping subdomains: the most natural one in which the DD subdomains coincide with the layer domains Ω_j^{per}, and an alternative one in which the subdomains are horizontal strips. We present in what follows the details of the first subdomain partitioning strategy mentioned above.

3.1 DD with subdomains Ω_j^{per}

A natural non-overlapping domain decomposition approach to the solution of equations (2.1) consists of solving subdomain problems in $\Omega_j^{per}, j = 0, \ldots, N+1$ with matching Robin transmission boundary conditions on the common subdomain interfaces Γ_j for $j = 0, \ldots, N$. Indeed, this procedure amounts to computing α-quasiperiodic subdomain solutions:

$$\begin{aligned}
\Delta u_j + k_j^2 u_j &= 0 \quad \text{in} \quad \Omega_j^{per}, \qquad (3.1)\\
(\partial_{n_0} u_0 + \partial_{n_0} u^{inc}) + Z_{1,0}(u_0 + u^{inc}) &= -\partial_{n_1} u_1 + Z_{1,0} u_1 \text{ on } \Sigma_{0,1} := \Gamma_0\\
\partial_{n_1} u_1 + Z_{0,1} u_1 &= -(\partial_{n_0} u_0 + \partial_{n_0} u^{inc}) + Z_{0,1}(u_0 + u^{inc}) \text{ on } \Sigma_{1,0} := \Gamma_0\\
\partial_{n_j} u_j + Z_{j+1,j} u_j &= -\partial_{n_{j+1}} u_{j+1} + Z_{j+1,j} u_{j+1} \text{ on } \Sigma_{j,j+1} := \Gamma_j,\ 1 \le j \le N\\
\partial_{n_{j+1}} u_{j+1} + Z_{j,j+1} u_{j+1} &= -\partial_{n_j} u_j + Z_{j,j+1} u_j \text{ on } \Sigma_{j+1,j} := \Gamma_j, 1 \le j \le N.
\end{aligned}$$

where $Z_{j+1,j} : H^{1/2}(\Sigma_{j,j+1}) \to H^{-1/2}(\Sigma_{j,j+1})$, $Z_{j,j+1} : H^{1/2}(\Sigma_{j+1,j}) \to H^{-1/2}(\Sigma_{j+1,j})$ are certain transmission operators for $0 \le j \le N$, and $\partial_{n_j} = n_j \cdot \nabla$. In addition, we require that u_0 and u_{N+1} are radiative. We have chosen to double index the interfaces between layer subdomains: the first index j refers to the index of the layer Ω_j, whereas the second index ℓ denotes the index of the layer Ω_ℓ adjacent to the layer Ω_j so that $\Sigma_{j,\ell}$ is the interface between Ω_j and Ω_ℓ. Here and in what follows $H^s(\Gamma)$ denote Sobolev spaces of α-quasiperiodic functions/distributions defined on the periodic interface Γ; the definition of these spaces is given in terms of Fourier series [26].

Heuristically, in order to give rise to rapidly convergent iterative DD, the transmission operators $Z_{j+1,j}$ ought to be good approximations of the restriction to $\Sigma_{j+1,j} = \Sigma_{j,j+1}$ of the DtN operator associated with the α-quasiperiodic Helmholtz equation in the domain Ω_{j+1} with wavenumber k_{j+1}. This requirement explains why the indices are reversed in the definition of the transmission operators. In addition, the transmission operators $Z_{j+1,j}$ and $Z_{j,j+1}$ ought to be selected to meet the following two criteria: (1) the subdomain boundary value problems that incorporate these transmission operators in the form of generalized Robin boundary conditions are well-posed for all frequencies, and (2) the DD matching of the generalized Robin data on the interfaces of material discontinuity (which coincide with the layer boundaries) is equivalent to the original transmission conditions (2.1) on the same interfaces.

Specifically, with regards to the issue (1) above, we require that for a given layer domain Ω_j with $1 \leq j \leq N$, the following α-quasiperiodic boundary value problem is well-posed:

$$\begin{aligned} \Delta w_j + k_j^2 w_j &= 0 \quad \text{in } \Omega_j^{per} \\ \partial_{n_j} w_j + Z_{j-1,j} w_j &= g_{j,j-1} \quad \text{on } \Sigma_{j,j-1} \\ \partial_{n_j} w_j + Z_{j+1,j} w_j &= g_{j,j+1} \quad \text{on } \Sigma_{j,j+1} \end{aligned} \tag{3.2}$$

where $g_{j,j-1}$ and $g_{j,j+1}$ are generic α-quasiperiodic functions defined on $\Sigma_{j,j-1}$ and $\Sigma_{j,j+1}$ respectively. The following coercivity properties

$$\Im\langle Z_{j-1,j}\varphi_{j,j-1},\ \varphi_{j,j-1}\rangle < 0 \quad \text{and} \quad \Im\langle Z_{j+1,j}\varphi_{j,j+1},\ \varphi_{j,j+1}\rangle < 0, \tag{3.3}$$

for all $\varphi_{j,j-1} \in H^{1/2}(\Sigma_{j,j-1}),\ \varphi_{j,j+1} \in H^{1/2}(\Sigma_{j,j+1})$ in terms of the $H^{1/2}$ and $H^{-1/2}$ duality pairings $\langle\cdot,\cdot\rangle$ are sufficient conditions for guaranteeing the well posedness of the boundary value problems (3.2). Indeed, this can be established easily by an application of the Green's identities in the domain Ω_j^{per}. In the case of the semi-infinite domain Ω_0, we require that the following α-quasiperiodic boundary value problem is well-posed:

$$\begin{aligned} \Delta w_0 + k_0^2 w_0 &= 0 \quad \text{in } \Omega_0^{per} \\ \partial_{n_0} w_0 + Z_{1,0}\ w_0 &= g_{0,1} \quad \text{on } \Sigma_{0,1} \end{aligned} \tag{3.4}$$

where $g_{0,1}$ is a α-quasiperiodic function defined on $\Sigma_{0,1}$. The coercivity property

$$\Im\langle Z_{1,0}\varphi_{0,1},\ \varphi_{0,1}\rangle < 0, \quad \text{for all } \varphi_{0,1} \in H^{1/2}(\Sigma_{0,1}), \tag{3.5}$$

suffices to establish the well posedness of the boundary value (3.4). The latter fact can be established via the same arguments as those in Theorem 3.1 in [26]. A similar coercivity condition imposed on the operator $Z_{N,N+1}$ ensures the well posedness of the analogous α-quasiperiodic boundary value problem on the semi-infinite domain Ω_{N+1}.

Returning to the requirement (2) above, we ask that the DD matching of the generalized Robin data

$$\begin{aligned} \partial_{n_j} u_j + Z_{j+1,j} u_j &= -\partial_{n_{j+1}} u_{j+1} + Z_{j+1,j} u_{j+1} \quad \text{on} \quad \Sigma_{j,j+1},\ 1 \leq j \leq N \\ \partial_{n_{j+1}} u_{j+1} + Z_{j,j+1} u_{j+1} &= -\partial_{n_j} u_j + Z_{j,j+1} u_j \quad \text{on} \quad \Sigma_{j+1,j}, 1 \leq j \leq N \end{aligned}$$

is equivalent to the continuity conditions

$$u_j = u_{j+1} \qquad \text{and} \qquad \partial_{n_j} u_j = -\partial_{n_{j+1}} u_{j+1} \quad \text{on} \quad \Gamma_j = \Sigma_{j,j+1} = \Sigma_{j+1,j}, 1 \leq j \leq N.$$

It can be immediately seen that the equivalence in part (2) is guaranteed provided that $Z_{j,j+1} + Z_{j+1,j} : H^{1/2}(\Gamma_j) \to H^{-1/2}(\Gamma_j)$ is an injective operator. Under the assumption that the coercivity properties (3.3) hold, it follows that

$$\Im\langle (Z_{j,j+1} + Z_{j+1,j})\varphi,\ \varphi\rangle < 0, \quad \text{for all } \varphi \in H^{1/2}(\Gamma_j),$$

and thus the operators $Z_{j,j+1} + Z_{j+1,j}$ are injective for all $1 \leq j \leq N$. Thus, the coercivity properties (3.3) ensure that both requirements (1) and (2) above are met. We postpone the discussion on the selection of the transmission operators $Z_{j,j+1}$ and $Z_{j+1,j}$ and we formulate the DD system (3.1) in matrix operator form. To that end, we define certain RtR operators associated with the boundary value problems (3.2). Specifically, we define the RtR map $\mathcal{S}^j$ in the following manner:

$$\mathcal{S}^j \begin{bmatrix} g_{j,j-1} \\ g_{j,j+1} \end{bmatrix} = \begin{bmatrix} \mathcal{S}^j_{j-1,j-1} & \mathcal{S}^j_{j-1,j+1} \\ \mathcal{S}^j_{j+1,j-1} & \mathcal{S}^j_{j+1,j+1} \end{bmatrix} \begin{bmatrix} g_{j,j-1} \\ g_{j,j+1} \end{bmatrix} := \begin{bmatrix} (\partial_{n_j} w_j - Z_{j,j-1} w_j)|_{\Sigma_{j,j-1}} \\ (\partial_{n_j} w_j - Z_{j,j+1} w_j)|_{\Sigma_{j,j+1}} \end{bmatrix}. \tag{3.6}$$

Also, associated with the boundary value problem (3.4) posed in the semi-infinite domain Ω_0 we define the RtR map $\mathcal{S}^0$ in the form

$$\mathcal{S}^0_{1,1} g_{0,1} := (\partial_{n_0} w_0 - Z_{0,1} w_0)|_{\Sigma_{0,1}}. \tag{3.7}$$

The RtR map $\mathcal{S}^{N+1}_{N,N}$ corresponding to the domain Ω_{N+1} is defined in a similar manner to $\mathcal{S}^0_{1,1}$ but for a boundary data $g_{N+1,N}$ defined on $\Sigma_{N+1,N}$.

With these notations in place, the DD formulation (3.1) seeks to find the generalized Robin data associated with each interface $\Gamma_j = \Sigma_{j,j+1} = \Sigma_{j+1,j}$

$$f_j = \begin{bmatrix} f_{j,j+1} \\ f_{j+1,j} \end{bmatrix} := \begin{bmatrix} (\partial_{n_j} u_j + Z_{j+1,j} u_j)|_{\Sigma_{j,j+1}} \\ (\partial_{n_{j+1}} u_{j+1} + Z_{j,j+1} u_{j+1})|_{\Sigma_{j+1,j}} \end{bmatrix}, \ 0 \leq j \leq N$$

as the solution of the following $(2N+2) \times (2N+2)$ operator linear system

$$\mathcal{A} f = b \tag{3.8}$$

where $f = [f_0\ f_1\ \ldots f_N]^\top$ and the right-hand-side vector $b = [b_0\ b_1\ \ldots\ b_N]^\top$ has zero components $b_\ell = [0\ 0]^\top,\ 1 \leq \ell \leq N$ with the exception of the first component

$$b_0 = \begin{bmatrix} -(\partial_{n_0} u^{inc} + Z_{1,0}\ u^{inc})|_{\Sigma_{0,1}} \\ -(\partial_{n_0} u^{inc} - Z_{0,1} u^{inc})|_{\Sigma_{1,0}} \end{bmatrix}.$$

and the DD Schwarz iteration matrix $\mathcal{A}$ is a tridiagonal block operator matrix whose explicit form is

$$\mathcal{A} = \begin{bmatrix} D_0 & U_0 & 0 & \ldots & 0 \\ L_0 & D_1 & U_1 & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ \ldots & L_{j-1} & D_j & U_j & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ \ldots & \ldots & L_{N-2} & D_{N-1} & U_{N-1} \\ \ldots & \ldots & \ldots & L_{N-1} & D_N \end{bmatrix} \tag{3.9}$$

where

$$D_j := \begin{bmatrix} I & \mathcal{S}^{j+1}_{j,j} \\ \mathcal{S}^j_{j+1,j+1} & I \end{bmatrix}, \quad U_j = \begin{bmatrix} \mathcal{S}^{j+1}_{j,j+2} & 0 \\ 0 & 0 \end{bmatrix}, \quad L_j = \begin{bmatrix} 0 & 0 \\ 0 & \mathcal{S}^{j+1}_{j+2,j} \end{bmatrix}. \tag{3.10}$$

We present in what follows a different strategy of domain decomposition whereby the subdomains are horizontal slabs.

3.2 DD with slab subdomains

An alternative DD possibility is to partition the computational domain using horizontal slabs. We restrict ourselves to cases where the layer domains $\Omega_j^{per},\ 1 \le j \le N$ are tall enough so that each periodic interface $\Gamma_j,\ 0 \le j \le N$ can be contained in a horizontal strip that does not intersect any other interface $\Gamma_\ell,\ \ell \neq j$. Under this assumption, these horizontal slabs constitute the DD subdomains—see Figure 2 for a depiction of the partitioning in the case of four layers (i.e. $N = 2$). In general, however, a domain decomposition into horizontal slabs might require that an interface Γ_j intersect a (flat) boundary of a slab; we leave this challenging scenario for future considerations.

Assuming that there exist real numbers $c_0 > c_1 > \ldots > c_{N+1}$ such that for all $0 \le j \le N$ we have that $c_j > \overline{F}_j + \max F_j(x_1)$ and $c_{j+1} < \overline{F}_j + \min F_j(x_1)$, then we can partition $\mathbb{R}^2$ into a union of nonoverlapping horizontal strips $\mathbb{R}^2 = \cup_{j=0}^{N+2}\Omega_j^\flat$, where the slab domains are defined as $\Omega_0^\flat := \{(x_1,x_2) : x_2 \ge c_0\}$, $\Omega_j^\flat := \{(x_1,x_2) : c_j \le x_2 \le c_{j-1}\},\ 1 \le j \le N+1$, and $\Omega_{N+2}^\flat := \{(x_1,x_2) : x_2 \le c_{N+1}\}$. Using the domain decomposition into layered slabs we seek α-quasiperiodic solutions v_j of the following system

$$\begin{aligned}
\Delta v_j + k_j(x)^2 v_j &= 0 \qquad \text{in} \quad \Omega_j^{\flat,per},\ 1 \le j \le N+1 \\
[v_j] = 0, \quad \left[\partial_{n_j} v_j\right] &= 0 \quad \text{on } \Gamma_{j-1},\ 1 \le j \le N+1 \\
-(\partial_{x_2} v_0 + \partial_{x_2} u^{inc}) + Z_{1,0}^\flat(v_0 + u^{inc}) &= -\partial_{x_2} v_1 + Z_{1,0}^\flat v_1 \text{ on } \Sigma_{0,1}^\flat, \\
\partial_{x_2} v_1 + Z_{0,1}^\flat v_1 &= (\partial_{x_2} v_0 + \partial_{x_2} u^{inc}) + Z_{0,1}^\flat(v_0 + u^{inc}) \text{ on } \Sigma_{1,0}^\flat \\
-\partial_{x_2} v_j + Z_{j+1,j}^\flat v_j &= -\partial_{x_2} v_{j+1} + Z_{j+1,j}^\flat v_{j+1} \text{ on } \Sigma_{j,j+1}^\flat,\ 1 \le j \le N+1 \\
\partial_{x_2} v_{j+1} + Z_{j,j+1}^\flat v_{j+1} &= \partial_{x_2} v_j + Z_{j,j+1}^\flat v_j \text{ on } \Sigma_{j+1,j}^\flat, 1 \le j \le N+1,
\end{aligned} \tag{3.11}$$

where $k_0(x) := k_0$, $k_{N+2}(x) := k_{N+1}$, and

$$k_j(x) := \begin{cases} k_{j-1},\ x_2 > \overline{F}_{j-1} + F_{j-1}(x_1), \\ k_j,\ x_2 < \overline{F}_{j-1} + F_{j-1}(x_1), \end{cases} \qquad 1 \le j \le N+1.$$

In equations (3.11) we have $\Sigma_{j,j+1}^\flat = \Sigma_{j+1,j}^\flat := \{(x_1,c_j), 0 \le x_1 \le d\},\ 0 \le j \le N+1$ and $[v_j]$ denotes the jump of the function v_j across the interface Γ_{j-1}. We require that the transmission operators have the following mapping properties $Z_{j+1,j}^\flat : H^{1/2}(\Sigma_{j,j+1}^\flat) \to H^{-1/2}(\Sigma_{j,j+1}^\flat)$ and $Z_{j+1,j}^\flat : H^{1/2}(\Sigma_{j+1,j}^\flat) \to H^{-1/2}(\Sigma_{j,j+1}^\flat)$ and satisfy coercivity properties similar to those in equations (3.3). The coercivity properties of the transmission operators $Z_{j-1,j}^\flat$ and $Z_{j+1,j}^\flat$ are needed to ensure the well-posedness of the following subdomain equations

$$\begin{aligned}
\Delta v_j + k_j(x)^2 v_j &= 0 \qquad \text{in} \quad \Omega_j^{\flat,per}, \\
[v_j] = 0, \quad \left[\partial_{n_j} v_j\right] &= 0 \quad \text{on } \Gamma_{j-1} \\
\partial_{x_2} v_j + Z_{j-1,j}^\flat v_j &= g_{j,j-1}^\flat \text{ on } \Sigma_{j,j-1}^\flat, \\
-\partial_{x_2} v_j + Z_{j+1,j}^\flat v_j &= g_{j,j+1}^\flat \text{ on } \Sigma_{j+1,j}^\flat,
\end{aligned} \tag{3.12}$$

for all $1 \le j \le N+1$ as well as those posed in the semi-infinite domains $\Omega_0^{\flat,per}$ and $\Omega_{N+1}^{\flat,per}$ respectively. Associated to the Helmholtz transmission problem (3.12) is the RtR operator defined below

$$\mathcal{S}^{\flat,j} \begin{bmatrix} g_{j,j-1}^\flat \\ g_{j,j+1}^\flat \end{bmatrix} = \begin{bmatrix} \mathcal{S}_{j-1,j-1}^{\flat,j} & \mathcal{S}_{j-1,j+1}^{\flat,j} \\ \mathcal{S}_{j+1,j-1}^{\flat,j} & \mathcal{S}_{j+1,j+1}^{\flat,j} \end{bmatrix} \begin{bmatrix} g_{j,j-1}^\flat \\ g_{j,j+1}^\flat \end{bmatrix} := \begin{bmatrix} (\partial_{x_2} v_j - Z_{j,j-1}^\flat v_j)|_{\Sigma_{j,j-1}^\flat} \\ (-\partial_{x_2} v_j - Z_{j,j+1}^\flat v_j)|_{\Sigma_{j,j+1}^\flat} \end{bmatrix}. \tag{3.13}$$

