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On analyticity of scattered fields in layered structures with interfacial graphene

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Abstract

Two-dimensional materials such as graphene have become crucial components of most state-of-the-art plasmonic devices. The possibility of not only generating plasmons in the terahertz regime, but also tuning them in real time via chemical doping or electrical gating make them compelling materials for engineers seeking to build accurate sensors. Thus, the faithful modeling of the propagation of linear waves in a layered, periodic structure with such materials at the interfaces is of paramount importance in many branches of the applied sciences. In this paper, we present a novel formulation of the problem featuring surface currents to model the two-dimensional materials which not only is free of the artificial singularities present in related approaches, but also can be used to deliver a proof of existence, uniqueness, and analytic dependence of solutions. We advocate for a surface integral formulation which is phrased in terms of well-chosen Impedance–Impedance Operators that are immune to the Dirichlet eigenvalues which plague the Dirichlet–Neumann Operators that appear in classical formulations. With a High-Order Perturbation of Surfaces approach we are able to give a straightforward demonstration of this new well-posedness result which only requires the verification that a finite collection of explicitly stated transcendental expressions be nonzero. We further illustrate the utility of this formulation by displaying results of a High-Order Spectral numerical implementation which is flexible, rapid, and robust.

KEYWORDS
graphene, Helmholtz equation, High-Order perturbation of surfaces methods, Impedance–Impedance Operators, layered media, two-dimensional materials

1 | INTRODUCTION

Graphene is a single layer of carbon atoms first isolated experimentally in 2004[1,2] which resulted in the awarding of the 2010 Nobel Prize in Physics to Geim[3] and Novoselov.[4] One of the noteworthy properties of graphene is that its plasmons are excited in the terahertz regime[5] which is of extraordinary interest to engineers. For a complete introduction to graphene including applications, modeling, and device design, we direct the interested reader to the survey article of Bludov et al[6] and the text of Goncalves and Peres.[7]

For this reason, the capability of simulating linear waves interacting with a periodic, layered structure with graphene present at the interfaces is supremely important in many branches of science and engineering. Examples, with or without graphene, are easy to find from acoustics (e.g., remote sensing,[8] nondestructive testing,[9] and underwater acoustics[10]), to electromagnetics (e.g., extraordinary optical transmission,[11] surface enhanced spectroscopy,[12] and surface plasmon resonance [SPR] biosensing[13,14]), to elastodynamics (e.g., full waveform inversion[15,16] and hazard assessment[17,18]). In regards to the SPR phenomena which arises in many areas of nanophotonics,[19–21] due to the strength of the plasmonic effect (the field enhancement can be several orders of magnitude) and its quite sensitive nature (the enhancement is typically only seen over a range of tens of nanometers), such simulations must be very robust and of high accuracy for applications of interest. For this reason, we have a particular interest in High-Order Spectral (HOS) algorithms[22–24] which deliver high fidelity solutions with great efficiency.

1.1 | Overview of numerical approaches

Engineers and scientists have used all of the classical numerical algorithms for the simulation of this problem (e.g., Finite Difference Methods,[25,26] Finite Element Methods,[27,28] Discontinuous Galerkin Methods,[29] Spectral Element Methods,[30] and Spectral Methods[22–24,31,32]). However, such *volumetric* approaches are greatly disadvantaged with an unnecessarily large number of unknowns for the piecewise homogeneous problems we consider here.

Surface methods can be orders of magnitude faster when compared to the volumetric algorithms discussed above primarily due to the greatly reduced number of degrees of freedom required to resolve a computation, in addition to the *exact* enforcement of far-field boundary conditions. Consequently, these approaches are an extremely important alternative and are becoming more widely used by practitioners. Paramount among these interfacial methods are those based upon Integral Equations (IEs),[33–42] however, these face difficulties. Most have been addressed in recent years through (i) the use of sophisticated quadrature rules to deliver HOS accuracy, (ii) the design of preconditioned iterative solvers with suitable acceleration,[43] and (iii) new strategies to avoid periodizing the Green function.[33,36,39] Consequently, they are a compelling alternative (see, e.g., the survey article of Ref. 42 for more details), however, two properties render them noncompetitive for the *parameterized* problems we consider as compared with the methods we advocate here:

1. For geometries specified by the real value ε (here the deviation of the interface shapes from flat), 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.
2. The dense, nonsymmetric positive definite systems of linear equations which must be inverted with each simulation.

As we advocated in Refs. 44, 45 a "High-Order Perturbation of Surfaces" (HOPS) approach can effectively address these concerns. More specifically, we argued for the method of Field Expansions (FE) which traces its roots to the low-order calculations of Rayleigh[46] and Rice.[47] The High-Order version was first investigated by Bruno and Reitich[48–51] and later enhanced and stabilized by the author and Reitich[52,53] with the method of Transformed Field Expansions (TFE). These formulations maintain the advantageous properties of classical IE formulations (e.g., surface formulation and exact enforcement of far-field conditions) while avoiding the shortcomings listed above:

1. As HOPS methods are built upon expansions in the deformation parameter, ε, once the Taylor coefficients are known for the scattering quantities, it is simply a matter of summing these (rather than beginning a new simulation) for any given choice of ε to recover the returns.
2. Due to the perturbative nature of the scheme, at every Taylor order one need only invert a single, sparse operator corresponding to the flat-interface, order-zero approximation of the problem.

Regardless of the strategy employed, the precise formulation of the problem can strongly influence the performance of any of these numerical methods. Of particular note, when there are internal layers present in the structure, a wise formulation will avoid the "Dirichlet eigenvalues" present for such domains. In short, if Dirichlet traces are used as data at these interfaces, "artificial" singularities can be introduced which are not exhibited by the full, coupled system. More specifically, many formulations utilize Dirichlet–Neumann Operators (DNOs) (e.g., Refs. 54–56) where one can *explicitly* compute layer thicknesses where the underlying Dirichlet problem delivers a nonunique solution. One approach to eliminating this artificial source of singularity is to utilize "Impedance–Impedance Operators" (IIOs) as advocated by Gillman et al.[54] On interior layers, these IIOs can be constructed to be unitary so that not only are their eigenvalues nonzero, they are restricted to the unit circle in the complex plane giving a very well-conditioned algorithm.[57,58]

1.2 | New contributions

In this publication, we demonstrate how a formulation of this layered media problem as a linear system of equations, $\mathbf{AV} = \mathbf{R}$, cf. (15), in terms of well-chosen IIOs can deliver a rigorous demonstration of the existence, uniqueness, and analyticity of solutions with respect to the interface deformation parameter ε, $\mathbf{V} = \sum_{n=0}^{\infty} \mathbf{V}_n \varepsilon^n$. More specifically, our problem statement includes surface currents at the layer interfaces which are often used to model the effects of graphene (or other two-dimensional materials).[59,60] By fortuitous combinations of the boundary conditions and identification of new unknowns (impedances), the problem is rewritten in terms of generic IIOs. This contrasts with the most natural strategy of using Dirichlet and Neumann traces as unknowns in the unmodified boundary conditions which, in turn, leads to the introduction of DNOs that may cease to exist due to Dirichlet eigenvalues of the governing equations. With a careful choice of *particular* IIOs, an existence, uniqueness, and analyticity theorem can be proven using the method of TFE[53,61]: Unique solutions $\mathbf{V}_n$ exist and satisfy the estimate $\|\mathbf{V}_n\|_{X^s} \leq CB^n$, cf. Theorem 2. This result is novel in the presence of surface currents and should not only be of interest to the community, but also points to a stable and highly accurate numerical algorithm. While the result can be definitively stated for the case of two layers and one interface in the absence of a surface current, for three or more layers, or in the presence of surface currents, a sequence of explicitly stated transcendental equations must all be nonzero to deduce the theorem. While this state of affairs is not ideal, the conditions are readily verified given a particular configuration.

Regarding the algorithm, we report on a numerical realization of our novel formulation complete with implementation details and a validation by the Method of Manufactured Solutions (MMS).[62–64] With this code we not only revisited a well-known simulation from the literature,[6] but also investigated a natural generalization which demonstrates compelling behavior which should be of interest to engineers designing sensing devices.

The rest of the paper is organized as follows: In Section 2, we recall the governing equations for scattering of linear waves by a laterally invariant periodic layered medium featuring surface currents in either Transverse Electric (TE) or Transverse Magnetic (TM) polarization, with a particular discussion of transparent boundary conditions in Section 2.1. In Section 3, we describe a nonoverlapping Domain Decomposition Method in terms of IIOs. The main existence, uniqueness, and analyticity theorem is stated and proven in Section 4. The key to this proof is the analysis of the linearized operator which is given in Section 5. We close with numerical results in Section 6. We give implementation details in Section 6.1, describe validation by the MMS in Section 6.2, and investigate graphene surface plasmons (GSPs) on single and double sheets of graphene in Section 6.3. We also describe details of our formulation in an extensive set of appendices. We compute the IIOs relevant to our considerations explicitly in the case of infinitesimal interface deformations in Appendix A (with particular reference to the upper, lower, and inner layers in Appendix Sections A.1, A.2, and A.3, respectively). The analyticity of the IIOs with respect to boundary perturbations is stated in Appendix B, while the analogous results for the magnitude of the normal vector and components of our linearized operator are given in Appendices C and D, respectively. We close with consideration of the particular cases of $M = 1$ interface (two layers) and $M = 2$ interfaces (three layers) in Appendices E and F, respectively.

2 | GOVERNING EQUATIONS

We now generalize the two-layer formulation of our problem found in Ref. 56 by considering a multiply layered, y-invariant, medium with M interfaces at

$$z = a^{(m)} + g^{(m)}(x), \quad 1 \leq m \leq M,$$

which are d-periodic

$$g^{(m)}(x + d) = g^{(m)}(x), \quad 1 \leq m \leq M,$$

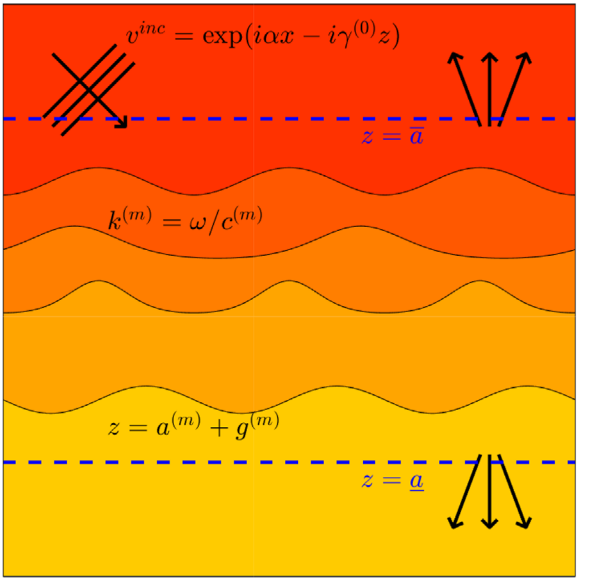


FIGURE 1 Five-layer problem configuration with layer interfaces $z = a^{(m)} + g^{(m)}(x)$, and artificial boundaries $z = \overline{a}$ and $z = \underline{a}$

separating $(M+1)$-many layers which define the domains

$$S^{(0)} := \{(x,z) | z > a^{(1)} + g^{(1)}(x)\},$$
$$S^{(m)} := \{(x,z) | a^{(m+1)} + g^{(m+1)}(x) < z < a^{(m)} + g^{(m)}(x)\}, \qquad 1 \le m \le M-1,$$
$$S^{(M)} := \{(x,z) | z < a^{(M)} + g^{(M)}(x)\},$$

with (upward pointing) normals

$$N^{(m)} := (-\partial_x g^{(m)}(x), 1)^T, \quad 1 \le m \le M;$$

see Figure 1.

The $(M+1)$ domains are filled with homogeneous materials of permittivities $\epsilon^{(m)}$ $(0 \le m \le M)$ where the uppermost layer must be a dielectric so that $\epsilon^{(0)} \in \mathbf{R}^+$. We assume that polarized monochromatic plane-wave radiation of incidence angle θ, frequency ω, and wavenumber $k^{(0)} = \sqrt{\epsilon^{(0)}} k_0$, $k_0 := \omega/c_0$ (c_0 is the speed of light), illuminates the structure from above

$$\underline{v}^{\text{inc}} = e^{i(-\omega t + \alpha x - \gamma^{(0)} z)}, \quad \alpha = k^{(0)} \sin(\theta), \quad \gamma^{(0)} = k^{(0)} \cos(\theta).$$

It is straightforward to generalize the governing equations derived in Ref. 56 to $(M+1)$ many layers by choosing as unknowns, $v^{(m)}(x,z)$, the laterally quasiperiodic

$$v^{(m)}(x+d, z) = e^{i\alpha d} v^{(m)}(x,z), \quad 0 \le m \le M, \tag{1}$$

transverse components of either the electric or magnetic fields. These reduced fields satisfy the Helmholtz equations

$$\Delta v^{(m)} + \epsilon^{(m)} k_0^2 v^{(m)} = 0, \quad \text{in } S^{(m)}, \quad 0 \le m \le M, \tag{2}$$

where $k^{(m)} = \sqrt{\epsilon^{(m)}} k_0$, which are coupled through the Dirichlet and Neumann boundary conditions at $z = a^{(m)} + g^{(m)}(x)$, $1 \leq m \leq M$,

$$v^{(m-1)} - v^{(m)} + \left|N^{(m)}\right|^{-1} p^{(m)} \tau^{(m)} \partial_{N^{(m)}} v^{(m)} = \xi^{(m)}, \tag{3a}$$

$$\tau^{(m-1)} \partial_{N^{(m)}} v^{(m-1)} - \tau^{(m)} \partial_{N^{(m)}} v^{(m)} + \left|N^{(m)}\right| s^{(m)} v^{(m)} = \tau^{(m-1)} \nu^{(m)}, \tag{3b}$$

where for TE or s and TM or p polarizations,

$$\tau^{(m)} = \begin{cases} 1, & \text{TE}, \\ 1/\epsilon_m, & \text{TM}, \end{cases} \quad s^{(m)} = \begin{cases} i k_0 \hat{\sigma}^{(m)}, & \text{TE}, \\ 0, & \text{TM}, \end{cases} \quad p^{(m)} = \begin{cases} 0, & \text{TE}, \\ \hat{\sigma}^{(m)}/(i k_0), & \text{TM}, \end{cases}$$

and

$$\begin{aligned} \xi^{(1)}(x) &:= -v^{\text{inc}}(x, a^{(1)} + g^{(1)}(x)) \\ &= -e^{i(\alpha x - \gamma^{(0)}(a^{(1)} + g^{(1)}(x)))}, \end{aligned} \tag{3c}$$

$$\begin{aligned} \nu^{(1)}(x) &:= -\left[\partial_{N^{(1)}} v^{\text{inc}}(x, z)\right]_{z = a^{(1)} + g^{(1)}(x)} \\ &= \left(i\gamma^{(0)} + (i\alpha)\partial_x g^{(1)}\right) e^{i(\alpha x - \gamma^{(0)}(a^{(1)} + g^{(1)}(x)))}. \end{aligned} \tag{3d}$$

In our model, we will enforce that $\xi^{(m)} \equiv \nu^{(m)} \equiv 0$ $(2 \leq m \leq M)$, however, as we see, it is no impediment to the method if we set these to any nonzero function. We point out the nondimensional surface currents $\hat{\sigma}^{(m)}$ which will be used to model the presence of a two-dimensional material.[59,60]

Remark 1. The correct modeling of the electromagnetic properties of graphene is still an open question . Many choices can reasonably be made for the surface current to accurately emulate the presence of a graphene sheet, and for this we choose a Drude model[6,7] of the form

$$\hat{\sigma}_D = \frac{\sigma_D}{\epsilon_0 c_0}, \quad \sigma_D = \sigma_0 \left(\frac{4E_F}{\pi}\right) \frac{1}{\hbar\gamma - i\hbar\omega}, \quad \sigma_0 = \frac{\pi e^2}{2h}, \tag{4}$$

where $e < 0$ is the electron charge, γ is the relaxation rate, and $E_F > 0$ is the (local) Fermi level position. For instance, in Ref. 6 the authors chose values $E_F = 0.45$ eV and $\Gamma := \hbar\gamma = 2.6$ meV.

