A Stable High-Order Perturbation of Surfaces Method for Numerical Simulation of Diffraction Problems in Triply Layered Media

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Abstract

The accurate numerical simulation of linear waves interacting with periodic layered media is a crucial capability in engineering applications. In this contribution we study the stable and high-order accurate numerical simulation of the interaction of linear, time-harmonic waves with a periodic, triply layered medium with irregular interfaces. In contrast with volumetric approaches, High-Order Perturbation of Surfaces (HOPS) algorithms are inexpensive interfacial methods which rapidly and recursively estimate scattering returns by perturbation of the interface shape. In comparison with Boundary Integral/Element Methods, the stable HOPS algorithm we describe here does not require specialized quadrature rules, periodization strategies, or the solution of dense non-symmetric positive definite linear systems. In addition, the algorithm is provably stable as opposed to other classical HOPS approaches. With numerical experiments we show the remarkable efficiency, fidelity, and accuracy one can achieve with an implementation of this algorithm.

Keywords: High-Order Spectral Methods, Time-Harmonic Linear Wave Scattering, Periodic Layered Media, High-Order Perturbation of Surfaces Methods

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1. Introduction

The accurate numerical simulation of linear waves interacting with periodic layered media is a crucial capability in many areas of scientific and industrial interest. Examples exist in areas such as geophysics [1, 2], materials science [3], imaging [4], oceanography [5], and nanoplasmonics [6, 7, 8]. The latter includes topics as diverse as extraordinary optical transmission [9], surface enhanced spectroscopy [10], and surface plasmon resonance biosensing [11, 12, 13, 14, 15, 16]. For each application, it is necessary to approximate the scattering returns of such models in a fast, highly accurate, and reliable fashion.

While all of the classical numerical algorithms (e.g., Finite Differences and Finite/Spectral Element methods) have been brought to bear upon this problem (see, particularly, the work of Dobson [17, 18] and Bao [19, 20, 21] on Finite Element solution of the doubly layered problem), we have recently argued [22, 23, 24, 25] that such *volumetric* approaches are greatly disadvantaged with an unnecessarily large number of unknowns for the layered media problems we consider here. Interfacial methods based upon Integral Equations (IEs) [26], for instance [27, 28, 29, 30, 31, 32], are a natural candidate but, as we have pointed out [22, 23, 24, 25], these also face difficulties. Most of these have been addressed in recent years through (i.) the use of sophisticated quadrature rules to deliver High-Order Spectral accuracy, (ii.) the design of preconditioned iterative solvers with suitable acceleration [33], and (iii.) new strategies to avoid periodizing the Green function [27, 28, 29, 30, 31, 32]. Consequently, they are a compelling alternative (see, e.g., the survey article of [34] for more details), however, two properties render them non-competitive for the *parameterized* problems we consider as compared with the methods we advocate here. First, for configurations characterized by the real value ε (for us the heights/slopes of the irregular interfaces), an IE solver will return the scattering returns only for a *particular* value of ε . If this value is changed then the solver must be run again. Second, the dense, non-symmetric positive definite systems of linear equations generated by IEs which must be inverted with each simulation. We note that the “Rigorous Coupled Wave Analysis” (RCWA) [35, 36] is very popular amongst practitioners for the problem we consider here. While it is very convenient to code and can be very fast if implemented with care, non-trivial interface shapes are modeled as thin layers using a staircase approximation which is, necessarily, a low-order approximation.

38 A “High Order Perturbation of Surfaces” (HOPS) approach can effec-
39 tively address these concerns. More specifically, in [23, 24, 25] we put forth
40 the method of Field Expansions (FE) which traces its roots to the low-order
41 calculations of Rayleigh [37] and Rice [38]. This was extended to a high-order
42 algorithm by Bruno & Reitich [39, 40, 41] and later enhanced and stabilized
43 by Nicholls and Reitich [42, 43, 44], and Nicholls and Malcolm [45, 23, 25].
44 These formulations are particularly compelling as they maintain the advan-
45 tageous properties of classical IE formulations (e.g., surface formulation and
46 exact enforcement of far-field and quasiperiodicity conditions) while avoid-
47 ing the shortcomings listed above. First, since the methods are built upon
48 expansions in the boundary parameter, ε , once the Taylor coefficients are
49 known for the scattering quantities, it is simply a matter of summing these
50 (rather than beginning a new simulation) for any given choice of ε to recover
51 the returns. Second, due to the nature of the scheme, at every perturbation
52 order one need only invert a single, sparse operator corresponding to the
53 flat-interface, order-zero approximation of the problem.

54 However, Nicholls and Reitich [46] showed that, like other classical HOPS
55 schemes, the FE method depends upon strong *cancellations* for its conver-
56 gence which can result in quite ill-conditioned simulations. We refer the
57 interested reader to [46, 47, 48, 42, 43] for the initial description of this
58 phenomena, and the additional exhaustive and illuminating simulations of
59 Wilkening and Vasan [49].

60 In response to these observations, Nicholls and Reitich described an alter-
61 native HOPS scheme, the method of Transformed Field Expansions (TFE),
62 which does *not* possess strong cancellations [46, 47, 48, 42, 43]. In fact, the
63 resulting recursions can be used in a *rigorous* proof of the strong convergence
64 of the perturbation expansions in a Sobolev space [46, 48], **which was later**
65 **extended to Lipschitz profiles in [50]**. In addition, the TFE recursions were
66 implemented to reveal a stable and highly accurate numerical scheme for the
67 simulation of scattering returns by singly layered periodic gratings [47, 43].

68 This work was generalized by Nicholls and Shen to the case of irregular
69 bounded obstacles in two [51] and three dimensions [52], who later delivered
70 a rigorous numerical analysis of the method [53]. Subsequently, He, Nicholls,
71 and Shen [54] devised a highly non-trivial extension to the case of periodic
72 gratings separating *two* materials of different dielectric constants. Here, of
73 course, one must be concerned not only with a reflected field and its far-field
74 boundary condition (upward propagating) at positive infinity, but also with a
75 transmitted field which satisfies a different condition (downward propagating)

76 at negative infinity. In this contribution we make the further extension to
77 the case of *three* layers which introduces the added complication of waves
78 propagating both “up” and “down” in a vertically bounded layer in between.
79 This difficulty manifests itself in the governing equations (and our numerical
80 algorithm) through the complication of a *coupled* system of three boundary
81 value problems (at each wavenumber in the spatial variable).

82 More specifically, to begin we introduce artificial boundaries above and
83 below the interfaces of the structure, which truncate the unbounded domain.
84 We use Dirichlet–Neumann operators at each of these artificial boundaries
85 to enforce the outgoing wave conditions *transparently* and without reflection
86 [55, 56, 57, 58, 59, 60, 61, 62, 63, 64]. Our spectrally accurate method involves
87 the novelty of a modified Legendre–Galerkin approach where the standard
88 basis is supplemented with additional connecting basis functions across the
89 layer boundaries in the spirit of the work by He, Nicholls, and Shen [54]
90 for two layers. However, our contribution is more subtle than what appears
91 in the aforementioned publication; for more details we refer the reader to
92 Section 5.

93 The organization of the paper is as follows: In Section 2 we recall the
94 governing equations of an electromagnetic field incident upon a periodic, two–
95 dimensional, triply layered irregular grating structure. In Section 3 we derive
96 the TFE recursions in this triply layered context, and discuss a Legendre–
97 Galerkin method to solve the resulting *coupled* boundary value problems in
98 Sections 4 and 5. Extensive numerical results are provided in Section 6,
99 followed by concluding remarks in Section 7.

100 2. Governing Equations

The geometry we consider is displayed in Figure 1: A z –invariant, triply
layered structure. Dielectrics occupy all three domains, the upper (with
refractive index n^u) fills the region

$$S_g^u := \{y > \bar{g} + g(x)\},$$

the middle (with refractive index n^v) occupies

$$S_{g,h}^v := \{\bar{h} + h(x) < y < \bar{g} + g(x)\},$$

while the lower (with index of refraction n^w) fills

$$S_h^w := \{z < \bar{h} + h(x)\}.$$

Figure 1: A depiction of the triply layered grating structure with layer interfaces at $y = \bar{g} + g(x)$ and $y = \bar{h} + h(x)$.

The gratings are d -periodic so that $g(x+d) = g(x)$ and $h(x+d) = h(x)$. The structure is illuminated from above by monochromatic plane-wave incident radiation of frequency ω , aligned with the grooves

$$\underline{\mathbf{E}}^{inc}(x, y, t) = \mathbf{A}e^{i\alpha x - i\beta^u y - i\omega t}, \quad \underline{\mathbf{H}}^{inc}(x, y, t) = \mathbf{B}e^{i\alpha x - i\beta^u y - i\omega t}.$$

We consider the reduced electric and magnetic fields

$$\mathbf{E}(x, y) = e^{i\omega t} \underline{\mathbf{E}}(x, y, t), \quad \mathbf{H}(x, y) = e^{i\omega t} \underline{\mathbf{H}}(x, y, t),$$

101 which, like the reduced scattered fields, are α -quasiperiodic due to the inci-
 102 dent radiation. To close the problem, we specify that the scattered radiation
 103 is “outgoing” (upward propagating in S_g^u and downward propagating in S_h^w).

It is well known (see, e.g., Petit [65]) that in this two-dimensional setting, the time-harmonic Maxwell equations decouple into two scalar Helmholtz problems which govern the transverse electric (TE) and transverse magnetic (TM) polarizations. We define the invariant (z) direction of the scattered (electric or magnetic) fields by

$$u = u(x, y), \quad v = v(x, y), \quad w = w(x, y),$$

104 in S_g^u , $S_{g,h}^v$, and S_h^w , respectively. The incident radiation in the upper layer
 105 is specified by u^{inc} .

We find that we must seek outgoing, α -quasiperiodic solutions of

$$\Delta u + k_u^2 u = 0, \quad \text{in } S_g^u, \quad (1a)$$

$$\Delta v + k_v^2 v = 0, \quad \text{in } S_{g,h}^v, \quad (1b)$$

$$\Delta w + k_w^2 w = 0, \quad \text{in } S_h^w, \quad (1c)$$

$$u - v = -u^{inc}, \quad y = \bar{g} + g(x), \quad (1d)$$

$$v - w = 0, \quad y = \bar{h} + h(x), \quad (1e)$$

$$\partial_{N_g} u - \tau^2 \partial_{N_g} v = -\partial_{N_g} u^{inc}, \quad y = \bar{g} + g(x), \quad (1f)$$

$$\partial_{N_h} v - \sigma^2 \partial_{N_h} w = 0, \quad y = \bar{h} + h(x), \quad (1g)$$

where $k_m = n^m \omega / c_0 = \omega / c^m$, $m \in \{u, v, w\}$, c_0 is the speed of light, $N_g = (-\partial_x g, 1)^T$, $N_h = (-\partial_x h, 1)^T$, and

$$\tau^2 = \begin{cases} 1 & \text{TE} \\ (k_u/k_v)^2 = (n^u/n^v)^2 & \text{TM}, \end{cases}$$

and

$$\sigma^2 = \begin{cases} 1 & \text{TE} \\ (k_v/k_w)^2 = (n^v/n^w)^2 & \text{TM}. \end{cases}$$

106 2.1. Transparent Boundary Conditions

Following the standard TFE methodology [47, 43, 54] we introduce artificial boundaries and transparent boundary conditions to solve (1) (see also the work of Dobson [17, 18], Bao [19, 20, 21], and He, Min, and Nicholls [66] for such developments in the setting of Finite/Spectral Element solution of layered medium problems). More precisely, we introduce the planes $y = a > \bar{g} + |g|_{L^\infty}$ and $y = b < \bar{h} - |h|_{L^\infty}$, and define the domains

$$S^a := \{y > a\}, \quad S^b := \{y < b\}, \\ S_g^{a,u} := \{\bar{g} + g(x) < y < a\}, \quad S_h^{w,b} := \{b < y < \bar{h} + h(x)\};$$

107 see Figure 2.