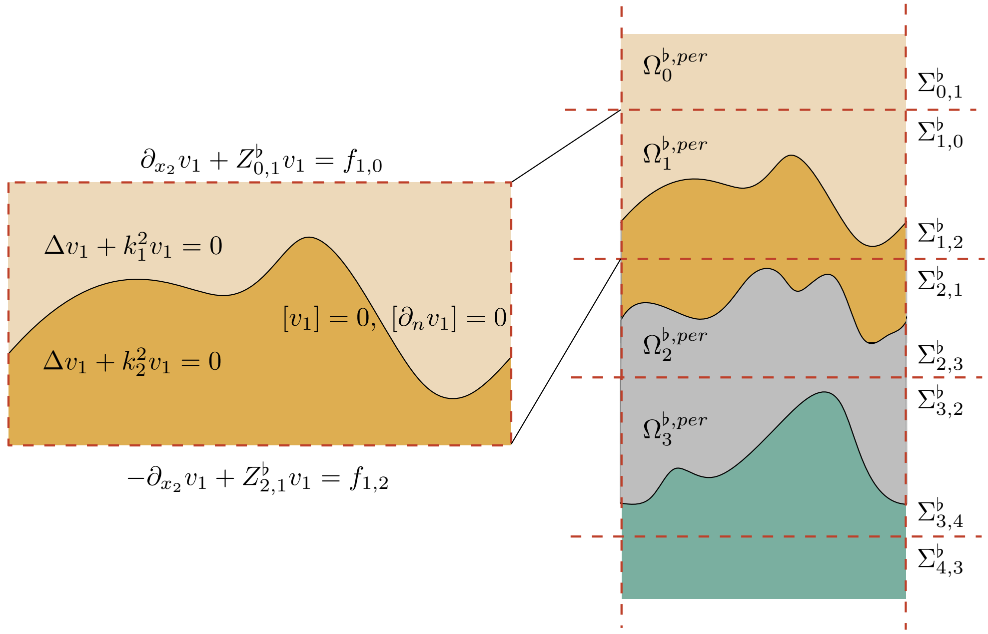

Figure 2: Slab domain decomposition.

The DD formulation (3.11) then seeks to find the generalized Robin data associated with each interface $\Sigma^\flat_{j,j+1} = \Sigma^\flat_{j+1,j}$

$$f^\flat_j = \begin{bmatrix} f^\flat_{j,j+1} \\ f^\flat_{j+1,j} \end{bmatrix} \quad := \quad \begin{bmatrix} (-\partial_{x_2} v_j + Z^\flat_{j+1,j} v_j)|_{\Sigma_{j,j+1}} \\ (\partial_{x_2} v_{j+1} + Z^\flat_{j,j+1} v_{j+1})|_{\Sigma_{j+1,j}} \end{bmatrix}, \; 0 \leq j \leq N+1,$$

as the solution of the following $(2N+4) \times (2N+4)$ operator linear system

$$\mathcal{A}^\flat f^\flat = b^\flat \tag{3.14}$$

where the DD Schwarz iteration matrix $\mathcal{A}^\flat$ is similar to that defined in equation (3.9), $f^\flat = [f^\flat_0 \; f^\flat_1 \; \ldots f^\flat_{N+1}]^\top$ and the right-hand-side vector $b^\flat = [b^\flat_0 \; b^\flat_1 \; \ldots \; b^\flat_{N+1}]^\top$ has zero components $b^\flat_\ell = [0 \; 0]^\top, \; 1 \leq \ell \leq N+1$ with the exception of the first component

$$b^\flat_0 = \begin{bmatrix} (\partial_{x_2} u^{inc} - Z^\flat_{1,0} \; u^{inc})|_{\Sigma_{0,1}} \\ (\partial_{x_2} u^{inc} + Z^\flat_{0,1} u^{inc})|_{\Sigma_{1,0}} \end{bmatrix}.$$

Having described two possible DD strategies for the solution of quasiperiodic Helmholtz transmission problems (2.1), we now present a methodology based on Fourier calculus to construct quasi-optimal transmission operators.

4 Construction of quasi-optimal transmission operators based on shape perturbation series

We present in what follows a perturbative method to construct quasi-optimal transmission operators $Z_{j,j+1}$ and $Z_{j+1,j}$ for $0 \leq j \leq N$ corresponding to the DD formulation (3.1). To this end, given a generic d-periodic profile function $F(x_1)$ we define the periodic interface $\Gamma := \{(x_1, F(x_1)),\ 0 \leq x_1 \leq d\}$ and the semi-infinite domains $\Omega^{+,per} := \{(x_1, x_2), 0 \leq x_1 \leq d,\ F(x_1) \leq x_2\}$ and respectively $\Omega^{-,per} := \{(x_1, x_2), 0 \leq x_1 \leq d,\ F(x_1) \geq x_2\}$. We assume that the profile function $F(x_1)$ can be expressed in the form $F(x_1) = \varepsilon \widetilde{F}(x_1)$, where the d-periodic function $\widetilde{F}(x_1)$ is smooth (it actually suffices that the profile function is Lipschitz [8, 15]). We employ a perturbative approach [25] to construct approximations of the DtN operator $Y^{\pm}(k, F)g := \pm\partial_n v|_{\Gamma}$ corresponding to the following boundary value problem in the domains $\Omega^{\pm,per}$:

$$
\begin{aligned}
\Delta v^{\pm} + k^2 v^{\pm} &= 0, \quad \text{in } \Omega^{\pm,per}, \\
v^{\pm} &= g, \quad \text{on } \Gamma,
\end{aligned}
\tag{4.1}
$$

where $v^{\pm}$ are radiative in the domains $\Omega^{\pm,per}$, g is a α-quasiperiodic function defined on Γ, and $n(x) = (F'(x), -1)$ is the normal to Γ pointing into the domain $\Omega^{-,per}$. Under the assumptions above, the DtN operators $Y^{\pm}(k, F)$ are analytic in the shape perturbation variable ε [25], and thus we seek the operator $Y^{\pm}(k, F)$ in the form of the perturbation series

$$
Y^{\pm}(k, F) = \sum_{n=0}^{\infty} Y_n^{\pm}(k, \widetilde{F})\varepsilon^n,
\tag{4.2}
$$

where the operators $Y_n^{\pm}(k, \widetilde{F}) : H^{1/2}(\Gamma) \to H^{-1/2}(\Gamma)$ can be computed via explicit recursive formulas [25] with the Method of Operator Expansions (OE) (see also [21, 22]). Let us denote by $\rho(k, F)$ the radius of convergence of the perturbation series (4.2). Following [25], we present next the recursive formulas that lead to closed form expressions of the operators $Y_n^{\pm}(k, \widetilde{F})$. First, given an α-quasiperiodic function $\varphi \in H^{1/2}(\Gamma)$ which can be represented as

$$
\varphi(x_1) = \sum_{p \in \mathbb{Z}} \varphi_p e^{i\alpha_p x_1},
$$

we define the Fourier multiplier operator

$$
\beta_D(k)[\varphi](x_1) := \sum_{p \in \mathbb{Z}} \beta_{k,p}\varphi_p e^{i\alpha_p x_1},\ \ \beta_{k,p} := (k^2 - \alpha_p^2)^{1/2}.
\tag{4.3}
$$

Then, it can be shown that the operators $Y_n^{\pm}(k, \widetilde{F})$ in the perturbation series (4.2) can be computed via the OE recursion

$$
\begin{aligned}
Y_0^{\pm}(k, \widetilde{F})[\varphi] &= (-i\beta_D(k))[\varphi], \\
Y_n^{\pm}(k, \widetilde{F})[\varphi] &= \pm k^2 \widetilde{F}_n(x_1)(\pm i\beta_D(k))^{n-1}\varphi \pm \partial_{x_1}\left[\widetilde{F}_n(x_1)\partial_{x_1}(\pm i\beta_D(k))^{n-1}\varphi\right] \\
&- \sum_{m=0}^{n-1} Y_m^{\pm}(k, \widetilde{F})\left[\widetilde{F}_{n-m}(\pm i\beta_D(k))^{n-m}\varphi\right],
\end{aligned}
\tag{4.4}
$$

where $\widetilde{F}_\ell(x_1) := \frac{\widetilde{F}(x_1)^\ell}{\ell!}$. We note that given that all the operators $Y_n^{\pm}(k, \widetilde{F})$ have the same mapping properties, that is $Y_n^{\pm}(k, \widetilde{F}) : H^{1/2}(\Gamma) \to H^{-1/2}(\Gamma)$ for all $0 \leq n$, the recursions (4.4) possess significant subtractive cancellations. More stable expressions of the operators $Y_n^{\pm}(k, \widetilde{F}), 1 \leq n \leq 2$, were proposed in [25]. Specifically, using the commutator

$$
\left[\beta_D(k), \widetilde{F}\right][\varphi] := \beta_D(k)[\widetilde{F}\varphi] - \widetilde{F}\beta_D(k)[\varphi]
$$

it can be shown that the low-order term corrections $Y_n^{\pm}(k,\widetilde{F}),\ n=1,2$, can be expressed in the equivalent form

$$Y_1^{\pm}(k,\widetilde{F})[\varphi] = (D\widetilde{F})\ (D\varphi) - \left[\beta_D(k),\widetilde{F}\right][\beta_D(k)\varphi], \tag{4.5}$$

and

$$Y_2^{\pm}(k,\widetilde{F})[\varphi] = i\beta_D(k)\left(-\left[\beta_D(k),\widetilde{F}^2/2\right][\beta_D(k)\varphi] + \widetilde{F}\left[\beta_D(k),\widetilde{F}\right][\beta_D(k)\varphi]\right), \tag{4.6}$$

where $D=\partial_{x_1}$. The stability of the recursions (4.5) and (4.6) can be attributed to the fact that the commutators featured in those formulas are actually bounded operators in the space $H^{1/2}(\Gamma)$. However, the calculation of high-order correction terms $Y_n^{+}(k,\widetilde{F}),\ n\geq 3$ via the stable recursions above becomes quite cumbersome. As such, a different strategy based on changes of variables (that straighten out the boundary Γ) and DtN corresponding to variable coefficient Helmholtz equations in half-planes is advocated in [25] for stable computations of DtN maps. Given that our motivation is to construct readily computable DD transmission operators that are approximations of DtN operators, we will restrict to low-order terms $Y_n^{+}(k,F)$ in the perturbation series (4.2), which, as discussed above, can be computed by explicit and stable recursions.

In order to meet the coercivity requirements (3.3), we *complexify* the wavenumber k in the form $\kappa=k+i\sigma,\sigma>0$ and we define

$$Y^{L,\pm}(\kappa,F) := \sum_{\ell=0}^{L} Y_\ell^{\pm}(\kappa,\widetilde{F})\varepsilon^\ell,\ L\leq 2, \tag{4.7}$$

using formulas (4.5) and (4.6) for the definition of the operators in equation (4.7). Indeed, we establish the following result.

Lemma 4.1 *Provided that $\varepsilon<\rho(k,F)$ is small enough, the following coercivity property holds*

$$\Im\langle Y^{L,\pm}(\kappa,F)\varphi,\ \varphi\rangle < 0$$

for all $\varphi\in H^{1/2}(\Gamma)$.

Proof. By the construction of the Fourier multiplier operator $-i\beta_D(\kappa)$ we have that

$$\Im\langle Y_0^{\pm}(\kappa,\widetilde{F})\varphi,\ \varphi\rangle = -\sum_{p\in\mathbb{Z}}\Re(\kappa^2-\alpha_p^2)^{1/2}|\varphi_p|^2 < 0,$$

for all $\varphi\in H^{1/2}(\Gamma_0)$, given that $\Re(\kappa^2-\alpha_p^2)^{1/2}>0$ for all $p\in\mathbb{Z}$. Using the fact that $\left|\langle Y_\ell^{\pm}(\kappa,\widetilde{F})\varphi,\ \varphi\rangle\right| \lesssim \|\varphi\|^2_{H^{1/2}(\Gamma)}$ we obtain

$$\Im\langle Y^{L,\pm}(\kappa,F)\varphi,\ \varphi\rangle \leq \Im\langle Y_0^{\pm}(\kappa,\widetilde{F})\varphi,\ \varphi\rangle + C\varepsilon\|\varphi\|^2_{H^{1/2}(\Gamma)} < 0$$

for ε small enough. ∎

We are now in the position to construct quasi-optimal transmission operators $Z_{j-1,j}$ and $Z_{j+1,j}$. We assume without loss of generality that each grating profile $F_j(x_1)=\varepsilon\widetilde{F}_j(x_1),\ 0\leq j\leq N$, and we select transmission operators in the form

$$Z^{s,L}_{j-1,j} := Y^{L,+}(\kappa_{j-1},\widetilde{F}_{j-1}),\ 1\leq j\leq N+1, \qquad Z^{s,L}_{j+1,j} := Y^{L,-}(\kappa_{j+1},\widetilde{F}_j), 0\leq j\leq N, \tag{4.8}$$

where $\kappa_j = k_j + i\sigma_j,\ \sigma_j > 0$ and k_j is the wavenumber corresponding to the layer domain Ω_j. We note that the transmission operators given in equation (4.8) correspond to semi-infinite, and not bounded layers. As such, the width of the layers is not incorporated in the definition of the transmission operators defined in equation (4.8).

It is also possible to employ the high-order shape deformation technique to construct transmission operators that are approximations of DtN operators corresponding to bounded periodic layers [23]. Indeed, in the case of a bounded interior layer domain Ω_j we consider the boundary value problem

$$\begin{aligned} \Delta v_j + k_j^2 v_j &= 0, \quad \text{in } \Omega_j^{per}, \\ v_j &= g_{j,j-1}, \quad \text{on } \Sigma_{j,j-1}, \\ v_j &= g_{j,j+1}, \quad \text{on } \Sigma_{j,j+1}, \end{aligned} \tag{4.9}$$

for which we define the DtN operator $\mathbf{Y}_j(k_j)\begin{bmatrix} g_{j,j-1} \\ g_{j,j+1}\end{bmatrix} := \begin{bmatrix}\partial_{n_j} v_j|_{\Sigma_{j,j-1}} \\ \partial_{n_j} v_j|_{\Sigma_{j,j+1}}\end{bmatrix}$. We mention that (a) the DtN operators $\mathbf{Y}_j(k_j)$ are 2×2 matrix operators $\mathbf{Y}_j(k_j) = \begin{bmatrix} Y_{j-1,j-1}(k_j) & Y_{j-1,j+1}(k_j) \\ Y_{j+1,j-1}(k_j) & Y_{j+1,j+1}(k_j)\end{bmatrix}$, and (b) the same DtN operators are not properly defined for all wavenumbers k_j. Assuming that $F_{j-1}(x_1) = \varepsilon\widetilde{F_{j-1}}(x_1)$ and respectively $F_j(x_1) = \varepsilon\widetilde{F_j}(x_1)$ where $\widetilde{F_{j-1}}(x_1)$ and $\widetilde{F_j}(x_1)$ are smooth, the DtN operator $\mathbf{Y}_j(k_j)$ can be expressed in terms of the perturbation series

$$\mathbf{Y}_j(k_j) = \sum_{\ell=0}^{\infty} \mathbf{Y}_{j,\ell}(k_j)\varepsilon^\ell. \tag{4.10}$$