2.1 | Transparent boundary conditions

Regarding far-field boundary conditions, we choose the upward/downward propagating wave conditions (UPC/DPC).[65] For this, we introduce the planes

$$z = \overline{a} > a^{(1)} + \left|g^{(1)}\right|_{L^\infty}, \quad z = \underline{a} < a^{(M)} - \left|g^{(M)}\right|_{L^\infty},$$

define the domains

$$\overline{S} := \{z > \overline{a}\}, \quad \underline{S} := \{z < \underline{a}\},$$

and note that we can find unique quasiperiodic solutions of the relevant Helmholtz problems on each of these domains given generic Dirichlet data, say $\phi(x)$ and $\mu(x)$. For this, we use the Rayleigh expansions[46] which state that

$$v^{(0)}(x,z) = \sum_{p=-\infty}^{\infty} \hat{\phi}_p e^{i\alpha_p x + i\gamma_p^{(0)}(z-\overline{a})}, \qquad \text{in } \overline{S},$$

$$v^{(M)}(x,z) = \sum_{p=-\infty}^{\infty} \hat{\mu}_p e^{i\alpha_p x - i\gamma_p^{(M)}(z-\underline{a})}, \qquad \text{in } \underline{S},$$

where

$$\hat{\phi}_p = \frac{1}{d}\int_0^d \phi(x) e^{-i\alpha_p x}\, dx$$

for $p \in \mathbf{Z}$, $m \in \{0, \dots, M\}$,

$$\alpha_p := \alpha + \left(\frac{2\pi}{d}\right)p, \quad \gamma_p^{(m)} := \sqrt{\epsilon^{(m)}k_0^2 - \alpha_p^2}, \quad \mathrm{Im}\left\{\gamma_p^{(m)}\right\} \geq 0.$$

We note that if $\epsilon^{(m)} \in \mathbf{R}^+$ then

$$\gamma_p^{(m)} := \begin{cases} \sqrt{\epsilon^{(m)}k_0^2 - \alpha_p^2}, & p \in \mathcal{U}^{(m)}, \\ i\sqrt{\alpha_p^2 - \epsilon^{(m)}k_0^2}, & p \notin \mathcal{U}^{(m)}, \end{cases}$$

and the set of propagating modes is

$$\mathcal{U}^{(m)} := \left\{p \in \mathbf{Z} \mid \alpha_p^2 \leq \epsilon^{(m)}k_0^2\right\}.$$

We point out that

$$v^{(0)}(x,\overline{a}) = \sum_{p=-\infty}^{\infty} \hat{\phi}_p e^{i\alpha_p x} = \phi(x),$$

$$v^{(M)}(x,\underline{a}) = \sum_{p=-\infty}^{\infty} \hat{\mu}_p e^{i\alpha_p x} = \mu(x).$$

With these formulas, we can compute the *outward-pointing*Neumann data at the artificial boundaries

$$-\partial_z v^{(0)}(x,\overline{a}) = \sum_{p=-\infty}^{\infty} -(i\gamma_p^{(0)})\hat{\phi}_p e^{i\alpha_p x} =: T^{(0)}[\phi(x)],$$

$$\partial_z v^{(M)}(x,\underline{a}) = \sum_{p=-\infty}^{\infty} (-i\gamma_p^{(M)})\hat{\mu}_p e^{i\alpha_p x} =: T^{(M)}[\mu(x)],$$

which define the order-one Fourier multipliers, $\{T^{(0)}, T^{(M)}\}$.

With these operators, it is not difficult to see that quasiperiodic, upward propagating solutions to the Helmholtz equation

$$\Delta v^{(0)} + \epsilon^{(0)} k_0^2 v^{(0)} = 0, \quad z > a^{(1)} + g^{(1)}(x),$$

equivalently solve

$$\Delta v^{(0)} + \epsilon^{(0)} k_0^2 v^{(0)} = 0, \qquad a^{(1)} + g^{(1)}(x) < z < \overline{a}, \tag{5a}$$

$$\partial_z v^{(0)} + T^{(0)}[v^{(0)}] = 0, \qquad z = \overline{a}. \tag{5b}$$

Similarly, one can show that quasiperiodic, downward propagating solutions to the Helmholtz equation

$$\Delta v^{(M)} + \epsilon^{(M)} k_0^2 v^{(M)} = 0, \quad z < a^{(M)} + g^{(M)}(x),$$

equivalently solve

$$\Delta v^{(M)} + \epsilon^{(M)} k_0^2 v^{(M)} = 0, \qquad \underline{a} < z < a^{(M)} + g^{(M)}(x), \tag{6a}$$

$$\partial_z v^{(M)} - T^{(M)}[v^{(M)}] = 0, \qquad z = \underline{a}. \tag{6b}$$

Remark 2. We point out that the conditions (5b) and (6b) specify solutions which satisfy the UPC and DPC of definition 2.6 in Arens.[65] It is these two conditions which guarantee the uniqueness of solutions on the unbounded domains $\{z > \overline{a}\}$ and $\{z < \underline{a}\}$.

3 | A NONOVERLAPPING DOMAIN DECOMPOSITION METHOD

There are many equivalent formulations of our governing equations, (1), (2), (3), (5b), and (6b), but several classical approaches contain unnecessary flaws which we would prefer to avoid. In particular, when utilizing a nonoverlapping Domain Decomposition Method, as we choose to do here, one must be careful to select interface unknowns which do not induce needless singularities. Principally what we have in mind are the "Dirichlet eigenvalues" which arise when Dirichlet data are selected as a boundary unknown on an interior layer. To fix this, we follow the lead of Després[58,66–68] by pursuing IIOs which can be constructed to exist at all values of $k^{(m)}$.

To begin, we consider the order-r Fourier multiplier operators, $\{Y^{(m)}, Z^{(m)}\}$,

$$Y^{(m)}[\phi] := \sum_{p=-\infty}^{\infty} Y_p^{(m)} \hat{\phi}_p e^{i\alpha_p x}, \quad Z^{(m)}[\phi] := \sum_{p=-\infty}^{\infty} Z_p^{(m)} \hat{\phi}_p e^{i\alpha_p x},$$

$$\left|Y_p^{(m)}\right|, \left|Z_p^{(m)}\right| \sim \left(1 + |p|^2\right)^{r/2}, \quad r \in \{0, 1\},$$

acting on the generic function $\phi(x)$ with (generalized) Fourier coefficients $\hat{\phi}_p$ defined in Section 2.1, and rearrange the boundary conditions (3) by the matrices

$$P^{(m)} := \begin{pmatrix} -Y^{(m)} & -I \\ Z^{(m)} & -I \end{pmatrix}.$$

These we require to be invertible (so that all steps can be reversed) which can be accomplished by insisting that $(Y^{(m)} + Z^{(m)})$ be invertible.

Applying the operators $P^{(m)}$ to (3) and changing to the new set of (impedance) unknowns

$$\begin{aligned}
U^{(m),\ell}(x) &:= -\tau^{(m)} \partial_{N^{(m+1)}} v^{(m)} - Y^{(m+1)}[v^{(m)}], && 0 \le m \le M-1, \\
U^{(m),u}(x) &:= \tau^{(m)} \partial_{N^{(m)}} v^{(m)} - Z^{(m)}[v^{(m)}], && 1 \le m \le M, \\
\tilde{U}^{(m),\ell}(x) &:= -\tau^{(m)} \partial_{N^{(m+1)}} v^{(m)} + Z^{(m+1)}[v^{(m)}], && 0 \le m \le M-1, \\
\tilde{U}^{(m),u}(x) &:= \tau^{(m)} \partial_{N^{(m)}} v^{(m)} + Y^{(m)}[v^{(m)}], && 1 \le m \le M,
\end{aligned}$$

the equations, (3), become

$$U^{(m-1),\ell} + \tilde{U}^{(m),u} + F^{(m)} U^{(m),u} + \tilde{F}^{(m)} \tilde{U}^{(m),u} = \zeta^{(m)}, \qquad 1 \le m \le M, \tag{7a}$$

$$\tilde{U}^{(m-1),\ell} + U^{(m),u} + G^{(m)} U^{(m),u} + \tilde{G}^{(m)} \tilde{U}^{(m),u} = \psi^{(m)}, \qquad 1 \le m \le M. \tag{7b}$$

In these

$$\begin{aligned}
\zeta^{(m)}(x) &:= -\tau^{(m-1)} \nu^{(m)} - Y^{(m)}[\xi^{(m)}], && 1 \le m \le M, \\
\psi^{(m)}(x) &:= -\tau^{(m-1)} \nu^{(m)} + Z^{(m)}[\xi^{(m)}], && 1 \le m \le M,
\end{aligned}$$

and

$$F^{(m)} := -Y^{(m)} \left[p^{(m)} \left| N^{(m)} \right|^{-1} Y^{(m)} + s^{(m)} \left| N^{(m)} \right| I \right] (Y^{(m)} + Z^{(m)})^{-1}, \tag{8a}$$

$$\tilde{F}^{(m)} := -Y^{(m)} \left[p^{(m)} \left| N^{(m)} \right|^{-1} Z^{(m)} - s^{(m)} \left| N^{(m)} \right| I \right] (Y^{(m)} + Z^{(m)})^{-1}, \tag{8b}$$

$$G^{(m)} := Z^{(m)}\left[p^{(m)}\left|N^{(m)}\right|^{-1}Y^{(m)} + s^{(m)}\left|N^{(m)}\right|I\right](Y^{(m)} + Z^{(m)})^{-1}, \tag{8c}$$

$$\tilde{G}^{(m)} := Z^{(m)}\left[p^{(m)}\left|N^{(m)}\right|^{-1}Z^{(m)} - s^{(m)}\left|N^{(m)}\right|I\right](Y^{(m)} + Z^{(m)})^{-1}. \tag{8d}$$

We can simplify these equations with the introduction of suitable surface integral operators, in this case IIOs.

Definition 1. Given an integer $s \geq 0$ and any $\delta > 0$, if $g^{(1)} \in C^{s+3/2+\delta}$ then, for order-r ($r = 0, 1$) Fourier multipliers $\{Y^{(1)}, Z^{(1)}\}$, if a unique quasiperiodic solution exists of

$$\Delta v^{(0)} + \epsilon^{(0)} k_0^2 v^{(0)} = 0, \qquad a^{(1)} + g^{(1)} < z < \overline{a}, \tag{9a}$$

$$\partial_z v^{(0)} + T^{(0)}[v^{(0)}] = 0, \qquad z = \overline{a}, \tag{9b}$$

$$-\tau^{(0)}\partial_{N^{(1)}} v^{(0)} - Y^{(1)} v^{(0)} = U^{(0),\ell}, \qquad z = a^{(1)} + g^{(1)}, \tag{9c}$$

we define the Upper IIO

$$Q[U^{(0),\ell}] = Q(\overline{a}, a^{(1)}, g^{(1)})[U^{(0),\ell}] := \tilde{U}^{(0),\ell} = -\tau^{(0)}\partial_{N^{(1)}} v^{(0)} + Z^{(1)} v^{(0)}. \tag{10}$$

Definition 2. Given an integer $s \geq 0$ and any $\delta > 0$, if $g^{(M)} \in C^{s+3/2+\delta}$ then, for order-r ($r = 0, 1$) Fourier multipliers $\{Y^{(M)}, Z^{(M)}\}$, if a unique quasiperiodic solution exists of

$$\Delta v^{(M)} + \epsilon^{(M)} k_0^2 v^{(M)} = 0, \qquad \underline{a} < z < a^{(M)} + g^{(M)}, \tag{11a}$$

$$\tau^{(M)}\partial_{N^{(M)}} v^{(M)} - Z^{(M)} v^{(M)} = U^{(M),u}, \qquad z = a^{(M)} + g^{(M)}, \tag{11b}$$

$$\partial_z v^{(M)} - T^{(M)}[v^{(M)}] = 0, \qquad z = \underline{a}, \tag{11c}$$

we define the Lower IIO

$$S[U^{(M),u}] = S(\underline{a}, a^{(M)}, g^{(M)})[U^{(M),u}] := \tilde{U}^{(M),u} = \tau^{(M)}\partial_{N^{(M)}} v^{(M)} + Y^{(M)} v^{(M)}. \tag{12}$$

Definition 3. Given an integer $s \geq 0$ and any $\delta > 0$, if $g^{(m)}, g^{(m+1)} \in C^{s+3/2+\delta}$ then, for order-r ($r = 0, 1$) Fourier multipliers $\{Y^{(m)}, Y^{(m+1)}, Z^{(m)}, Z^{(m+1)}\}$, if a unique quasiperiodic solution exists of

$$\Delta v^{(m)} + \epsilon^{(m)} k_0^2 v^{(m)} = 0, \qquad a^{(m+1)} + g^{(m+1)} < z < a^{(m)} + g^{(m)}, \tag{13a}$$

$$\tau^{(m)}\partial_{N^{(m)}}v^{(m)} - Z^{(m)}v^{(m)} = U^{(m),u}, \qquad z = a^{(m)} + g^{(m)}, \tag{13b}$$

$$-\tau^{(m)}\partial_{N^{(m+1)}}v^{(m)} - Y^{(m+1)}v^{(m)} = U^{(m),\ell}, \qquad z = a^{(m+1)} + g^{(m+1)}, \tag{13c}$$

we define an Inner IIO

$$\begin{aligned} R^{(m)}\left[\begin{pmatrix} U^{(m),u} \\ U^{(m),\ell} \end{pmatrix}\right] &= R^{(m)}(a^{(m)}, g^{(m)}, a^{(m+1)}, g^{(m+1)})\left[\begin{pmatrix} U^{(m),u} \\ U^{(m),\ell} \end{pmatrix}\right] \\ &= \begin{pmatrix} R^{(m),uu} & R^{(m),u\ell} \\ R^{(m),\ell u} & R^{(m),\ell\ell} \end{pmatrix}\left[\begin{pmatrix} U^{(m),u} \\ U^{(m),\ell} \end{pmatrix}\right] \\ &:= \begin{pmatrix} \tilde{U}^{(m),u} \\ \tilde{U}^{(m),\ell} \end{pmatrix} = \begin{pmatrix} \tau^{(m)}\partial_{N^{(m)}}v^{(m)} + Y^{(m)}v^{(m)} \\ -\tau^{(m)}\partial_{N^{(m+1)}}v^{(m)} + Z^{(m+1)}v^{(m)} \end{pmatrix}. \end{aligned} \tag{14}$$

Remark 3. For use in Section 5 we describe, in Appendix A, formulas for these IIOs when the grating interfaces are *infinitesimal* which we model by quasiperiodic solutions in the case $g^{(m)} \equiv 0$. Furthermore, for use in Section 4 we state analyticity properties of these IIOs in Appendix B.

Remark 4. As far as we are aware, it is still an open problem to determine which particular choices of operators $\{Y^{(m)}, Z^{(m)}\}$ deliver unique solutions. However, it is known that if

$$\operatorname{Im}\left\{\int_0^d (Y^{(m)}\varphi)\overline{\varphi}\,dx\right\} > 0, \quad \operatorname{Im}\left\{\int_0^d (Z^{(m)}\varphi)\overline{\varphi}\,dx\right\} > 0,$$

then (9), (11), and (13) are well-posed (see, e.g.,[58]). However, we will provide more precise and readily verified, though more complicated, characterizations in (A1), (A3), and (A7).