The transparent boundary conditions are based upon the Rayleigh expansions [37] which can be used to solve the problems on S^a and S^b explicitly with generic Dirichlet data, say $\zeta(x)$ and $\psi(x)$, at the artificial boundaries $\{y = a\}$ and $\{y = b\}$, respectively. More precisely we have

$$u = u(x, y) = \sum_{p=-\infty}^{\infty} \hat{\zeta}_p e^{i\alpha_p x + i\beta_p^u (y-a)}, \quad y > a,$$

Figure 2: A depiction of the truncated triply layered grating structure with layer interfaces at $y = \bar{g} + g(x)$ and $y = \bar{h} + h(x)$, and artificial boundaries at $y = a$ and $y = b$.

and

$$w = w(x, y) = \sum_{p=-\infty}^{\infty} \hat{\psi}_p e^{i\alpha_p x - i\beta_p^w (y-b)}, \quad y < b,$$

where, for $p \in \mathbf{Z}$ and $m \in \{u, w\}$,

$$\alpha_p := \alpha + (2\pi/d)p, \quad \beta_p^m := \begin{cases} \sqrt{(k_m)^2 - \alpha_p^2} & p \in \mathcal{U}^m \\ i\sqrt{\alpha_p^2 - (k_m)^2} & p \notin \mathcal{U}^m \end{cases},$$

and the set of propagating modes is given by

$$\mathcal{U}^m := \{p \in \mathbf{Z} \mid \alpha_p^2 < (k_m)^2\}.$$

Notice that

$$u(x, a) = \sum_{p=-\infty}^{\infty} \hat{\zeta}_p e^{i\alpha_p x} = \zeta(x), \quad w(x, b) = \sum_{p=-\infty}^{\infty} \hat{\psi}_p e^{i\alpha_p x} = \psi(x).$$

With these solution formulas we can compute the Neumann data at the artificial boundaries

$$\partial_y u(x, a) = \sum_{p=-\infty}^{\infty} (i\beta_p^u) \hat{\zeta}_p e^{i\alpha_p x}, \quad \partial_y w(x, b) = \sum_{p=-\infty}^{\infty} (-i\beta_p^w) \hat{\psi}_p e^{i\alpha_p x},$$

which permit us to define the Dirichlet–Neumann Operators (DNOs)

$$T_1[\zeta] := \sum_{p=-\infty}^{\infty} (i\beta_p^u) \hat{\zeta}_p e^{i\alpha_p x}, \quad T_3[\psi] := \sum_{p=-\infty}^{\infty} (-i\beta_p^w) \hat{\psi}_p e^{i\alpha_p x},$$

108 which are order-one Fourier multipliers.

Using these we can state (1) *equivalently* on the *bounded* domain $\{b < y < a\}$ as

$$\Delta u + k_u^2 u = 0, \quad \text{in } S_g^{a,u}, \quad (2a)$$

$$\Delta v + k_v^2 v = 0, \quad \text{in } S_{g,h}^v, \quad (2b)$$

$$\Delta w + k_w^2 w = 0, \quad \text{in } S_h^{w,b}, \quad (2c)$$

$$u - v = -u^{inc}, \quad y = \bar{g} + g(x), \quad (2d)$$

$$v - w = 0, \quad y = \bar{h} + h(x), \quad (2e)$$

$$\partial_{N_g} u - \tau^2 \partial_{N_g} v = -\partial_{N_g} u^{inc}, \quad y = \bar{g} + g(x), \quad (2f)$$

$$\partial_{N_h} v - \sigma^2 \partial_{N_h} w = 0, \quad y = \bar{h} + h(x), \quad (2g)$$

$$\partial_y u - T_1[u] = 0, \quad y = a, \quad (2h)$$

$$\partial_y w - T_3[w] = 0, \quad y = b, \quad (2i)$$

109 which we use as the starting point for our numerical method.

110 3. Transformed Field Expansions

111 In this section, we present the Transformed Field Expansion (TFE) algo-
 112 rithm. First, we introduce a domain flattening change of variables known as
 113 σ –coordinates [67] in the oceanographic literature, and the C–method [68]
 114 in the electromagnetics community. Then, we consider a boundary pertur-
 115 bation algorithm to solve the resulting equations which leads to the provably
 116 convergent TFE recursions.

117 *3.1. The Change of variables*

We define the change of variables:

$$\begin{aligned}
x' &= x, \\
y_1 &= a \left(\frac{y - (\bar{g} + g)}{a - (\bar{g} + g)} \right) + \bar{g} \left(\frac{a - y}{a - (\bar{g} + g)} \right), & \bar{g} + g < y < a, \\
y_2 &= \bar{h} \left(\frac{y - (\bar{g} + g)}{(\bar{h} + h) - (\bar{g} + g)} \right) + \bar{g} \left(\frac{(\bar{h} + h) - y}{(\bar{h} + h) - (\bar{g} + g)} \right), & \bar{h} + h < y < \bar{g} + g, \\
y_3 &= b \left(\frac{y - (\bar{h} + h)}{b - (\bar{h} + h)} \right) + \bar{h} \left(\frac{b - y}{b - (\bar{h} + h)} \right) & b < y < \bar{h} + h,
\end{aligned}$$

which maps

$$S_g^{a,u} \rightarrow S_0^{a,u}, \quad S_{g,h}^v \rightarrow S_{0,0}^v, \quad S_h^{w,b} \rightarrow S_0^{w,b}.$$

We note that

$$b \leq y_3 \leq \bar{h} \leq y_2 \leq \bar{g} \leq y_1 \leq a.$$

A long calculation, presented in Appendix A, shows that (2) transforms under this change of variables to the following system of equations to be solved.

$$\Delta_{x',y_1} u + k_u^2 u = \mathcal{R}_1, \quad \text{in } S_0^{a,u}, \quad (3a)$$

$$\Delta_{x',y_2} v + k_v^2 v = \mathcal{R}_2, \quad \text{in } S_{0,0}^v, \quad (3b)$$

$$\Delta_{x',y_3} w + k_w^2 w = \mathcal{R}_3, \quad \text{in } S_0^{w,b}, \quad (3c)$$

$$u - v = -e^{i\alpha x'} e^{-i\beta u(\bar{g}+g)}, \quad y_1 = y_2 = \bar{g}, \quad (3d)$$

$$v - w = 0, \quad y_2 = y_3 = \bar{h}, \quad (3e)$$

$$\partial_{y_1} u - \tau^2 \partial_{y_2} v = \mathcal{J}_1, \quad y_1 = y_2 = \bar{g}, \quad (3f)$$

$$\partial_{y_2} v - \sigma^2 \partial_{y_3} w = \mathcal{J}_2, \quad y_2 = y_3 = \bar{h}, \quad (3g)$$

$$\partial_{y_1} u - T_1[u] = -\frac{g}{a - \bar{g}} T_1[u], \quad y_1 = a, \quad (3h)$$

$$\partial_{y_3} w - T_3[w] = -\frac{h}{b - \bar{h}} T_3[w], \quad y_3 = b, \quad (3i)$$

where

$$\mathcal{R}_i = \frac{1}{E_i^2} [\partial_{x'} R_i^x + \partial_{y_i} R_i^x + R_i].$$

118 We refer the reader to Appendix A for the particular forms for the right hand
 119 sides $\{\mathcal{R}_1, \mathcal{R}_2, \mathcal{R}_3, \mathcal{J}_1, \mathcal{J}_2\}$.

120 *3.2. Boundary Perturbation*

We now consider a boundary perturbation method to solve the transformed governing equations, (3). To begin, we expand the fields in power series

$$\{u, v, w\} = \sum_{n=0}^{\infty} \{u_n, v_n, w_n\}(x, y) \varepsilon^n.$$

Inserting these expansions into (3) and equating at order $\mathcal{O}(\varepsilon^n)$ delivers

$$\Delta_{x',y_1} u_n + k_u^2 u_n = \mathcal{R}_{1,n}, \quad \text{in } S_0^{a,u}, \quad (4a)$$

$$\Delta_{x',y_2} v_n + k_v^2 v_n = \mathcal{R}_{2,n}, \quad \text{in } S_{0,0}^v, \quad (4b)$$

$$\Delta_{x',y_3} w_n + k_w^2 w_n = \mathcal{R}_{3,n}, \quad \text{in } S_0^{w,b}, \quad (4c)$$

$$u_n - v_n = -e^{i\alpha x'} e^{-i\beta \bar{g}} \frac{(-i\beta f_g)^n}{n!}, \quad y_1 = y_2 = \bar{g}, \quad (4d)$$

$$v_n - w_n = 0, \quad y_2 = y_3 = \bar{h}, \quad (4e)$$

$$\partial_{y_1} u_n - \tau^2 \partial_{y_2} v_n = \mathcal{J}_{1,n}, \quad y_1 = y_2 = \bar{g}, \quad (4f)$$

$$\partial_{y_2} v_n - \sigma^2 \partial_{y_3} w_n = \mathcal{J}_{2,n}, \quad y_2 = y_3 = \bar{h}, \quad (4g)$$

$$\partial_{y_1} u_n - T_1[u_n] = -\frac{f_g}{a - \bar{g}} T_1[u_{n-1}], \quad y_1 = a, \quad (4h)$$

$$\partial_{y_3} w_n - T_3[w_n] = -\frac{f_h}{b - \bar{h}} T_3[w_{n-1}], \quad y_3 = b. \quad (4i)$$

In these we have defined

$$\mathcal{R}_{i,n} = \frac{1}{E_i^2} [\partial_{x'} R_{i,n}^x + \partial_{y_i} R_{i,n}^x + R_{i,n}],$$

121 [and the remaining terms are specified in Appendix A.](#)