The OE method gives the terms in the series as [23]

$$\begin{aligned} \mathbf{Y}_{j,0}(k_j) &= i\beta_D(k_j)\begin{bmatrix} \coth(ih_j\beta_D(k_j)) & -\operatorname{csch}(ih_j\beta_D(k_j)) \\ -\operatorname{csch}(ih_j\beta_D(k_j)) & \coth(ih_j\beta_D(k_j))\end{bmatrix}, \\ \mathbf{Y}_{j,n}(k_j) &= -(\mathbf{C}_n(\widetilde{F}_{j-1}) + \mathbf{C}_n(\widetilde{F}_j))\frac{k_j^2}{i\beta_D(k_j)} - D(\mathbf{C}_n(\widetilde{F}_{j-1}) + \mathbf{C}_n(\widetilde{F}_j))\frac{1}{i\beta_D(k_j)}D \\ &- \sum_{m=0}^{n-1}\mathbf{Y}_{j,m}(k_j)\left[\mathbf{S}_{n-m}(\widetilde{F}_{j-1}) + \mathbf{S}_{n-m}(\widetilde{F}_j)\right], \end{aligned} \tag{4.11}$$

where $h_j = \overline{F}_{j-1} - \overline{F}_j$ and

$$\mathbf{C}_n(\widetilde{F}_{j-1}) := \widetilde{F}_{j-1,n}\begin{bmatrix}\operatorname{shch}_{n+1}(ih_j\beta_D(k_j)) & (-1)^{n+1}\operatorname{shch}_{n+1}(0) \\ 0 & 0\end{bmatrix}\frac{(i\beta_D(k_j))^n}{\sinh(ih_j\beta_D(k_j))},$$

$$\mathbf{C}_n(\widetilde{F}_j) := \widetilde{F}_{j,n}\begin{bmatrix} 0 & 0 \\ -\operatorname{shch}_{n+1}(0) & (-1)^n\operatorname{shch}_{n+1}(ih_j\beta_D(k_j))\end{bmatrix}\frac{(i\beta_D(k_j))^n}{\sinh(ih_j\beta_D(k_j))},$$

as well as

$$\mathbf{S}_n(\widetilde{F}_{j-1}) := \widetilde{F}_{j-1,n}\begin{bmatrix}\operatorname{shch}_n(ih_j\beta_D(k_j)) & (-1)^n\operatorname{shch}_n(0) \\ 0 & 0\end{bmatrix}\frac{(i\beta_D(k_j))^n}{\sinh(ih_j\beta_D(k_j))},$$

$$\mathbf{S}_n(\widetilde{F}_j) := \widetilde{F}_{j,n}\begin{bmatrix} 0 & 0 \\ \operatorname{shch}_n(0) & (-1)^n\operatorname{shch}_n(ih_j\beta_D(k_j))\end{bmatrix}\frac{(i\beta_D(k_j))^n}{\sinh(ih_j\beta_D(k_j))},$$

where

$$\operatorname{shch}_n(z) = \frac{e^z - (-1)^n e^{-z}}{2} = \begin{cases} \cosh(z), & n \text{ even} \\ \sinh(z), & n \text{ odd.} \end{cases}$$

Remark 4.2 *We note that the operators* (4.11) *can be evaluated in a straightforward manner in Fourier space. However, unlike formulas* (4.5) *and* (4.6)*, the recursions* (4.11) *do not avoid subtractive cancellations, and, as such, are prone to instabilities for rougher profiles* $\widetilde{F}_{j-1}$ *and* $\widetilde{F}_j$*. In order to bypass these instabilities, an alternative strategy based on changes of variables that straighten out the boundaries is proposed in [14] for robust perturbative evaluations of layer DtN. Nevertheless, the latter strategy requires numerical solutions for the evaluation of the terms in the perturbation series of the DtN operators* $\mathbf{Y}_j(k_j)$*. As such, the evaluation of the DtN operators* $\mathbf{Y}_j(k_j)$ *via the straightening of boundaries strategy in [14] becomes more involved than the straightforward one given by the recursions* (4.11)*. Consequently, we advocate for the use of the simple recursions* (4.11) *to construct approximations of DtN operators, and we point out their limitations in the case of rough profiles.*

Again, the complexification of the wavenumber $\kappa_j = k_j + i\sigma_j, \sigma_j > 0$ leads to corresponding Fourier multipliers $\mathbf{Y}_{j,n}(\kappa_j),\ n \geq 0$ that are well defined for all values h_j. Therefore, we define the 2×2 matrix operators

$$\mathbf{Y}_j^L(\kappa_j) = \sum_{\ell=0}^{L} \mathbf{Y}_{j,\ell}(\kappa_j)\varepsilon^\ell = \begin{bmatrix} Y^L_{j-1,j-1}(\kappa_j) & Y^L_{j-1,j+1}(\kappa_j) \\ Y^L_{j+1,j-1}(\kappa_j) & Y^L_{j+1,j+1}(\kappa_j) \end{bmatrix},\ \kappa_j = k_j + i\sigma_j,\ \sigma_j > 0.$$

As an alternative to (4.8) we can select the transmission operators corresponding to the layer $\Omega_j,\ 1 \leq j \leq N$ in the form

$$Z^L_{j,j-1} := Y^L_{j-1,j-1}(\kappa_j),\ 1 \leq j \leq N, \qquad Z^L_{j,j+1} := Y^L_{j+1,j+1}(\kappa_j),\ 1 \leq j \leq N, \tag{4.12}$$

as well as

$$Z^L_{0,1} := Y^+_L(\kappa_0, \widetilde{F}_0), \qquad Z^L_{N+1,N} := Y^-_L(\kappa_{N+1}, \widetilde{F}_N). \tag{4.13}$$

Again, under the assumption that the shape perturbation parameter ε is small enough (and in particular smaller than the radius of convergence of the perturbation series (4.10)), the arguments in the proof of Lemma 4.1 can be easily adapted to derive coercivity properties of the type (3.3) for the transmission operators $Z^L_{j,j-1}$ and $Z^L_{j,j+1}$ defined in equation (4.12).

Finally, the transmission operators $Z^\flat_{j,j+1}$ corresponding to the DD with slab subdomains (3.11) are simply selected to be complexified versions of half-space DtN operators, that is

$$Z^\flat_{j,j+1} = Z^\flat_{j+1,j} := -i\beta_D(\kappa_j), \quad 0 \leq j \leq N. \tag{4.14}$$

We refer to the DD formulations (3.1) and respectively (3.11) corresponding to the choice of transmission operators presented in this section as quasi-optimal DD (QO DD) in what follows. We refer to the operator QO DD Schwartdary integral equations.

5 Boundary integral operator formulations

5.1 Robin-To-Robin operators

At the heart of a DD implementation is the computation of the RtR maps. We present in this Section explicit representations of RtR maps in terms of boundary integral operators associated with quasiperiodic Green functions that will serve as the basis of the implementation of the DD formulations considered in this paper. For a given wavenumber k, we define the α quasiperiodic Green function

$$G_k^q(x_1,x_2)=\sum_{n\in\mathbb{Z}}e^{-i\alpha nd}G_k(x_1+nd,x_2) \tag{5.1}$$

where $G_k(x_1,x_2)=\frac{i}{4}H_0^{(1)}(k|\mathbf{x}|),\ \mathbf{x}=(x_1,x_2)$. We also define $\alpha_r:=\alpha+\frac{2\pi}{d}r$ and $\beta_r=(k^2-\alpha_r^2)^{1/2}$, with the same convention on the square root used throughout this paper. The series (5.1) converges for wavenumbers k for which none of the coefficients β_r is equal to zero—that is wavenumbers which are not Wood frequencies. In the case of wavenumber k that is a Wood frequency, shifted quasiperiodic Green functions can be used instead [4, 26].

We assume that the interface Γ is defined as $\Gamma:=\{(x_1,F(x_1)):0\leq x_1\leq d\}$ where F is a C^2 periodic function of principal period equal to d. Given a density φ defined on Γ (which can be extended by α-quasiperiodicity to arguments $(x_1,F(x_1)),x_1\in\mathbb{R}$) we define the single and double layer potentials corresponding to a wavenumber k

$$[SL_k\varphi](\mathbf{x}):=\int_\Gamma G_k^q(\mathbf{x}-\mathbf{y})\varphi(\mathbf{y})ds(\mathbf{y}),\quad [DL_k\varphi](\mathbf{x}):=\int_\Gamma\frac{\partial G_k^q(\mathbf{x}-\mathbf{y})}{\partial\mathbf{n}(\mathbf{y})}\varphi(\mathbf{y})ds(\mathbf{y}), \tag{5.2}$$

for $\mathbf{x}\notin\Gamma$ and $\mathbf{x}=(x_1,x_2)$ such that $0\leq x_1\leq d$. It is immediate to see that the quantities $[SL_k\varphi](\mathbf{x})$ and $[DL_k\varphi](\mathbf{x})$ are α-quasiperiodic outgoing solutions of the Helmholtz equation corresponding to wavenumber k in the domains $\{\mathbf{x}:x_2>F(x_1)\}$ and $\{\mathbf{x}:x_2<F(x_1)\}$ respectively. The Dirichlet and Neumann boundary values of the single and double layer potentials give rise to the four boundary integral operators associated with quasiperiodic Helmholtz problems. Denoting by $n(\mathbf{x})=(-F'(x_1),1),\ \mathbf{x}=(x_1,F(x_1)),\ 0\leq x_1\leq d$ the (non-unit) normal to Γ pointing into the domain $\{\mathbf{x}:x_2>F(x_1)\}$ we define the single layer boundary integral operator

$$[S_k(\varphi)](\mathbf{x}):=\lim_{\varepsilon\to 0}[SL_k\varphi](\mathbf{x}\pm\varepsilon n(\mathbf{x}))=\int_0^d G_k^q(x-y,F(x)-F(y))\varphi((y,F(y)))\ (1+(F'(y))^2)^{1/2}dy, \tag{5.3}$$

with $\mathbf{x}=(x,F(x))$. Similarly, we also define the *weighted* single layer operator in the form

$$[S_k^w(\varphi)](\mathbf{x}):=\int_0^d G_k^q(x-y,F(x)-F(y))\varphi((y,F(y)))dy,\quad \mathbf{x}=(x,F(x)). \tag{5.4}$$

We also have

$$\lim_{\varepsilon\to 0}\nabla[SL_k\varphi](\mathbf{x}\pm\varepsilon n(\mathbf{x}))\cdot n(\mathbf{x})=\mp\frac{1}{2}\varphi(\mathbf{x})\ (1+(F'(x))^2)^{1/2}+[K_k^\top(\varphi)](\mathbf{x}),\quad \mathbf{x}=(x,F(x)), \tag{5.5}$$

where the adjoint double layer operator in equation (5.5) can be expressed explicitly as

$$[K_k^\top(\varphi)](\mathbf{x})=\int_\Gamma\frac{\partial G_k^q(\mathbf{x}-\mathbf{y})}{\partial n(\mathbf{x})}\varphi(\mathbf{y})ds(y),\quad \mathbf{x}\in\Gamma. \tag{5.6}$$

We also define a weighted version of the adjoint double layer operators in the form

$$[(K_k^w)^\top(\varphi)](\mathbf{x})=\int_0^d\frac{\partial G_k^q(\mathbf{x}-\mathbf{y})}{\partial n(\mathbf{x})}\varphi((y,F(y)))dy,\quad \mathbf{x}\in\Gamma. \tag{5.7}$$

In addition, applying the same machinery to the double layer potentials we can define the double layer operator

$$\lim_{\varepsilon\to 0}[DL_k\varphi](\mathbf{x}\pm\varepsilon n(\mathbf{x})) = \pm\frac{1}{2}\varphi(\mathbf{x}) + [K_k(\varphi)](\mathbf{x}), \quad \mathbf{x}=(x,F(x)) \tag{5.8}$$

as well as the hypersingular operators

$$\lim_{\varepsilon\to 0}\nabla[DL_k\varphi](\mathbf{x}\pm\varepsilon n(\mathbf{x}))\cdot\mathbf{n}(\mathbf{x}) = [N_k(\varphi)](\mathbf{x}), \quad \mathbf{x}=(x,F(x)). \tag{5.9}$$

Weighted versions of the double layer and hyper singular operators are defined accordingly [10]. In what follows we express RtR operators associated with quasiperiodic Helmholtz problems using the boundary integral operators introduced above.

We start with the analysis of the case of one interface Γ_0 (that is $N=0$) separating two semi-infinite domains under the assumption that Γ_0 is the graph of a smooth and periodic function. The motivation for this is that the particularly simple case of one interface already contains the main difficulties related to the analysis of the well-posedness of QO DD. Our analysis relies on the boundary integral operator of the RtR operators. Using the α-quasiperiodic boundary integral operators above, we are now in the position to compute the RtR operators $\mathcal{S}^j$, $(j=0,1)$ corresponding to the semi-infinite domains Ω_j, $(j=0,1)$. We note that in this case we have $Z^{s,L}_{0,1}=Z^L_{0,1}=Y^{L,+}(\kappa_0,\widetilde{F}_0)$, and $Z^{s,L}_{1,0}=Z^L_{1,0}=Y^{L,-}(\kappa_1,\widetilde{F}_0)$. We start with the calculation of the RtR operator $\mathcal{S}^0$ corresponding to problem (3.4) by seeking its solution w_0 in the form

$$w_0(\mathbf{x}) := [SL_k\varphi_0](\mathbf{x}), \quad \mathbf{x}\notin\Gamma_0,$$

for a density function φ_0 defined on Γ_0. We have then that

$$\partial_{n_0}w_0 = \frac{1}{2}\varphi_0\,|\mathbf{x}'| + K^\top_{\Gamma_0,k_0}\varphi_0, \quad w_0 = S_{\Gamma_0,k_0}\varphi_0, \quad \mathbf{x}'=(1,F_0'(x))$$

where the operators $K^\top_{\Gamma_0,k_0}$ are defined just as in equation (5.6) but with normal n_0 pointing into Ω_0^- (the exterior of Ω_0). Here and in what follows we introduce an additional subscript to make explicit the curve that is the domain of integration of the boundary integral operators. Accordingly, the function w_0 satisfy the generalized Robin boundary condition on Γ_0 is equivalent to the density function φ_0 solving the following BIE

$$\frac{1}{2}\varphi_0\,|\mathbf{x}'| + K^\top_{\Gamma_0,k_0}\varphi_0 + Z^L_{1,0}S_{\Gamma_0,k_0}\varphi_0 = g_{0,1} \quad \text{on } \Gamma_0.$$

Defining the weighted density $\varphi_0^w := \varphi_0\,|\mathbf{x}'|$ on Γ_0, we see that φ_0^w is in turn a solution of the following weighted BIE:

$$\left(\frac{1}{2}I + (K^w_{\Gamma_0,k_0})^\top + Z^L_{1,0}S^w_{\Gamma_0,k_0}\right)\varphi_0^w = g_{0,1} \quad \text{on } \Gamma_0. \tag{5.10}$$

Given that $w_0 = S^w_{\Gamma_0,k_0}\varphi_0^w$ on Γ_0, we immediately obtain from equation (5.10) that the RtR operator $\mathcal{S}^0_{1,1}$ defined in equation (3.7) can be expressed through the following explicit formula

$$\mathcal{S}^0_{1,1} = I - (Z^L_{0,1}+Z^L_{1,0})S^w_{\Gamma_0,k_0}\left(\frac{1}{2}I + (K^w_{\Gamma_0,k_0})^\top + Z^L_{1,0}S^w_{\Gamma_0,k_0}\right)^{-1}. \tag{5.11}$$

Our next goal is to establish the robustness of the formulation (5.11). We assume in what follows that the parameter ε in the shape Γ_0 given by $F_0(x_1)=\varepsilon\widetilde{F}_0(x_1)$ is smaller than the minimum of the radii ρ_j of convergence of the boundary perturbation expansion series of the DtN operators $Y^\pm(k_j,F_0)$, cf. (4.2). We establish the following theorem

Theorem 5.1 *Assuming that the profile function $\widetilde{F_0}(x_1)$ is periodic and C^2, and the shape parameter ε is small enough, the operator*

$$\mathcal{A}_{1,0} := \frac{1}{2}I + (K^w_{\Gamma_0,k_0})^\top + Z^L_{1,0}S^w_{\Gamma_0,k_0} : H^{-1/2}(\Gamma_0) \to H^{-1/2}(\Gamma_0)$$

is invertible with continuous inverse.