In terms of this notation the boundary conditions, (7), become

$$\begin{aligned} &U^{(m-1),\ell} + F^{(m)}U^{(m),u} + (I + \tilde{F}^{(m)})\{R^{(m),uu}[U^{(m),u}] + R^{(m),u\ell}[U^{(m),\ell}]\} \\ &\quad = \zeta^{(m)}, \quad 1 \le m \le M-1, \\ &U^{(M-1),\ell} + F^{(M)}U^{(M),u} + (I + \tilde{F}^{(M)})S[U^{(M),u}] = \zeta^{(M)}, \end{aligned}$$

and

$$\begin{aligned} &Q[U^{(0),\ell}] + (I + G^{(1)})U^{(1),u} + \tilde{G}^{(1)}(R^{(1),uu}[U^{(1),u}] + R^{(1),u\ell}[U^{(1),\ell}]) = \psi^{(1)}, \\ &R^{(m-1),\ell u}[U^{(m-1),u}] + R^{(m-1),\ell\ell}[U^{(m-1),\ell}] + (I + G^{(m)})U^{(m),u} \\ &\quad + \tilde{G}^{(m)}(R^{(m),uu}[U^{(m),u}] + R^{(m),u\ell}[U^{(m),\ell}]) = \psi^{(m)}, \quad 2 \le m \le M-1, \\ &R^{(M-1),\ell u}[U^{(M-1),u}] + R^{(M-1),\ell\ell}[U^{(M-1),\ell}] + (I + G^{(M)})U^{(M),u} \\ &\quad + \tilde{G}^{(M)}S[U^{(M),u}] = \psi^{(M)}. \end{aligned}$$

We write this more compactly as

$$\mathbf{A}\mathbf{V} = \mathbf{R}, \tag{15}$$

where

$$\mathbf{V} := \begin{pmatrix} U^{(0),\ell} \\ U^{(1),u} \\ U^{(1),\ell} \\ \vdots \\ U^{(M-1),u} \\ U^{(M-1),\ell} \\ U^{(M),u} \end{pmatrix}, \quad \mathbf{R} := \begin{pmatrix} \zeta^{(1)} \\ \psi^{(1)} \\ \vdots \\ \zeta^{(M)} \\ \psi^{(M)} \end{pmatrix}.$$

Also

$$\mathbf{A} = \begin{pmatrix} \mathbf{D}^{(1)} & \mathbf{U}^{(1)} & 0 & 0 & \cdots & 0 \\ \mathbf{L}^{(2)} & \mathbf{D}^{(2)} & \mathbf{U}^{(2)} & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & 0 & 0 \\ 0 & 0 & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \mathbf{L}^{(M-1)} & \mathbf{D}^{(M-1)} & \mathbf{U}^{(M-1)} \\ 0 & \cdots & 0 & 0 & \mathbf{L}^{(M)} & \mathbf{D}^{(M)} \end{pmatrix}, \tag{16a}$$

where

$$\mathbf{U}^{(m)} = \begin{pmatrix} (I + \tilde{F}^{(m)})R^{(m),u\ell} & 0 \\ \tilde{G}^{(m)}R^{(m),u\ell} & 0 \end{pmatrix}, \quad 1 \le m \le M-1, \tag{16b}$$

and

$$\mathbf{L}^{(m)} = \begin{pmatrix} 0 & 0 \\ 0 & R^{(m-1),\ell u} \end{pmatrix}, \quad 2 \le m \le M, \tag{16c}$$

and

$$\mathbf{D}^{(1)} = \begin{pmatrix} I & F^{(1)} + (I + \tilde{F}^{(1)})R^{(1),uu} \\ Q & (I + G^{(1)}) + \tilde{G}^{(1)}R^{(1),uu} \end{pmatrix}, \tag{16d}$$

$$\mathbf{D}^{(m)} = \begin{pmatrix} I & F^{(m)} + (I + \tilde{F}^{(m)})R^{(m),uu} \\ R^{(m-1),\ell\ell} & (I + G^{(m)}) + \tilde{G}^{(m)}R^{(m),uu} \end{pmatrix}, \qquad 2 \le m \le M-1, \tag{16e}$$

$$\mathbf{D}^{(M)} = \begin{pmatrix} I & F^{(M)} + (I + \tilde{F}^{(M)})S \\ R^{(M-1),\ell\ell} & (I + G^{(M)}) + \tilde{G}^{(M)}S \end{pmatrix}. \tag{16f}$$

4 | ANALYTICITY OF SOLUTIONS

We pursue the existence, uniqueness, and analyticity of solutions of our governing equations, (15), by a perturbative approach. For this, we will demonstrate that the operator, $\mathbf{A}$, and data, $\mathbf{R}$, are analytic with respect to interface deformations, $g^{(m)}$, and use the regular perturbation theory outlined in Ref. 55 to establish the analyticity of $\mathbf{V}$. More precisely, if we assume that

$$g^{(m)}(x) = \varepsilon f^{(m)}(x), \quad 1 \leq m \leq M,$$

for ε sufficiently small and $f^{(m)}$ smooth enough (at least $C^{3/2+\delta}$ for any $\delta > 0$; see Theorem 2), view (15) as

$$\mathbf{A}(\varepsilon)\mathbf{V}(\varepsilon) = \mathbf{R}(\varepsilon) \tag{17}$$

show that $\mathbf{A}$ and $\mathbf{R}$ are analytic with respect to ε so that

$$\mathbf{A}(\varepsilon) = \sum_{n=0}^{\infty} \mathbf{A}_n \varepsilon^n, \quad \mathbf{R}(\varepsilon) = \sum_{n=0}^{\infty} \mathbf{R}_n \varepsilon^n,$$

then we can seek a solution

$$\mathbf{V} = \mathbf{V}(\varepsilon) = \sum_{n=0}^{\infty} \mathbf{V}_n \varepsilon^n, \tag{18}$$

which will be shown to converge strongly in an appropriate function space. Upon insertion of (18) into (17) we find, at order $\mathcal{O}(\varepsilon^n)$,

$$\mathbf{A}_0 \mathbf{V}_n = \mathbf{R}_n - \sum_{\ell=0}^{n-1} \mathbf{A}_{n-\ell} \mathbf{V}_\ell,$$

or

$$\mathbf{V}_n = \mathbf{A}_0^{-1} \left[\mathbf{R}_n - \sum_{\ell=0}^{n-1} \mathbf{A}_{n-\ell} \mathbf{V}_\ell \right]. \tag{19}$$

For this, we take advantage of the fact that the IIOs introduced above depend analytically upon ε provided that the $f^{(m)}$ are smooth enough. These assertions are made more concrete in the theorems presented in Appendix B.

In regard to Equation (15) it is not difficult to show that

$$\mathbf{R}_n = \begin{pmatrix} \zeta_n^{(1)} \\ \psi_n^{(1)} \\ \vdots \\ \zeta_n^{(M)} \\ \psi_n^{(M)} \end{pmatrix}, \tag{20}$$

where

$$\zeta_n^{(1)}(x) = -\tau^{(0)}\nu_n^{(1)} - Y^{(1)}\left[\xi_n^{(1)}\right],$$

$$\psi_n^{(1)}(x) = -\tau^{(0)}\nu_n^{(1)} + Z^{(1)}\left[\xi_n^{(1)}\right],$$

and $\zeta^{(m)} \equiv \psi^{(m)} \equiv 0$, $2 \le m \le M$. In these

$$\xi_n^{(1)}(x) = -e^{i(\alpha x - \gamma^{(0)}a^{(1)})}(-i\gamma^{(0)})^n \frac{\left(f^{(1)}(x)\right)^n}{n!},$$

$$\nu_n^{(1)}(x) = (i\gamma^{(0)})\xi_n^{(1)}(x) + (i\alpha)(\partial_x f)\xi_{n-1}^{(1)},$$

and $\xi_{-1}^{(1)} \equiv 0$. In addition

$$\mathbf{A}_n = \begin{pmatrix} \mathbf{D}_n^{(1)} & \mathbf{U}_n^{(1)} & 0 & 0 & \cdots & 0 \\ \mathbf{L}_n^{(2)} & \mathbf{D}_n^{(2)} & \mathbf{U}_n^{(2)} & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & 0 & 0 \\ 0 & 0 & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \mathbf{L}_n^{(M-1)} & \mathbf{D}_n^{(M-1)} & \mathbf{U}_n^{(M-1)} \\ 0 & \cdots & 0 & 0 & \mathbf{L}_n^{(M)} & \mathbf{D}_n^{(M)} \end{pmatrix}, \tag{21}$$

where, for $n = 0$,

$$\mathbf{U}_0^{(m)} = \begin{pmatrix} \left(I + \tilde{F}_0^{(m)}\right)R_0^{(m),u\ell} & 0 \\ \tilde{G}_0^{(m)}R_0^{(m),u\ell} & 0 \end{pmatrix}, \qquad 1 \le m \le M-1, \tag{22a}$$

$$\mathbf{L}_0^{(m)} = \begin{pmatrix} 0 & 0 \\ 0 & R_0^{(m-1),\ell u} \end{pmatrix}, \qquad 2 \le m \le M, \tag{22b}$$

$$\mathbf{D}_0^{(1)} = \begin{pmatrix} I & F_0^{(1)} + \left(I + \tilde{F}_0^{(1)}\right)R_0^{(1),uu} \\ Q_0 & \left(I + G_0^{(1)}\right) + \tilde{G}_0^{(1)}R_0^{(1),uu} \end{pmatrix}, \tag{22c}$$

$$\mathbf{D}_0^{(m)} = \begin{pmatrix} I & F_0^{(m)} + \left(I + \tilde{F}_0^{(m)}\right)R_0^{(m),uu} \\ R_0^{(m-1),\ell\ell} & \left(I + G_0^{(m)}\right) + \tilde{G}_0^{(m)}R_0^{(m),uu} \end{pmatrix}, \qquad 2 \le m \le M-1, \tag{22d}$$

$$\mathbf{D}_0^{(M)} = \begin{pmatrix} I & F_0^{(M)} + \left(I + \tilde{F}_0^{(M)}\right)S_0 \\ R_0^{(M-1),\ell\ell} & \left(I + G_0^{(M)}\right) + \tilde{G}_0^{(M)}S_0 \end{pmatrix}, \tag{22e}$$

and

$$F_0^{(m)} := -Y^{(m)}[p^{(m)}Y^{(m)} + s^{(m)}](Y^{(m)} + Z^{(m)})^{-1}, \tag{23a}$$

$$\tilde{F}_0^{(m)} := -Y^{(m)}[p^{(m)}Z^{(m)} - s^{(m)}](Y^{(m)} + Z^{(m)})^{-1}, \tag{23b}$$

$$G_0^{(m)} := Z^{(m)}[p^{(m)}Y^{(m)} + s^{(m)}](Y^{(m)} + Z^{(m)})^{-1}, \tag{23c}$$

$$\tilde{G}_0^{(m)} := Z^{(m)}[p^{(m)}Z^{(m)} - s^{(m)}](Y^{(m)} + Z^{(m)})^{-1}. \tag{23d}$$

Meanwhile, for $n > 0$,

$$\mathbf{U}_n^{(m)} = \begin{pmatrix} R_n^{(m),u\ell} & 0 \\ 0 & 0 \end{pmatrix} + \sum_{q=0}^{n} \begin{pmatrix} \tilde{F}_{n-q}^{(m)} R_q^{(m),u\ell} & 0 \\ \tilde{G}_{n-q}^{(m)} R_q^{(m),u\ell} & 0 \end{pmatrix}, \qquad 1 \le m \le M-1, \tag{24a}$$

$$\mathbf{L}_n^{(m)} = \begin{pmatrix} 0 & 0 \\ 0 & R_n^{(m-1),\ell u} \end{pmatrix}, \qquad 2 \le m \le M, \tag{24b}$$

$$\mathbf{D}_n^{(1)} = \begin{pmatrix} 0 & F_n^{(1)} + R_n^{(1),uu} \\ Q_n & G_n^{(1)} \end{pmatrix} + \sum_{q=0}^{n} \begin{pmatrix} 0 & \tilde{F}_{n-q}^{(1)} R_q^{(1),uu} \\ 0 & \tilde{G}_{n-q}^{(1)} R_q^{(1),uu} \end{pmatrix}, \tag{24c}$$

$$\mathbf{D}_n^{(m)} = \begin{pmatrix} 0 & F_n^{(m)} + R_n^{(m),uu} \\ R_n^{(m-1),\ell\ell} & G_n^{(m)} \end{pmatrix} + \sum_{q=0}^{n} \begin{pmatrix} 0 & \tilde{F}_{n-q}^{(m)} R_q^{(m),uu} \\ 0 & \tilde{G}_{n-q}^{(m)} R_q^{(m),uu} \end{pmatrix}, \qquad 2 \le m \le M-1, \tag{24d}$$

$$\mathbf{D}_n^{(M)} = \begin{pmatrix} 0 & F_n^{(M)} + S_n \\ R_n^{(M-1),\ell\ell} & G_n^{(M)} \end{pmatrix} + \sum_{q=0}^{n} \begin{pmatrix} 0 & \tilde{F}_{n-q}^{(M)} S_q \\ 0 & \tilde{G}_{n-q}^{(M)} S_q \end{pmatrix}, \tag{24e}$$

where, from (8),

$$F_n^{(m)} := -Y^{(m)}\left[p^{(m)}\left|N^{(m)}\right|_n^{-1} Y^{(m)} + s^{(m)}\left|N^{(m)}\right|_n\right](Y^{(m)} + Z^{(m)})^{-1}, \tag{25a}$$

$$\tilde{F}_n^{(m)} := -Y^{(m)}\left[p^{(m)}\left|N^{(m)}\right|_n^{-1} Z^{(m)} - s^{(m)}\left|N^{(m)}\right|_n\right](Y^{(m)} + Z^{(m)})^{-1}, \tag{25b}$$

$$G_n^{(m)} := Z^{(m)}\left[p^{(m)}\left|N^{(m)}\right|_n^{-1} Y^{(m)} + s^{(m)}\left|N^{(m)}\right|_n\right](Y^{(m)} + Z^{(m)})^{-1}, \tag{25c}$$

$$\tilde{G}_n^{(m)} := Z^{(m)}\left[p^{(m)}\left|N^{(m)}\right|_n^{-1} Z^{(m)} - s^{(m)}\left|N^{(m)}\right|_n\right](Y^{(m)} + Z^{(m)})^{-1}, \tag{25d}$$

and the forms for $|N^{(m)}|_n$ and $|N^{(m)}|_n^{-1}$ are given in (C1) and (C2), respectively.
The relevant result from Ref. 55 states the following.

Theorem 1. *Given two Banach spaces X and Y, suppose that:*

1. $\mathbf{R}_n \in Y$ *for all* $n \geq 0$, *and there exist constants* $C_R > 0$, $B_R > 0$ *such that*

$$\|\mathbf{R}_n\|_Y \leq C_R B_R^n.$$

2. $\mathbf{A}_n : X \to Y$ *for all* $n \geq 0$, *and there exist constants* $C_A > 0$, $B_A > 0$ *such that*

$$\|\mathbf{A}_n\|_{X \to Y} \leq C_A B_A^n,$$

where $\|\cdot\|_{X\to Y}$ *is the operator norm.*

3. $\mathbf{A}_0^{-1} : Y \to X$, *and there exists a constant* $C_e > 0$ *such that*

$$\left\|\mathbf{A}_0^{-1}\right\|_{Y \to X} \leq C_e.$$

Then, Equation (17) has a unique solution, (18), and there exist constants $C_V > 0$ and $B_V > 0$ such that

$$\|\mathbf{V}_n\|_X \leq C_V B_V^n \tag{26}$$

for all $n \geq 0$ and any

$$C_V \geq 2 C_e C_R, \quad B_V \geq \max\{B_R, 2B_A, 4C_e C_A B_A\}.$$

This implies that, for any $0 \leq \rho < 1$, (18), converges for all ε such that $B\varepsilon < \rho$, that is, $\varepsilon < \rho/B$.

To begin, we recall the classical L^2-based Sobolev classes of d-periodic *surface* functions with s-many weak derivatives ($s \geq 0$)[69,70]

$$H^s(d) := \left\{\xi(x) \in L^2(d) \mid \|\xi\|_{H^s} < \infty\right\},$$

where

$$\|\xi\|_{H^s}^2 = \sum_{p=-\infty}^{\infty} \left|\hat{\xi}_p\right|^2 \langle p \rangle^{2s}, \quad \langle p \rangle^2 := 1 + |p|^2.$$

These spaces can be defined for $s < 0$ by specifying that H^{-s} be the dual of H^s.[69,70] In addition, we remember, for integer $s \geq 0$, the space $C^s(d)$ of continuous functions with s-many continuous derivatives. If s is not an integer then these refer to the classical Hölder spaces.[69,71] We will also require the vector-valued version of these spaces,

$$X^s(d) := \left\{ \mathbf{V} := \begin{pmatrix} U^{(0),\ell} \\ U^{(1),u} \\ \vdots \\ U^{(M-1),\ell} \\ U^{(M),u} \end{pmatrix} \middle| U^{(m-1),\ell} \in H^s(d); U^{(m),u} \in H^{s+t}(d); 1 \leq m \leq M \right\},$$

where we define the extra smoothness sometimes mandated in TM polarization,

$$t := \begin{cases} 0, & \text{TE or TM } (r = 0), \\ 1, & \text{TM } (r = 1), \end{cases} \tag{27}$$

and

$$Y^s(d) := \left\{ \mathbf{V} := \begin{pmatrix} U^{(0),\ell} \\ U^{(1),u} \\ \vdots \\ U^{(M-1),\ell} \\ U^{(M),u} \end{pmatrix} \middle| U^{(m-1),\ell}, U^{(m),u} \in H^s(d); 1 \leq m \leq M \right\}.$$

These spaces have the norms

$$\|\mathbf{V}\|_{X^s}^2 := \sum_{m=1}^{M} \left\{ \left\| U^{(m-1),\ell} \right\|_{H^s}^2 + \left\| U^{(m),u} \right\|_{H^{s+t}}^2 \right\},$$

and

$$\|\mathbf{V}\|_{Y^s}^2 := \sum_{m=1}^{M} \left\{ \left\| U^{(m-1),\ell} \right\|_{H^s}^2 + \left\| U^{(m),u} \right\|_{H^s}^2 \right\}.$$

We will need the following result on analyticity of the norm of the vector $|N^{(m)}|$, its reciprocal $|N^{(m)}|^{-1}$, and the functions $\{F^{(m)}, \tilde{F}^{(m)}, G^{(m)}, \tilde{G}^{(m)}\}$. The proof is presented in Appendix C.