Using the quasiperiodicity of the solutions, we make the following (generalized) Fourier series expansions,

$$\begin{aligned} \{u_n, v_n, w_n\} &= \sum_{p=-\infty}^{\infty} \{u_n^p(y), v_n^p(y), w_n^p(y)\} e^{i\alpha_p x}, \\ \mathcal{R}_{i,n}(x, y) &= \sum_{p=-\infty}^{\infty} \mathcal{R}_{i,n}^p(y) e^{i\alpha_p x}, \quad \mathcal{J}_{i,n}(x) = \sum_{p=-\infty}^{\infty} \mathcal{J}_{i,n}^p e^{i\alpha_p x}, \end{aligned}$$

for $i = 1, 2, 3$. Insertion of these into (4) delivers

$$\partial_y^2 u_n^p(y) + (k_u^2 - \alpha_p^2)u_n^p(y) = \mathcal{R}_{1,n}^p(y), \quad \bar{g} < y < a, \quad (5a)$$

$$\partial_y^2 v_n^p(y) + (k_v^2 - \alpha_p^2)v_n^p(y) = \mathcal{R}_{2,n}^p(y), \quad \bar{h} < y < \bar{g}, \quad (5b)$$

$$\partial_y^2 w_n^p(y) + (k_w^2 - \alpha_p^2)w_n^p(y) = \mathcal{R}_{3,n}^p(y), \quad b < y < \bar{h}, \quad (5c)$$

$$u_n^p(\bar{g}) - v_n^p(\bar{g}) = -e^{-i\beta\bar{g}} \frac{(-i\beta f_g)^n}{n!} =: \zeta_n^p, \quad (5d)$$

$$v_n^p(\bar{h}) - w_n^p(\bar{h}) = 0, \quad (5e)$$

$$\partial_y u_n^p(\bar{g}) - \tau^2 \partial_y v_n^p(\bar{g}) = \mathcal{J}_{1,n}^p, \quad (5f)$$

$$\partial_y v_n^p(\bar{h}) - \sigma^2 \partial_y w_n^p(\bar{h}) = \mathcal{J}_{2,n}^p, \quad (5g)$$

$$\partial_y u_n^p - i\beta_p^u u_n^p = -\frac{f_g}{a - \bar{g}} T_1^p[u_{n-1}^p] =: \mathcal{B}_{1,n}^p, \quad y = a, \quad (5h)$$

$$\partial_y w_n^p + i\beta_p^w w_n^p = -\frac{f_h}{b - \bar{h}} T_2^p[w_{n-1}^p] =: \mathcal{B}_{2,n}^p, \quad y = b. \quad (5i)$$

122 4. A Weak formulation of the Boundary Value Problem

In order to homogenize (5) for our weak formulation we decompose the solutions $\{u_n^p, v_n^p, w_n^p\}$ as

$$\{u_n^p, v_n^p, w_n^p\} = \{\tilde{u}_n^p, \tilde{v}_n^p, \tilde{w}_n^p\} + \{\check{u}_n^p, \check{v}_n^p, \check{w}_n^p\},$$

where $\{\tilde{u}_n^p, \tilde{v}_n^p, \tilde{w}_n^p\}$ solve (5) with $\mathcal{R}_{i,n}^p \equiv 0$, while $\{\check{u}_n^p, \check{v}_n^p, \check{w}_n^p\}$ solve (5) with $\mathcal{B}_{i,n}^p \equiv \zeta_n^p \equiv \mathcal{J}_{i,n}^p \equiv 0$. More specifically, dropping the $\{n, p\}$ indices, we write

$$\partial_y^2 \tilde{u}(y) + (k_u^2 - \alpha^2)\tilde{u}(y) = 0, \quad \bar{g} < y < a \quad (6a)$$

$$\partial_y^2 \tilde{v}(y) + (k_v^2 - \alpha^2)\tilde{v}(y) = 0, \quad \bar{h} < y < \bar{g} \quad (6b)$$

$$\partial_y^2 \tilde{w}(y) + (k_w^2 - \alpha^2)\tilde{w}(y) = 0, \quad b < y < \bar{h} \quad (6c)$$

$$\tilde{u}(\bar{g}) - \tilde{v}(\bar{g}) = \zeta, \quad (6d)$$

$$\tilde{v}(\bar{h}) - \tilde{w}(\bar{h}) = 0, \quad (6e)$$

$$\partial_y \tilde{u}(\bar{g}) - \tau^2 \partial_y \tilde{v}(\bar{g}) = \mathcal{J}_1, \quad (6f)$$

$$\partial_y \tilde{v}(\bar{h}) - \sigma^2 \partial_y \tilde{w}(\bar{h}) = \mathcal{J}_2, \quad (6g)$$

$$\partial_y \tilde{u} - i\beta^u \tilde{u} = \mathcal{B}_1, \quad y = a, \quad (6h)$$

$$\partial_y \tilde{w} + i\beta^w \tilde{w} = \mathcal{B}_2, \quad y = b. \quad (6i)$$

Due to their simplicity, (6) can be solved explicitly so it remains to solve for $\{\tilde{u}, \tilde{v}, \tilde{w}\}$ which we accomplish by a High-Order Spectral method. For the latter we set

$$\begin{aligned}\tilde{u} &= M_1 e^{i\beta^u y} + N_1 e^{-i\beta^u y}, & \tilde{v} &= M_2 e^{i\beta^v y} + N_2 e^{-i\beta^v y}, \\ \tilde{w} &= M_3 e^{i\beta^w y} + N_3 e^{-i\beta^w y}\end{aligned}$$

123 which we substitute into (6), and then find explicit forms for M_i and N_i .

For $\{\tilde{u}_n^p, \tilde{v}_n^p, \tilde{w}_n^p\}$ we consider the following equations

$$\partial_y^2 \tilde{u}(y) + (k_u^2 - \alpha^2) \tilde{u}(y) = \mathcal{R}_1(y), \quad \bar{g} < y < a \quad (7a)$$

$$\partial_y^2 \tilde{v}(y) + (k_v^2 - \alpha^2) \tilde{v}(y) = \mathcal{R}_2(y), \quad \bar{h} < y < \bar{g} \quad (7b)$$

$$\partial_y^2 \tilde{w}(y) + (k_w^2 - \alpha^2) \tilde{w}(y) = \mathcal{R}_3(y), \quad b < y < \bar{h} \quad (7c)$$

$$\tilde{u}(\bar{g}) - \tilde{v}(\bar{g}) = 0, \quad (7d)$$

$$\tilde{v}(\bar{h}) - \tilde{w}(\bar{h}) = 0, \quad (7e)$$

$$\partial_y \tilde{u}(\bar{g}) - \tau^2 \partial_y \tilde{v}(\bar{g}) = 0, \quad (7f)$$

$$\partial_y \tilde{v}(\bar{h}) - \sigma^2 \partial_y \tilde{w}(\bar{h}) = 0, \quad (7g)$$

$$\partial_y \tilde{u} - i\beta^u \tilde{u} = 0, \quad y = a, \quad (7h)$$

$$\partial_y \tilde{w} + i\beta^w \tilde{w} = 0, \quad y = b. \quad (7i)$$

Our weak formulation of (7) is: Find $U \in H^1([b, a])$ such that

$$\begin{aligned}(\tilde{k}^2 U, \varphi) - (\partial_y U, \partial_y \varphi) + (1 - \tau^2) \partial_y v(\bar{g}) \bar{\varphi}(\bar{g}) + (\sigma^{-2} - 1) \partial_y v(\bar{h}) \bar{\varphi}(\bar{h}) \\ = (\mathcal{R}, \varphi) - i\beta_u u(a) \bar{\varphi}(a) - i\beta_w w(b) \bar{\varphi}(b), \quad \forall \varphi \in H^1([b, a]),\end{aligned}$$

where

$$\begin{aligned}U &= \begin{cases} u_N, & y \in I_1, \\ v_N, & y \in I_2, \\ w_N, & y \in I_3, \end{cases} \quad \varphi = \begin{cases} \varphi_1, & y \in I_1, \\ \varphi_2, & y \in I_2, \\ \varphi_3, & y \in I_3, \end{cases} \\ \mathcal{R} &= \begin{cases} \mathcal{R}_1, & y \in I_1, \\ \mathcal{R}_2, & y \in I_2, \\ \mathcal{R}_3, & y \in I_3, \end{cases} \quad \tilde{k} = \begin{cases} k_u, & y \in I_1, \\ k_v, & y \in I_2, \\ k_w, & y \in I_3, \end{cases}\end{aligned}$$

and

$$I_1 := \{\bar{g} < y < a\}, \quad I_2 := \{\bar{h} < y < \bar{g}\}, \quad I_3 := \{b < y < \bar{h}\}.$$

Following He, Nicholls, and Shen [54], we define the following finite dimensional function space $X_{N_y} \subset H^1([b, a])$ to specify a Legendre–Galerkin method,

$$X_{N_y} := \{\varphi_i \in P_{N_y}(I_i) \mid \partial_y \varphi_1(a) - i\beta^u \varphi_1(a) = 0, \partial_y \varphi_3(b) + i\beta^w \varphi_3(b) = 0\},$$

where P_{N_y} is the space of polynomials of degree less than N_y . The Legendre–Galerkin formulation becomes: Find $U_{N_y} \in X_{N_y}$ such that

$$\begin{aligned} (\tilde{k}^2 U_{N_y}, \varphi) - (\partial_y U_{N_y}, \partial_y \varphi) + (1 - \tau^2) \partial_y v_{N_y}(\bar{g}) \bar{\varphi}(\bar{g}) + (\sigma^{-2} - 1) \partial_y v_{N_y}(\bar{h}) \bar{\varphi}(\bar{h}) \\ = (I_{N_y} f, \varphi) - i\beta^u u_{N_y}(a) \bar{\varphi}(a) - i\beta^w u_{N_y}(b) \bar{\varphi}(b), \quad \forall \varphi \in X_{N_y}. \end{aligned}$$

where I_{N_y} is the projection operator onto P_{N_y} . Using integration–by–parts on each subdomain, we can obtain the alternate variational formulation: Find $U_{N_y} \in X_{N_y}$ such that

$$\begin{aligned} (\partial_y^2 U_{N_y}, \varphi) + \tilde{k}^2 (U_{N_y}, \varphi) + \partial_y u_{N_y}(\bar{g}) \bar{\varphi}(\bar{g}) - \tau^2 \partial_y v_{N_y}(\bar{g}) \bar{\varphi}(\bar{g}) \\ + \sigma^{-2} \partial_y v_{N_y}(\bar{h}) \bar{\varphi}(\bar{h}) - \partial_y w_{N_y}(\bar{h}) \bar{\varphi}(\bar{h}) = (I_{N_y} \mathcal{R}, \varphi), \quad \forall \varphi \in X_{N_y}. \end{aligned}$$

124 5. The Legendre–Galerkin Numerical Method

At this point we follow the spectral Legendre–Galerkin approach of Shen [69, 70, 54] and consider as basis functions *combinations* of Legendre polynomials, $L_j(s)$. For $y \in I_1$ we define

$$\begin{aligned} \phi_{1,j} := (1 + i) L_j \left(\frac{2(y - a)}{a - \bar{g}} + 1 \right) + a_{1,j} L_{j+1} \left(\frac{2(y - a)}{a - \bar{g}} + 1 \right) \\ + b_{1,j} L_{j+2} \left(\frac{2(y - a)}{a - \bar{g}} + 1 \right), \end{aligned}$$

such that

$$(\partial_y \phi_{1,j} - i\beta^u \phi_{1,j})(a) = 0, \quad \phi_{1,j}(\bar{g}) = 0,$$

for $j = 1, 2, \dots, N_y - 2$. Further, for $y \in I_2$, we denote

$$\begin{aligned} \phi_{2,j} := (1 + i) L_j \left(\frac{2(y - \bar{g})}{\bar{g} - \bar{h}} + 1 \right) + a_{2,j} L_{j+1} \left(\frac{2(y - \bar{g})}{\bar{g} - \bar{h}} + 1 \right) \\ + b_{2,j} L_{j+2} \left(\frac{2(y - \bar{g})}{\bar{g} - \bar{h}} + 1 \right), \end{aligned}$$

where

$$\phi_{2,j}(\bar{g}) = 0, \quad \phi_{2,j}(\bar{h}) = 0.$$

In a similar way we define, for $y \in I_3$,

$$\begin{aligned} \phi_{3,j} := (1 + i)L_j \left(\frac{2(y - \bar{h})}{\bar{h} - b} + 1 \right) + a_{3,j}L_{j+1} \left(\frac{2(y - \bar{h})}{\bar{h} - b} + 1 \right) \\ + b_{3,j}L_{j+2} \left(\frac{2(y - \bar{h})}{\bar{h} - b} + 1 \right), \end{aligned}$$

where

$$\partial_y \phi_{3,j}(b) + i\beta^w \phi_{3,j}(b) = 0, \quad \phi_{3,j}(\bar{h}) = 0.$$