Proof. Assuming that $\varepsilon < \rho_1$, where ρ_1 is the radius of convergence of the shape perturbation series of the DtN operator $Y^-(k_1, F_0)$, we have [25]

$$\|Y^-(k_1, F_0) - \sum_{\ell=0}^{L} Y^-_\ell(k_1, \widetilde{F}_0)\varepsilon^\ell\|_{H^{1/2}(\Gamma_0)\to H^{-1/2}(\Gamma_0)} \lesssim \varepsilon^{L+1}. \tag{5.12}$$

Given that

$$|(k_1^2 - \alpha_p^2)^{1/2} - ((k_1 + i\sigma_1)^2 - \alpha_p^2)^{1/2}| = \mathcal{O}(p^{-1}),\ p \to \infty$$

it follows that

$$Y^-_0(k_1, \widetilde{F}_0) - Y^-_0(\kappa_1, \widetilde{F}_0) = -i(\beta_D(k_1) - \beta_D(\kappa_1)) : H^{1/2}(\Gamma_0) \to H^{3/2}(\Gamma_0).$$

Using the stable commutator representations (4.5) and (4.6), together with the mapping properties of the commutators established in [25], we obtain

$$Y^-_1(k_1, \widetilde{F}_0) - Y^-_1(\kappa_1, \widetilde{F}_0) : H^{1/2}(\Gamma_0) \to H^{3/2}(\Gamma_0)$$

and respectively

$$Y^-_2(k_1, \widetilde{F}_0) - Y^-_2(\kappa_1, \widetilde{F}_0) : H^{1/2}(\Gamma_0) \to H^{3/2}(\Gamma_0).$$

In conclusion, we can express

$$\sum_{\ell=0}^{L} Y^-_\ell(k_1, \widetilde{F}_0)\varepsilon^\ell - Z^L_{1,0} = Z^{L,0}_{1,0} + Z^{L,1}_{1,0}$$

where

$$Z^{L,0}_{1,0} := \sum_{\ell=0}^{\min(L,2)} \left[Y^-_\ell(k_1, \widetilde{F}_0) - Y^-_\ell(\kappa_1, \widetilde{F}_0)\right]\varepsilon^\ell$$

and respectively

$$Z^{L,1}_{1,0} := \begin{cases} \sum_{\ell=3}^{L} \left[Y^-_\ell(k_1, \widetilde{F}_0) - Y^-_\ell(\kappa_1, \widetilde{F}_0)\right]\varepsilon^\ell,\ L \geq 3 \\ 0,\ L < 3 \end{cases}.$$

Clearly, we have that $Z^{L,0}_{1,0} : H^{1/2}(\Gamma_0) \to H^{3/2}(\Gamma_0)$ and $\|Z^{L,1}_{1,0}\|_{H^{1/2}(\Gamma_0)\to H^{1/2}(\Gamma_0)} \lesssim \varepsilon^3$. In conclusion, we can express the difference between the DtN operator $Y^-(k_1, F_0)$ and the QO DD transmission operator $Z^L_{1,0}$ in the form

$$Y^-(k_1, F_0) - Z^L_{1,0} = Z^{L,0}_{1,0} + Z^{L,1}_{1,0} + Z^{L,2}_{1,0} \tag{5.13}$$

where

$$Z^{L,2}_{1,0} := Y^-(k_1, F_0) - \sum_{\ell=0}^{L} Y^-_\ell(k_1, \widetilde{F}_0)\varepsilon^\ell.$$

Taking into account estimate (5.12), we have established that the operators on the right-hand side of equation (5.13) have the following properties

$$Z_{1,0}^{L,0} : H^{1/2}(\Gamma_0) \to H^{3/2}(\Gamma_0), \quad \|Z_{1,0}^{L,1} + Z_{1,0}^{L,2}\|_{H^{1/2}(\Gamma_0)\to H^{1/2}(\Gamma_0)} \lesssim \varepsilon^{\min(L,2)+1}. \tag{5.14}$$

Now, we can express the operator $\mathcal{A}_{1,0}$ in the form

$$\begin{aligned} \mathcal{A}_{1,0} &= \left[\frac{1}{2}I + Y^-(k_1, F_0)S^w_{\Gamma_0,k_1}\right] \\ &+ \left[(K^w_{\Gamma_0,k_0})^\top + (Z^L_{1,0} - Y^-(k_1, F_0))S^w_{\Gamma_0,k_0} + Y^-(k_1, F_0)(S^w_{\Gamma_0,k_0} - S^w_{\Gamma_0,k_1})\right]. \end{aligned}$$

Given that

$$Y^-(k_1, F_0)S^w_{\Gamma_0,k_1} = \frac{1}{2}I + (K^w_{\Gamma_0,k_1})^\top$$

where the operator $(K^w_{\Gamma_0,k_1})^\top$ is defined with respect to $-n_0$, we express the operator $\mathcal{A}_{1,0}$ in the form

$$\mathcal{A}_{1,0} = I + \mathcal{A}^0_{1,0} + \mathcal{K}_{1,0},$$

where

$$\mathcal{K}_{1,0} := (K^w_{\Gamma_0,k_0})^\top + (K^w_{\Gamma_0,k_1})^\top - Z^{L,0}_{1,0} S^w_{\Gamma_0,k_0} + Y^-(k_1, F_0)(S^w_{\Gamma_0,k_0} - S^w_{\Gamma_0,k_1})$$

and

$$\mathcal{A}^0_{1,0} := -(Z^{L,1}_{1,0} + Z^{L,2}_{1,0})S^w_{\Gamma_0,k_0}.$$

Under the assumption that Γ_0 is C^2 periodic, the following classical properties

$$(K^w_{\Gamma_0,k_j})^\top : H^{-1/2}(\Gamma_0) \to H^{1/2}(\Gamma_0), \quad S^w_{\Gamma_0,k_0} - S^w_{\Gamma_0,k_1} : H^{-1/2}(\Gamma_0) \to H^{5/2}(\Gamma_0)$$

together with those established in (5.14) imply that

$$\mathcal{K}_{1,0} : H^{-1/2}(\Gamma_0) \to H^{1/2}(\Gamma_0).$$

On the other hand, the estimates established in (5.14) imply that

$$\|\mathcal{A}^0_{1,0}\|_{H^{-1/2}(\Gamma_0)\to H^{-1/2}(\Gamma_0)} \lesssim \varepsilon^{\min(L,2)+1}.$$

In conclusion, the operator $\mathcal{A}_{1,0} : H^{-1/2}(\Gamma_0) \to H^{-1/2}(\Gamma_0)$ is a compact perturbation of the operator $I + \mathcal{A}^0_{1,0}$, and the latter can be shown to be invertible in the space $H^{-1/2}(\Gamma_0)$ via Neumann series arguments provided that ε is small enough. The invertibility of the operator $\mathcal{A}_{1,0}$ can be established then via the Fredholm theory provided that the same operator is injective. The latter, in turn, follows from the well-posedness of the Helmholtz boundary value problem (3.4). Indeed, if $\varphi_0 \in Ker(\mathcal{A}_{1,0})$, then the function w_0 defined as the single layer potential applied to the function φ_0 is a solution of the boundary value problem (3.4) in Ω_0 with zero generalized Robin boundary conditions on Γ_0. This implies that $w_0 = 0$ in Ω_0, and hence $w_0 = 0$ on Γ_0. Now, w_0 is also a radiative solution of the Helmholtz equation in Ω_1 with zero Dirichlet boundary values on Γ_0. Consequently, $w_0 = 0$ in Ω_1 as well. Finally, given that $\varphi_0 = [\partial_{n_0} w_0]$ on Γ_0, we obtain that $\varphi_0 = 0$ on Γ_0, which completes the proof of the theorem. ∎

Using the same techniques as in the proof of Theorem 5.1, we represent the RtR operator $\mathcal{S}^0_{1,1}$ in the form

$$\begin{aligned}\mathcal{S}^0_{1,1} &= \left(\frac{1}{2}I - Y^-(k_1,F_0)S^w_{\Gamma_0,k_1}\right)\mathcal{A}^{-1}_{1,0} + \left(\frac{1}{2}I - Y^+(k_0,F_0)S^w_{\Gamma_0,k_0}\right)\mathcal{A}^{-1}_{1,0}\\ &- \left(Z^L_{0,1} - Y^+(k_0,F_0)\right)S^w_{\Gamma_0,k_0}\mathcal{A}^{-1}_{1,0} - \left(Z^L_{1,0} - Y^-(k_1,F_0)\right)S^w_{\Gamma_0,k_1}\mathcal{A}^{-1}_{1,0}\\ &+ \mathcal{A}^0_{1,0}\mathcal{A}^{-1}_{1,0} + \mathcal{K}_{1,0}\mathcal{A}^{-1}_{1,0} + Z^L_{1,0}\left(S^w_{\Gamma_0,k_1} - S^w_{\Gamma_0,k_0}\right)\mathcal{A}^{-1}_{1,0}.\end{aligned}$$

Again, using results established in the proof of Theorem 5.1, we use the representation just derived above to express the operator $\mathcal{S}^0_{1,1}$ in the form

$$\mathcal{S}^0_{1,1} = \mathcal{S}^{0,0}_{1,1} + \mathcal{K}^0_0 \tag{5.15}$$

where $\mathcal{K}^0_0 : H^{-1/2}(\Gamma_0) \to H^{1/2}(\Gamma_0)$ and thus $\mathcal{K}^0_0$ is a compact operator in $H^{-1/2}(\Gamma_0)$, and $\mathcal{S}^{0,0}_{1,1} : H^{-1/2}(\Gamma_0) \to H^{-1/2}(\Gamma_0)$ has small norm

$$\|\mathcal{S}^{0,0}_{1,1}\|_{H^{-1/2}(\Gamma_0)\to H^{-1/2}(\Gamma_0)} \lesssim \varepsilon^{\min(L,2)+1}. \tag{5.16}$$

A similar result can be established for the representation of the RtR operator $\mathcal{S}^1_{0,0}$ in the form $\mathcal{S}^1_{0,0} = \mathcal{S}^{1,0}_{0,0} + \mathcal{K}^1_0$, where the operators in the latter decomposition have the same mapping properties as those of the operators $\mathcal{S}^{0,0}_{1,1}$ and $\mathcal{K}^0_0$.

5.2 Invertibility of the QO DD formulation (3.1) in the case of one interface

We are now in a position to establish the well-posedness of the DD formulation in the case of one interface:

Theorem 5.2 *Assuming that the profile function $\widetilde{F_0}(x_1)$ is periodic and C^2, the QO DD operator matrix*

$$\mathcal{A} = \begin{bmatrix} I & \mathcal{S}^1_{0,0} \\ \mathcal{S}^0_{1,1} & I \end{bmatrix}$$

is invertible with continuous inverse in the space $H^{-1/2}(\Gamma_0) \times H^{-1/2}(\Gamma_0)$ provided that the shape parameter ε is small enough.

Proof. First, using the decompositions $\mathcal{S}^j_{j+1,j+1} = \mathcal{S}^{j,0}_{j+1,j+1} + \mathcal{K}^j_0,\ j = 0,1$ (here we assume that the value of $j+1$ is actually that of $j+1(mod\ 2)$), where

$$\|\mathcal{S}^{j,0}_{j+1,j+1}\|_{H^{-1/2}(\Gamma_0)\to H^{-1/2}(\Gamma_0)} \lesssim \varepsilon^{\min(L,2)+1},\ j=0,1$$

and $\mathcal{K}^j_0 : H^{-1/2}(\Gamma_0) \to H^{-1/2}(\Gamma_0),\ j = 0,1$ are compact, it follows that

$$\mathcal{A} = \begin{bmatrix} I & \mathcal{S}^{1,0}_{0,0} \\ \mathcal{S}^{0,0}_{1,1} & I \end{bmatrix} + \begin{bmatrix} 0 & \mathcal{K}^0_0 \\ \mathcal{K}^1_0 & 0 \end{bmatrix}.$$

Neumann series arguments yield the fact that the matrix operator $\begin{bmatrix} I & \mathcal{S}^{1,0}_{0,0} \\ \mathcal{S}^{0,0}_{1,1} & I \end{bmatrix}$ is invertible in the space $H^{-1/2}(\Gamma_0) \times H^{-1/2}(\Gamma_0)$, while the matrix operator $\begin{bmatrix} 0 & \mathcal{K}^0_0 \\ \mathcal{K}^1_0 & 0 \end{bmatrix}$ is compact in the same functional space $H^{-1/2}(\Gamma_0) \times H^{-1/2}(\Gamma_0)$. Consequently, the QO DD operator $\mathcal{A}$ is Fredholm of index zero in the space $H^{-1/2}(\Gamma_0) \times H^{-1/2}(\Gamma_0)$, and thus the result of the theorem is established once we prove the injectivity of the operator $\mathcal{A}$. Now let $(\varphi_0, \varphi_1) \in Ker(\mathcal{A})$ and define u_0 and u_1 be α-quasiperiodic radiative solutions of the following Helmholtz boundary value problems

$$\begin{aligned} \Delta u_0 + k_0^2 u_0 &= 0 \quad \text{in } \Omega_0 \\ \partial_{n_0} u_0 + Z_{1,0}^L u_0 &= \varphi_0 \quad \text{on } \Gamma_0, \end{aligned}$$

and

$$\begin{aligned} \Delta u_1 + k_1^2 u_1 &= 0 \quad \text{in } \Omega_1 \\ \partial_{n_1} u_1 + Z_{0,1}^L u_1 &= \varphi_1 \quad \text{on } \Gamma_0. \end{aligned}$$

The requirement $(\varphi_0, \varphi_1) \in Ker(\mathcal{A})$ translates into the following system of equations on Γ_0

$$\begin{aligned} \partial_{n_0} u_0 + Z_{1,0}^L u_0 &= -\partial_{n_1} u_1 + Z_{1,0}^L u_1 \\ \partial_{n_1} u_1 + Z_{0,1}^L u_1 &= -\partial_{n_0} u_0 + Z_{0,1}^L u_0. \end{aligned}$$

Using the injectivity of the operator $Z_{1,0}^L + Z_{0,1}^L$, we obtain immediately that $u_0 = u_1$ and $\partial_{n_0} u_0 = -\partial_{n_1} u_1$ on Γ_0. Hence, $u_j = 0$ in Ω_j for $j = 0, 1$, and in conclusion $\varphi_j = 0$ on Γ_0 for $j = 0, 1$. ■

Remark 5.3 *We note that in the case when Γ_0 is flat, the RtR operators $\mathcal{S}^j_{j+1,j+1}, j = 0, 1$ are actually compact in the space $H^{-1/2}(\Gamma_0)$.*

We turn our attention to the analysis of the QO DD (3.1) in the case of multiple interfaces separating several layers.

5.3 Invertibility of the QO DD formulation (3.1) in the case of multiple interfaces

We begin by expressing the RtR operators $\mathcal{S}^j$ defined in equation (3.6) via boundary integral operators. We present our derivations in the case of transmission operators $Z^{s,L}_{j-1,j}$ and $Z^{s,L}_{j+1,j}$ defined in equation (4.8); analogous results can be established in the case of transmission operators $Z^L_{j-1,j}$ and $Z^L_{j+1,j}$ defined in equation (4.12). We note that the Helmholtz problems (3.2) can be all expressed in the generic form

$$\begin{aligned} \Delta w + k^2 w &= 0, \quad \text{in } \Omega^{per}, \\ \partial_n w + Z_t\, w &= g_t, \quad \text{on } \Gamma_t, \\ \partial_n w + Z_b\, w &= g_b, \quad \text{on } \Gamma_b, \end{aligned} \tag{5.17}$$

where g_t, g_b are α-quasiperiodic functions; for instance, $Z_t := Z^{s,L}_{j-1,j}$ and $Z_b = Z^{s,L}_{j+1,j}$ in the case when $\Omega^{per} = \Omega^{per}_j$. Thus, the RtR operators $\mathcal{S}^j, 1 \leq j < N$, defined in equation (3.6) are all related to the following RtR operator associated with the Helmholtz boundary value problems (5.17):

$$\mathcal{S} \begin{bmatrix} g_t \\ g_b \end{bmatrix} = \begin{bmatrix} \mathcal{S}_{t,t} & \mathcal{S}_{t,b} \\ \mathcal{S}_{b,t} & \mathcal{S}_{b,b} \end{bmatrix} \begin{bmatrix} g_t \\ g_b \end{bmatrix} := \begin{bmatrix} (\partial_n w - Z_t'\, w)|_{\Gamma_t} \\ (\partial_n w - Z_b'\, w)|_{\Gamma_b} \end{bmatrix}, \tag{5.18}$$

where $Z_t' = Z^{s,L}_{j,j-1}$ and $Z_b' = Z^{s,L}_{j,j+1}$ in the case when $\Omega^{per} = \Omega^{per}_j$. Seeking a solution w of equations (5.17) in the form

$$w = SL_{k,t}\varphi_t + SL_{k,b}\varphi_b,$$

where $SL_{k,t}$ and $SL_{k,b}$ denote the quasiperiodic single layer potentials whose domains of integration are Γ_t and Γ_b, we arrive at the following expression for the RtR operator $\mathcal{S}$:

$$\mathcal{S} = \begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix} - \begin{bmatrix} Z_t + Z_t' & 0 \\ 0 & Z_b + Z_b' \end{bmatrix} \begin{bmatrix} S^w_{k,t,t} & S^w_{k,b,t} \\ S^w_{k,t,b} & S^w_{k,b,b} \end{bmatrix} \times \begin{bmatrix} 1/2I + (K^w_{k,t,t})^\top + Z_t S^w_{k,t,t} & (K^w_{k,b,t})^\top + Z_t S^w_{k,b,t} \\ (K^w_{k,t,b})^\top + Z_b S^w_{k,t,b} & 1/2I + (K^w_{k,b,b})^\top + Z_b S^w_{k,b,b} \end{bmatrix}^{-1}. \tag{5.19}$$

We note that in equation (5.19), the subscripts in the notation $S^w_{k,b,t}$ signify that, in equation (5.3), the target point is $\mathbf{x} \in \Gamma_t$ and the integration point is $\mathbf{y} \in \Gamma_b$. The invertibility of the operators featured in equation (5.19) can be established using similar reasoning to that in the proof of Theorem 5.1 under similar assumptions on the regularity of the profiles g_t and g_b, and the smallness of the shape perturbation parameter ε. Using similar arguments to those that led to establishing property (5.15), and the fact that the off-diagonal operators in equation (5.19) feature boundary integral operators whose kernels are smooth, it can be shown after somewhat tedious calculations that (i) the off-diagonal operators $\mathcal{S}_{t,b}$ and $\mathcal{S}_{b,t}$ have the following mapping properties:

$$\mathcal{S}_{t,b} : H^{-1/2}(\Gamma_b) \to H^{1/2}(\Gamma_t), \quad \mathcal{S}_{b,t} : H^{-1/2}(\Gamma_t) \to H^{1/2}(\Gamma_b),$$

and (ii) the diagonal operators $\mathcal{S}_{t,t}$ and $\mathcal{S}_{t,b}$ can be decomposed in the form

$$\mathcal{S}_{t,t} = \mathcal{S}^0_{t,t} + \mathcal{S}^1_{t,t}, \quad \|\mathcal{S}^0_{t,t}\|_{H^{-1/2}(\Gamma_t)\to H^{-1/2}(\Gamma_t)} \lesssim \varepsilon^{\min(L,2)+1}, \quad \mathcal{S}^1_{t,t} : H^{-1/2}(\Gamma_t) \to H^{1/2}(\Gamma_t),$$

as well as

$$\mathcal{S}_{b,b} = \mathcal{S}^0_{b,b} + \mathcal{S}^1_{b,b}, \quad \|\mathcal{S}^0_{b,b}\|_{H^{-1/2}(\Gamma_b)\to H^{-1/2}(\Gamma_b)} \lesssim \varepsilon^{\min(L,2)+1}, \quad \mathcal{S}^1_{b,b} : H^{-1/2}(\Gamma_b) \to H^{1/2}(\Gamma_b).$$