Lemma 1. *Given an integer $s \geq 0$, an integer $r \in \{0, 1\}$, and any $\delta > 0$, if t is defined by (27), $f^{(m)} \in C^{s+r+3/2+\delta}$ and $W \in H^{s+t}(d)$, then the expansions*

$$\left|N^{(m)}\right|(\varepsilon) = \sum_{n=0}^{\infty} \left|N^{(m)}\right|_n \varepsilon^n, \quad \left|N^{(m)}\right|^{-1}(\varepsilon) = \sum_{n=0}^{\infty} \left|N^{(m)}\right|_n^{-1} \varepsilon^n,$$

$$F^{(m)}(\varepsilon) = \sum_{n=0}^{\infty} F_n^{(m)} \varepsilon^n, \quad \tilde{F}^{(m)}(\varepsilon) = \sum_{n=0}^{\infty} \tilde{F}_n^{(m)} \varepsilon^n,$$

$$G^{(m)}(\varepsilon) = \sum_{n=0}^{\infty} G_n^{(m)} \varepsilon^n, \quad \tilde{G}^{(m)}(\varepsilon) = \sum_{n=0}^{\infty} \tilde{G}_n^{(m)} \varepsilon^n,$$

converge strongly satisfying the estimates

$$\left\| \left| N^{(m)} \right|_n \right|_{C^{s+r+3/2+\delta}} < K_N \frac{D_N^{n-1}}{(n+1)^2}, \qquad \left\| \left| N^{(m)} \right|_n^{-1} \right|_{C^{s+r+3/2+\delta}} < \tilde{K}_N \frac{\tilde{D}_N^{n-1}}{(n+1)^2},$$

$$\left\| F_n^{(m)}[W] \right\|_{H^s} < K_F \frac{D_F^{n-1}}{(n+1)^2} \|W\|_{H^{s+t}}, \qquad \left\| \tilde{F}_n^{(m)}[W] \right\|_{H^s} < \tilde{K}_F \frac{\tilde{D}_F^{n-1}}{(n+1)^2} \|W\|_{H^{s+t}},$$

$$\left\| G_n^{(m)}[W] \right\|_{H^s} < K_G \frac{D_G^{n-1}}{(n+1)^2} \|W\|_{H^{s+t}}, \qquad \left\| \tilde{G}_n^{(m)}[W] \right\|_{H^s} < \tilde{K}_G \frac{\tilde{D}_G^{n-1}}{(n+1)^2} \|W\|_{H^{s+t}}$$

for universal constants $K_N, \tilde{K}_N, K_F, \tilde{K}_F, K_G, \tilde{K}_G > 0$ *and* $D_N, \tilde{D}_N, D_F, \tilde{D}_F, D_G, \tilde{D}_G > 0$.

Beyond this, we require the analyticity of the constituent parts of the operator $\mathbf{A} = \mathbf{A}(\varepsilon)$; the proof is presented in Appendix D.

Lemma 2. *Given an integer* $s \geq 0$, *an integer* $r \in \{0, 1\}$, *and any* $\delta > 0$, *if* t *is defined by (27),* $f^{(m)} \in C^{s+r+3/2+\delta}$ *and* $\mathbf{W} \in H^s \times H^{s+t}$, *then the expansions*

$$\mathbf{D}^{(m)}(\varepsilon) = \sum_{n=0}^{\infty} \mathbf{D}_n^{(m)} \varepsilon^n, \quad \mathbf{L}^{(m)}(\varepsilon) = \sum_{n=0}^{\infty} \mathbf{L}_n^{(m)} \varepsilon^n, \quad \mathbf{U}^{(m)}(\varepsilon) = \sum_{n=0}^{\infty} \mathbf{U}_n^{(m)} \varepsilon^n,$$

converge strongly satisfying the estimates

$$\left\| \mathbf{D}_n^{(m)}[\mathbf{W}] \right\|_{H^s \times H^s} < C_D \frac{B_D^{n-1}}{(n+1)^2} \|\mathbf{W}\|_{H^s \times H^{s+t}}, \qquad \forall\, n > 0,$$

$$\left\| \mathbf{L}_n^{(m)}[\mathbf{W}] \right\|_{H^s \times H^s} < C_L \frac{B_L^{n-1}}{(n+1)^2} \|\mathbf{W}\|_{H^s \times H^{s+t}}, \qquad \forall\, n > 0,$$

$$\left\| \mathbf{U}_n^{(m)}[\mathbf{W}] \right\|_{H^s \times H^s} < C_U \frac{B_U^{n-1}}{(n+1)^2} \|\mathbf{W}\|_{H^s \times H^{s+t}}, \qquad \forall\, n > 0$$

for universal constants $C_D, C_L, C_U, B_D, B_L, B_U > 0$.

With these, we can prove our primary result.

Theorem 2. *Given an integer* $s \geq 0$, *an integer* $r \in \{0, 1\}$, *and any* $\delta > 0$, *if* t *is defined by (27), suppose that*

1. $f^{(m)} \in C^{s+r+3/2+\delta}(d)$ *for all* $1 \leq m \leq M$;
2. $(Y^{(m)} + Z^{(m)})$ *is invertible for all* $1 \leq m \leq M$;
3. $\Delta_p^{(m)} \neq 0$ *for all* $p \in \mathbf{Z}$, $0 \leq m \leq M$, *(see (A1), (A3), (A7));*
4. *For the recursion (A10) we have, for all* $p \in \mathbf{Z}$,

$$Y_p^{(m+1)} S(2h) \neq \tau^{(m)} C(2h), \qquad 1 \leq m \leq M-1,$$

$$Z_p^{(m)} S(2h) \neq \tau^{(m)} C(2h), \qquad 1 \leq m \leq M-1,$$

(see (A11)),
5. $(I + G_0^{(m)})$ *is invertible for all* $1 \leq m \leq M$.

Then Equation (17) has a unique solution (18) and there exist constants $C > 0$ *and* $B > 0$ *such that*

$$\|\mathbf{V}_n\|_{X^s} \leq CB^n$$

for all $n \geq 0$. *This implies that, for any* $0 \leq \rho < 1$, *(18) converges for all* ε *such that* $B\varepsilon < \rho$, *that is,* $\varepsilon < \rho/B$.

Remark 5. The reasons for the assorted hypotheses above are

1. The interfaces $f^{(m)}$ are smooth enough so that the IIOs, Q, S, and $R^{(m)}$, $1 \leq m \leq (M-1)$ are all analytic (see Appendix B).
2. The operators $P^{(m)}$ are invertible so that the surface formulations are equivalent (see Section 3).
3. The configuration is such that the flat-interface IIOs are all well-defined (cf. (A1), (A3), and (A7) in Appendix A).
4. The configuration is such that the choices in the quasi-optimal domain decomposition can be made uniquely (cf. (A10) and (A11) in Appendix A).
5. The currents satisfy polarization-dependent constraints such that the linear operators $(I + G_0^{(m)})$ are *invertible* (see Section 5). Notice that in the absence of currents this is trivially satisfied.

Proof. We can establish this result by simply invoking Theorem 1 which requires the verification of its three hypotheses. To begin we choose

$$X = X^s(d), \quad Y = Y^s(d).$$

Showing that the data $\mathbf{R}_n$ satisfies Hypothesis 1 of Theorem 1 is straightforward and follows the calculations of lemma 4.17 of Ref. 55 quite closely.

From (16a), it is clear that $\mathbf{A}_n$ is simply composed of the operators $\mathbf{D}_n^{(m)}$, $\mathbf{U}_n^{(m)}$, and $\mathbf{L}_n^{(m)}$ which are effectively estimated in Lemma 2. With this the estimates in Hypothesis 2 of Theorem 1 are readily satisfied. We recall that this fundamental result (Lemma 2) is built upon Theorems B1, B2, and B3 regarding the analyticity of the IIOs, Q, S, and $R^{(m)}$ (under Hypotheses 1 and 3), and Lemma 1 concerning analyticity of the functions $|N^{(m)}|$ and $|N^{(m)}|^{-1}$, and the operators $F_n^{(m)}$, $\tilde{F}_n^{(m)}$, $G_n^{(m)}$, and $\tilde{G}_n^{(m)}$.

All that remains is the estimate on the inverse of $\mathbf{A}_0$ which is provided in Section 5 and depends on the quasi-optimal domain decomposition which is ensured by Hypotheses 4 and 5. ■

Remark 6. The smoothness we require of the interfacial profiles is low enough to accommodate many configurations of applied interest. With a much more involved theoretical investigation the author believes that $f^{(m)} \in C^{1,\alpha}$ and perhaps even $f^{(m)}$ Lipschitz would likely deliver the same results; see Ref. 72 for more details on a possible approach.

5 | INVERTIBILITY OF THE LINEARIZED OPERATOR

We will now demonstrate that if the operators $\{Y^{(m)}, Z^{(m)}\}$ are chosen via the recursion (A10) then the operator $\mathbf{A}_0$ is invertible and Theorem 1 can be applied to solve (17). We note the Quasi-Optimal Domain Decomposition outlined in Remarks A1, A2, and A3 that defines the recursions

$$Z^{(1)} = \tau^{(0)}\left(i\gamma_D^{(0)}\right), \tag{28a}$$

$$Z^{(m+1)} = \frac{-(\tau^{(m)})^2\left(\gamma_p^{(m)}\right)^2 S(2h) - \tau^{(m)} Z^{(m)} C(2h)}{-\tau^{(m)} C(2h) + Z^{(m)} S(2h)}, \qquad m = 1, \dots M-1, \tag{28b}$$

and

$$Y^{(M)} = \tau^{(M)}\left(i\gamma_D^{(M)}\right), \tag{29a}$$

$$Y^{(m)} = \frac{-(\tau^{(m)})^2\left(\gamma_p^{(m)}\right)^2 S(2h) - \tau^{(m)} Y^{(m+1)} C(2h)}{-\tau^{(m)} C(2h) + Y^{(m+1)} S(2h)}, \qquad m = M-1, \dots, 1, \tag{29b}$$

which render $Q(0) \equiv S(0) \equiv R^{(m),uu}(0) \equiv R^{(m),\ell\ell}(0) \equiv 0$. With these choices, we see from (22) that

$$\mathbf{D}^{(m)}(0) = \begin{pmatrix} I & F_0^{(m)} \\ 0 & I + G_0^{(m)} \end{pmatrix}, \quad 0 \le m \le M,$$

which is the identity matrix in the absence of surface currents, and invertible in their presence by Hypothesis 5. In fact,

$$\mathbf{D}^{(m)}(0)^{-1} = \begin{pmatrix} I & -F_0^{(m)}\left(I + G_0^{(m)}\right)^{-1} \\ 0 & \left(I + G_0^{(m)}\right)^{-1} \end{pmatrix}, \quad 0 \le m \le M. \tag{30}$$

In this way, the choices are "optimal," however, these selections do not eliminate either the operator $\mathbf{L}^{(m)}$ or $\mathbf{U}^{(m)}$, nor does this work for nontrivial configurations $\varepsilon > 0$. For this reason, the choices are only "quasi-optimal."

Based upon these developments, we require only the following result to establish the existence and mapping properties of the linearized operator $\mathbf{A}_0$.

Lemma 3. *Given any integer $s \ge 0$, if*

$$\Delta_p^{(m)} \neq 0, \quad \forall\, p \in \mathbf{Z}, \quad \forall\, 1 \le m \le M-1,$$

see (A7), the operators $R^{(m),u\ell}(0)$ and $R^{(m),\ell u}(0)$ are compact for $1 \le m \le M-1$.

Proof. We describe the proof for $R^{(m),u\ell}(0)$ and note that the corresponding demonstration for $R^{(m),\ell u}(0)$ is quite similar. We follow the proof of lemma 4.8 in Ref. 55 which uses the method of Kress[70] by considering the limit of finite dimensional range operators (which are compact, see theorem 2.23 of Ref. 70). These are shown to be norm convergent to $R^{(m),u\ell}(0)$ thereby rendering it compact. Our scheme for generating these approximations is to consider the P-truncations in Fourier space,

$$R_P^{(m),u\ell}(0)[\phi(x)] := \sum_{|p|\le P} \left(\frac{-\tau^{(m)}(Y_p^{(m)} + Z_p^{(m)})}{\Delta_p^{(m)}} \right) \hat{\phi}_p e^{i\alpha_p x},$$

cf. (A8b), where

$$\Delta_p^{(m)} = \left((\tau^{(m)})^2 \left(\gamma_p^{(m)} \right)^2 - Z_p^{(m)} Y_p^{(m+1)} \right) S(2h) + \tau^{(m)} \left(Z_p^{(m)} + Y_p^{(m+1)} \right) C(2h),$$

cf. (A7). It is not difficult to show that the recursions (28) and (29), beginning with the order-one Fourier multipliers

$$Z^{(1)} = \tau^{(0)} \left(i\gamma_D^{(0)} \right), \quad Y^{(M)} = \tau^{(M)} \left(i\gamma_D^{(M)} \right),$$

generate a full sequence of order-one Fourier multipliers, $\{Y^{(m)}, Z^{(m)}\}$. With this, it is not hard to demonstrate that, for P sufficiently large,

$$\left| \frac{(Y_p^{(m)} + Z_p^{(m)})}{\Delta_p^{(m)}} \right| \sim e^{-\kappa|p|}, \quad |p| > P$$

for some $\kappa > 0$ since $\Delta_p^{(m)}$ grows exponentially. Thus,

$$\begin{aligned} \left\| \left(R^{(m),u\ell}(0) - R_P^{(m),u\ell}(0) \right) \phi \right\|_{H^s}^2 &= \sum_{|p|>P} \left| \tau^{(m)} \right|^2 \left| \frac{Y_p^{(m)} + Z_p^{(m)}}{\Delta_p^{(m)}} \right|^2 \left| \hat{\phi}_p \right|^2 \\ &\le \sum_{|p|>P} \left| \tau^{(m)} \right|^2 C^2 e^{-2\kappa|p|} \left| \hat{\phi}_p \right|^2 \\ &\le \tilde{C} e^{-2\kappa\langle P \rangle} \|\phi\|_{H^s}^2, \end{aligned}$$

which must go to zero as $P^2 \to \infty$ showing norm convergence. ■

At last we can state and prove the last result for our existence theorem.