Note that these basis functions vanish at the mean interface levels $y = \bar{g}$ and $y = \bar{h}$. For this reason (c.f., [54]), we introduce additional basis functions which are nonzero at $y = \bar{g}$ and $y = \bar{h}$:

$$\eta_1(y) = \begin{cases} c_1(y - \bar{g}) + 1, & \bar{g} \leq y \leq a, \\ c_2(y - \bar{g}) + 1, & \bar{h} \leq y \leq \bar{g}, \\ 0, & b \leq y \leq \bar{h}, \end{cases}$$

and

$$\eta_2(y) = \begin{cases} 0, & \bar{g} \leq y \leq a, \\ c_3(y - \bar{h}) + 1, & \bar{h} \leq y \leq \bar{g}, \\ c_4(y - \bar{h}) + 1, & b \leq y \leq \bar{h}, \end{cases}$$

chosen such that

$$\begin{aligned} (\partial_y \eta_1 - i\beta^u \eta_1)(a) &= 0, & \eta_1(\bar{h}) &= 0, \\ (\partial_y \eta_2 + i\beta^w \eta_2)(b) &= 0, & \eta_2(\bar{g}) &= 0. \end{aligned}$$

It is easy to show that

$$c_1 = \frac{i\beta^u}{1 - i\beta^u(a - \bar{g})}, \quad c_2 = \frac{1}{\bar{g} - \bar{h}}, \quad c_3 = \frac{1}{\bar{h} - \bar{g}}, \quad c_4 = -\frac{i\beta^w}{1 + i\beta^w(b - \bar{h})}.$$

With these we define the basis functions defined on all $\{b < y < a\}$

$$\tilde{\phi}_j(y) = \begin{cases} \phi_{1,j}(y), & \bar{g} < y < a, \\ 0, & b < y < \bar{g}, \end{cases} \quad j = 0, \dots, N_y - 2,$$

and

$$\tilde{\phi}_{N_y-1+j}(y) = \begin{cases} 0, & \bar{g} < y < a \\ \phi_{2,j}(y), & \bar{h} < y < \bar{g}, \\ 0, & b < y < \bar{h}, \end{cases} \quad j = 0, \dots, N_y - 2,$$

and

$$\tilde{\phi}_{2N_y-2+j}(y) = \begin{cases} 0, & \bar{h} < y < a \\ \phi_{3,j}(y), & b < y < \bar{h}, \end{cases} \quad j = 0, \dots, N_y - 2,$$

and, finally,

$$\tilde{\phi}_{3N_y-3}(y) = \eta_1(y), \quad \tilde{\phi}_{3N_y-2}(y) = \eta_2(y).$$

Our numerical approximation proceeds by seeking

$$u^{N_y}(y) := \sum_{j=0}^{3N_y-2} \hat{u}_j \tilde{\phi}_j(y),$$

and setting

$$\begin{aligned} \mathbf{u} &= (\hat{u}_0, \dots, \hat{u}_{N_y-2})^T, \\ \mathbf{v} &= (\hat{u}_{N_y-1}, \dots, \hat{u}_{2N_y-3})^T, \\ \mathbf{w} &= (\hat{u}_{2N_y-2}, \dots, \hat{u}_{3N_y-4})^T, \\ \mathbf{f} &= (\hat{f}_0, \dots, \hat{f}_{3N_y-4})^T, \end{aligned}$$

where

$$\hat{f}_j := (I_{N_y} f, \tilde{\phi}_j), \quad j = 0, \dots, 3N_y - 2.$$

We also define the following block matrices

$$\begin{aligned} (A_{11})_{ij} &= (\partial_y^2 \tilde{\phi}_j, \tilde{\phi}_i)_{I_1} + k^2 (\tilde{\phi}_j, \tilde{\phi}_i)_{I_1}, \\ (C_{11})_{ij} &= (\partial_y^2 \tilde{\phi}_{N_y-1+j}, \tilde{\phi}_{N_y-1+i})_{I_1} + k^2 (\tilde{\phi}_{N_y-1+j}, \tilde{\phi}_{N_y-1+i})_{I_2}, \\ (B_{11})_{ij} &= (\partial_y^2 \tilde{\phi}_{2N_y-2+j}, \tilde{\phi}_{2N_y-2+i})_{I_3} + k^2 (\tilde{\phi}_{2N_y-2+j}, \tilde{\phi}_{2N_y-2+i})_{I_3}, \end{aligned}$$

where $0 \leq i, j \leq N_y - 2$. We make the column vectors

$$\begin{aligned} a_{12} &= (\partial_y^2 \tilde{\phi}_{3N_y-3} + k^2 \tilde{\phi}_{3N_y-3}, \tilde{\phi}_j)_{I_1}, \\ c_{12} &= (\partial_y^2 \tilde{\phi}_{3N_y-3} + k^2 \tilde{\phi}_{3N_y-3}, \tilde{\phi}_{N_y-1+j})_{I_2}, \\ d_{12} &= (\partial_y^2 \tilde{\phi}_{3N_y-2} + k^2 \tilde{\phi}_{3N_y-2}, \tilde{\phi}_{N_y-1+j})_{I_2}, \\ b_{12} &= (\partial_y^2 \tilde{\phi}_{3N_y-2} + k^2 \tilde{\phi}_{3N_y-2}, \tilde{\phi}_{2N_y-2+j})_{I_3}, \end{aligned}$$

and row vectors

$$\begin{aligned}
a_{21} &= (\partial_y^2 \tilde{\phi}_j + k^2 \tilde{\phi}_j, \tilde{\phi}_{3N_y-3})_{I_1} + \partial_y \tilde{\phi}_j(\bar{g}), \\
c_{21} &= (\partial_y^2 \tilde{\phi}_{N_y-1+j} + k^2 \tilde{\phi}_{N_y-1+j}, \tilde{\phi}_{3N_y-3})_{I_2} - \tau^2 \partial_y \tilde{\phi}_{N_y-1+j}(\bar{g}), \\
d_{21} &= (\partial_y^2 \tilde{\phi}_{N_y-1+j} + k^2 \tilde{\phi}_{N_y-1+j}, \tilde{\phi}_{3N_y-2})_{I_2} + \sigma^{-2} \partial_y \tilde{\phi}_{N_y-1+j}(\bar{h}), \\
b_{21} &= (\partial_y^2 \tilde{\phi}_{2N_y-2+j} + k^2 \tilde{\phi}_{2N_y-2+j}, \tilde{\phi}_{3N_y-2})_{I_3} - \partial_y \tilde{\phi}_{2N_y-2+j}(\bar{h}),
\end{aligned}$$

for $0 \leq j \leq N_y - 2$. Finally, we set

$$\begin{aligned}
a_{22} &= (\partial_y^2 \tilde{\phi}_{3N_y-3} + k^2 \tilde{\phi}_{3N_y-3}, \tilde{\phi}_{3N_y-3}) + \partial_y \tilde{\phi}_{3N_y-3}(\bar{g}^+) - \tau^2 \partial_y \tilde{\phi}_{3N_y-3}(\bar{g}^-), \\
a_{33} &= (\partial_y^2 \tilde{\phi}_{3N_y-2} + k^2 \tilde{\phi}_{3N_y-2}, \tilde{\phi}_{3N_y-2}) + \sigma^{-2} \partial_y \tilde{\phi}_{3N_y-2}(\bar{h}^+) - \partial_y \tilde{\phi}_{3N_y-2}(\bar{h}^-), \\
a_{23} &= (\partial_y^2 \tilde{\phi}_{3N_y-2} + k^2 \tilde{\phi}_{3N_y-2}, \tilde{\phi}_{3N_y-3}) \\
&\quad + [\partial_y \tilde{\phi}_{3N_y-2}(\bar{g}^+) - \tau^2 \partial_y \tilde{\phi}_{3N_y-2}(\bar{g}^-)] \tilde{\phi}_{3N_y-3}(\bar{g}), \\
a_{32} &= (\partial_y^2 \tilde{\phi}_{3N_y-3} + k^2 \tilde{\phi}_{3N_y-3}, \tilde{\phi}_{3N_y-2}) \\
&\quad + [\sigma^{-2} \partial_y \tilde{\phi}_{3N_y-3}(\bar{h}^+) - \partial_y \tilde{\phi}_{3N_y-3}(\bar{h}^-)] \tilde{\phi}_{3N_y-2}(\bar{h}).
\end{aligned}$$

With these our Legendre–Galerkin scheme becomes the following system of $3N_y - 1$ equations:

$$\begin{pmatrix} A_{11} & 0 & 0 & a_{12} & 0 \\ 0 & C_{11} & 0 & c_{12} & d_{12} \\ 0 & 0 & B_{11} & 0 & b_{12} \\ a_{21}^T & c_{21}^T & 0 & a_{22} & a_{23} \\ 0 & d_{21}^T & b_{21} & a_{32} & a_{33} \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \\ \mathbf{w} \\ \hat{u}_{3N_y-3} \\ \hat{u}_{3N_y-2} \end{pmatrix} = \begin{pmatrix} \mathbf{f} \\ \hat{f}_{3N_y-3} \\ \hat{f}_{3N_y-2} \end{pmatrix}.$$

125 6. Numerical simulations

126 We conducted numerical experiments with an implementation of the al-
 127 gorithm outlined above. To begin, we demonstrated the accuracy of the
 128 boundary value problem solver (7) at the core of our approach versus an ex-
 129 act solution. We followed this by exhibiting the fidelity of our full scattering
 130 solver using the “energy defect” as our indicator of convergence.

131 6.1. Simulations of a Simplified Model

To begin our numerical experiments we considered the approximation of the “reduced” boundary value problem (7) at the heart of our full solver.