We are now in the position to prove the following theorem

Theorem 5.4 *Assuming that the transmission problem* (2.1) *is well-posed, the profiles $\widetilde{F}_j(x)$ are all periodic and C^2 for $0 \le j \le N$, and that the shape parameter ε corresponding to the grating profiles $F_j(x) = \varepsilon\widetilde{F}_j(x),\ 0 \le j \le N$ is small enough, the QO DD Schwarz iteration operator $\mathcal{A}^s$ defined in equation* (3.9) *is invertible in the space $H^{-1/2}(\Gamma_0) \times H^{-1/2}(\Gamma_0) \times \ldots \times H^{-1/2}(\Gamma_N) \times H^{-1/2}(\Gamma_N)$.*

Proof. Assuming that ε is smaller than all the radii of convergence of the shape perturbation series of the DtN operators $Y^+(k_{j+1}, \Gamma_{j-1}),\ 1 \le j \le N+1$ and $Y^-(k_j, \Gamma_j),\ 0 \le j \le N$, we use the results established above to express the diagonal blocks of the RtR operators $\mathcal{S}^j,\ 1 \le j \le N$ in the form

$$\mathcal{S}^j_{\ell,\ell} = \mathcal{S}^{j,0}_{\ell,\ell} + \mathcal{S}^{j,1}_{\ell,\ell}, \quad \ell \in \{j-1, j+1\}$$

where

$$\|\mathcal{S}^{j,0}_{\ell,\ell}\|_{H^{-1/2}(\Gamma_\ell)\to H^{-1/2}(\Gamma_\ell)} \lesssim \varepsilon^{\min 2, L+1}, \quad \mathcal{S}^{j,1}_{\ell,\ell} : H^{-1/2}(\Gamma_\ell) \to H^{1/2}(\Gamma_\ell).$$

Similar decomposition can be performed on the RtR operators $\mathcal{S}^0$ and $\mathcal{S}^{N+1}$. In addition, the off diagonal blocks of the RtR operators $\mathcal{S}^j,\ 1 \le j \le N$ can be shown to have the following mapping property

$$\mathcal{S}^j_{\ell,\ell'} : H^{-1/2}(\Gamma_{\ell'}) \to H^{1/2}(\Gamma_\ell), \quad \{\ell, \ell'\} = \{j-1, j+1\}.$$

Then, we can express the QO DD operator $\mathcal{A}^s$ in the form

$$\mathcal{A}^s = \mathcal{A}^{s,0} + \mathcal{A}^{s,1}$$

where

$$\mathcal{A}^{s,0} := \begin{bmatrix} I & \mathcal{S}^{1,0}_{0,0} & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & \ldots & 0 & 0 \\ \mathcal{S}^{0,0}_{1,1} & I & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & \ldots & 0 & 0 \\ 0 & 0 & I & \mathcal{S}^{2,0}_{1,1} & \ldots & 0 & 0 & 0 & 0 & \ldots & 0 & 0 \\ 0 & 0 & \mathcal{S}^{1,0}_{2,2} & I & \ldots & 0 & 0 & 0 & 0 & \ldots & 0 & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \\ 0 & 0 & 0 & 0 & \ldots & 0 & I & \mathcal{S}^{j+1,0}_{j,j} & 0 & \ldots & 0 & 0 \\ 0 & 0 & 0 & 0 & \ldots & 0 & \mathcal{S}^{j,0}_{j+1,j+1} & I & 0 & \ldots & 0 & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & I & \mathcal{S}^{N+1,0}_{N,N} \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \mathcal{S}^{N,0}_{N+1,N+1} & I \end{bmatrix},$$

and the matrix operator $\mathcal{A}^{s,1}$ is compact in the space $H^{-1/2}(\Gamma_0) \times H^{-1/2}(\Gamma_0) \times \ldots \times H^{-1/2}(\Gamma_N) \times H^{-1/2}(\Gamma_N)$. Given the bounds established above on the operators that are non-diagonal entries in the matrix operator $\mathcal{A}^{s,0}$, we conclude that the operator $\mathcal{A}^{s,0}$ is invertible in the space $H^{-1/2}(\Gamma_0) \times H^{-1/2}(\Gamma_0) \times \ldots \times H^{-1/2}(\Gamma_N) \times H^{-1/2}(\Gamma_N)$. Thus, the invertibility of the operator $\mathcal{A}^s$ is equivalent to its injectivity. The latter, in turn, follows from the well-posedness of the transmission problem (2.1) just as in the proof of Theorem 5.1. ■

5.4 Invertibility of the slab subdomain QO DD formulation (3.11)

We now consider a representation of the RtR operators associated with the Helmholtz transmission boundary value problem (3.12). We assume for simplicity that none of the wavenumbers are Wood frequencies. Then, we look for the solution v_j of the boundary value problem (3.12) in the form

$$v_j(\mathbf{x}) = \begin{cases} [SL_{k_{j-1},\Sigma^\flat_{j,j-1}}\varphi_{j,j-1}](\mathbf{x}) + [SL_{k_{j-1},\Gamma_{j-1}}\varphi](\mathbf{x}) + [DL_{k_{j-1},\Gamma_{j-1}}\psi](\mathbf{x}), & x_2 > \overline{F}_{j-1} + F_{j-1}(x_1), \\ [SL_{k_j,\Sigma^\flat_{j+1,j}}\varphi_{j+1,j}](\mathbf{x}) + [SL_{k_j,\Gamma_{j-1}}\varphi](\mathbf{x}) + [DL_{k_j,\Gamma_{j-1}}\psi](\mathbf{x}), & x_2 < \overline{F}_{j-1} + F_{j-1}(x_1), \end{cases} \tag{5.20}$$

where the double layer potentials on the interface Γ_{j-1} are defined with respect to the unit normal pointing towards the domain Ω_j. The enforcement of the boundary conditions in (3.12) leads to the following system of BIEs

$$\begin{aligned}
&\left(\frac{1}{2}I + K^{\top}_{k_{j-1},\Sigma^{\flat}_{j,j-1}} + Z^{\flat}_{j-1,j}S_{k_{j-1},\Sigma^{\flat}_{j,j-1}}\right)\varphi_{j,j-1} + \left(\partial_{x_2}SL_{k_{j-1},\Gamma_{j-1},\Sigma^{\flat}_{j-1,j}} + Z^{\flat}_{j-1,j}SL_{k_{j-1},\Gamma_{j-1},\Sigma^{\flat}_{j-1,j}}\right)\varphi \\
&\qquad + \left(\partial_{x_2}DL_{k_{j-1},\Gamma_{j-1},\Sigma^{\flat}_{j-1,j}} + Z^{\flat}_{j-1,j}DL_{k_{j-1},\Gamma_{j-1},\Sigma^{\flat}_{j-1,j}}\right)\psi = g^{\flat}_{j,j-1} \\
&\left(\frac{1}{2}I + K^{\top}_{k_j,\Sigma^{\flat}_{j+1,j}} + Z^{\flat}_{j+1,j}S_{k_j,\Sigma^{\flat}_{j+1,j}}\right)\varphi_{j+1,j} + \left(-\partial_{x_2}SL_{k_j,\Gamma_{j-1},\Sigma^{\flat}_{j+1,j}} + Z^{\flat}_{j+1,j}SL_{k_j,\Gamma_{j-1},\Sigma^{\flat}_{j+1,j}}\right)\varphi \\
&\qquad + \left(-\partial_{x_2}DL_{k_j,\Gamma_{j-1},\Sigma^{\flat}_{j+1,j}} + Z^{\flat}_{j+1,j}DL_{k_j,\Gamma_{j-1},\Sigma^{\flat}_{j+1,j}}\right)\psi = g^{\flat}_{j+1,j} \\
&\left(\partial_{n_j}SL_{k_{j-1},\Sigma^{\flat}_{j,j-1},\Gamma_{j-1}}\right)\varphi_{j,j-1} - \left(\partial_{n_j}SL_{k_j,\Sigma^{\flat}_{j+1,j},\Gamma_{j-1}}\right)\varphi_{j+1,j} + \left(I + K^{\top}_{k_{j-1},\Gamma_{j-1}} - K^{\top}_{k_j,\Gamma_{j-1}}\right)\varphi \\
&\qquad + \left(N_{k_{j-1},\Gamma_{j-1}} - N_{k_j,\Gamma_{j-1}}\right)\psi = 0 \\
&-\left(SL_{k_{j-1},\Sigma^{\flat}_{j,j-1},\Gamma_{j-1}}\right)\varphi_{j,j-1} + \left(SL_{k_j,\Sigma^{\flat}_{j+1,j},\Gamma_{j-1}}\right)\varphi_{j+1,j} + \left(S_{k_j,\Gamma_{j-1}} - S_{k_{j-1},\Gamma_{j-1}}\right)\varphi \\
&\qquad + \left(I + K_{k_j,\Gamma_{j-1}} - K_{k_{j-1},\Gamma_{j-1}}\right)\psi = 0
\end{aligned} \tag{5.21}$$

which can be shown to be equivalent to the Helmholtz transmission problem (3.12). In addition, it is relatively straightforward to show that the RtR operator $S^{\flat,j}$ associated with the Helmholtz boundary value (3.12), and explicitly defined in equation (3.13), is a compact operator in the space $H^{-1/2}(\Sigma^{\flat}_{j,j-1})\times H^{-1/2}(\Sigma^{\flat}_{j+1,j})$ under the assumption that the periodic function F_{j-1} is C^2 or better. Thus, the block operators in the representation $S^{\flat,j} = \begin{bmatrix} \mathcal{S}^{\flat,j}_{j-1,j-1} & \mathcal{S}^{\flat,j}_{j-1,j+1} \\ \mathcal{S}^{\flat,j}_{j+1,j-1} & \mathcal{S}^{\flat,j}_{j+1,j+1}\end{bmatrix}$ are themselves compact operators in appropriate function spaces. In conclusion, the DD operator $\mathcal{A}^{\flat}$ corresponding to the QO DD formulation (3.12) is a compact perturbation of the identity. Thus, its invertibility can be established analogously to that of the DD operator in Theorem 5.4 under the assumption that the original Helmholtz transmission problem (3.12) is well-posed. We note that the well-posedness of the QO DD formulation (3.11) holds regardless of the roughness of the profiles Γ_j, as long as the flat interfaces do not intersect the interfaces of material discontinuity.

6 Numerical results

6.1 Nyström discretization

Our numerical methods to solve equations (3.8) and (3.14) rely on Nyström discretizations of the boundary integral operators that feature in the computation of the RtR operators given in Section 5. A key ingredient in the evaluation of quasiperiodic boundary integral operators is the efficient evaluation of the quasiperiodic Green function G^q_k defined in equation (5.1). For frequencies that are away from Wood frequencies, we employ the recently introduced Windowed Green Function Method [3–5]. Specifically, let $\chi(r)$ be a smooth cutoff function equal to 1 for $r < 1/2$ and equal to 0 for $r > 1$ and define the windowed Green functions

$$G^{q,A}_k(x,x_2) = \sum_{m\in\mathbb{Z}} e^{-i\alpha md}G_k(x_1+md,x_2)\chi(r_m/A), \quad r_m = ((x_1+md)^2+x_2^2)^{1/2}. \tag{6.1}$$

The functions $G^{q,A}_k$ converge superalgebraically fast to G^q_k as $A\to\infty$ when k is not a Wood frequency [3–5]. Consequently, we make use of the functions $G^{q,A}_k$ for large A in the definition of the quasiperiodic boundary integral operators. In the case of wavenumber k which is a Wood frequency, we use shifted Green functions and their associated boundary integral operators [3]. Given that the functions $G_k^{q,A}$ exhibit the same singularities as the free-space Green's functions G_k, the four quasiperiodic boundary integral operators (5.4), (5.7), (5.8), (5.9) are discretized using trigonometric collocation and the singular quadratures of Martensen-Kussmaul (MK) that rely on logarithmic splitting of the kernels [17, 20]. The full description of these discretizations is provided in [3]. Since the transmission operators considered in this paper are Fourier multipliers, their discretization is straightforward in the context of this trigonometric interpolation framework.

In summary, using Nyström discretizations of the boundary integral operators based on trigonometric interpolation with n equispaced points, we produce $\mathbb{C}^{n\times n}$ Nyström discretization matrices of the four quasiperiodic boundary integral operators (5.4), (5.7), (5.8), (5.9). Using these Nyström discretization matrices of the quasiperiodic boundary integral operators within the integral representations of the RtR operators presented in Sections 5.2 and 5.3 (cf. formulas (5.11) and (5.19)), we obtain Nyström discretization matrices $\mathcal{S}^{j,n}$ of the corresponding RtR operators $\mathcal{S}^j$ for various choices of transmission operators. For instance, in the case when the transmission operators $Z^L_{j,j-1}$ and $Z^L_{j,j+1}$ defined as in equation (4.12), the RtR Nyström discretization matrices $\mathcal{S}^{j,n}$ of the continuous RtR operators $\mathcal{S}^j$ are expressed in $\mathbb{C}^{2n\times 2n}$ block form

$$\mathcal{S}^{j,n} = \begin{bmatrix} \mathcal{S}^{j,n}_{j-1,j-1} & \mathcal{S}^{j,n}_{j-1,j} \\ \mathcal{S}^{j,n}_{j,j-1} & \mathcal{S}^{j,n}_{j,j} \end{bmatrix}.$$

We note that the RtR representation formulas (5.11) and (5.19) require inverting boundary integral operators. Inverting their Nyström discretization matrices can be performed in practice via direct solvers (when warranted by the size of the problem) or more generally by iterative solvers such as GMRES. Either procedure leads to the formal construction of a $2(N+1)n \times 2(N+1)n$ Nyström discretization matrix of the continuous Schwarz iteration matrix $\mathcal{A}$ defined in equation (3.9) which, in the case of layered transmission operators (4.12) and (4.13), is expressed in the block form

$$\mathcal{A}_n = \begin{bmatrix} D_0^n & U_0^n & 0_n & \dots & 0_n \\ L_0^n & D_1^n & U_1^n & \dots & 0_n \\ \dots & \dots & \dots & \dots & \dots \\ \dots & L_{j-1}^n & D_j^n & U_j^n & \dots \\ \dots & \dots & \dots & \dots & \dots \\ 0_n & \dots & L_{N-2}^n & D_{N-1}^n & U_{N-1}^n \\ 0_n & 0_n & \dots & L_{N-1}^n & D_N^n \end{bmatrix} \tag{6.2}$$

where

$$D_j^n := \begin{bmatrix} I_n & \mathcal{S}^{j+1,n}_{j,j} \\ \mathcal{S}^{j,n}_{j+1,j+1} & I_n \end{bmatrix} \quad U_j^n = \begin{bmatrix} \mathcal{S}^{j+1,n}_{j,j+2} & 0_n \\ 0_n & 0_n \end{bmatrix} \quad L_j^n = \begin{bmatrix} 0_n & 0_n \\ 0_n & \mathcal{S}^{j+1,n}_{j+2,j} \end{bmatrix}. \tag{6.3}$$

We denote the case of semi-infinite transmission operators (4.8) by $\mathcal{A}_n^s$, and the case of slab layers by $\mathcal{A}_n^\flat$ (which has dimensions $2(N+2)n \times 2(N+2)n$). None of the matrices $\mathcal{A}_n$, $\mathcal{A}_n^s$, or $\mathcal{A}_n^\flat$ are stored in practice; instead, the solution of the discrete DD systems featuring these matrices is performed via Krylov subspace iterative solvers such as GMRES. Thus, it is the application of the matrices $\mathcal{A}_n$ and $\mathcal{A}_n^s$ on $2(N+1)n$ vectors (which are discretizations of the generalized Robin data $f_j,\ 0 \le j \le N$) that is effected in practice via $N+2$ subdomain solutions. Similarly, the application of the matrices $\mathcal{A}_n^\flat$ on $2(N+2)n$ vectors requires $N+3$ subdomain solutions. The main scope of the numerical results presented in this paper is to study the performance of GMRES solvers involving the DD discretization matrices $\mathcal{A}_n$, $\mathcal{A}_n^s$, and $\mathcal{A}_n^\flat$.