Theorem 3. *Given any integer $s \ge 0$, if*

$$\Delta_p^{(m)} \ne 0, \quad \forall\, p \in \mathbf{Z}, \quad \forall\, 1 \le m \le M-1,$$

see (A7), then the operator $\mathbf{A}_0 : X^s(d) \to Y^s(d)$ *is invertible and*

$$\mathbf{A}_0^{-1} : Y^s(d) \to X^s(d).$$

Proof. From (16a), we write $\mathbf{A}_0 = \mathbf{A}(0) = \mathbf{D}(0) + \mathbf{K}(0)$, where

$$\mathbf{D}(0) = \begin{pmatrix} \mathbf{D}^{(1)}(0) & 0 & 0 & 0 & \cdots & 0 \\ 0 & \mathbf{D}^{(2)}(0) & 0 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & 0 & 0 \\ 0 & 0 & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & 0 & \mathbf{D}^{(M-1)}(0) & 0 \\ 0 & \cdots & 0 & 0 & 0 & \mathbf{D}^{(M)}(0) \end{pmatrix},$$

and

$$\mathbf{K}(0) = \begin{pmatrix} 0 & \mathbf{U}^{(1)}(0) & 0 & 0 & \cdots & 0 \\ \mathbf{L}^{(2)}(0) & 0 & \mathbf{U}^{(2)}(0) & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & 0 & 0 \\ 0 & 0 & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \mathbf{L}^{(M-1)}(0) & 0 & \mathbf{U}^{(M-1)}(0) \\ 0 & \cdots & 0 & 0 & \mathbf{L}^{(M)}(0) & 0 \end{pmatrix}.$$

It is clear that

$$\mathbf{D}(0)^{-1} = \begin{pmatrix} \mathbf{D}^{(1)}(0)^{-1} & 0 & 0 & 0 & \cdots & 0 \\ 0 & \mathbf{D}^{(2)}(0)^{-1} & 0 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & 0 & 0 \\ 0 & 0 & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & 0 & \mathbf{D}^{(M-1)}(0)^{-1} & 0 \\ 0 & \cdots & 0 & 0 & 0 & \mathbf{D}^{(M)}(0)^{-1} \end{pmatrix},$$

so that the existence and mapping properties of $\mathbf{D}(0)^{-1}$ can be demonstrated by an examination of each of the $\mathbf{D}^{(m)}(0)^{-1}$. In the case of our quasi-optimal choice of IIOs, we have already observed that

$$\mathbf{D}^{(m)}(0)^{-1} = \begin{pmatrix} I & -F_0^{(m)}\left(I + G_0^{(m)}\right)^{-1} \\ 0 & \left(I + G_0^{(m)}\right)^{-1} \end{pmatrix},$$

cf. (30). Given $\mathbf{W} = (W^\ell, W^u) \in H^s \times H^s$ (note that these operators act on lower/upper traces at the mth *interface* rather than upon upper/lower traces on a *layer*) we can estimate

$$\begin{aligned} \left\|\mathbf{D}^{(m)}(0)^{-1}[\mathbf{W}]\right\|_{H^s \times H^{s+t}} &\le \left\|W^\ell - F_0^{(m)}\left(I + G_0^{(m)}\right)^{-1} W^u\right\|_{H^s} + \left\|\left(I + G_0^{(m)}\right)^{-1} W^u\right\|_{H^{s+t}} \\ &\le \left\|W^\ell\right\|_{H^s} + \left\|F_0^{(m)}\left(I + G_0^{(m)}\right)^{-1} W^u\right\|_{H^s} + \left\|\left(I + G_0^{(m)}\right)^{-1} W^u\right\|_{H^{s+t}} \end{aligned}$$

$$\leq \left\| W^{\ell} \right\|_{H^s} + \| W^u \|_{H^s} + \| W^u \|_{H^s}$$

$$\leq C \| \mathbf{W} \|_{H^s \times H^s},$$

which implies that $\mathbf{D}(0)^{-1} : Y^s(d) \to X^s(d)$.

Due to the compactness of the operators $R^{(m),u\ell}(0)$ and $R^{(m),\ell u}(0)$, the block operator $\mathbf{K}(0)$ is also compact. Appealing to the Fredholm theory, we have that $\mathbf{A}(0)$ is invertible.[37] ■

6 | NUMERICAL RESULTS

In this section, we put this new formulation into action by presenting some preliminary numerical results on scattering of linear waves by a triply layered medium (see Appendix F) with sheets of graphene at one or both of the interfaces. We begin by briefly describing the algorithm, continue with a short numerical validation, and then finish with simulations of the absorbance of two test configurations.

6.1 | Implementation

Our novel algorithm for solving the layered media problems presented in this section utilizes the surface formulation of the governing equations in terms of IIOs parameterized by the interface height/slope ε,

$$\mathbf{A}(\varepsilon)\mathbf{V}(\varepsilon) = \mathbf{R}(\varepsilon),$$

cf. (17). As in Section 4, we seek a solution of the form (18) which is truncated after $N \geq 0$ orders

$$\mathbf{V}(\varepsilon) \approx \mathbf{V}^N(\varepsilon) := \sum_{n=0}^{N} \mathbf{V}_n \varepsilon^n. \tag{31}$$

These must solve (19) for $0 \leq n \leq N$ where the $\mathbf{A}_n$ are given in (21) and the $\mathbf{R}_n$ are specified in (20). In these, we must specify how one computes the operators $\{F_n^{(m)}, \tilde{F}_n^{(m)}, G_n^{(m)}, \tilde{G}_n^{(m)}\}$ and the IIOs $\{Q_n, R_n^{(m)}, S_n\}$. For the former, the considerations are the same as those described in Ref. 57 save that we now consider choices $\{Y^{(m)}, Z^{(m)}\}$ which are not necessarily those of Després[66–68] ($Y^{(m)} = Z^{(m)} = i\eta$, $\eta \in \mathbf{R}^+$), and the terms in (25) are more involved. However, once the terms $|N^{(m)}|_n$ and $|N^{(m)}|_n^{-1}$ are derived, see (C1) and (C2), these forms are straightforward.

For the latter, we simulated the IIOs using the method of TFE[53,61,73] where almost all of the relevant details are specified in Ref. 57. In summary, we used a spectral Fourier–Chebyshev methodology[22–24] where

$$\mathbf{V}_n(x,z) \approx \mathbf{V}_n^{N_x,N_z}(x,z) := \sum_{p=-N_x/2}^{N_x/2-1} \sum_{q=0}^{N_z} \hat{\mathbf{V}}_{n,p,q} T_q(z/h) e^{i\alpha_p x},$$

and T_q is the qth Chebyshev polynomial. To find the Fourier–Chebyshev coefficients, $\{\hat{\mathbf{V}}_{n,p,q}\}$, we took a collocation approach and demanded that the governing equations be true at the gridpoints

$$\{x_j = j(d/N_x) \mid 0 \le j \le N_x - 1\}, \quad \{z_r = h\cos(\pi r/N_z) \mid 0 \le r \le N_z\}.$$

Using fast Fourier and Chebyshev transforms,[22–24] the resulting equations can be solved efficiently and stably.

An important question is how the Taylor series, (31), in ε is summed, for instance, the approximation

$$\hat{\mathbf{V}}^N_{p,q}(\varepsilon) := \sum_{n=0}^{N} \hat{\mathbf{V}}_{n,p,q}\varepsilon^n$$

of $\hat{\mathbf{V}}_{p,q}(\varepsilon)$. For this task, the classical analytic continuation technique of Padé approximation[74] has been used for HOPS methods with great success[49,73] and we advocate its use here. Padé approximation seeks to estimate the truncated Taylor series $\hat{\mathbf{V}}^N_{p,q}(\varepsilon)$ by the rational function

$$[L/M](\varepsilon) := \frac{a^L(\varepsilon)}{b^M(\varepsilon)} = \frac{\sum_{\ell=0}^{L} a_\ell \varepsilon^\ell}{1 + \sum_{m=1}^{M} b_m \varepsilon^m}, \quad L + M = N,$$

and

$$[L/M](\varepsilon) = \hat{\mathbf{V}}^N_{p,q}(\varepsilon) + \mathcal{O}(\varepsilon^{L+M+1});$$

well-known formulas for the coefficients $\{a_\ell, b_m\}$ can be found in Ref. 74. This approximant has remarkable properties of enhanced convergence, and we refer the interested reader to section 2.2 of Baker and Graves-Morris[74] and the insightful calculations of section 8.3 of Bender and Orszag[75] for a thorough discussion of the capabilities and limitations of Padé approximants.

6.2 | Validation by the MMS

Regarding the validation of our scheme, we utilized the MMS.[62–64] To summarize this scheme, consider the generic system of partial differential equations subject to general boundary conditions

$$\mathcal{P}v = 0, \qquad \text{in } \Omega,$$
$$\mathcal{B}v = 0, \qquad \text{at } \partial\Omega.$$

It is usually just as easy to implement a numerical algorithm to solve the nonhomogeneous version of this set of equations

$$\mathcal{P}v = \mathcal{F}, \qquad \text{in } \Omega,$$
$$\mathcal{B}v = \mathcal{J}, \qquad \text{at } \partial\Omega.$$

To test a code, one can begin with the "manufactured solution," $\tilde{v}$, and set

$$\mathcal{F}_v := \mathcal{P}\tilde{v}, \quad \mathcal{J}_v := \mathcal{J}\tilde{v}.$$

Thus, given the pair $\{\mathcal{F}_v, \mathcal{J}_v\}$ we have an *exact*solution of the nonhomogeneous problem, namely, $\tilde{v}$. While this does not guarantee a correct implementation, if the function $\tilde{v}$ is chosen to imitate the behavior of anticipated solutions (e.g., satisfying the boundary conditions exactly) then this can give us confidence in our algorithm.

For the current implementation, we focused upon the three-layer problem ($M = 2$) with layers $m = 0, 1, 2$ denoted, for simplicity, by the letters $\{u, v, w\}$, respectively (cf. Appendix F). We considered the quasiperiodic, outgoing solutions of the Helmholtz equation (9a)

$$u_r(x, z) := A_r^u e^{i\alpha_r x + i\gamma_r^u z}, \quad r \in \mathbf{Z}, \quad A_r^u \in \mathbf{C},$$

and their counterparts for (11a)

$$w_r(x, z) := A_r^w e^{i\alpha_r x - i\gamma_r^w z}, \quad r \in \mathbf{Z}, \quad A_r^w \in \mathbf{C}.$$

Furthermore, we considered the quasiperiodic solutions of the Helmholtz equation (13a)

$$v_r(x, z) := A_r^v e^{i\alpha_r x + i\gamma_r^v z} + B_r^v e^{i\alpha_r x - i\gamma_r^v z}, \quad r \in \mathbf{Z}, \quad A_r^v, B_r^v \in \mathbf{C}.$$

We selected two simple sinusoidal profiles

$$g^{(u)}(x) = \varepsilon f^{(u)}(x) = \varepsilon \cos(2x), \quad g^{(\ell)}(x) = \varepsilon f^{(\ell)}(x) = \varepsilon \sin(2x), \tag{32}$$

and defined, for any choice of the layer half-thickness $\bar{h}$, the Dirichlet and Neumann traces

$$\begin{aligned}
\xi_r^{(u)}(x) &:= u_r(x, \bar{h} + g^{(u)}(x)), \quad \nu_r^{(u)}(x) := (-\partial_{N^{(u)}} u_r)(x, \bar{h} + g^{(u)}(x)),\\
\xi_r^{(v),h}(x) &:= v_r(x, \bar{h} + g^{(u)}(x)), \quad \nu_r^{(v),h}(x) := (\partial_{N^{(u)}} v_r)(x, \bar{h} + g^{(u)}(x)),\\
\xi_r^{(v),-h}(x) &:= v_r(x, -\bar{h} + g^{(\ell)}(x)), \quad \nu_r^{(v),-h}(x) := (-\partial_{N^{(\ell)}} v_r)(x, -\bar{h} + g^{(\ell)}(x)),\\
\xi_r^{(w)}(x) &:= w_r(x, -\bar{h} + g^{(\ell)}(x)), \quad \nu_r^{(w)}(x) := (\partial_{N^{(\ell)}} w_r)(x, -\bar{h} + g^{(\ell)}(x)).
\end{aligned}$$

From these we defined, for any choices of the operators $\{Y^{(u)}, Z^{(u)}, Y^{(\ell)}, Z^{(\ell)}\}$, the impedances

$$U_r := \tau^{(u)} \nu^{(u)} - Y^{(u)}[\xi^{(u)}], \quad \tilde{U}_r := \tau^{(u)} \nu^{(u)} + Z^{(u)}[\xi^{(u)}], \tag{33a}$$

$$V_r^u := \tau^{(v)} \nu^{(v),h} - Z^{(u)}[\xi^{(v),h}], \quad \tilde{V}_r^u := \tau^{(v)} \nu^{(v),h} + Y^{(u)}[\xi^{(v),h}], \tag{33b}$$

$$V_r^\ell := \tau^{(v)} \nu^{(v),-h} - Y^{(\ell)}[\xi^{(v),-h}], \quad \tilde{V}_r^\ell := \tau^{(v)} \nu^{(v),-h} + Z^{(\ell)}[\xi^{(v),-h}], \tag{33c}$$

$$W_r := \tau^{(w)}\nu^{(w)} - Z^{(\ell)}[\xi^{(w)}], \quad \tilde{W}_r := \tau^{(w)}\nu^{(w)} + Y^{(\ell)}[\xi^{(w)}]. \tag{33d}$$

We chose the following physical parameters:

$$\begin{gathered} d = 2\pi, \quad \alpha = 0.1, \quad \epsilon^{(u)} = 1.1, \quad \epsilon^{(v)} = e, \quad \epsilon^{(w)} = \pi, \\ \hat{\sigma}^{(u)} = 0.2, \quad \hat{\sigma}^{(\ell)} = 0.45, \\ A_r^u = -3\,\delta_{r,3}, \quad A_r^w = 4\,\delta_{r,3}, \quad A_r^v = -e\,\delta_{r,3}, \quad B_r^v = \pi\,\delta_{r,3}, \end{gathered} \tag{34}$$

(where $\delta_{r,s}$ is the Kronecker delta) in TM polarization, and the numerical parameters

$$N_x = 64, \quad N_z = 24, \quad N = 10, \quad a = 1/10, \quad b = 1/10. \tag{35}$$

To test the performance and capabilities of our formulation, we made three choices of the operators $\{Y^{(u)}, Z^{(u)}, Y^{(\ell)}, Z^{(\ell)}\}$. The first was that of Després[66–68]

$$Y^{(u)} = Z^{(u)} = Y^{(\ell)} = Z^{(\ell)} = i\eta, \quad \eta = \left(\frac{\sqrt{\epsilon^{(u)}} + \sqrt{\epsilon^{(w)}}}{2} \right) k_0 \in \mathbf{R}^+, \tag{36}$$

while the second was a slight generalization of this

$$Y^{(u)} = i\eta, \quad Z^{(u)} = 1.1\,Y^{(u)}, \quad Y^{(\ell)} = 1.23\,Y^{(u)}, \quad Z^{(\ell)} = 0.98\,Y^{(u)}, \tag{37}$$

which is also guaranteed to produce well-posed IIOs. Finally, we chose our quasi-optimal selections from Appendix F

$$Y_p^{(\ell)} = \tau^{(w)}(i\gamma_p^{(w)}), \quad Y_p^{(u)} = \frac{-(\tau^{(v)})^2(\gamma_p^{(v)})^2 T(2h) - \tau^{(v)}\tau^{(w)}(i\gamma_p^{(w)})}{-\tau^{(v)} + \tau^{(w)}(i\gamma_p^{(w)})T(2h)}, \tag{38a}$$

and

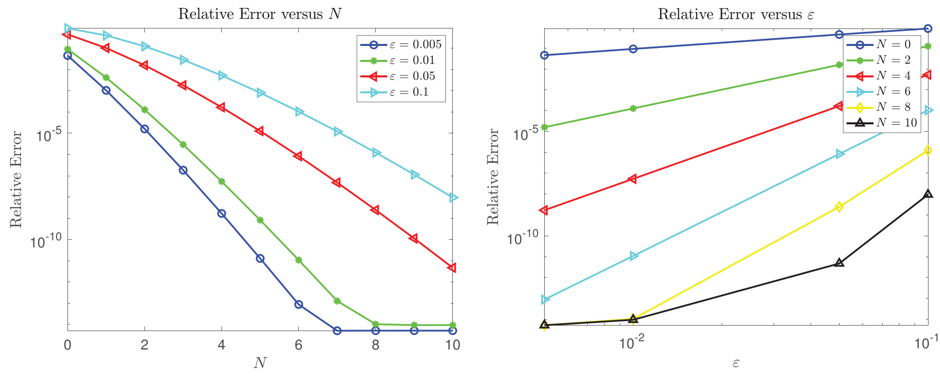
$$Z_p^{(u)} = \tau^{(u)}(i\gamma_p^{(u)}), \quad Z_p^{(\ell)} = \frac{-(\tau^{(v)})^2(\gamma_p^{(v)})^2 T(2h) - \tau^{(v)}\tau^{(u)}(i\gamma_p^{(u)})}{-\tau^{(v)} + \tau^{(u)}(i\gamma_p^{(u)})T(2h)}. \tag{38b}$$

To illuminate the behavior of our scheme, we studied four choices

$$\varepsilon = 0.005, 0.01, 0.05, 0.1$$

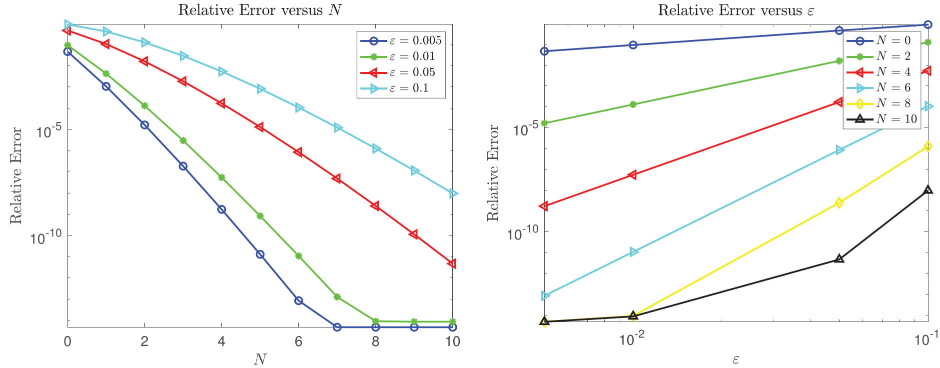
in (32). For this, we supplied the "exact" input data, $\{U_r, V_r^u, V_r^\ell, W_r\}$, from (33) to our HOPS algorithm to simulate solutions of the IIO formulation of the three-layer scattering problem. We compared the output of this, $\{\tilde{U}_r^{\text{approx}}, \tilde{V}_r^{u,\text{approx}}, \tilde{V}_r^{\ell,\text{approx}}, \tilde{W}_r^{\text{approx}}\}$, with the "exact" output, $\{\tilde{U}_r, \tilde{V}_r^u, \tilde{V}_r^\ell, \tilde{W}_r\}$, by computing the relative error

$$\text{Error}_{\text{rel}} := \left|\tilde{U}_r - \tilde{U}_r^{\text{approx}}\right|_{L^\infty} / \left|\tilde{U}_r\right|_{L^\infty}.$$



(a) Error versus perturbation order, N. **(b)** Error versus perturbation size, ε.