With this we displayed the convergence performance we anticipated for the full algorithm proposed in Section 5. For this we considered the following problem.

$$\partial_y^2 u(y) + k_u^2 u(y) = \mathcal{F}_1(y), \quad \bar{g} < y < a \quad (8a)$$

$$\partial_y^2 v(y) + k_v^2 v(y) = \mathcal{F}_2(y), \quad \bar{h} < y < \bar{g} \quad (8b)$$

$$\partial_y^2 w(y) + k_w^2 w(y) = \mathcal{F}_3(y), \quad b < y < \bar{h} \quad (8c)$$

$$u(\bar{g}) - v(\bar{g}) = 0, \quad (8d)$$

$$v(\bar{h}) - w(\bar{h}) = 0, \quad (8e)$$

$$\partial_y u(\bar{g}) - \tau^2 \partial_y v(\bar{g}) = 0, \quad (8f)$$

$$\partial_y v(\bar{h}) - \sigma^2 \partial_y w(\bar{h}) = 0, \quad (8g)$$

$$\partial_y u - i\beta^u u = 0, \quad y = a, \quad (8h)$$

$$\partial_y w + i\beta^w w = 0, \quad y = b. \quad (8i)$$

To test the convergence of our algorithm we began by considering the following functions and parameters which we used to define an exact solution:

$$\begin{aligned} u &= \exp(y)(y-a)^2(y-b)^2, & v &= \exp(y)(y-a)^2(y-b)^2, \\ w &= \exp(y)(y-a)^2(y-b)^2, \\ a &= 2.5, & \bar{g} &= 1, & \bar{h} &= 0, & b &= -2, & \tau &= 1, & \sigma &= 1, \\ k_u &= 5.0, & k_v &= 1.0, & k_w &= 1.1, \\ \beta_u &= -2 + 2i, & \beta_w &= 1 - i. \end{aligned} \quad (9)$$

132 One can check that the functions u , v , and w satisfy the homogeneous bound-
133 ary conditions in (8). One can also easily find the corresponding terms $\mathcal{F}_1, \mathcal{F}_2$,
134 and $\mathcal{F}_3$ which make u , v , and w exact solutions.

As a second example, we considered $\tau \neq 1$ and $\sigma \neq 1$, which was meant to model a TM simulation:

$$\begin{aligned} u &= \tau^2 \sigma^2 \exp(y)(y-a)^2(y-b)^2(y-\bar{g})(y-\bar{h}), \\ v &= \sigma^2 \exp(y)(y-a)^2(y-b)^2(y-\bar{g})(y-\bar{h}), \\ w &= \exp(y)(y-a)^2(y-b)^2(y-\bar{g})(y-\bar{h}), \\ a &= 5, & \bar{g} &= 3, & \bar{h} &= 0, & b &= -2, & \tau &= 2, & \sigma &= 4, \\ k_u &= 3.0, & k_v &= 1 + i, & k_w &= 2.0, \\ \beta_u &= 2 + i, & \beta_w &= 1 - i. \end{aligned} \quad (10)$$

135 To test numerical convergence, we defined the relative L^2 error

$$\frac{\|u_{\text{ex}} - u_{N_y}\|_{L^2}}{\|u_{\text{ex}}\|_{L^2}}, \quad (11)$$

136 where u_{ex} is the exact solution (c.f. (9) and (10)) and u_{N_y} is the numerical solution of (8). Figures 3 and 4 display the spectral rate of convergence

Figure 3: Relative L^2 error, (11), of our Legendre–Galerkin approximation of (8) with parameter choices (9) versus number of basis functions N_y .

137 which our Legendre–Galerkin method achieved in this simplified setting.

139 6.2. Simulations of a Triply Layered Medium: Smooth Interfaces

140 We now display results of simulations of a triply layered medium whose
 141 scattering returns are governed by (2). As exact solutions are unavailable,
 142 to display the spectral accuracy of our Legendre–Galerkin scheme we use the
 143 widely–accepted diagnostic of “energy defect”; see e.g. [65, 16, 39, 40, 41].

To describe this we consider the Rayleigh expansions [37] in the upper and lower layers

$$u(x, y) = \sum_{p=-\infty}^{\infty} \hat{u}_p e^{i\alpha_p x + i\beta_p^u y}, \quad w(x, y) = \sum_{p=-\infty}^{\infty} \hat{w}_p e^{i\alpha_p x - i\beta_p^w y},$$

Figure 4: Relative L^2 error, (11), of our Legendre–Galerkin approximation of (8) with parameter choices (10) versus number of basis functions N_y .

and, from these, define the efficiencies

$$e_p^u := \frac{\beta_p^u}{\beta^u} |\hat{u}_p|^2, \quad p \in \mathcal{U}^u,$$

$$e_p^w := \frac{\beta_p^w}{\beta^w} |\hat{w}_p|^2, \quad p \in \mathcal{U}^w.$$

The efficiencies measure the energy at wavenumber p propagated away from the grating interface, and if all materials in the structure are lossless ($n^m \in \mathbf{R}$), we obtain conservation of energy. More precisely, in TE mode

$$\sum_{p \in \mathcal{U}^u} e_p^u + \sum_{p \in \mathcal{U}^w} e_p^w = 1,$$

while in TM mode

$$\sum_{p \in \mathcal{U}^u} e_p^u + \left(\frac{k_u^2}{k_w^2} \right) \sum_{p \in \mathcal{U}^w} e_p^w = 1.$$

In particular, we can define the “energy defect” [65] for TE polarization as

$$\delta_{\text{TE}} := 1 - \sum_{p \in \mathcal{U}^u} e_p^u - \sum_{p \in \mathcal{U}^w} e_p^w,$$

and for TM polarization as

$$\delta_{\text{TM}} := 1 - \sum_{p \in \mathcal{U}^u} e_p^u - \left(\frac{k_u^2}{k_w^2} \right) \sum_{p \in \mathcal{U}^w} e_p^w,$$

144 which should be zero for an exact solution.

We conducted a sequence of simulations to show the spectral accuracy of our proposed Legendre–Galerkin algorithm. For a series of smooth interface tests, we used the following parameters

$$\begin{aligned} a = 5, \quad \bar{g} = 2, \quad \bar{h} = 1, \quad b = -2, \quad \alpha = 0.1, \\ d = 2\pi, \quad g(x) = \sin(x), \quad h(x) = \sin(x/2). \end{aligned} \quad (12)$$

145 For numerical parameters we used N to denote the perturbation order, N_x
146 the number of Fourier modes in x , and N_y the number of Galerkin coefficients
147 in y . Finally, ε was the boundary deformation height/slope, while k_u , k_v , and
148 k_w were the [wavenumbers](#) in the upper, middle, and lower layers, respectively.

149 In [Figures 5 and 6](#) we display the energy defect versus number of per-
150 turbation orders retained for the parameter choices $N_x = N_y = 24$ and
151 $(k_u, k_v, k_w) = (1.5, 2.5, 3.5)$. We show this for TE and TM modes with var-
152 ious values of ε . The figures show the spectral convergence of the energy
153 defect as the perturbation order N is refined. We also found that the energy
154 defect decays more quickly to machine precision for smaller choices of ε .

155 We repeated this experiment for fixed value of N while varying the spatial
156 discretization parameters N_x and N_y . The results are displayed in [Figures 7](#)
157 and [8](#) for $N = 20$ and various values of N_x and N_y . Once again, we chose
158 $(k_u, k_v, k_w) = (1.5, 2.5, 3.5)$ and performed simulations for TE and TM modes
159 for a selection of ε . Once again we saw the spectral convergence of the energy
160 defect, this time versus the number of Fourier and Legendre coefficients.

161 We then focused on the behavior of our method as ε was increased. For
162 this we fixed $N_x = 22$ and $N_y = 24$, and once again choose $(k_u, k_v, k_w) =$
163 $(1.5, 2.5, 3.5)$. We conducted numerical experiments in both TE and TM
164 polarizations, and display the results in [Figures 9 and 10](#). These figures depict
165 the energy defect versus the perturbation size ε with various perturbation

Figure 5: Energy defect versus perturbation order, N , for smooth interface configuration (12): TE mode.

orders N . As expected, smaller errors are realized for smaller choices of ε and larger values of N .

Finally, in Figures 11 and 12 we computed the energy defect for fixed $\varepsilon = 0.01$, $N = 15$, $N_x = 20$, and $N_y = 40$ (for TE and TE modes) with various choices of [wavenumber](#). If the collection of [wavenumbers](#) was not large (e.g. $(k_u, k_v, k_w) = (1.5, 2.5, 3.5)$), then we observed rapid convergence to machine precision. However, as we increased to larger values of k_m our convergence deteriorated due to the severe under-resolution of our parameter choices. To address this latter concern we revisited these computations and found that if we refined our spatial discretization then we could recover the striking convergence we saw for the smallest values of (k_u, k_v, k_w) . To be more specific, as we display in Figure 13, if we chose $N_x = 30$ and $N_y = 60$ we realized accuracies of 10^{-14} to 10^{-15} for the moderate values $(k_u, k_v, k_w) = (11.5, 12.5, 13.5)$. Furthermore, if we chose $N_x = 40$ and $N_y = 100$ then we realized errors on the order of 10^{-14} for the large values $(k_u, k_v, k_w) = (41.5, 42.5, 43.5)$.

Figure 6: Energy defect versus perturbation order, N , for smooth interface configuration (12): TM mode.

182 6.3. Simulations of a Triply Layered Medium: Rough Interfaces

We repeated the first simulation of the previous section specified in (12) with the smooth profiles replaced by the much rougher profiles

$$f_r(x) = (2 \times 10^{-4}) x^4 (2\pi - x)^4 - c_0,$$

$$f_L(x) = \begin{cases} -\frac{2}{\pi}x + 1, & 0 \leq x \leq \pi, \\ \frac{2}{\pi}x - 3, & \pi \leq x \leq 2\pi, \end{cases}$$

(with c_0 chosen such that f_r has zero mean) which possess C^4 (but not C^5) and Lipschitz regularity, respectively [48]. For our experiments we used their Fourier series representations

$$f_r(x) = \sum_{k=1}^{\infty} \frac{96(2k^2\pi^2 - 21)}{125k^8} \cos(kx)$$

$$f_L(x) = \sum_{k=1}^{\infty} \frac{8}{\pi^2(2k-1)^2} \cos((2k-1)x),$$

Figure 7: Energy defect versus number of modes, $\sqrt{N_x N_y}$, for smooth interface configuration (12): TE mode.

which we truncated after wavenumber $P = 40$,

$$f_{r,P}(x) = \sum_{k=1}^P \frac{96(2k^2\pi^2 - 21)}{125k^8} \cos(kx)$$

$$f_{L,P}(x) = \sum_{k=1}^{P/2} \frac{8}{\pi^2(2k-1)^2} \cos((2k-1)x).$$

The specific details of our numerical simulations are given by the following parameters.

$$a = 5, \quad \bar{g} = 2, \quad \bar{h} = 1, \quad b = -2, \quad \alpha = 0.1,$$

$$d = 2\pi, \quad g(x) = f_{r,40}(x) \quad h(x) = f_{L,40}(x). \quad (13)$$

183 In addition, we picked $(k_u, k_v, k_w) = (1.5, 2.5, 3.5)$, $\varepsilon = 0.05$, $N = 15$, and
 184 three choices of (N_x, N_y) . In Figure 14 we display the results of these exper-
 185 iments and show that, provided with sufficient resolution, our new approach

Figure 8: Energy defect versus number of modes, $\sqrt{N_x N_y}$, for smooth interface configuration (12): TM mode.

186 is equally applicable to configurations with finite and even Lipschitz smooth-
187 ness. In Figures 15 and 16 we show the real and imaginary parts of the
188 scattered solution. The layer interfaces are depicted in dashed red lines.
189 To further investigate the capabilities of our algorithm, we revisit this com-
190 putation with different values of P , more precisely $P = 20, 40, 80, 160$. The
191 results of this study are summarized in Figure 17 which show that, while the
192 accuracy deteriorates a small amount as P increases (representing a more
193 faithful representation of the very rough interfaces), it remains quite small
194 throughout the entire range of P and shows no sign of producing divergent
195 results regardless of how large P is chosen.