As it is well documented, the choice of the transmission operators in DD formulations of Helmholtz transmission problems is motivated by optimizing the exchange of information between adjacent layers/subdomains. However, for high-frequency/high-contrast periodic layered media, there is significant global exchange of information amongst all layers, which cannot be captured by local transmission operators alone. One widely used remedy to deal with the global inter-layer communication is based on sweeping preconditioners. Sweeping preconditioners achieve an approximate block LU factorization of the DD matrix $\mathcal{A}_n$ (or $\mathcal{A}_n^s$ and $\mathcal{A}_n^\flat$). In the case of DD for layered media, the sweeping preconditioners can be easily constructed on the basis of a very elegant matrix interpretation [29] which we describe briefly next. The *exact* LU factorization of the block tridiagonal matrix $\mathcal{A}_n$ takes on the form

$$\mathcal{A}_n = \begin{bmatrix} T_0 & \dots & \dots & \dots \\ L_0^n & T_1 & \dots & \dots \\ \dots & \dots & \dots & \dots \\ \dots & L_{N-2}^n & T_{N-1} & 0_n \\ \dots & \dots & L_{N-1}^n & T_N \end{bmatrix} \begin{bmatrix} I_n & T_0^{-1}U_0^n & \dots & \dots \\ 0_n & I_n & T_1^{-1}U_1^n & \dots \\ \dots & \dots & \dots & \dots \\ \dots & \dots & I_n & T_{N-1}^{-1}U_{N-1}^n \\ \dots & \dots & \dots & I_n \end{bmatrix}$$

where

$$\begin{aligned} T_0 &= D_0^n \\ T_j &= D_j^n - L_{j-1}^n T_{j-1}^{-1} U_{j-1}^n,\ j \geq 1. \end{aligned}$$

An approximate LU factorization of the matrix $\mathcal{A}_n$ can be derived on the premise that optimal transmission operators ought to act like perfectly transparent boundary conditions. This would entail that the block operators $\mathcal{S}_{j+1,j+1}^{j,n}$ and $\mathcal{S}_{j-1,j-1}^{j,n}$ be identically zero, which means that all the diagonal blocks D_j are approximated by the identity matrix I_n. Given that $L_{j-1}^n U_{j-1}^n = 0_n$, a very simple approximate LU factorization of the matrix $\mathcal{A}_n$ is provided by

$$\mathcal{A}_n \approx \mathcal{B}_n := \begin{bmatrix} I_n & \dots & \dots & \dots \\ L_0^n & I_n & \dots & \dots \\ \dots & \dots & \dots & \dots \\ \dots & L_{N-2}^n & I_n & 0_n \\ \dots & \dots & L_{N-1}^n & I_n \end{bmatrix} \begin{bmatrix} I_n & U_0^n & \dots & \dots \\ 0_n & I_n & U_1^n & \dots \\ \dots & \dots & \dots & \dots \\ \dots & \dots & I_n & U_{N-1}^n \\ \dots & \dots & \dots & I_n \end{bmatrix}. \tag{6.4}$$

Clearly, solving $\mathcal{B}_n x_n = f_n$ is straightforward as it does not involve any inversions of (smaller) block matrices. Indeed, this is done through the forward sweep

$$\begin{aligned} y_0^n &= f_0^n, \\ y_j^n &= f_j^n - L_{j-1}^n y_{j-1}^n,\ 1 \leq j \leq N, \end{aligned}$$

followed by the backward sweep

$$\begin{aligned} x_N^n &= y_N^n, \\ x_{N-j}^n &= y_{N-j}^n - U_{N-j}^n x_{N-j+1}^n,\ 1 \leq j \leq N. \end{aligned}$$

Accordingly, the application of the double sweep preconditioner $\mathcal{B}_n^{-1}$ on a $2(N+1)n$ vector requires $2N$ additional subdomain solutions. In conclusion, a matrix-vector product associated with the matrix $\mathcal{B}_n^{-1}\mathcal{A}_n$ requires $3N+2$ subdomain solutions, the same as $(\mathcal{B}_n^s)^{-1}\mathcal{A}_n^s$, while $(\mathcal{B}_n^\flat)^{-1}\mathcal{A}_n^\flat$ requires $3N+5$ subdomain solutions.

Remark 6.1 *The exact LU factorization can also be employed for the solution of QO DD linear systems involving the matrix $\mathcal{A}_n$ provided that the RtR discretization matrices $\mathcal{S}^{j,n}$, $0 \leq j \leq N$ are assembled—see [26] for details of such a direct DD approach. The sweeping preconditioner methodology presented in this paper is more flexible, as the RtR matrices $\mathcal{S}^{j,n}$, $0 \leq j \leq N$ need not be assembled, and subdomain solutions themselves can be obtained via iterative solvers. Because of this, the sweeping preconditioner above can be viewed as a matrix-free preconditioner.*

As presented above, the double sweep preconditioner is a sequential algorithm. It is possible to resort to other matrix-free preconditioning strategies that exhibit more parallelism. For instance, Symmetric Gauss-Seidel (SGS) preconditioners can be applied to great effect [30]. These preconditioners take on the form

$$P_n := L_n^{-1} + U_n^{-1} - I \tag{6.5}$$

where L_n is a matrix whose lower triangular entries (that is those corresponding to indices (ℓ, j) such that $j \leq \ell$) coincide with those of $\mathcal{A}_n$, and the rest of its entries are equal to zero. U_n is a matrix whose upper triangular entries (that is those corresponding to indices (ℓ, j) such that $\ell \leq j$) coincide with those of $\mathcal{A}_n$, and the rest of its entries are equal to zero, and I denotes the identity matrix of the same size as $\mathcal{A}_n$. Denoting $g_n := L_n^{-1} f_n$ and $h_n := U_n^{-1} f_n$, the components of g_n and h_n are computed via the relations

$$\begin{aligned}
g^n_{j,t} &= f^n_{j,t} & h^n_{j,b} &= f^n_{j,b} & & 0 \leq j \leq N\\
g^n_{0,b} &= f^n_{0,b} - \mathcal{S}^{0,n} g^n_{0,t} & h^n_{N,t} &= f^n_{N,t} - \mathcal{S}^{N+1,n} h^n_{N,b} & &\\
g^n_{j,b} &= f^n_{j,b} - S^{j,n}_{j+1,j+1} f^n_{j,t} & h^n_{N-j,t} &= f^n_{N-j,t} - S^{N-j+1,n}_{N-j,N-j} f^n_{N-j,b} & &\\
&\quad - S^{j,n}_{j+1,j-1} g^n_{j-1,b} & &\quad - S^{N-j+1,n}_{N-j,N-j+1} h^n_{N-j+1,t} & & 1 \leq j \leq N
\end{aligned}$$

where $f^n_j = [f^n_{j,t}\ f^n_{j,b}]^\top$, $g^n_j = [g^n_{j,t}\ g^n_{j,b}]^\top$, and $h^n_j = [h^n_{j,t}\ h^n_{j,b}]^\top$. Again here, the application of a RtR block matrix requires a subdomain solution.

6.2 QO DD solvers and sweeping preconditioners

We present in this section various numerical examples that illustrate the iterative behavior of the QO DD solvers using sweeping preconditioners. We consider both smooth and Lipschitz grating profiles that exhibit various degrees of roughness—as measured by the ratio of the height to the period, as well as by the oscillatory nature of the profile. Specifically, we consider the smooth profile $\widetilde{F}^s(x_1) := 2.5 \cos x_1$, the rough profile $\widetilde{F}^r(x_1) = 2.5\ \pi(0.4\cos(x_1) - 0.2\cos(2x_1) + 0.4\cos(3x_1))$, and structures with interfaces $x_2 = -\ell H + \varepsilon \widetilde{F}^m(x_1), 0 \leq \ell \leq N,\ 0 < H,\ m \in \{s, r\}$. We consider Lipschitz grating profiles $\widetilde{F}^L$ depicted in Figure 3 of period 2π and height ε (note that the second profile in Figure 3 is not the graph of a 2π periodic function).

In the numerical results in this section we report the numbers of iterations required by the QO DD solvers to reach relative GMRES residuals of 10^{-4} and 10^{-6}. Specifically, we used GMRES to solve the linear systems corresponding to discretization matrices $\mathcal{A}_n$ and $\mathcal{A}^s_n$ corresponding to the QO DD formulation (3.9) with transmission operators defined in equations (4.8) and (4.12) respectively, and $\mathcal{A}^\flat_n$ corresponding to the QO DD formulation with slab subdomains (3.11). We also specify in the table headers the various approximation orders L in the definition of the transmission operators (4.8) and (4.12) that enter the QO DD formulations (3.9). As previously discussed, higher values of the approximation parameter L lead to ill-conditioning in the calculations of transmission operators. We also investigate the effectiveness of the sweeping preconditioner applied to the

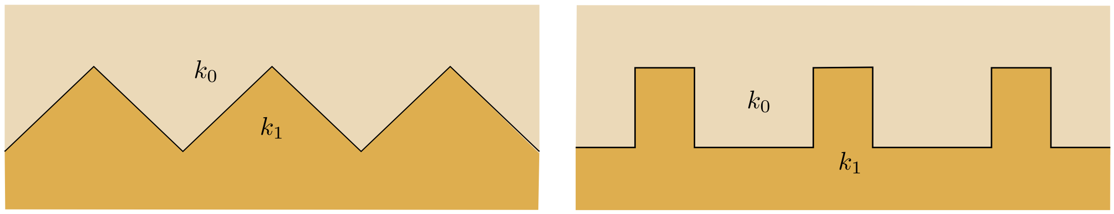

Figure 3: Lipschitz grating profiles of period 2π and height ε.

QO DD discretization matrices. For this we present the numbers of GMRES iterations needed with the sweeping preconditioner under the table header $\mathcal{B}_n^{-1}\mathcal{A}_n$ (and its analogues $(\mathcal{B}_n^s)^{-1}\mathcal{A}_n^s$ and $(\mathcal{B}_n^\flat)^{-1}\mathcal{A}_n^\flat$).

In the numerical experiments presented here we chose discretization sizes n and windowing parameters A for the quasiperiodic Green function $G_k^{q,A}$ in equation (6.1) so that the solutions produced by DD based on Nyström discretizations of the RtR operators exhibit accuracies of the order 10^{-4} (or better) as measured by conservation of energy metrics. Specifically, we selected the windowing parameter $A = 120$ and the discretization size $n = 256$ in all the results presented in this section, with the exception of the experiments involving perfectly conducting inclusions, where we chose a larger windowing parameter $A = 300$. The Nyström discretization matrices of the RtR maps were produced following the calculations presented in Section 5 using direct linear algebra solvers to invert the discretization matrices corresponding to boundary integral operators. In all the numerical results presented in this section we considered normal incidence, that is the quasiperiodic parameter $\alpha = 0$. Qualitatively similar results are obtained for other values of α. Finally, unless specified, the wavenumbers considered in the numerical experiments are not Wood frequencies.

In our previous contribution [26] similar quasiperiodic transmission problems were treated via a *direct* solver based on a DD approach with classical Robin data exchange. That approach relied on the LU factorization of the matrices $\mathcal{A}_n$, and, as such, it required that the RtR matrices $\mathcal{S}^{j,n}$ be assembled. In contrast, the QO DD approach presented in this paper bypasses that need, and hence it is more flexible for high frequency applications.

6.2.1 Two layers

We start the presentation of our numerical results with the case of two semi-infinite layers separated by a periodic interface. We present in Table 1 numbers of GMRES iterations required by the QO DD Nyström discretization matrices $\mathcal{A}_n$ to reach GMRES relative residuals of 10^{-6} in the case of a deep, smooth and rough grating interface separating two high-contrast media. Commensurate energy errors were produced by the Nyström discretizations of the QO DD linear system. The wavenumbers considered in these results correspond to periodic transmission problems of periods that consist of $5, 10, 20$, and 80 wavelengths espectively. We remark that using transmission operators $Z_{0,1}^2$ and $Z_{1,0}^2$ in the QO DD algorithm gives rise to numbers of GMRES iterations that scale very mildly with respect to the increasing frequencies. We continue in Table 2 with numerical examples concerning a deep Lipschitz grating separating two high-contrast media. In the case of Lipschitz interfaces, we used transmission operators $Z_{0,1}^0$ and $Z_{1,0}^0$ respectively; we observed that the use of higher-order transmission operators $Z_{0,1}^L$ and $Z_{1,0}^L$ with $1 \leq L \leq 2$ does not lead to improved iterative convergence of the QO DD solvers. According to the results presented in Figure 4, the numbers of GMRES

Interface	$k_0 = 1.3, k_1 = 4.3$		$k_0 = 2.3, k_1 = 8.3$		$k_0 = 4.3, k_1 = 16.3$		$k_0 = 16.3, k_1 = 64.3$	
	$\mathcal{A}_n, L = 0$	$\mathcal{A}_n, L = 2$	$\mathcal{A}_n, L = 0$	$\mathcal{A}_n, L = 2$	$\mathcal{A}_n, L = 0$	$\mathcal{A}_n, L = 2$	$\mathcal{A}_n, L = 0$	$\mathcal{A}_n, L = 2$
smooth	14	12	16	12	19	14	21	14
rough	19	17	22	15	24	17	28	18

Table 1: Numbers of GMRES iterations required by QO DD formulations to reach relative residuals of 10^{-6} for configurations consisting of 2 layers, where the interface Γ_0 is given by deep grating profiles $F_\ell(x_1) = 2.5\cos x_1$ (top panel) and $F_\ell(x_1) = 2.5\pi(0.4\cos(x_1) - 0.2\cos(2x_1) + 0.4\cos(3x_1))$ (bottom panel), and various values of wavenumbers $k_\ell, \ell = 0, 1$.

Profile	$k_0 = 1.3, k_1 = 4.3$	$k_0 = 2.3, k_1 = 8.3$	$k_0 = 4.3, k_1 = 16.3$	$k_0 = 16.3, k_1 = 64.3$
	$\mathcal{A}_n, L = 0$	$\mathcal{A}_n, L = 0$	$\mathcal{A}_n, L = 0$	$\mathcal{A}_n, L = 0$
sawtooth	15	16	18	20
binary	17	19	21	25

Table 2: Numbers of GMRES iterations required by QO DD formulations to reach relative residuals of 10^{-6} for configurations consisting of 2 layers, where the interface Γ_0 is given by the Lipschitz grating profiles depicted in Figure 3 with height to period ratio equal to 1 (top panel corresponds to the sawtooth grating and the bottom panel corresponds to the binary grating), and various values of wavenumbers $k_\ell, \ell = 0, 1$.

iterations required by the QO DD formulation appear to be growing logarithmically with respect to the frequency in the case of deep Lipschitz interfaces.

6.2.2 Three layers.

We devote the next set of results to configurations consisting of three layers separated by two periodic interfaces. We present in Table 3 numbers of GMRES iterations required by the QO DD discretization matrices $\mathcal{A}_n$ to reach relative residuals of 10^{-4} for increasingly rougher (yet smooth) grating profiles separating high-contrast periodic layers. We remark that for small values of the roughness parameter ε (i.e. $\varepsilon = 0.1,\ 0.5$), the numbers of iterations do not appear to depend on the increased contrast. For larger values of the parameter ε (i.e. $\varepsilon = 1$), the numbers of iterations grow with the frequency, yet the growth rate is modest. We also point out that the use of transmission operators $Z^2_{j,j+1}$ (which are higher-order approximations of the DtN operators) appears to be beneficial to the iterative behavior of the QO DD algorithm.

6.2.3 Many layers.

We investigate next the iterative behavior of the QO DD solvers and the effectiveness of the sweeping preconditioners in the case of configurations that involve large numbers of layers. In the case when the height of the interfaces is small enough (i.e. the height parameter $\varepsilon = 0.02$), we see in Table 5 that the sweeping preconditioner applied to the QO DD matrices $\mathcal{A}_n$ appears to be scalable, that is the numbers of GMRES iterations required for convergence does not depend on the number of layers or on the frequencies in each layer. We note that the transmission problems considered in Table 5 (as well as in Table 6-Table 8) range from 100 to 4,000 wavelengths—as measured by the

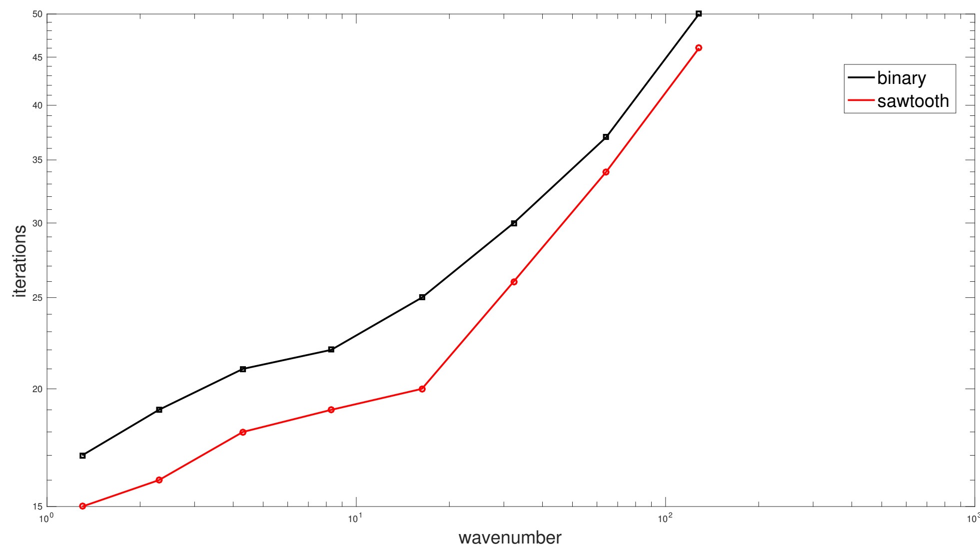

Figure 4: Numbers of GMRES iterations required by QO DD formulations to reach relative residuals of 10^{-6} for configurations consisting of 2 layers, where the interface Γ_0 is given by the Lipschitz grating profiles depicted in Figure 3 with height to period ratio equal to 1 for wavenumbers $k_0 = 2^\ell + 0.3,\ 0 \leq \ell \leq 7$ and $k_1 = 2^{2+\ell} + 0.3,\ 0 \leq \ell \leq 7$. The rate of growth of GMRES iterations appears to be logarithmic in these cases.