FIGURE 2 Plot of relative error with six choices of $N = 0, 2, 4, 6, 8, 10$ and four choices of $\varepsilon = 0.005, 0.01, 0.05, 0.1$ for IIO choice (36) with Taylor summation. Physical parameters (34) and numerical discretization (35)



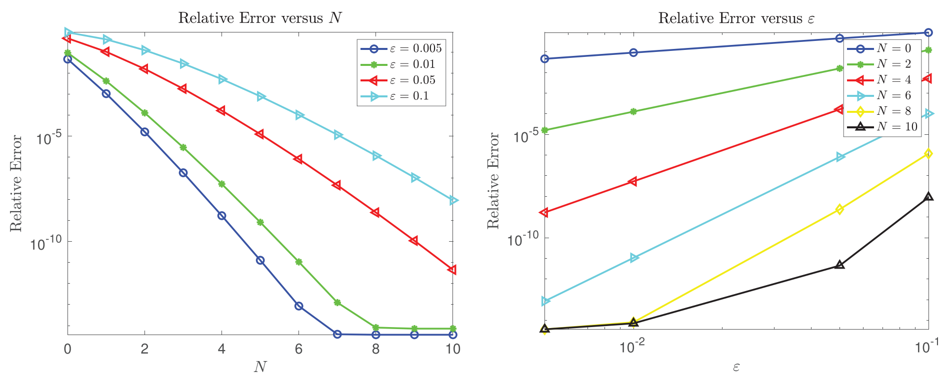
(a) Error versus perturbation order, N. **(b)** Error versus perturbation size, ε.

FIGURE 3 Plot of relative error with six choices of $N = 0, 2, 4, 6, 8, 10$ and four choices of $\varepsilon = 0.005, 0.01, 0.05, 0.1$ for IIO choice (37) with Taylor summation. Physical parameters (34) and numerical discretization (35)

We note that the choice to measure the defect in the upper-layer quantity, $\tilde{U}_r$, was arbitrary, and measuring the mismatch in any of the other output quantities produced similar results.

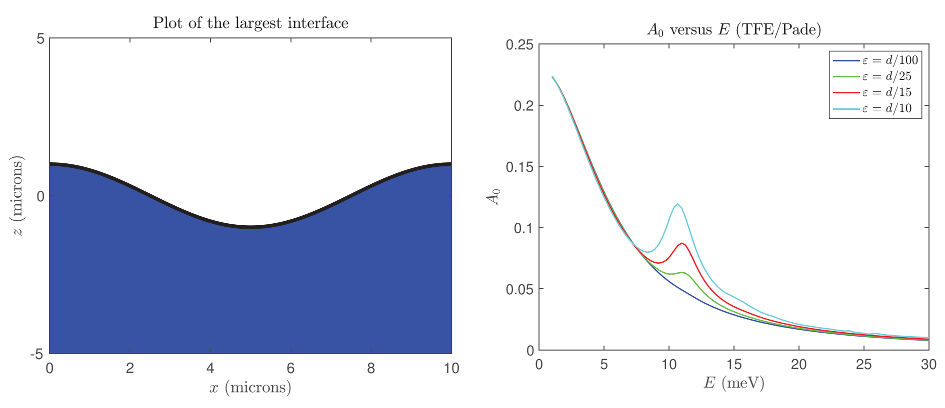
To begin our study, we selected the first choice of IIOs, (36), and we report our results in Figures 2(A) and (B). More specifically, Figure 2(A) displays both the rapid and stable decay of the relative error as N is increased, and how this rate of decay improves as ε is decreased. Figure 2(B) shows both how the error shrinks as ε becomes smaller, and that this rate is enhanced as N is increased.

We repeated this experiment for IIO choices (37) and (38). The results are shown in Figures 3(A) and (B), and Figures 4(A) and (B) for (37) and (38), respectively. As with the first choice, the error decays rapidly as N is increased (with a faster rate for ε smaller) and ε is decreased (more prominently for N larger). These simulations clearly demonstrate the highly efficient and accurate results which our new algorithm can deliver, even for a complicated three-layer structure with *different* currents at the two interfaces.



(a) Error versus perturbation order, N. **(b)** Error versus perturbation size, ε.

FIGURE 4 Plot of relative error with six choices of $N = 0, 2, 4, 6, 8, 10$ and four choices of $\varepsilon = 0.005, 0.01, 0.05, 0.1$ for IIO choice (38) with Taylor summation. Physical parameters (34) and numerical discretization (35)



(a) A diffraction grating composed of a dielectric (permittivity $\epsilon^{(u)} = 1$) overlaying a corrugated graphene sheet (with shape $z = \varepsilon f(x)$, $\varepsilon = d/10$) mounted on a second dielectric (permittivity $\epsilon^{(w)} = 11$).

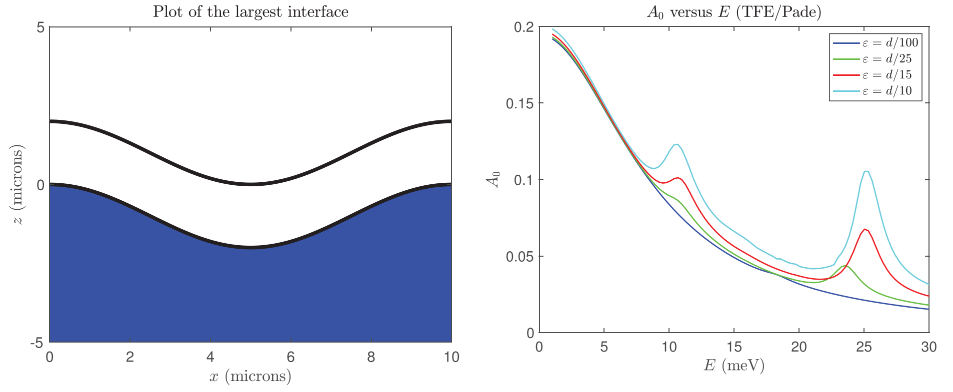
(b) Absorption versus energy for the dielectric–graphene–dielectric configuration with graphene sheet shaped by $z = \varepsilon f(x)$ for $\varepsilon = d/100, d/25, d/15, d/10$.

FIGURE 5 Depiction of the dielectric-graphene-dielectric configuration together with its absorption spectrum

Remark 7. We note that typical MMS simulations implemented in MATLAB[76] (without particular regard for computational performance) on the author's laptop (Apple MacBook Air Dual-Core Intel Core i7, 2.2 GHz, with 8 GB memory running macOS BigSur 11.1) took less than 1/20 of a second. Reliable timings of different portions of the algorithm were difficult to obtain.

6.3 | GSPs on single and double graphene sheets

We conclude with a demonstration of our algorithm's ability to investigate both a simulation already appearing in the literature, and a new one based upon a natural generalization. The former



(a) A diffraction grating composed of a dielectric (permittivity $\epsilon^{(u)} = 1$) overlaying a corrugated graphene sheet (with shape $z = \varepsilon f^{(u)}(x)$, $\varepsilon = d/10$) on top of a layer of the same dielectric (permittivity $\epsilon^{(u)} = 1$) overlaying a second corrugated graphene sheet (with shape $z = \varepsilon g^{(\ell)}(x)$, $\varepsilon = d/10$) mounted on a second dielectric (permittivity $\epsilon^{(w)} = 11$).

(b) Absorption versus energy for the dielectric–graphene–dielectric–graphene–dielectric configuration with graphene sheets shaped by $z = \varepsilon f^{(u)}(x)$ and $z = \varepsilon f^{(\ell)}(x)$ for $\varepsilon = d/100, d/25, d/15, d/10$.

FIGURE 6 Depiction of the dielectric-graphene-dielectric-graphene-dielectric configuration together with its absorption spectrum

we include to further build confidence in the fidelity of our scheme, while the latter is displayed to give a brief indication of the wide array of structures that we could simulate.

To begin, we revisited the calculations found in section 7.2 of Ref. 56 which replicated the simulation found in the survey paper of Bludov et al.[6] In section 9 of this latter work, the authors took up the topic of scattering of electromagnetic waves by corrugated sheets of graphene, and specialized to sinusoidal sheets in section 9.4. More specifically, they investigated one-dimensional, sinusoidally perturbed graphene sheets in TM polarization with interface profile shaped by

$$g(x) = \varepsilon f(x) = \varepsilon \sin(2\pi x/d).$$

They chose physical parameters

$$d = 10 \text{ microns}, \quad \epsilon^{(u)} = 1, \quad \epsilon^{(w)} = 11, \quad \alpha = 0,$$

and then used a Drude model, (4), for the graphene.[6]

The output of the simulation were plots of the (specular) reflectance, transmission, and absorbance

$$R_0 = |\hat{u}_0|^2, \quad T_0 = (\gamma^{(w)}/\gamma^{(u)})|\hat{w}_0|^2, \quad A_0 = 1 - R_0 - T_0,$$

cf. (E1), versus energy of the incident radiation, $E = hc_0/\lambda$, for four choices of the interface deformation

$$\varepsilon = d/100, d/25, d/15, d/10$$

(See Figure 5A for the geometry for the largest deformation.) We attempted to replicate their absorbance curve using our new algorithm and display our results in Figure 5(B). We note the remarkable *qualitative* agreement with the figure of Ref. 6, in particular the GSPR (Graphene Surface Plasmon Resonance) excited around 11 meV as predicted.

Beyond this, we explored a natural generalization of this geometry which is readily simulated with the implementation of our new formulation. More specifically, we inserted a *second* layer of *free-standing* graphene above the structure just considered. Please see Figure 6(A) for a depiction of the configuration in the case of the largest deformation $\varepsilon = d/10$. In Figure 6(B), we display results of our simulation which shows not only the original GSP near 11 meV, but also a new, stronger, GSP near 25 meV. It is the goal of future work to investigate this new GSP, whether it can be "moved," whether more can be induced, and so forth. We note here that this investigation can be readily conducted in a rapid and robust fashion with the formulation and implementation presented here.

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DATA AVAILABILITY STATEMENT

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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APPENDIX A: INFINITESIMAL INTERFACE IMPEDANCE–IMPEDANCE OPERATORS (IIOs)

In this section, we give explicit formulas for the IIOs introduced in Section 3 in the case of *infinitesimal* grating interfaces which we model by quasiperiodic solutions in the case $g^{(m)} \equiv 0$.

A.1 | The upper layer

We begin with the upper layer where it is easy to see that the solution of (9a) and (9b) is

$$v^{(0)}(x,z) = \sum_{p=-\infty}^{\infty} A_p e^{i\alpha_p x + i\gamma_p^{(0)}(z-a^{(1)})}.$$

The boundary condition (9c) demands that

$$\widehat{U^{(0),\ell}}_p = -\tau^{(0)}(i\gamma_p^{(0)})A_p - Y_p^{(1)} A_p,$$

so that

$$v^{(0)}(x,z) = \sum_{p=-\infty}^{\infty} \frac{\widehat{U^{(0),\ell}}_p}{-\tau^{(0)}(i\gamma_p^{(0)}) - Y_p^{(1)}} e^{i\alpha_p x + i\gamma_p^{(0)}(z-a^{(1)})}.$$

Thus, from (10),

$$\begin{aligned} Q(0)[U^{(0),\ell}] &= -\tau^{(0)}\partial_z v^{(0)}(x,a^{(1)}) + Z^{(1)} v^{(0)}(x,a^{(1)}) \\ &= \sum_{p=-\infty}^{\infty} \left(\frac{-\tau^{(0)}(i\gamma_p^{(0)}) + Z_p^{(1)}}{-\tau^{(0)}(i\gamma_p^{(0)}) - Y_p^{(1)}} \right) \widehat{U^{(0),\ell}}_p e^{i\alpha_p x}, \end{aligned}$$

which gives the order-zero Fourier multiplier

$$Q(0) = \left(\frac{-\tau^{(0)}\left(i\gamma_D^{(0)}\right) + Z^{(1)}}{-\tau^{(0)}\left(i\gamma_D^{(0)}\right) - Y^{(1)}} \right),$$

provided that, for all $p \in \mathbf{Z}$,

$$\Delta_p^{(0)} := -\tau^{(0)}\left(i\gamma_D^{(0)}\right) - Y_p^{(1)} \tag{A1}$$

is not zero.

Remark A1. We note that if we choose

$$Z^{(1)} = \tau^{(0)}\left(i\gamma_D^{(0)}\right), \tag{A2}$$

then $Q(0) \equiv 0$.

A.2 | The lower layer

In a similar manner, in the lower layer one can show that the solution of (11a) and (11b) is

$$v^{(M)}(x,z) = \sum_{p=-\infty}^{\infty} D_p e^{i\alpha_p x - i\gamma_p^{(M)}(z-a^{(M)})}.$$

The boundary condition (11b) demands that

$$\widehat{U^{(M),u}}_p = \tau^{(M)}(-i\gamma_p^{(M)})D_p - Z_p^{(M)}D_p,$$

so that

$$v^{(M)}(x,z) = \sum_{p=-\infty}^{\infty} \frac{\widehat{U^{(M),u}}_p}{\tau^{(M)}(-i\gamma_p^{(M)}) - Z_p^{(M)}} e^{i\alpha_p x - i\gamma_p^{(M)}(z-a^{(M)})}.$$

Thus, from (12),

$$\begin{aligned} S(0)[U^{(M),u}] &= \tau^{(M)}\partial_z v^{(M)}(x,a^{(M)}) + Y^{(M)}v^{(M)}(x,a^{(M)}) \\ &= \sum_{p=-\infty}^{\infty} \left(\frac{\tau^{(M)}(-i\gamma_p^{(M)}) + Y_p^{(M)}}{\tau^{(M)}(-i\gamma_p^{(M)}) - Z_p^{(M)}} \right) \widehat{U^{(M),u}}_p e^{i\alpha_p x}, \end{aligned}$$

which gives the order-zero Fourier multiplier

$$S(0) = \left(\frac{\tau^{(M)}(-i\gamma_D^{(M)}) + Y^{(M)}}{\tau^{(M)}(-i\gamma_D^{(M)}) - Z^{(M)}} \right),$$

if we demand that, for all $p \in \mathbf{Z}$,

$$\Delta_p^{(M)} := \tau^{(M)}(-i\gamma_p^{(M)}) - Z_p^{(M)} \tag{A3}$$

be nonzero.

Remark A2. We note that if we choose

$$Y^{(M)} = \tau^{(M)}\left(i\gamma_D^{(M)}\right), \tag{A4}$$

then $S(0) \equiv 0$.