196 To close our study we reconsider the smooth profile configuration, (12),
197 but replace the choice of k_v with 42.5 meant to simulate a device with “high-
198 contrast media.” In Figure 18 we report the results of this experiment and
199 see, once again, that given sufficient resolution we can realize results with
200 excellent accuracy.

Figure 9: Energy defect versus perturbation size, ϵ , for smooth interface configuration (12): TE mode.

7. Conclusions

We have described a High-Order Perturbation of Surfaces (HOPS) algorithm for electromagnetic scattering in a triply layered periodic medium. We equivalently restated the governing Helmholtz equations for this layered medium on a *bounded* domain using Dirichlet-Neumann operators at artificial boundaries above and below the structure. Utilizing a suitable change of variables, we were able to study the governing equations on a *separable* geometry with *flat* interfaces. Introducing boundary perturbations, we expressed the scattered field in a Taylor series and derived a sequence of linear problems to be solved at each perturbation order for the n -th order term in this expansion, resulting in a Transformed Field Expansions (TFE) algorithm. Accurate numerical simulations of these TFE recursions were performed with a Legendre-Galerkin method based on a novel weak formulation. Our numerical simulations show the spectral convergence which our new algorithm can achieve.

Our developments clearly point towards several extensions of great im-

Figure 10: Energy defect versus perturbation size, ϵ , for smooth interface configuration (12): TM mode.

portance. In particular, our approach must be generalized to an arbitrary number of layers. While the extension is, in some sense, straightforward given the developments of this contribution, the algorithmic differences are significant and we will describe them in a future publication. In addition, the current approach, which models the scattering of *scalar* waves relevant to acoustics, must be extended to the *vector* wave scattering problems of electromagnetics (in three dimensions) and linear elastodynamics.

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228

Appendix A. Derivation of the Transformed Equations

229

Figure 11: Energy defect versus perturbation order, N , for smooth interface configuration (12): TE mode.

230 In this section we give a full derivation of the transformed version of the
 231 governing equations (2) presented in Section 3.1.

Remark 1. As our problem geometry features three distinct layers, two of which are similar (the upper and lower) and one of which (the middle) has quite different character, the notation can become cumbersome. In order to simplify and shorten our presentation we give formulas for the upper and lower layers together, while separating the middle layer formulas from these. To achieve this we assign the upper and lower layers indices $i = 1$ and $i = 3$, respectively, and define the middle layer by $i = 2$. In addition we use the following notation for the geometrical aspects of each domain: In the upper layer

$$u_1 := u, \quad \xi_1 := a, \quad \bar{\varphi}_1 := \bar{g}, \quad \varphi_1(x) := g(x), \quad g(x) = \varepsilon \psi_1(x),$$

the latter in anticipation of our boundary perturbation methodology. In the lower domain we define

$$u_3 := w, \quad \xi_3 := b, \quad \bar{\varphi}_3 := \bar{h}, \quad \varphi_3(x) := h(x), \quad h(x) = \varepsilon \psi_3(x).$$

Figure 12: Energy defect versus perturbation order, N , for smooth interface configuration (12): TM mode.

In the middle layer ($i = 2$) we find it more useful to simply define

$$u_2 := v, \quad g(x) = \varepsilon f_g(x), \quad h(x) = \varepsilon f_h(x),$$

232 where we note that $\{f_g, f_h\}$ are just different names for $\{\psi_1, \psi_3\}$ defined
 233 above. In these, $\{\psi_1 = f_g, \psi_3 = f_h\}$ are the order one boundary perturbation
 234 *shapes*.

Returning to our change of variables, by the chain rule we find

$$\partial_x = \partial_{x'} + (\partial_x y_i) \partial_{y_i} \tag{A.1a}$$

$$\partial_y = (\partial_y y_i) \partial_{y_i}, \tag{A.1b}$$

for $i = 1, 2, 3$. For $i = 1, 3$, we have

$$(x', y_i) = \left(x, \xi_i \left(\frac{y - (\bar{\varphi}_i + \varphi_i)}{\xi_i - (\bar{\varphi}_i + \varphi_i)} \right) + \bar{\varphi}_i \left(\frac{\xi_i - y}{\xi_i - (\bar{\varphi}_i + \varphi_i)} \right) \right),$$

Figure 13: Energy defect versus perturbation order, N , for two higher wavenumber combinations for smooth interface configuration (12): TE mode.

and noting that

$$\begin{aligned}
[\xi_i - (\bar{\varphi}_i + \varphi_i)]\partial_x &= [\xi_i - (\bar{\varphi}_i + \varphi_i)]\partial_{x'} + [\xi_i - (\bar{\varphi}_i + \varphi_i)]\partial_x y_i \partial_{y_i} \\
&= [\xi_i - (\bar{\varphi}_i + \varphi_i)]\partial_{x'} + \partial_x \left([\xi_i - (\bar{\varphi}_i + \varphi_i)] y_i \right) \partial_{y_i} \\
&\quad - y_i \partial_x [\xi_i - (\bar{\varphi}_i + \varphi_i)] \partial_{y_i},
\end{aligned}$$

we discover that

$$\begin{aligned}
[\xi_i - (\bar{\varphi}_i + \varphi_i)]\partial_x &= [\xi_i - (\bar{\varphi}_i + \varphi_i)]\partial_{x'} + \partial_{x'} \varphi_i (y_i - \xi_i) \partial_{y_i}, \\
[\xi_i - (\bar{\varphi}_i + \varphi_i)]\partial_y &= (\xi_i - \bar{\varphi}_i) \partial_{y_i}.
\end{aligned}$$

On the other hand, for $i = 2$,

$$(x', y_2) = \left(x', \bar{h} \left(\frac{y - (\bar{g} + g)}{(\bar{h} + h) - (\bar{g} + g)} \right) + \bar{g} \left(\frac{(\bar{h} + h) - y}{(\bar{h} + h) - (\bar{g} + g)} \right) \right).$$

Figure 14: Energy defect versus perturbation order, N , for rough interface configuration (13): TE mode.

Setting $M(x) = (\bar{h} + h) - (\bar{g} + g)$, we deduce that

$$\begin{aligned}
M\partial_x &= M\partial_{x'} + M(\partial_x y_2)\partial_{y_2} = M\partial_{x'} + \left[\partial_x(My_2) - (\partial_x M)y_2 \right] \partial_{y_2} \\
&= M\partial_{x'} + \left[\bar{h}(-\partial_x g) + \bar{g}\partial_x h - (\partial_x h - \partial_x g)y_2 \right] \partial_{y_2} \\
&= M\partial_{x'} + [-\bar{h}\partial_x g + \bar{g}\partial_x h - \partial_x h y_2 + \partial_x g y_2] \partial_{y_2} \\
&= M\partial_{x'} + [\partial_x g(y_2 - \bar{h}) - \partial_x h(y_2 - \bar{g})] \partial_{y_2}.
\end{aligned}$$

Hence, we obtain that

$$M\partial_x = M\partial_{x'} + [\partial_x g(y_2 - \bar{h}) - \partial_x h(y_2 - \bar{g})] \partial_{y_2}.$$

Similarly, noting that

$$M\partial_y = M\partial_y y_2 \partial_{y_2} = \partial_y(My_2) \partial_{y_2} = (\bar{h} - \bar{g}) \partial_{y_2},$$

we find that

$$M\partial_y = (\bar{h} - \bar{g}) \partial_{y_2}.$$

Figure 15: Plot of the real part of the scattered field for rough interface configuration (13): TE mode. Layer interfaces depicted in dashed red lines.

For $i = 1, 3$, setting

$$C_i = [\xi_i - (\bar{\varphi}_i + \varphi_i)], \quad D_i = \frac{\partial \varphi_i}{\partial x'}(y_i - \xi_i), \quad E_i = (\xi_i - \bar{\varphi}_i),$$

and

$$C_2 = M, \quad D_2 = \partial_x g(y_2 - \bar{h}) - \partial_x h(y_2 - \bar{g}), \quad E_2 = \bar{h} - \bar{g},$$

we rewrite (A.1) as

$$C_i \partial_x = C_i \partial_{x'} + D_i \partial_{y_i}, \quad C_i \partial_y = E_i \partial_{y_i}, \quad i = 1, 2, 3.$$

235

We now seek forms for the *second* derivatives

$$\begin{aligned} C^2 \partial_x^2 &= C \partial_x (C \partial_x) - C (\partial_x C) \partial_x, \\ C^2 \partial_y^2 &= C \partial_{y_i} (C \partial_{y_i}) - C (\partial_{y_i} C) \partial_{y_i}. \end{aligned}$$

Figure 16: Plot of the imaginary part of the scattered field for rough interface configuration (13): TE mode. Layer interfaces depicted in dashed red lines.

We note that

$$\begin{aligned}
 C\partial_x(C\partial_x) &= [C\partial_{x'} + D\partial_{y_i}][C\partial_{x'} + D\partial_{y_i}] \\
 &= C\partial_{x'}[C\partial_{x'}] + D\partial_{y_i}[C\partial_{x'}] + C\partial_{x'}[D\partial_{y_i}] + D\partial_{y_i}[D\partial_{y_i}] \\
 &= \partial_{x'}[C^2\partial_{x'}] - (\partial_{x'}C)[C\partial_{x'}] + \partial_{y_i}[CD\partial_{x'}] - (\partial_{y_i}D)[C\partial_{x'}] \\
 &\quad + \partial_{x'}[CD\partial_{y_i}] - (\partial_{x'}C)[D\partial_{y_i}] + \partial_{y_i}[D^2\partial_{y_i}] - (\partial_{y_i}D)[D\partial_{y_i}],
 \end{aligned}$$

and

$$C(\partial_x C)\partial_x = (\partial_{x'} C)[C\partial_{x'} + D\partial_{y_i}] = (\partial_{x'} C)[C\partial_{x'}] + (\partial_{x'} C)[D\partial_{y_i}],$$

and

$$C^2\partial_y^2 = C\partial_y(C\partial_y) - C(\partial_y C)\partial_y = E^2\partial_{y_i}^2.$$

Hence, we deduce that the Laplacian transforms as

$$\begin{aligned}
 C^2\Delta &= \partial_{x'}[C^2\partial_{x'}] - (\partial_{x'}C)[C\partial_{x'}] + \partial_{y_i}[CD\partial_{x'}] - (\partial_{y_i}D)[C\partial_{x'}] \\
 &\quad + \partial_{x'}[CD\partial_{y_i}] - (\partial_{x'}C)[D\partial_{y_i}] + \partial_{y_i}[D^2\partial_{y_i}] - (\partial_{y_i}D)[D\partial_{y_i}] \\
 &\quad - (\partial_{x'}C)[C\partial_{x'}] - (\partial_{x'}C)[D\partial_{y_i}] + E^2\partial_{y_i}^2.
 \end{aligned}$$

Figure 17: Energy defect versus perturbation order, N , for rough interface configuration (13) with $P = 20, 40, 80, 160$: TE mode.