Profile	ε	$k_0 = 1.3, k_1 = 4.3, k_2 = 16.3$				$k_0 = 2.3, k_1 = 8.3, k_2 = 32.3$				$k_0 = 4.3, k_1 = 16.3, k_3 = 64.3$			
		$\mathcal{A}_n, L=0$	$\mathcal{B}_n^{-1}\mathcal{A}_n, L=0$	$\mathcal{A}_n, L=2$	$\mathcal{B}_n^{-1}\mathcal{A}_n, L=2$	$\mathcal{A}_n, L=0$	$\mathcal{B}_n^{-1}\mathcal{A}_n, L=0$	$\mathcal{A}_n, L=2$	$\mathcal{B}_n^{-1}\mathcal{A}_n, L=2$	$\mathcal{A}_n, L=0$	$\mathcal{B}_n^{-1}\mathcal{A}_n, L=0$	$\mathcal{A}_n, L=2$	$\mathcal{B}_n^{-1}\mathcal{A}_n, L=2$
smooth	0.1	9	9	9	9	9	9	9	9	9	9	9	9
smooth	0.5	13	11	11	11	14	12	11	11	14	12	11	11
smooth	1	20	17	16	14	23	19	16	14	27	23	19	16
rough	0.1	10	9	10	9	11	11	11	11	10	9	9	9
rough	0.5	18	15	13	11	18	15	14	13	19	15	17	14
rough	1	30	25	20	19	38	33	22	21	56	49	24	22

Table 3: Numbers of GMRES iterations required by QO DD formulations to reach relative residuals of 10^{-4} for configurations consisting of 3 layers, where the interfaces $\Gamma_\ell, 0 \leq \ell \leq 1$ are given by grating profiles $F_\ell(x_1) = -\ell H + 2.5\varepsilon \cos x_1, H = 3.3, 0 \leq \ell \leq 1$ (top panel) and $F_\ell(x_1) = -\ell H + 2.5\pi\varepsilon(0.4\cos(x_1) - 0.2\cos(2x_1) + 0.4\cos(3x_1)), H = 3.3, 0 \leq \ell \leq 1$ (bottom panel) for various values of the height parameter ε, under normal incidence, and various values of wavenumbers k_ℓ.

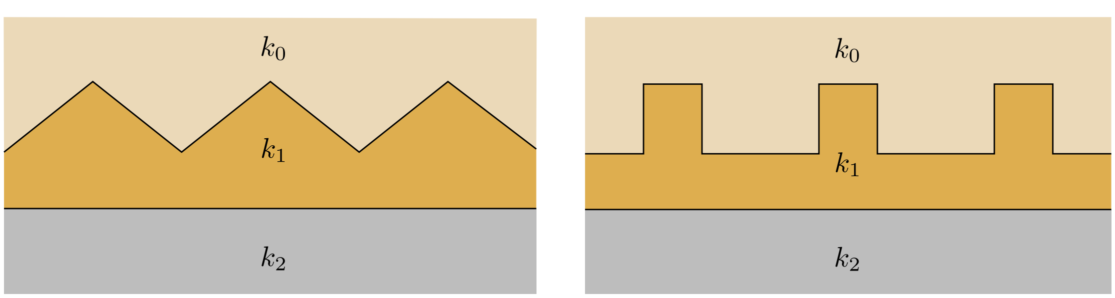

Figure 5: Three layer configurations with Lipschitz upper layer grating profiles of period 2π and height ε.

Profile	ε	$k_0 = 1.3, k_1 = 4.3, k_2 = 16.3$		$k_0 = 2.3, k_1 = 8.3, k_2 = 32.3$		$k_0 = 4.3, k_1 = 16.3, k_3 = 64.3$	
		$\mathcal{A}_n, L = 0$	$\mathcal{B}_n^{-1}\mathcal{A}_n, L = 0$	$\mathcal{A}_n, L = 0$	$\mathcal{B}_n^{-1}\mathcal{A}_n, L = 0$	$\mathcal{A}_n, L = 0$	$\mathcal{B}_n^{-1}\mathcal{A}_n, L = 0$
sawtooth	0.25	15	13	18	15	22	18
sawtooth	1.25	16	14	18	16	21	18
sawtooth	2.5	18	16	19	17	21	19
binary	0.25	18	17	21	18	25	23
binary	1.25	18	17	21	18	26	23
binary	2.5	18	17	25	22	28	25

Table 4: Numbers of GMRES iterations required by QO DD formulations to reach relative residuals of 10^{-4} for configurations consisting of 3 layers as depicted in Figure 5. The smallest distance between the grating profiles Γ_0 and Γ_1 was taken to be equal to 1.3. The results corresponding to the top sawtooth grating are presented in the top panel, and the results corresponding to the top binary grating are presented in the bottom panel. We considered various values of the height parameter ε for the top grating profiles. for various values of the height parameter ε, under normal incidence, and various values of wavenumbers k_ℓ.

Profile	N	$k_\ell = \ell + 1.3, 0 \le \ell \le N$				$k_\ell = 2\ell + 1.3, 0 \le \ell \le N$				$k_\ell = 4\ell + 1.3, 0 \le \ell \le N$			
		$\mathcal{A}_n, L = 0$	$\mathcal{B}_n^{-1}\mathcal{A}_n, L = 0$	$\mathcal{A}_n, L = 2$	$\mathcal{B}_n^{-1}\mathcal{A}_n, L = 2$	$\mathcal{A}_n, L = 0$	$\mathcal{B}_n^{-1}\mathcal{A}_n, L = 0$	$\mathcal{A}_n, L = 2$	$\mathcal{B}_n^{-1}\mathcal{A}_n, L = 2$	$\mathcal{A}_n, L = 0$	$\mathcal{B}_n^{-1}\mathcal{A}_n, L = 0$	$\mathcal{A}_n, L = 2$	$\mathcal{B}_n^{-1}\mathcal{A}_n, L = 2$
smooth	9	58	13	58	13	62	13	62	13	61	12	61	12
smooth	19	115	14	115	14	119	14	119	14	118	14	118	14
smooth	29	164	14	164	14	171	14	171	14	168	14	168	14
rough	9	60	13	60	13	58	14	58	14	61	14	61	14
rough	19	119	14	115	14	119	16	117	14	117	14	150	14
rough	29	167	14	161	14	166	15	164	14	183	14	167	14

Table 5: Numbers of GMRES iterations required by preconditioned/unpreconditioned QO DD formulations to reach relative residuals of 10^{-4} for configurations consisting of $N + 2$ layers for various values of N, where the interfaces $\Gamma_\ell, 0 \le \ell \le N$ are given by grating profiles $F_\ell(x_1) = -\ell H + 2.5\varepsilon \cos x_1, H = 3.3, 0 \le \ell \le N$ with $\varepsilon = 0.02$ (top panel) and $F_\ell(x_1) = -\ell H + 2.5\pi\varepsilon(0.4\cos(x_1) - 0.2\cos(2x_1) + 0.4\cos(3x_1)), H = 3.3, 0 \le \ell \le N$ with $\varepsilon = 0.02$ (bottom panel), under normal incidence, and various values of wavenumbers k_ℓ.

number of wavelengths across the period of each interface; the discretization size ranges from 5,000 to 15,000 unknowns. As the roughness parameter is increased from $\varepsilon = 0.02$ to $\varepsilon = 0.1$, we see in Table 6 that the numbers of GMRES iterations remain fixed when the sweeping preconditioner is applied to the DD matrices $\mathcal{A}_n^s$, but not in its counterpart case involving the DD matrices $\mathcal{A}_n$. Furthermore, QO DD solvers based on higher-order transmission operators (that is values of the parameter $L \ge 1$ in the definition of the transmission operators $Z^L_{j,j-1}$,$Z^L_{j,j+1}$, and respectively $Z^{s,L}_{j,j-1}$ and $Z^{s,L}_{j,j+1}$) perform only marginally better than those based on zeroth-order transmission operators (that is $L = 0$ in the definition of the aforementioned transmission operators) in the case of small roughness parameters ε. Based on our numerical experience, we observed that the iterative behavior of the QO DD solvers and the sweeping preconditioners depicted in Table 5 and Table 6 is not sensitive to the width H of the layers or the shape of the grating profiles. Furthermore, qualitatively similar behavior was observed in the cases when the interfaces Γ_ℓ are Lipschitz.

As the roughness of the gratings Γ_ℓ increases, the sweeping preconditioner $(\mathcal{B}_n^s)^{-1}\mathcal{A}_n^s$ is still effective, yet the number of iterations required grows mildly with the number of layers as well as with increased frequencies/contrasts—see Table 7. Remarkably, there are important benefits in the reduction of GMRES iterations by incorporating higher-order transmission operators $Z^{s,2}_{j,j-1}$ and $Z^{s,2}_{j,j+1}$ over the zeroth-order ones $Z^{s,0}_{j,j-1}$ and $Z^{s,0}_{j,j+1}$ in the preconditioned QO DD formulations. Also, the sweeping preconditioner is less effective for QO DD formulations based on transmission

Profile	N	$k_\ell = \ell + 1.3, 0 \le \ell \le N$				$k_\ell = 2\ell + 1.3, 0 \le \ell \le N$				$k_\ell = 4\ell + 1.3, 0 \le \ell \le N$			
		$\mathcal{A}_n, L=2$	$\mathcal{B}_n^{-1}\mathcal{A}_n, L=2$	$\mathcal{A}_n^s, L=2$	$(\mathcal{B}_n^s)^{-1}\mathcal{A}_n^s, L=2$	$\mathcal{A}_n, L=2$	$\mathcal{B}_n^{-1}\mathcal{A}_n, L=2$	$\mathcal{A}_n^s, L=2$	$(\mathcal{B}_n^s)^{-1}\mathcal{A}_n^s, L=2$	$\mathcal{A}_n, L=2$	$\mathcal{B}_n^{-1}\mathcal{A}_n, L=2$	$\mathcal{A}_n^s, L=2$	$(\mathcal{B}_n^s)^{-1}\mathcal{A}_n^s, L=2$
smooth	9	60	18	60	15	58	17	58	14	57	15	57	14
smooth	19	109	20	109	18	110	20	110	15	104	19	104	14
smooth	29	156	22	156	18	161	25	159	16	157	24	154	14
rough	9	64	18	61	14	59	19	59	15	60	20	55	14
rough	19	117	26	111	16	119	30	108	16	125	33	107	14
rough	29	170	36	156	16	179	48	155	15	188	54	152	14

Table 6: Numbers of GMRES iterations required by various preconditioned/unpreconditioned QO DD formulations to reach relative residuals of 10^{-4} for configurations consisting of $N+2$ layers for various values of N, where the interfaces $\Gamma_\ell, 0 \le \ell \le N$ are given by grating profiles $F_\ell(x_1) = -\ell H + 2.5\varepsilon \cos x_1, H = 3.3, 0 \le \ell \le N$ with $\varepsilon = 0.1$ (top panel) and $F_\ell(x_1) = -\ell H + 2.5\pi\varepsilon(0.4\cos(x_1) - 0.2\cos(2x_1) + 0.4\cos(3x_1)), H = 3.3, 0 \le \ell \le N$ with $\varepsilon = 0.1$ (bottom panel), under normal incidence, and various values of wavenumbers k_ℓ.

Profile	N	$k_\ell = \ell + 1.3, 0 \le \ell \le N$					$k_\ell = 2\ell + 1.3, 0 \le \ell \le N$					$k_\ell = 4\ell + 1.3, 0 \le \ell \le N$				
		$\mathcal{A}_n, L=0$	$\mathcal{B}_n^{-1}\mathcal{A}_n, L=0/2$	$(\mathcal{B}_n^s)^{-1}\mathcal{A}_n^s, L=0/2$	SGS	$(\mathcal{B}_n^\flat)^{-1}\mathcal{A}_n^\flat$	$\mathcal{A}_n, L=0$	$\mathcal{B}_n^{-1}\mathcal{A}_n, L=0/2$	$(\mathcal{B}_n^s)^{-1}\mathcal{A}_n^s, L=0/2$	SGS	$(\mathcal{B}_n^\flat)^{-1}\mathcal{A}_n^\flat$	$\mathcal{A}_n, L=0$	$\mathcal{B}_n^{-1}\mathcal{A}_n, L=0/2$	$(\mathcal{B}_n^s)^{-1}\mathcal{A}_n^s, L=0/2$	SGS	$(\mathcal{B}_n^\flat)^{-1}\mathcal{A}_n^\flat$
smooth	9	88	44/41	44/25	18	32	94	53/48	53/25	17	29	100	61/55	61/25	16	26
smooth	19	199	101/98	100/34	23	36	224	147/134	145/39	25	30	247	156/133	123/47	29	28
smooth	29	324	152/144	149/40	26	41	359	273/260	261/52	32	30	387	270/215	254/63	40	30
rough	9	121	58/57	57/28	19	23	129	82/66	84/30	20	28	141	71/67	79/34	21	30
rough	19	253	130/120	124/48	31	30	317	221/182	218/60	44	32	388	187/160	162/78	53	34
rough	29	390	206/177	190/68	46	32	502	296/233	251/75	57	34	862	389/354	375/86	69	37

Table 7: Numbers of GMRES iterations required by various preconditioned/unpreconditioned QO DD formulations to reach relative residuals of 10^{-4} for configurations consisting of $N+2$ layers for various values of N, where the interfaces $\Gamma_\ell, 0 \le \ell \le N$ are given by grating profiles $F_\ell(x_1) = -\ell H + 2.5\varepsilon \cos x_1, H = 3.3, 0 \le \ell \le N$ with $\varepsilon = 0.5$ (top panel) and $F_\ell(x_1) = -\ell H + 2.5\pi\varepsilon(0.4\cos(x_1) - 0.2\cos(2x_1) + 0.4\cos(3x_1)), H = 3.3, 0 \le \ell \le N$ with $\varepsilon = 0.5$ (bottom panel), under normal incidence, and various values of wavenumbers k_ℓ.

operators $Z^2_{j,j-1}$ and $Z^2_{j,j+1}$ (i.e. $\mathcal{B}_n^{-1}\mathcal{A}_n$) for rough interface profiles. The Symmetric Gauss-Seidel preconditioners (6.5) applied to the formulation $\mathcal{A}_n^s$ with transmission operators $Z^{s,2}_{j,j-1}$ and $Z^{s,2}_{j,j+1}$—referred to as *SGS* in Table 7, appear to perform better than the sweeping preconditioners. Finally, it can be seen from the results presented in Table 7 that QO DD solvers based on the formulation $(\mathcal{B}_n^\flat)^{-1}\mathcal{A}_n^\flat$ (which, given that the depth of the layers is larger than the profile roughness, is applicable in the case presented in Table 7) require small numbers of GMRES iterations for convergence, whose growth with respect to the number of layers or contrast is very mild. We mention that further reductions in numbers of iterations (about 25%) can be garnered from application of *SGS* preconditioners to $\mathcal{A}_n^\flat$.

In the case of very large gratings Γ_ℓ (whose height/period ratios are close to 1), the sweeping preconditioners $(\mathcal{B}_n^s)^{-1}\mathcal{A}_n^s$ (denoted by the acronym *SW*) become less effective–see Table 8. Nevertheless, the use of higher-order transmission operators $Z^{s,2}_{j,j-1}$ and $Z^{s,2}_{j,j+1}$ is again beneficial. We also remark that the Symmetric Gauss-Seidel preconditioners (6.5) (referred to as *SGS*) perform better than the sweeping preconditioners. We mention that due the ratio between the profile roughness and the width of the layers, the slab DD formulation (3.11) is not possible in this case: a strip domain decomposition would necessarily require that the flat subdomain interfaces intersect the gratings Γ_ℓ. Nevertheless, once the layers width is large enough with respect to profile roughness so that the DD formulation (3.11) is possible, the sweeping preconditioners $(\mathcal{B}_n^\flat)^{-1}\mathcal{A}_n^\flat$ are effective—see Table 9.

According to the results presented in Tables 5–9, the sweeping preconditioners $\mathcal{B}_n^{-1}$ and especially $(\mathcal{B}_n^s)^{-1}$ can effectively reduce the numbers of GMRES iterations required for the solution of

Profile	N	$k_\ell = \ell + 1.3, 0 \leq \ell \leq N$					$k_\ell = 2\ell + 1.3, 0 \leq \ell \leq N$					$k_\ell = 4\ell + 1.3, 0 \leq \ell \leq N$				
		$\mathcal{A}_n^s, L=0$	$SW, L=0$	$\mathcal{A}_n^s, L=2$	$SW, L=2$	SGS	$\mathcal{A}_n^s, L=0$	$SW, L=0$	$\mathcal{A}_n^s, L=2$	$SW, L=2$	SGS	$\mathcal{A}_n^s, L=0$	$SW, L=0$	$\mathcal{A}_n^s, L=2$	$SW, L=2$	SGS
smooth	9	195	137	83	57	32	260	191	92	66	39	310	280	135	87	48
smooth	19	522	312	171	109	63	696	524	253	204	108	1080	812	390	281	168
rough	9	266	164	103	76	45	390	254	121	84	59	481	416	166	125	88
rough	19	736	392	256	187	92	1145	658	354	247	166	1801	1223	461	312	245

Table 8: Numbers of GMRES iterations required by various preconditioned/unpreconditioned QO DD formulations to reach relative residuals of 10^{-4} for configurations consisting of $N+2$ layers for various values of N, where the interfaces $\Gamma_\ell, 0 \leq \ell \leq N$ are given by grating profiles $F_\ell(x_1) = -\ell H + 2.5\varepsilon \cos x_1, H = 3.3, 0 \leq \ell \leq N$ with $\varepsilon = 1$ (top panel) and $F_\ell(x_1) = -\ell H + 2.5\pi\varepsilon(0.4\cos(x_1) - 0.2\cos(2x_1) + 0.4\cos(3x_1)), H = 3.3, 0 \leq \ell \leq N$ with $\varepsilon = 1$ (bottom panel), under normal incidence, and various values of wavenumbers k_ℓ.