A.3 | An inner layer

Finally, in an inner layer it is convenient to define $h = (a^{(m)} - a^{(m+1)})/2$ and map $(a^{(m+1)}, a^{(m)})$ to $(-h, h)$. In this case, it can be shown that the solution of (13a) is

$$v^{(m)}(x,z) = \sum_{p=-\infty}^{\infty} \left\{A_p C(z) + D_p S(z)\right\} e^{i\alpha_p x}, \tag{A5}$$

where, if

$$\gamma_p^{(m)} = \gamma_p^{(m)\prime} + i\gamma_p^{(m)\prime\prime}, \quad \gamma_p^{(m)\prime}, \gamma_p^{(m)\prime\prime} \in \mathbf{R},$$

we define

$$C(z) := \begin{cases} \cos(\gamma_p^{(m)\prime} z), & \gamma_p^{(m)\prime\prime} = 0, \\ 1, & \gamma_p^{(m)} = 0, \\ \cosh(\gamma_p^{(m)\prime\prime} z), & \gamma_p^{(m)\prime} = 0, \end{cases} \quad S(z) := \begin{cases} \sin(\gamma_p^{(m)\prime} z)/\gamma_p^{(m)\prime}, & \gamma_p^{(m)\prime\prime} = 0, \\ z, & \gamma_p^{(m)} = 0, \\ \sinh(\gamma_p^{(m)\prime\prime} z)/\gamma_p^{(m)\prime\prime}, & \gamma_p^{(m)\prime} = 0. \end{cases}$$

These definitions can be used to establish that

$$C'(z) = -\left(\gamma_p^{(m)}\right)^2 S(z), \quad S'(z) = C(z), \tag{A6a}$$

$$C(-h) = C(h), \quad S(-h) = -S(h), \tag{A6b}$$

$$S(2z) = 2S(z)C(z), \quad C(2z) = C^2(z) - \left(\gamma_p^{(m)}\right)^2 S^2(z). \tag{A6c}$$

Using these, from (A5) we find

$$\partial_z v^{(m)}(x,z) = \sum_{p=-\infty}^{\infty} \left\{-\left(\gamma_p^{(m)}\right)^2 A_p S(z) + D_p C(z)\right\} e^{i\alpha_p x},$$

so that

$$U^{(m),u} = \sum_{p=-\infty}^{\infty} \left\{ \tau^{(m)}(-\left(\gamma_p^{(m)}\right)^2)S(h)A_p + \tau^{(m)}C(h)D_p \right.$$

$$\left. -Z_p^{(m)}C(h)A_p - Z_p^{(m)}S(h)D_p \right\} \mathrm{e}^{i\alpha_p x}$$

$$= \sum_{p=-\infty}^{\infty} \left\{ \left(-\tau^{(m)}\left(\gamma_p^{(m)}\right)^2 S(h) - Z_p^{(m)}C(h) \right) A_p \right.$$

$$\left. + \left(\tau^{(m)}C(h) - Z_p^{(m)}S(h) \right) D_p \right\} \mathrm{e}^{i\alpha_p x},$$

and

$$\tilde{U}^{(m),u} = \sum_{p=-\infty}^{\infty} \left\{ \tau^{(m)}(-\left(\gamma_p^{(m)}\right)^2)S(h)A_p + \tau^{(m)}C(h)D_p \right.$$

$$\left. +Y_p^{(m)}C(h)A_p + Y_p^{(m)}S(h)D_p \right\} \mathrm{e}^{i\alpha_p x}$$

$$= \sum_{p=-\infty}^{\infty} \left\{ \left(-\tau^{(m)}\left(\gamma_p^{(m)}\right)^2 S(h) + Y_p^{(m)}C(h) \right) A_p \right.$$

$$\left. + \left(\tau^{(m)}C(h) + Y_p^{(m)}S(h) \right) D_p \right\} \mathrm{e}^{i\alpha_p x},$$

and

$$U^{(m),\ell} = \sum_{p=-\infty}^{\infty} \left\{ -\tau^{(m)}(-\left(\gamma_p^{(m)}\right)^2)S(-h)A_p - \tau^{(m)}C(-h)D_p \right.$$

$$\left. -Y_p^{(m+1)}C(-h)A_p - Y_p^{(m+1)}S(-h)D_p \right\} \mathrm{e}^{i\alpha_p x}$$

$$= \sum_{p=-\infty}^{\infty} \left\{ \left(-\tau^{(m)}\left(\gamma_p^{(m)}\right)^2 S(h) - Y_p^{(m+1)}C(h) \right) A_p \right.$$

$$\left. + \left(-\tau^{(m)}C(h) + Y_p^{(m+1)}S(h) \right) D_p \right\} \mathrm{e}^{i\alpha_p x},$$

and

$$\tilde{U}^{(m),\ell} = \sum_{p=-\infty}^{\infty} \left\{ -\tau^{(m)}(-\left(\gamma_p^{(m)}\right)^2)S(-h)A_p - \tau^{(m)}C(-h)D_p \right.$$

$$\left. +Z_p^{(m+1)}C(-h)A_p + Z_p^{(m+1)}S(-h)D_p \right\} \mathrm{e}^{i\alpha_p x}$$

$$= \sum_{p=-\infty}^{\infty} \left\{ \left(-\tau^{(m)}\left(\gamma_p^{(m)}\right)^2 S(h) + Z_p^{(m+1)}C(h) \right) A_p \right.$$

$$+\left(-\tau^{(m)}C(h) - Z_p^{(m+1)}S(h)\right)D_p\Big\}e^{i\alpha_p x.}$$

From the calculations above, we learn that

$$\begin{pmatrix}\widehat{U^{(m),u}}_p\\ \widehat{U^{(m),\ell}}_p\end{pmatrix} = J_p^{(m)}\begin{pmatrix}A_p\\ D_p\end{pmatrix}, \quad \begin{pmatrix}\widehat{\tilde{U}^{(m),u}}_p\\ \widehat{\tilde{U}^{(m),\ell}}_p\end{pmatrix} = \tilde{J}_p^{(m)}\begin{pmatrix}A_p\\ D_p\end{pmatrix},$$

where

$$J_p^{(m)} = \begin{pmatrix} -\tau^{(m)}\left(\gamma_p^{(m)}\right)^2 S(h) - Z_p^{(m)}C(h)\tau^{(m)}C(h) - Z_p^{(m)}S(h)\\ -\tau^{(m)}\left(\gamma_p^{(m)}\right)^2 S(h) - Y_p^{(m+1)}C(h) - \tau^{(m)}C(h) + Y_p^{(m+1)}S(h)\end{pmatrix},$$

$$\tilde{J}_p^{(m)} = \begin{pmatrix} -\tau^{(m)}\left(\gamma_p^{(m)}\right)^2 S(h) + Y_p^{(m)}C(h)\tau^{(m)}C(h) + Y_p^{(m)}S(h)\\ -\tau^{(m)}\left(\gamma_p^{(m)}\right)^2 S(h) + Z_p^{(m+1)}C(h) - \tau^{(m)}C(h) - Z_p^{(m+1)}S(h)\end{pmatrix}.$$

Thus, for (14), if we express

$$\begin{pmatrix}\tilde{U}^{(m),u}\\ \tilde{U}^{(m),\ell}\end{pmatrix} = R(0)\left[\begin{pmatrix}U^{(m),u}\\ U^{(m),\ell}\end{pmatrix}\right] = \sum_{p=-\infty}^{\infty}\widehat{R(0)}_p\begin{pmatrix}\widehat{U^{(m),u}}_p\\ \widehat{U^{(m),\ell}}_p\end{pmatrix}e^{i\alpha_p x},$$

then, at each wavenumber $p \in \mathbf{Z}$, we have

$$\widehat{R(0)}_p J_p^{(m)} = \tilde{J}_p^{(m)} \quad \Rightarrow \quad \widehat{R(0)}_p = \tilde{J}_p^{(m)}(J_p^{(m)})^{-1.}$$

Clearly, a crucial calculation is the determinant of $J_p^{(m)}$ which, using the identities above, (A6), can be shown to be

$$\Delta_p^{(m)} := \det J_p^{(m)} = \left((\tau^{(m)})^2\left(\gamma_p^{(m)}\right)^2 - Z_p^{(m)}Y_p^{(m+1)}\right)S(2h)$$
$$+\tau^{(m)}\left(Z_p^{(m)} + Y_p^{(m+1)}\right)C(2h), \quad 1 \le m \le M-1. \quad \text{(A7)}$$

If this can be shown to be nonzero then this IIO will be well-defined. Provided that this is true we can use (A6) to show that

$$R^{(m)}(0)\left[\begin{pmatrix}U^{(m),u}\\ U^{(m),\ell}\end{pmatrix}\right] = \begin{pmatrix}R^{uu}(0) & R^{u\ell}(0)\\ R^{\ell u}(0) & R^{\ell\ell}(0)\end{pmatrix}\left[\begin{pmatrix}U^{(m),u}\\ U^{(m),\ell}\end{pmatrix}\right]$$
$$= \sum_{p=-\infty}^{\infty}\begin{pmatrix}R_p^{uu}(0) & R_p^{u\ell}(0)\\ R_p^{\ell u}(0) & R_p^{\ell\ell}(0)\end{pmatrix}\left[\begin{pmatrix}\widehat{U^{(m),u}}_p\\ \widehat{U^{(m),\ell}}_p\end{pmatrix}\right]e^{i\alpha_p x},$$

where

$$R_p^{uu}(0) = \frac{\left((\tau^{(m)})^2 \left(\gamma_p^{(m)} \right)^2 + Y_p^{(m)} Y_p^{(m+1)} \right) S(2h) + \tau^{(m)} \left(Y_p^{(m+1)} - Y_p^{(m)} \right) C(2h)}{\Delta_p^{(m)}}, \tag{A8a}$$

$$R_p^{u\ell}(0) = \frac{-\tau^{(m)} \left(Y_p^{(m)} + Z_p^{(m)} \right)}{\Delta_p^{(m)}}, \tag{A8b}$$

$$R_p^{\ell u}(0) = \frac{-\tau^{(m)} \left(Y_p^{(m+1)} + Z_p^{(m+1)} \right)}{\Delta_p^{(m)}}, \tag{A8c}$$

$$R_p^{\ell\ell}(0) = \frac{\left((\tau^{(m)})^2 \left(\gamma_p^{(m)} \right)^2 + Z_p^{(m)} Z_p^{(m+1)} \right) S(2h) + \tau^{(m)} \left(Z_p^{(m)} - Z_p^{(m+1)} \right) C(2h)}{\Delta_p^{(m)}.} \tag{A8d}$$

Remark A3. We note that if we select

$$\left((\tau^{(m)})^2 \left(\gamma_p^{(m)} \right)^2 + Y_p^{(m)} Y_p^{(m+1)} \right) S(2h) + \tau^{(m)} \left(Y_p^{(m+1)} - Y_p^{(m)} \right) C(2h) = 0, \tag{A9a}$$

$$\left((\tau^{(m)})^2 \left(\gamma_p^{(m)} \right)^2 + Z_p^{(m)} Z_p^{(m+1)} \right) S(2h) + \tau^{(m)} \left(Z_p^{(m)} - Z_p^{(m+1)} \right) C(2h) = 0, \tag{A9b}$$

then $R_p^{uu}(0) \equiv R_p^{\ell\ell}(0) \equiv 0$. This amounts to two equations for four unknowns, however, we anticipate our subsequent developments by recalling that we have already hinted at the choices

$$Z^{(1)} = \tau^{(0)} \left(i\gamma_D^{(0)} \right), \quad Y^{(M)} = \tau^{(M)} \left(i\gamma_D^{(M)} \right), \tag{A10a}$$

cf. (A2) and (A4), so that $Q(0) \equiv S(0) \equiv 0$, and endeavor to select $Y^{(m)}$ from $Y^{(m+1)}$ (a backward recurrence from $Y^{(M)}$) and $Z^{(m+1)}$ from $Z^{(m)}$ (a forward recurrence from $Z^{(1)}$). With this in mind we write these as

$$Y_p^{(m)} = \frac{-(\tau^{(m)})^2 \left(\gamma_p^{(m)} \right)^2 S(2h) - \tau^{(m)} Y_p^{(m+1)} C(2h)}{-\tau^{(m)} C(2h) + Y_p^{(m+1)} S(2h)}, \qquad m = M-1, \dots, 1, \tag{A10b}$$

$$Z_p^{(m+1)} = \frac{-(\tau^{(m)})^2 \left(\gamma_p^{(m)} \right)^2 S(2h) - \tau^{(m)} Z_p^{(m)} C(2h)}{-\tau^{(m)} C(2h) + Z_p^{(m)} S(2h)}, \qquad m = 1, \dots, M-1. \tag{A10c}$$

In order that these recursions can be carried out we assume that, for all $p \in \mathbf{Z}$,

$$Y_p^{(m+1)} S(2h) \neq \tau^{(m)} C(2h), \qquad 1 \leq m \leq M-1, \tag{A11a}$$

$$Z_p^{(m)} S(2h) \neq \tau^{(m)} C(2h), \qquad 1 \leq m \leq M-1. \tag{A11b}$$

Remark A4. One final comment on these recursion formulas is that overflow can result from computing the factors $S(2h)$ and $C(2h)$ when h becomes large. This can be avoided by rescaling (A10), for instance, by either $S(2h)$ or $C(2h)$.

APPENDIX B: ANALYTICITY OF IIOS

In this section, we state theorems of analyticity for the three IIOs which play a role in this paper. We do not give proofs as these results are rather standard given the state-of-the-art in the field.[55]

Theorem B1. *Given an integer $s \geq 0$ and any $\delta > 0$, if $f^{(1)} \in C^{s+3/2+\delta}(d)$ and*

$$\Delta_p^{(0)} \neq 0, \quad \forall\, p \in \mathbf{Z},$$

cf. (A1), then, for order-r ($r = 0, 1$) Fourier multipliers $\{Y^{(1)}, Z^{(1)}\}$, the series

$$Q(\varepsilon f^{(1)}) = \sum_{n=0}^{\infty} Q_n(f^{(1)}) \varepsilon^n,$$

converges strongly as an operator from $H^s(d)$ to $H^s(d)$. More precisely,

$$\|Q_n\|_{H^s \to H^s} \leq C_Q \frac{B_Q^{n-1}}{(n+1)^2}, \quad n > 0 \tag{B1}$$

for universal constants $C_Q, B_Q > 0$.

Theorem B2. *Given an integer $s \geq 0$ and any $\delta > 0$, if $f^{(M)} \in C^{s+3/2+\delta}(d)$ and*

$$\Delta_p^{(M)} \neq 0, \quad \forall\, p \in \mathbf{Z},$$

cf. (A3), then, for order-r ($r = 0, 1$) Fourier multipliers $\{Y^{(M)}, Z^{(M)}\}$, the series

$$S(\varepsilon f^{(M)}) = \sum_{n=0}^{\infty} S_n(f^{(M)}) \varepsilon^n,$$

converges strongly as an operator from $H^s(d)$ to $H^s(d)$. More precisely

$$\|S_n\|_{H^s \to H^s} \leq C_S \frac{B_S^{n-1}}{(n+1)^2}, \quad n > 0 \tag{B2}$$

for universal constants $C_S, B_S > 0$.

Theorem B3. *Given an integer $s \geq 0$ and any $\delta > 0$, if $f^{(m)}, f^{(m+1)} \in C^{s+3/2+\delta}(d)$ and*

$$\Delta_p^{(m)} \neq 0, \quad \forall\, p \in \mathbf{Z},$$

cf. (A7), then, for order-r ($r = 0, 1$) Fourier multipliers $\{Y^{(m)}, Y^{(m+1)}, Z^{(m)}, Z^{(m+1)}\}$, the series

$$\begin{pmatrix} R^{(m),uu}(\varepsilon f^{(m)}, \varepsilon f^{(m+1)}) & R^{(m),u\ell}(\varepsilon f^{(m)}, \varepsilon f^{(m+1)}) \\ R^{(m),\ell u}(\varepsilon f^{(m)}, \varepsilon f^{(m+1)}) & R^{(m),\ell\ell}(\varepsilon f^{(m)}, \varepsilon f^{(m+1)}) \end{pmatrix} = \sum_{n=0}^{\infty} \begin{pmatrix} R_n^{(m),uu}(f^{(m)}, f^{(m+1)}) & R_n^{(m),u\ell}(f^{(m)}, f^{(m+1)}) \\ R^{(m),\ell u}(f^{(m)}, f^{(m+1)}) & R_n^{(m),\ell\ell}(f^{(m)}, f^{(m+1)}) \end{pmatrix} \varepsilon^n$$

converges strongly as an operator from $H^s(d) \times H^s(d)$ to $H^s(d) \times H^s(d)$. More precisely,

$$\max\left\{ \left\| R_n^{(m),uu} \right\|_{H^s \to H^s}, \left\| R_n^{(m),u\ell} \right\|_{H^s \to H^s}, \left\| R_n^{(m),\ell u} \right\|_{H^s \to H^s}, \left\| R_n^{(m),\ell\ell} \right\|_{H^s \to H^s} \right\} \leq C_R \frac{B_R^{n-1}}{(n+1)^2}, \quad n > 0 \tag{B3}$$

for universal constants $C_R, B_R > 0$.