Noting that $\partial_{x'}C = -\partial_{y_i}D$, we derive that solutions of the Helmholtz equation satisfy

$$\begin{aligned}
0 &= C^2 \Delta u_i + C^2 k^2 u_i \\
&= \partial_{x'}[C^2 \partial_{x'} u_i] + \partial_{y_i}[CD \partial_{x'} u_i] + \partial_{x'}[CD \partial_{y_i} u_i] - (\partial_{x'} C)[D \partial_{y_i} u_i] \\
&\quad + \partial_{y_i}[D^2 \partial_{y_i} u_i] - (\partial_{x'} C)[C \partial_{x'} u_i] + E^2 \partial_{y_i}^2 u_i + C^2 k^2 u_i.
\end{aligned}$$

Setting $C^2(x) = E^2 + F(x)$, we find that

$$\begin{aligned}
\partial_{x'}[E^2 \partial_{x'} u_i] + E^2 \partial_{y_i}^2 u_i + E^2 k^2 u_i &= -\partial_{x'}[F \partial_{x'} u_i] - k^2 F u_i - \partial_{y_i}[CD \partial_{x'} u_i] \\
&\quad - \partial_{x'}[CD \partial_{y_i} u_i] + (\partial_{x'} C)[D \partial_{y_i} u_i] - \partial_{y_i}[D^2 \partial_{y_i} u_i] + (\partial_{x'} C)[C \partial_{x'} u_i],
\end{aligned}$$

Figure 18: Energy defect versus perturbation order, N , for smooth interface configuration (12) with $k_v = 42.5$: TE mode.

and hence we arrive at

$$\begin{aligned}
\partial_{x'}^2 u_i + \partial_{y_i}^2 u_i + k^2 u_i &= \frac{1}{E^2} \partial_{x'} [-F \partial_{x'} u_i - CD \partial_{y_i} u_i] \\
&+ \frac{1}{E^2} \partial_{y_i} [-CD \partial_{x'} u_i - D^2 \partial_{y_i} u_i] \\
&+ \frac{1}{E^2} \left[-k^2 F u_i + (\partial_{x'} C) [D \partial_{y_i} u_i + C \partial_{x'} u_i] \right]. \quad (\text{A.2})
\end{aligned}$$

236

Anticipating our boundary perturbation approach we introduce ε as specified in Remark 1 and rearrange the right hand side of (A.2). For $i = 1, 3$ we have

$$\begin{aligned}
C_i &= \xi_i - (\overline{\varphi}_i + \varepsilon \psi_i), & D_i &= \varepsilon \partial_{x'} \psi_i (y_i - \xi_i), \\
E_i &= \xi_i - \overline{\varphi}_i, & F_i &= \varepsilon^2 \psi_i^2 + \varepsilon \psi_i (2\overline{\varphi}_i - 2\xi_i).
\end{aligned}$$

Hence, (A.2) becomes

$$\partial_{x'}^2 u_i + \partial_{y_i}^2 u_i + k^2 u_i = \frac{1}{E_i^2} [\partial_{x'} R_i^x + \partial_{y_i} R_i^y + R_i],$$

where

$$\begin{aligned}
R_i^x &= -F_i \partial_{x'} u_i - C_i D_i \partial_{y_i} u_i \\
&= -(\varepsilon^2 \psi_i^2 + \varepsilon \psi_i (2\bar{\varphi}_i - 2\xi_i)) \partial_{x'} u_i - (\xi_i - \bar{\varphi}_i - \varepsilon \psi_i) (\varepsilon \partial_{x'} \psi_i) (y_i - \xi_i) \partial_{y_i} u_i \\
&= -\varepsilon \psi_i (2\bar{\varphi}_i - 2\xi_i) \partial_{x'} u_i - \varepsilon (\xi_i - \bar{\varphi}_i) \partial_{x'} \psi_i (y_i - \xi_i) \partial_{y_i} u_i \\
&\quad - \varepsilon^2 \psi_i^2 \partial_{x'} u_i + \varepsilon^2 \psi_i \partial_{x'} \psi_i (y_i - \xi_i) \partial_{y_i} u_i,
\end{aligned}$$

and

$$\begin{aligned}
R_i^y &= -C_i D_i \partial_{x'} u_i - D_i^2 \partial_{y_i} u_i \\
&= -(\xi_i - \bar{\varphi}_i - \varepsilon \psi_i) \varepsilon \partial_{x'} \psi_i (y_i - \xi_i) \partial_{x'} u_i - \varepsilon^2 (\partial_{x'} \psi_i)^2 (y_i - \xi_i)^2 \partial_{y_i} u_i \\
&= -\varepsilon (\xi_i - \bar{\varphi}_i) \partial_{x'} \psi_i (y_i - \xi_i) \partial_{x'} u_i + \varepsilon^2 \psi_i \partial_{x'} \psi_i (y_i - \xi_i) \partial_{x'} u_i \\
&\quad - \varepsilon^2 (\partial_{x'} \psi_i)^2 (y_i - \xi_i)^2 \partial_{y_i} u_i,
\end{aligned}$$

and

$$\begin{aligned}
R_i &= -k^2 F_i u_i + (\partial_{x'} C_i) [D_i \partial_{y_i} u_i + C_i \partial_{x'} u_i] \\
&= -k^2 \varepsilon \psi_i (\varepsilon \psi_i + 2\bar{\varphi}_i - 2\xi_i) u_i - \varepsilon \partial_{x'} \psi_i [\varepsilon \partial_{x'} \psi_i (y_i - \xi_i) \partial_{y_i} u_i \\
&\quad + (\xi_i - \bar{\varphi}_i - \varepsilon \psi_i) \partial_{x'} u_i] \\
&= -\varepsilon k^2 \psi_i (2\bar{\varphi}_i - 2\xi_i) u_i - \varepsilon \partial_{x'} \psi_i (\xi_i - \bar{\varphi}_i) \partial_{x'} u_i - \varepsilon^2 k^2 (\psi_i)^2 u_i \\
&\quad - \varepsilon^2 (\partial_{x'} \psi_i)^2 (y_i - \xi_i) \partial_{y_i} u_i + \varepsilon^2 \psi_i \partial_{x'} \psi_i \partial_{x'} u_i.
\end{aligned}$$

For $i = 2$ we have

$$\begin{aligned}
C_2 &= (\bar{h} - \bar{g}) + \varepsilon (f_h - f_g), \\
D_2 &= \varepsilon [\partial_{x'} f_g (y_2 - \bar{h}) - \partial_{x'} f_h (y_2 - \bar{g})], \\
E_2 &= \bar{h} - \bar{g}, \\
F_2 &= 2\varepsilon (f_h - f_g) (\bar{h} - \bar{g}) + \varepsilon^2 (f_h - f_g)^2,
\end{aligned}$$

and, for later use, we define $\tilde{D}_2 := \varepsilon D_2$. Hence, we find that

$$\begin{aligned}
R_2^x &= -2\varepsilon (f_h - f_g) (\bar{h} - \bar{g}) \partial_{x'} u_i - \varepsilon^2 (f_h - f_g)^2 \partial_{x'} u_i \\
&\quad - \varepsilon (\bar{h} - \bar{g}) \tilde{D} \partial_{y_2} u_i - \varepsilon^2 (f_h - f_g) \tilde{D} \partial_{y_2} u_i,
\end{aligned}$$

and

$$R_2^y = -\varepsilon (\bar{h} - \bar{g}) \tilde{D}_2 \partial_{x'} u_i - \varepsilon^2 (f_h - f_g) \tilde{D}_2 \partial_{x'} u_i - \varepsilon^2 \tilde{D}^2 \partial_{y_2} u_i,$$

and

$$R_2 = -2\varepsilon k^2(f_h - f_g)(\bar{h} - \bar{g})u_i - \varepsilon^2 k^2(f_h - f_g)^2 u_i + \varepsilon^2 \partial_{x'}(f_h - f_g) \tilde{D} \partial_{y_2} u_i \\ + \varepsilon \partial_{x'}(f_h - f_g)(\bar{h} - \bar{g}) \partial_{x'} u_i + \varepsilon^2 (f_h - f_g) \partial_{x'}(f_h - f_g) \partial_{x'} u_i.$$

237

For the boundary conditions we recall that

$$u^{inc}(x, y) = e^{i\alpha x - i\beta^u y},$$

and write (2d)–(2i) as

$$\begin{aligned} u_1 - u_2 &= -e^{i\alpha x - i\beta^u(\bar{g} + g(x))}, & y &= \bar{g} + g(x), \\ u_2 - u_3 &= 0, & y &= \bar{h} + h(x), \\ \partial_{N_g} u_1 - \tau^2 \partial_{N_g} u_2 &= (i\alpha \partial_x g(x) + i\beta^u) e^{i\alpha x - i\beta(\bar{g} + g(x))}, & y &= \bar{g} + g(x), \\ \partial_{N_h} u_2 - \sigma^2 \partial_{N_h} u_3 &= 0, & y &= \bar{h} + h(x), \\ \partial_y u_1 - T_1[u_1] &= 0, & y &= a, \\ \partial_y u_3 - T_3[u_3] &= 0, & y &= b. \end{aligned}$$

At $y = a$ and $y = b$, we find that

$$\partial_{y_i} u_i - \frac{C_i}{E_i} T_i[u_i] = 0,$$

for $i = 1, 3$, and this implies that

$$\partial_{y_i} u_i - T_i[u_i] = -\frac{\varphi_i}{\xi_i - \bar{\varphi}_i} T_i[u_i] = -\frac{\varepsilon \psi_i}{\xi_i - \bar{\varphi}_i} T_i[u_i].$$

At $y = \bar{g} + g(x)$ we deduce that

$$\partial_{N_g} u_1 - \tau^2 \partial_{N_g} u_2 = (i\alpha \partial_{x'} g + i\beta^u) e^{i\alpha x - i\beta^u(\bar{g} + g(x))}$$

which implies that

$$-\partial_{x'} g \partial_x u_1 + \partial_y u_1 - \tau^2 (-\partial_{x'} g \partial_x u_2 + \partial_y u_2) = (i\alpha \partial_{x'} g + i\beta^u) e^{i\alpha x - i\beta^u(\bar{g} + g(x))}.$$

Using the change of variables, we find that

$$\begin{aligned} -\varepsilon \partial_{x'} f_g \left[\partial_{x'} u_1 + \frac{\varepsilon \tilde{D}_1}{C_1} \partial_{y_1} u_1 \right] + \frac{E_1}{C_1} \partial_{y_1} u_1 - \tau^2 \left[-\varepsilon \partial_{x'} f_g \left(\partial_{x'} u_2 + \frac{\varepsilon \tilde{D}_2}{C_2} \partial_{y_2} u_2 \right) + \frac{E_2}{C_2} \partial_{y_2} u_2 \right] \\ = (\varepsilon i\alpha \partial_{x'} f_g + i\beta^u) e^{i\alpha x - i\beta^u(\bar{g} + g(x))}. \end{aligned}$$