Profile	N	$k_\ell = \ell + 1.3, 0 \leq \ell \leq N$			$k_\ell = 2\ell + 1.3, 0 \leq \ell \leq N$			$k_\ell = 4\ell + 1.3, 0 \leq \ell \leq N$		
		$(\mathcal{B}_n^s)^{-1}\mathcal{A}_n^s, L=2$	SGS	$(\mathcal{B}_n^\flat)^{-1}\mathcal{A}_n^\flat$	$(\mathcal{B}_n^s)^{-1}\mathcal{A}_n^s, L=2$	SGS	$(\mathcal{B}_n^\flat)^{-1}\mathcal{A}_n^\flat$	$(\mathcal{B}_n^s)^{-1}\mathcal{A}_n^s, L=2$	SGS	$(\mathcal{B}_n^\flat)^{-1}\mathcal{A}_n^\flat$
smooth	9	50	31	27	66	38	26	110	48	26
smooth	19	90	52	27	158	104	28	189	147	29
rough	9	73	44	26	98	66	28	150	84	29
rough	19	139	81	31	183	129	34	247	193	35

Table 9: Numbers of GMRES iterations required by various preconditioned QO DD formulations to reach relative residuals of 10^{-4} for configurations consisting of $N+2$ layers for various values of N, where the interfaces $\Gamma_\ell, 0 \leq \ell \leq N$ are given by grating profiles $F_\ell(x_1) = -\ell H + 2.5\cos x_1, H = 5.6, 0 \leq \ell \leq N$ (top panel) and $F_\ell(x_1) = -\ell H + 2.5\pi(0.4\cos(x_1) - 0.2\cos(2x_1) + 0.4\cos(3x_1)), H = 4.5, 0 \leq \ell \leq N$ (bottom panel), under normal incidence, and various values of wavenumbers k_ℓ.

QO DD algorithms for periodic transmission problems involving large number of layers, even in the case when the roughness of the interfaces of material discontinuity is pronounced. We have observed that these findings are virtually independent of the layer material properties (for instance, the numbers of GMRES iterations reported in these tables are about the same when we considered random wavenumbers in the same range) or the depth of the layers (as long as the original transmission problem is well posed). In addition, the sweeping preconditioners $(\mathcal{B}_n^\flat)^{-1}$, whenever applicable, are extremely efficient, even for very rough profiles Γ_ℓ.

As we have presented in Tables 5–9, the choice of the transmission operators plays an important role in the convergence properties of the ensuing DD algorithms. Besides the square root Fourier multiplier transmission operators presented in this paper, other transmission operators have been used in the DD arena. Notably, we mention the classical Robin transmission operators $Z = i\ I$ (the first transmission operators introduced for DD formulations of Helmholtz equations by Déspres [9]), as well as transmission operators of the form $Z = \mathcal{T}$ (related to the ones introduced in [19]), where the operator $\mathcal{T}$ is related to the Hilbert transform

$$\mathcal{T}(\varphi)(t) = i\ \partial_t \int_0^{2\pi} \mathcal{K}(t-\tau)\partial_\tau \varphi(\tau) d\tau + \varphi(t), \quad \mathcal{K}(t) := \frac{1}{\pi} \ln|1 - e^{it}|, \quad 0 \leq t \leq 2\pi, \tag{6.6}$$

where φ is a 2π periodic function. We note that these two choices of transmission operators give rise to unitary RtR maps, and thus they lead to DD formulations that are well-posed as long as the initial transmission problem (2.1) is well-defined. We illustrate in Figure 6 the numbers of iterations required by DD formulations that rely on the two above mentioned transmission operators. Specifically, we considered profiles defined by $F_\ell(x_1) = -\ell H + 2.5\varepsilon \cos x_1, H = 3.3, 0 \leq \ell \leq N$ with $\varepsilon = 0.1$ and we report numbers of GMRES iterations required by the DD with the transmission

k_ℓ	One layer inclusions		Two layer inclusions		Three layer inclusions		Four layer inclusions	
	$\mathcal{A}_n, L=0$	$\mathcal{B}_n^{-1}\mathcal{A}_n, L=0$	$\mathcal{A}_n, L=0$	$\mathcal{B}_n^{-1}\mathcal{A}_n, L=0$	$\mathcal{A}_n, L=0$	$\mathcal{B}_n^{-1}\mathcal{A}_n, L=0$	$\mathcal{A}_n, L=0$	$\mathcal{B}_n^{-1}\mathcal{A}_n, L=0$
$k_\ell = \ell + 1.3, \ell \notin I$ $k_\ell = \ell, \ell \in I$	62	17	71	23	81	30	111	40
$k_\ell = 2\ell + 1.3, \ell \notin I$ $k_\ell = 2\ell, \ell \in I$	60	17	69	24	85	31	132	46
$k_\ell = 4\ell + 1.3, \ell \notin I$ $k_\ell = 4\ell, \ell \in I$	57	18	76	28	89	36	141	49

Table 10: Numbers of GMRES iterations required by various QO DD formulations to reach relative residuals of 10^{-4} for configurations consisting of 11 layers with perfectly conducting inclusions depicted in Figure 8, where the interfaces $\Gamma_\ell, 0 \leq \ell \leq 9$ are given by grating profiles $F_\ell(x_1) = -\ell H + 2.5\varepsilon \cos x_1, H = 3, 0 \leq \ell \leq 9$ with $\varepsilon = 0.1$, under normal incidence, and various values of wavenumbers k_ℓ. The wavenumbers corresponding to layers with inclusions were selected to be Wood anomalies. Parameters $A = 300$, $M = 256$ were selected so that to lead to conservation of energy errors of the order 10^{-4}.

operators defined above to reach relative residuals of 10^{-4}. Comparing the results in Figure 6 with their counterparts in Table 6, we see that the use of DD with QO transmission operators $Z^{s,L}_{j,j-1}$ and $Z^L_{j,j+1}$ in conjunction with sweeping preconditioners can give rise to order of magnitude reductions in numbers of GMRES iterations. We mention that the sweeping preconditioner is ineffective in the cases presented in Figure 6. This finding is not surprising, given that the premise of sweeping preconditioners is that the transmission operators are good approximations of subdomain DtN maps. Finally, similar scenarios occur for rougher profiles.

Further insight on the superior performance of the DD algorithms based on QO transmission operators $Z^L_{j,j+1}$ can be garnered from the eigenvalue distribution depicted in Figure 7. We point out that the eigenvalues corresponding to the DD matrices $\mathcal{A}_n, L = 0$ are clustered around one, and the clustering is even more pronounced for the eigenvalues of the preconditioned matrix $\mathcal{B}_n^{-1}\mathcal{A}_n, L = 0$. In contrast, the distribution of the eigenvalues of the DD matrix corresponding to classical Robin transmission operators $Z = i\ I$ is not conducive to fast convergence of GMRES solvers.

6.2.4 Inclusions in periodic layers.

Finally, we present results concerning perfectly conducting inclusions embedded in layered media, see Figure 8. We present numerical experiments related to these configurations in Table 10 and 11. In order to showcase the versatility of our DD algorithm, we chose wavenumbers that are Wood frequencies in the layers that contain inclusions. We note that for these configurations the transmission operators that we use are approximations of DtN operators corresponding to homogeneous layers, and thus the presence of inclusions was not accounted in the construction of transmission operators. Nevertheless, we found that the sweeping preconditioner is still effective, yet the presence of multiple inclusions deteriorates somewhat its performance especially in the high-contrast media cases. The results in Table 10 correspond to cases where the contrast between the layers that contain inclusions and their adjacent layers is not significant (i.e., the quotients between the corresponding wavenumbers is close to unity). By contrast, the results in Table 11 correspond to high–contrast media (e.g., waveguides) where the wavenumbers in the layers that contain inclusions are much smaller than the wavenumbers in adjacent layers.

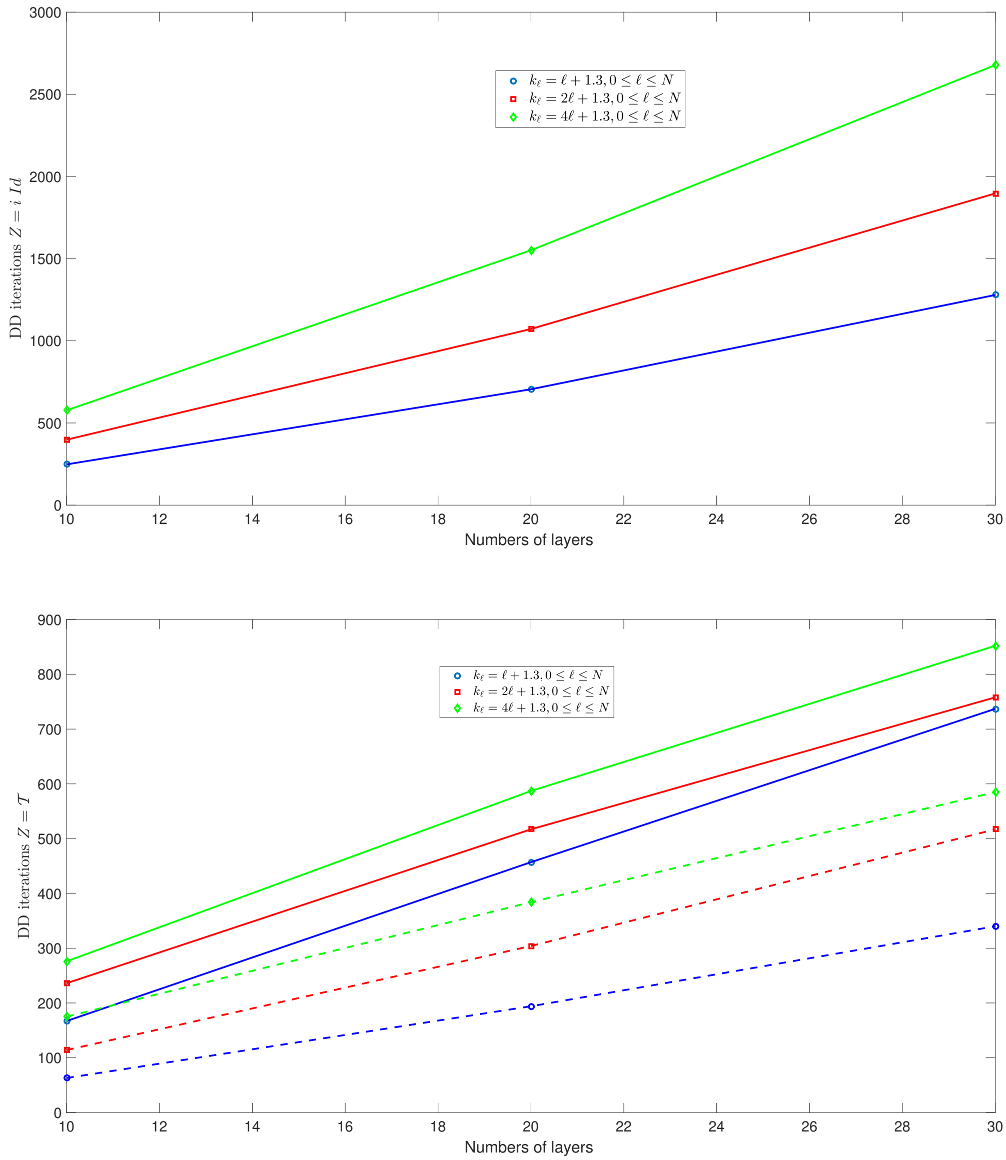

Figure 6: Numbers of GMRES iterations required to reach relative residuals of 10^{-4} by DD algorithms based on transmission operators $Z = iI$ (top) and $Z = \mathcal{T}$ (bottom) in the case when the profiles are given by the gratings $F_\ell(x_1) = -\ell H + 2.5\varepsilon \cos x_1, H = 3.3, 0 \le \ell \le N$ with $\varepsilon = 0.1$. In the case of transmission operators $Z = \mathcal{T}$ we plot with dashed lines the numbers of iterations required after the sweeping preconditioner is applied.

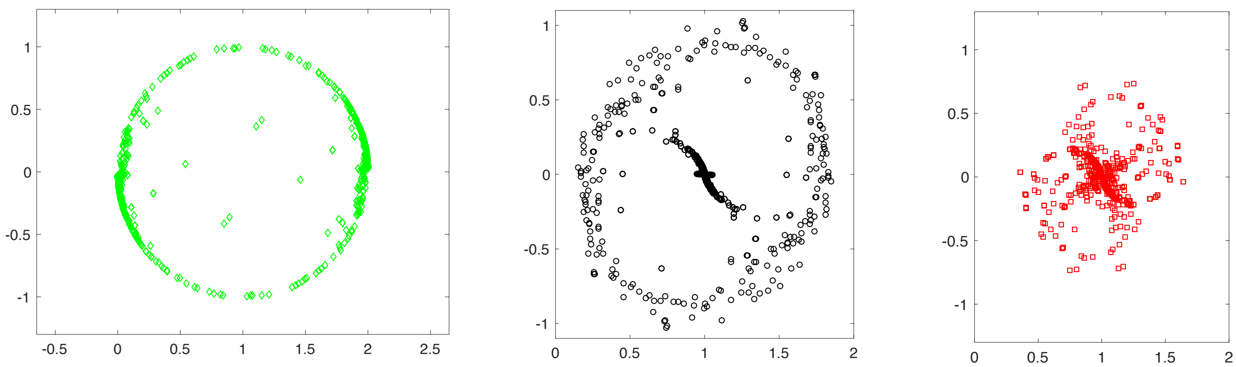

Figure 7: Eigenvalue distribution of QO DD formulations for $N = 9$, $k_\ell = \ell + 1.3, 0 \le \ell \le N$, $F_\ell(x_1) = -\ell H + 2.5\varepsilon \cos x_1, H = 3.3, 0 \le \ell \le N$ with $\varepsilon = 0.1$: $Z = i\ I$ (left), $\mathcal{A}_n, L = 0$ (center), and $\mathcal{B}_n^{-1}\mathcal{A}_n, L = 0$ (right).

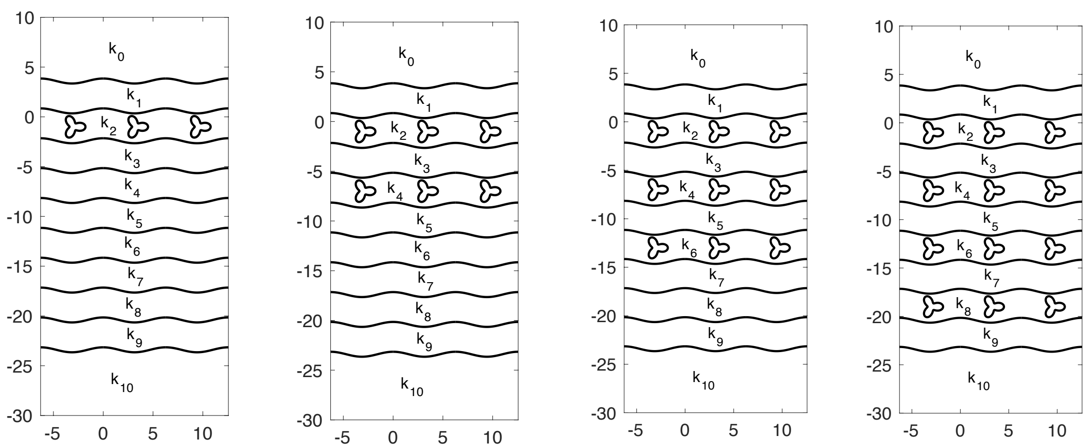

Figure 8: Periodic layer configurations with inclusions.

k_ℓ	One layer inclusions		Two layer inclusions		Three layer inclusions		Four layer inclusions	
	$\mathcal{A}_n, L = 0$	$\mathcal{B}_n^{-1}\mathcal{A}_n, L = 0$	$\mathcal{A}_n, L = 0$	$\mathcal{B}_n^{-1}\mathcal{A}_n, L = 0$	$\mathcal{A}_n, L = 0$	$\mathcal{B}_n^{-1}\mathcal{A}_n, L = 0$	$\mathcal{A}_n, L = 0$	$\mathcal{B}_n^{-1}\mathcal{A}_n, L = 0$
$k_\ell = \ell + 1.3, \ell \notin I$ $k_\ell = 1, \ell \in I$	50	15	39	18	41	22	33	21
$k_\ell = 2\ell + 1.3, \ell \notin I$ $k_\ell = 1, \ell \in I$	47	16	35	17	42	23	37	21
$k_\ell = 4\ell + 1.3, \ell \notin I$ $k_\ell = 1, \ell \in I$	43	14	33	16	23	15	21	15

Table 11: Numbers of GMRES iterations required by various QO DD formulations to reach relative residuals of 10^{-4} for configurations consisting of 11 layers with perfectly conducting inclusions depicted in Figure 8, where the interfaces $\Gamma_\ell, 0 \le \ell \le 9$ are given by grating profiles $F_\ell(x_1) = -\ell H + 2.5\varepsilon \cos x_1, H = 3, 0 \le \ell \le 9$ with $\varepsilon = 0.1$, under normal incidence, and various values of wavenumbers k_ℓ. The wavenumbers corresponding to layers with inclusions were selected to be Wood anomalies. Parameters $A = 300$, $M = 256$ were selected so that to lead to conservation of energy errors of the order 10^{-4}.

7 Conclusions

We have presented a sweeping preconditioner for the QO DD formulation of Helmholtz transmission problems in two dimensional periodic layered media. Our QO DD formulation is built upon transmission operators whose construction relies on low-order shape deformation expansions of periodic layer DtN operators. We used robust boundary integral equation formulations to represent the RtR operators, which were discretized via high-order Nyström discretizations. The sweeping preconditioners are particularly effective in the case when the subdomain partitions consist of horizontal layers, at least when the boundaries of the layers do not contain cross points. Extensions to cases when cross points are present, and to three dimensional cases are underway. We are also exploring strategies to parallelize the sweeping preconditioners.

Acknowledgments

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