Then, we obtain that

$$\frac{E_1}{C_1} \partial_{y_1} u_1 - \tau^2 \frac{E_2}{C_2} \partial_{y_2} u_2 = \mathcal{J}'_1,$$

where

$$\begin{aligned} \mathcal{J}'_1 := & \varepsilon(\partial_{x'} f_g)(\partial_{x'} u_1) + \varepsilon^2(\partial_{x'} f_g) \frac{\tilde{D}_1}{C_1} \partial_{y_1} u_1 - \varepsilon \tau^2 \partial_{x'} f_g \partial_{x'} u_2 - \varepsilon^2 \tau^2 \partial_{x'} f_g \frac{\tilde{D}_2}{C_2} \partial_{y_2} u_2 \\ & + (\varepsilon i \alpha \partial_{x'} f_g + i \beta^u) e^{i \alpha x - i \beta^u \bar{g}} e^{-i \beta^u g(x)}. \end{aligned}$$

Noting that

$$\begin{aligned} E_1 C_2 &= (a - \bar{g})(\bar{h} - \bar{g} + h - g) = (a - \bar{g})(\bar{h} - \bar{g}) + (a - \bar{g})(h - g), \\ E_2 C_1 &= (\bar{h} - \bar{g})(a - \bar{g} - g) = (a - \bar{g})(\bar{h} - \bar{g}) - g(\bar{h} - \bar{g}), \end{aligned}$$

we deduce that

$$\partial_{y_1} u_1 - \tau^2 \partial_{y_2} u_2 = \mathcal{J}_1,$$

where

$$\mathcal{J}_1 = \frac{C_1 C_2 \mathcal{J}'_1 - \varepsilon(a - \bar{g})(f_h - f_g) \partial_{y_1} u_1 - \varepsilon \tau^2 f_g(\bar{h} - \bar{g}) \partial_{y_2} u_2}{(a - \bar{g})(\bar{h} - \bar{g})}.$$

For later computations, the term $C_1 C_2 \mathcal{J}'_1$ can be written

$$C_1 C_2 \mathcal{J}'_1 = (a - \bar{g})(\bar{h} - \bar{g}) \mathcal{J}'_1 + \varepsilon \mathcal{J}'_1 \left((a - \bar{g})(f_h - f_g) - f_g(\bar{h} - \bar{g}) \right) - \varepsilon^2 f_g(f_h - f_g) \mathcal{J}'_1.$$

Similarly, at $y = \bar{h} + h(x)$, we find that

$$\partial_{N_h} u_2 - \sigma^2 \partial_{N_h} u_3 = 0,$$

which implies that

$$(-\partial_{x'} h \partial_x u_2 + \partial_y u_2) - \sigma^2 (-\partial_{x'} h \partial_x u_3 + \partial_y u_3) = 0.$$

By the change of variables, we deduce that

$$\begin{aligned} & -\varepsilon \partial_{x'} f_h \left[\partial_{x'} u_2 + \frac{\varepsilon \tilde{D}_2}{C_2} \partial_{y_2} u_2 \right] + \frac{E_2}{C_2} \partial_{y_2} u_2 \\ & - \sigma^2 \left[-\varepsilon \partial_{x'} f_h \left(\partial_{x'} u_3 + \frac{\varepsilon \tilde{D}_3}{C_3} \partial_{y_3} u_3 \right) + \frac{E_3}{C_3} \partial_{y_3} u_3 \right] = 0. \end{aligned}$$

Rearranging the equations, we obtain that

$$\frac{E_2}{C_2} \partial_{y_2} u_2 - \sigma^2 \frac{E_3}{C_3} \partial_{y_3} u_3 = \mathcal{J}_2',$$

where

$$\mathcal{J}_2' = \varepsilon(\partial_{x'} f_h)(\partial_{x'} u_2) + \varepsilon^2 \partial_{x'} f_h \frac{\tilde{D}_2}{C_2} \partial_{y_2} u_2 - \varepsilon \sigma^2 \partial_{x'} f_h \partial_{x'} u_3 - \varepsilon^2 \sigma^2 \partial_{x'} f_h \frac{\tilde{D}_3}{C_3} \partial_{y_3} u_3.$$

Noting that

$$\begin{aligned} E_2 C_3 &= (\bar{h} - \bar{g})(b - \bar{h} - h) = (\bar{h} - \bar{g})(b - \bar{h}) - (\bar{h} - \bar{g})h, \\ E_3 C_2 &= (b - \bar{h})(\bar{h} - \bar{g} + h - g) = (b - \bar{h})(\bar{h} - \bar{g}) + (b - \bar{h})(h - g), \end{aligned}$$

we deduce that

$$\partial_{y_2} u_2 - \sigma^2 \partial_{y_3} u_3 = \mathcal{J}_2,$$

where

$$\mathcal{J}_2 = \frac{C_2 C_3 \mathcal{J}_2' + \varepsilon f_h (\bar{h} - \bar{g}) \partial_{y_2} u_2 + \varepsilon \sigma^2 (b - \bar{h}) (f_h - f_g) \partial_{y_3} u_3}{(\bar{h} - \bar{g})(b - \bar{h})}.$$

For later computations, the term $C_2 C_3 \mathcal{J}_2'$ can be written

$$C_2 C_3 \mathcal{J}_2' = (b - \bar{h})(\bar{h} - \bar{g}) \mathcal{J}_2' + \varepsilon (b - \bar{h}) (f_h - f_g) \mathcal{J}_2' - \varepsilon f_h (\bar{h} - \bar{g}) \mathcal{J}_2' - \varepsilon^2 f_h (f_h - f_g) \mathcal{J}_2'.$$

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As we have a boundary perturbation method in mind, it is clearly important to expand these forms in power series in ε . These are recorded here for completeness. For $i = 1, 3$,

$$\begin{aligned} R_{i,n}^x &= -\psi_i(2\bar{\varphi}_i - 2\xi_i) \partial_{x'} u_{i,n-1} - (\xi_i - \bar{\varphi}_i) \partial_{x'} \psi_i (y_i - \xi_i) \partial_{y_i} u_{i,n-1} \\ &\quad - \psi_i^2 \partial_{x'} u_{i,n-2} + \psi_i \partial_{x'} \psi_i (y_i - \xi_i) \partial_{y_i} u_{i,n-2}, \\ R_{i,n}^y &= -(\xi_i - \bar{\varphi}_i) \partial_{x'} \psi_i (y_i - \xi_i) \partial_{x'} u_{i,n-1} + \psi_i \partial_{x'} \psi_i (y_i - \xi_i) \partial_{x'} u_{i,n-2} \\ &\quad - (\partial_{x'} \psi_i)^2 (y_i - \xi_i)^2 \partial_{y_i} u_{i,n-2}, \\ R_{i,n} &= -k^2 \psi_i (2\bar{\varphi}_i - 2\xi_i) u_{i,n-1} - \partial_{x'} \psi_i (\xi_i - \bar{\varphi}_i) \partial_{x'} u_{i,n-1} - k^2 (\psi_i)^2 u_{i,n-2} \\ &\quad - (\partial_{x'} \psi_i)^2 (y_i - \xi_i) \partial_{y_i} u_{i,n-2} + \psi_i \partial_{x'} \psi_i \partial_{x'} u_{i,n-2}, \end{aligned}$$

and

$$\begin{aligned}
R_{2,n}^x &= -2(f_h - f_g)(\bar{h} - \bar{g})\partial_{x'}u_{i,n-1} - (f_h - f_g)^2\partial_{x'}u_{i,n-2} \\
&\quad - (\bar{h} - \bar{g})\tilde{D}_2\partial_{y_2}u_{i,n-1} - (f_h - f_g)\tilde{D}_2\partial_{y_2}u_{i,n-2}, \\
R_{2,n}^y &= -(\bar{h} - \bar{g})\tilde{D}_2\partial_{x'}u_{i,n-1} - (f_h - f_g)\tilde{D}_2\partial_{x'}u_{i,n-2} - \tilde{D}_2^2\partial_{y_2}u_{i,n-2}, \\
R_{2,n} &= -2k^2(f_h - f_g)(\bar{h} - \bar{g})u_{i,n-1} - k^2(f_h - f_g)^2u_{i,n-2} \\
&\quad + \partial_{x'}(f_h - f_g)\tilde{D}_2\partial_{y_2}u_{i,n-2} \\
&\quad + \partial_{x'}(f_h - f_g)(\bar{h} - \bar{g})\partial_{x'}u_{i,n-1} + (f_h - f_g)\partial_{x'}(f_h - f_g)\partial_{x'}u_{i,n-2}.
\end{aligned}$$

For the boundary terms, we write

$$\begin{aligned}
\mathcal{J}_{1,n} &= \frac{C_1C_2\mathcal{J}'_{1,n} - (a - \bar{g})(f_h - f_g)\partial_{y_1}u_{1,n-1} - \tau^2f_g(\bar{h} - \bar{g})\partial_{y_2}u_{2,n-1}}{(a - \bar{g})(\bar{h} - \bar{g})}, \\
\mathcal{J}_{2,n} &= \frac{C_2C_3\mathcal{J}'_{2,n} + f_h(\bar{h} - \bar{g})\partial_{y_2}u_{2,n-1} + \sigma^2(b - \bar{h})(f_h - f_g)\partial_{y_3}u_{3,n-1}}{(\bar{h} - \bar{g})(b - \bar{h})},
\end{aligned}$$

where

$$\begin{aligned}
\mathcal{J}'_{1,n} &:= (\partial_{x'}f_g)(\partial_{x'}u_{1,n-1}) + (\partial_{x'}f_g)\frac{\tilde{D}_1}{C_1}\partial_{y_1}u_{1,n-2} \\
&\quad - \tau^2\partial_{x'}f_g\partial_{x'}u_{2,n-1} - \tau^2\partial_{x'}f_g\frac{\tilde{D}_2}{C_2}\partial_{y_2}u_{2,n-2} \\
&\quad + i\alpha\partial_{x'}f_ge^{i\alpha x' - i\beta^u\bar{g}}\frac{(-i\beta^uf_g)^{n-1}}{(n-1)!} + i\beta^ue^{i\alpha x' - i\beta^u\bar{g}}\frac{(-i\beta^uf_g)^n}{n!},
\end{aligned}$$

and

$$\begin{aligned}
\mathcal{J}'_{2,n} &= (\partial_{x'}f_h)(\partial_{x'}u_{2,n-1}) + \partial_{x'}f_h\frac{\tilde{D}_2}{C_2}\partial_{y_2}u_{2,n-2} \\
&\quad - \sigma^2\partial_{x'}f_h\partial_{x'}u_{3,n-1} - \sigma^2\partial_{x'}f_h\frac{\tilde{D}_3}{C_3}\partial_{y_3}u_{3,n-2},
\end{aligned}$$

and hence

$$\begin{aligned}
C_1C_2\mathcal{J}'_{1,n} &= (a - \bar{g})(\bar{h} - \bar{g})\mathcal{J}'_{1,n} + \mathcal{J}'_{1,n-1}\left((a - \bar{g})(f_h - f_g) - f_g(\bar{h} - \bar{g})\right) \\
&\quad - f_g(f_h - f_g)\mathcal{J}'_{1,n-2}, \\
C_2C_3\mathcal{J}'_{2,n} &= (b - \bar{h})(\bar{h} - \bar{g})\mathcal{J}'_{2,n} + (b - \bar{h})(f_h - f_g)\mathcal{J}'_{2,n-1} - f_h(\bar{h} - \bar{g})\mathcal{J}'_{2,n-1} \\
&\quad - f_h(f_h - f_g)\mathcal{J}'_{2,n-2}.
\end{aligned}$$

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