Remark B1. In previous work,[57,61 73] the theorems stated above have typically been phrased as, for example,

$$\|Q_n\|_{H^s \to H^s} \leq C_Q B_Q^n, \quad n \geq 0. \tag{B4}$$

This is essentially equivalent to (B1) as, for instance,

$$CB^n = CB(n+1)^2 \left(\frac{B}{\tilde{B}}\right)^{n-1} \frac{\tilde{B}^{n-1}}{(n+1)^2} = (CB)\mathcal{A}(n) \frac{\tilde{B}^{n-1}}{(n+1)^2},$$

where

$$\mathcal{A}(n) := (n+1)^2 \left(\frac{B}{\tilde{B}}\right)^{n-1},$$

which has a *unique* maximizer, say n^*, provided that $\tilde{B} > B$. With this maximizer we have

$$CB^n \leq \tilde{C} \frac{\tilde{B}^{n-1}}{(n+1)^2}, \quad \tilde{C} := CB\mathcal{A}(n^*).$$

Thus, if (B4) is true, then (B1) holds provided that we choose the constants slightly differently. In particular, $\tilde{B} > B$ so that the disk of analyticity may be slightly smaller.

APPENDIX C: ANALYTICITY OF MAGNITUDE OF THE NORMALS

We now present a brief demonstration of Lemma 1. Since

$$\left|N^{(m)}\right|^2 = 1 + \varepsilon^2(\partial_x f)^2,$$

we have

$$\left(\sum_{n=0}^{\infty}\left|N^{(m)}\right|_n \varepsilon^n\right)\left(\sum_{q=0}^{\infty}\left|N^{(m)}\right|_q \varepsilon^q\right) = 1 + \varepsilon^2(\partial_x f)^2,$$

or

$$\sum_{n=0}^{\infty}\varepsilon^n\left(\sum_{q=0}^{n}\left|N^{(m)}\right|_{n-q}\left|N^{(m)}\right|_q\right) = 1 + \varepsilon^2(\partial_x f)^2.$$

Thus, we can deduce that

$$\left|N^{(m)}\right|_0^2 = 1,$$

$$2\left|N^{(m)}\right|_0\left|N^{(m)}\right|_1 = 0,$$

$$2\left|N^{(m)}\right|_0\left|N^{(m)}\right|_2 = (\partial_{xf})^2 - \left|N^{(m)}\right|_1^2,$$

$$2\left|N^{(m)}\right|_0\left|N^{(m)}\right|_n = -\sum_{q=1}^{n-1}\left|N^{(m)}\right|_{n-q}\left|N^{(m)}\right|_q, \qquad n>2,$$

which gives

$$\left|N^{(m)}\right|_0 = 1, \tag{C1a}$$

$$\left|N^{(m)}\right|_1 = 0, \tag{C1b}$$

$$\left|N^{(m)}\right|_2 = \frac{1}{2}(\partial_x f)^2, \tag{C1c}$$

$$\left|N^{(m)}\right|_n = -\frac{1}{2}\sum_{q=1}^{n-1}\left|N^{(m)}\right|_{n-q}\left|N^{(m)}\right|_q, \qquad n > 2. \tag{C1d}$$

We now work by induction. At order $n = 0$ we have

$$K := \left\|\left|N^{(m)}\right|_0\right\|_{C^{s+r+3/2+\delta}} = 1.$$

The cases $n = 1, 2$ can be estimated by finite quantities and so we assume the estimate for $n < \bar{n}$ ($\bar{n} \geq 3$). We study

$$\begin{aligned}
\left\| \left| N^{(m)} \right|_{\bar{n}} \right|_{C^{s+r+3/2+\delta}} &\leq \frac{1}{2} \sum_{q=1}^{\bar{n}-1} \left\| \left| N^{(m)} \right|_{\bar{n}-q} \right|_{C^{s+r+3/2+\delta}} \left\| \left| N^{(m)} \right|_{q} \right|_{C^{s+r+3/2+\delta}} \\
&\leq \frac{1}{2} \sum_{q=1}^{\bar{n}-1} K \frac{D^{\bar{n}-q-1}}{(\bar{n}-q+1)^2} K \frac{D^{q-1}}{(q+1)^2} \\
&\leq K \left(\frac{1}{2} K \right) \frac{D^{\bar{n}-2}}{(\bar{n}+1)^2} \sum_{q=1}^{\bar{n}-1} \frac{(\bar{n}+1)^2}{(\bar{n}-q+1)^2 (q+1)^2} \\
&\leq K \left(\frac{1}{2} K \Sigma \right) \frac{D^{\bar{n}-2}}{(\bar{n}+1)^2},
\end{aligned}$$

and we are done if $D > K\Sigma/2$.

Regarding $|N^{(m)}|^{-1}$ we note that

$$\left| N^{(m)} \right| \left| N^{(m)} \right|^{-1} = 1,$$

so that

$$\left(\sum_{n=0}^{\infty} \left| N^{(m)} \right|_n \varepsilon^n \right) \left(\sum_{q=0}^{\infty} \left| N^{(m)} \right|_q^{-1} \varepsilon^q \right) = 1,$$

or

$$\sum_{n=0}^{\infty} \varepsilon^n \left(\sum_{q=0}^{n} \left| N^{(m)} \right|_{n-q} \left| N^{(m)} \right|_q^{-1} \right) = 1.$$

Thus, we can deduce that

$$\begin{aligned}
&\left| N^{(m)} \right|_0 \left| N^{(m)} \right|_0^{-1} = 1, \\
&\left| N^{(m)} \right|_0 \left| N^{(m)} \right|_n^{-1} = -\sum_{q=0}^{n-1} \left| N^{(m)} \right|_{n-q} \left| N^{(m)} \right|_q^{-1}, \qquad n>0,
\end{aligned}$$

which gives

$$\left| N^{(m)} \right|_0^{-1} = 1, \tag{C2a}$$

$$\left| N^{(m)} \right|_n^{-1} = -\sum_{q=0}^{n-1} \left| N^{(m)} \right|_{n-q} \left| N^{(m)} \right|_q^{-1}, \qquad n > 0. \tag{C2b}$$

Again we use induction. At order $n = 0$ we have

$$\tilde{K} := \left| \left| N^{(m)} \right|_0^{-1} \right|_{C^{s+r+3/2+\delta}} = 1.$$

Assuming the estimate for $n < \bar{n}$ we study

$$\begin{aligned}
\left| \left| N^{(m)} \right|_{\bar{n}}^{-1} \right|_{C^{s+r+3/2+\delta}} &\leq \sum_{q=0}^{\bar{n}-1} \left| \left| N^{(m)} \right|_{\bar{n}-q} \right|_{C^{s+r+3/2+\delta}} \left| \left| N^{(m)} \right|_{q}^{-1} \right|_{C^{s+r+3/2+\delta}} \\
&\leq \sum_{q=0}^{\bar{n}-1} K \frac{D^{\bar{n}-q-1}}{(\bar{n}-q+1)^2} \tilde{K} \frac{\tilde{D}^{q-1}}{(q+1)^2} \\
&\leq \tilde{K} K D \frac{\tilde{D}^{\bar{n}-2}}{(\bar{n}+1)^2} \sum_{q=0}^{\bar{n}-1} \left(\frac{D}{\tilde{D}} \right)^{\bar{n}-q-2} \frac{(\bar{n}+1)^2}{(\bar{n}-q+1)^2 (q+1)^2}.
\end{aligned}$$

If we now assume that $\tilde{D} > D$ then

$$\begin{aligned}
\left| \left| N^{(m)} \right|_{\bar{n}}^{-1} \right|_{C^{s+r+3/2+\delta}} &\leq \tilde{K} K D \frac{\tilde{D}^{\bar{n}-2}}{(\bar{n}+1)^2} \sum_{q=0}^{\bar{n}-1} \frac{(\bar{n}+1)^2}{(\bar{n}-q+1)^2 (q+1)^2} \\
&\leq \tilde{K} (K\Sigma) D \frac{\tilde{D}^{\bar{n}-2}}{(\bar{n}+1)^2},
\end{aligned}$$

and we are done if $\tilde{D} > DK\Sigma$.

Regarding the forms $F_n^{(m)}[W]$, $\tilde{F}_n^{(m)}[W]$, $G_n^{(m)}[W]$, and $\tilde{G}_n^{(m)}[W]$, we focus upon the first of these as the others can be handled in a similar fashion. We estimate

$$\begin{aligned}
\left\| F_n^{(m)}[W] \right\|_{H^s} &\leq \left\| -Y^{(m)} \left[p^{(m)} \left| N^{(m)} \right|_n^{-1} Y^{(m)} + s^{(m)} \left| N^{(m)} \right|_n I \right] (Y^{(m)} + Z^{(m)})^{-1} W \right\|_{H^s} \\
&\leq \left\| p^{(m)} \left| N^{(m)} \right|_n^{-1} Y^{(m)} (Y^{(m)} + Z^{(m)})^{-1} W \right\|_{H^{s+r}} \\
&\quad + \left\| s^{(m)} \left| N^{(m)} \right|_n (Y^{(m)} + Z^{(m)})^{-1} W \right\|_{H^s} \\
&\leq \left| p^{(m)} \right| \left| \left| N^{(m)} \right|_n^{-1} \right|_{C^{s+r}} \|W\|_{H^{s+r}} + \left| s^{(m)} \right| \left| \left| N^{(m)} \right|_n \right|_{C^s} \|W\|_{H^s} \\
&\leq \left\{ \left| p^{(m)} \right| \left| \left| N^{(m)} \right|_n^{-1} \right|_{C^{s+r}} + \left| s^{(m)} \right| \left| \left| N^{(m)} \right|_n \right|_{C^s} \right\} \|W\|_{H^{s+t}}.
\end{aligned}$$

In this final estimate, we see the need for the quantity t. If we are in Transverse Magnetic (TM) polarization and $r = 1$ then extra smoothness is required, otherwise there is no need. Finally, using our estimates on $|N^{(m)}|_n$ and $|N^{(m)}|_n^{-1}$ we have

$$\left\| F_n^{(m)}[W] \right\|_{H^s} \le \left\{ \left| p^{(m)} \right| \tilde{K}_N \frac{\tilde{D}_N^{n-1}}{(n+1)^2} + \left| s^{(m)} \right| K_N \frac{D_N^{n-1}}{(n+1)^2} \right\} \|W\|_{s+t},$$

and we are done if

$$D_F > \max\{\tilde{D}_N, D_N\}, \quad K_F > 2\max\left\{ \left| p^{(m)} \right| \tilde{K}_N, \left| s^{(m)} \right| K_N \right\}.$$

APPENDIX D: ANALYTICITY OF THE COMPONENTS OF THE LINEAR OPERATOR

The proof of Lemma 2 is elementary and simply requires an analysis of the forms (24). For brevity, we focus upon the single term

$$\mathbf{D}_n^{(m)} = \begin{pmatrix} 0 & F_n^{(m)} + R_n^{(m),uu} \\ R_n^{(m-1),\ell\ell} & G_n^{(m)} \end{pmatrix} + \sum_{q=0}^{n} \begin{pmatrix} 0 & \tilde{F}_{n-q}^{(m)} R_q^{(m),uu} \\ 0 & \tilde{G}_{n-q}^{(m)} R_q^{(m),uu} \end{pmatrix} \tag{D1}$$

for $2 \le m \le M-1$, cf. (24d). Regarding the estimate, we consider its action upon a generic function pair $\mathbf{W} = (W^\ell, W^u) \in H^s \times H^{s+t}$. (We note that these operators act on lower/upper traces at the mth *interface* rather than upon upper/lower traces on a *layer*.) This results in the following calculation:

$$\begin{aligned} \left\| \mathbf{D}_n^{(m)} \mathbf{W} \right\|_{H^s \times H^s} &\le \left\| (F_n^{(m)} + R_n^{(m),uu}) W^u + \sum_{q=0}^{n} \tilde{F}_{n-q}^{(m)} R_q^{(m),uu} W^u \right\|_{H^s} \\ &\quad + \left\| R_n^{(m-1),\ell\ell} W^\ell + G_n^{(m)} W^u + \sum_{q=0}^{n} \tilde{G}_{n-q}^{(m)} R_q^{(m),uu} W^u \right\|_{H^s} \\ &\le \left\| F_n^{(m)} W^u \right\|_{H^s} + \left\| R_n^{(m),uu} W^u \right\|_{H^s} + \sum_{q=0}^{n} \left\| \tilde{F}_{n-q}^{(m)} R_q^{(m),uu} W^u \right\|_{H^s} \\ &\quad + \left\| R_n^{(m-1),\ell\ell} W^\ell \right\|_{H^s} + \left\| G_n^{(m)} W^u \right\|_{H^s} + \sum_{q=0}^{n} \left\| \tilde{G}_{n-q}^{(m)} R_q^{(m),uu} W^u \right\|_{H^s}. \end{aligned}$$

Using the analyticity result for the IIO $R^{(m)}$, Theorem B3, and Lemma 1, we have

$$\begin{aligned} \left\| \mathbf{D}_n^{(m)} \mathbf{W} \right\|_{H^s \times H^s} &\le K_F \frac{D_F^{n-1}}{(n+1)^2} \|W^u\|_{H^{s+t}} + C_R \frac{B_R^{n-1}}{(n+1)^2} \|W^u\|_{H^s} \\ &\quad + \sum_{q=0}^{n} \tilde{K}_F \frac{\tilde{D}_F^{n-q-1}}{(n-q+1)^2} C_R \frac{B_R^{q-1}}{(q+1)^2} \|W^u\|_{H^{s+t}} \\ &\quad + C_R \frac{B_R^{n-1}}{(n+1)^2} \left\| W^\ell \right\|_{H^s} + K_G \frac{D_G^{n-1}}{(n+1)^2} \|W^u\|_{H^{s+t}} \end{aligned}$$

$$+\sum_{q=0}^{n} \tilde{K}_G \frac{\tilde{D}_G^{n-q-1}}{(n-q+1)^2} C_R \frac{B_R^{q-1}}{(q+1)^2} \|W^u\|_{H^{s+t}}.$$

Proceeding

$$\begin{aligned}
\left\|\mathbf{D}_n^{(m)}\mathbf{W}\right\|_{H^s\times H^s} &\leq K_F\|W^u\|_{H^{s+t}} \frac{D_F^{n-1}}{(n+1)^2} + C_R\|W^u\|_{H^s}\frac{B_R^{n-1}}{(n+1)^2} \\
&\quad + \tilde{K}_F C_R \|W^u\|_{H^{s+t}} \frac{B_D^{n-2}}{(n+1)^2} \\
&\quad\quad \times \sum_{q=0}^{n} \left(\frac{\tilde{D}_F}{B_D}\right)^{n-q-1} \left(\frac{B_R}{B_D}\right)^{q-1} \frac{(n+1)^2}{(n-q+1)^2(q+1)^2} \\
&\quad + C_R\left\|W^\ell\right\|_{H^s}\frac{B_R^{n-1}}{(n+1)^2} + K_G\|W^u\|_{H^{s+t}}\frac{D_G^{n-1}}{(n+1)^2} \\
&\quad + \tilde{K}_G C_R \|W^u\|_{H^{s+t}} \frac{B_D^{n-2}}{(n+1)^2} \\
&\quad\quad \times \sum_{q=0}^{n} \left(\frac{\tilde{D}_G}{B_D}\right)^{n-q-1} \left(\frac{B_R}{B_D}\right)^{q-1} \frac{(n+1)^2}{(n-q+1)^2(q+1)^2} \\
&\leq C_D \|\mathbf{W}\|_{H^s\times H^{s+t}} \frac{B_D^{n-1}}{(n+1)^2},
\end{aligned}$$

provided that

$$B_D \geq \max\{B_R, D_F, \tilde{D}_F, D_G, \tilde{D}_G\},$$

and

$$C_D \geq 6\max\{K_F, C_R, \tilde{K}_F C_R \Sigma, C_R, K_G, \tilde{K}_G C_R \Sigma\}.$$

APPENDIX E: TWO LAYERS

To illustrate our method, we consider the case of two layers ($M = 1$) where the governing equations, (15), simplify to

$$\begin{pmatrix} I & F + (I+\tilde{F})S \\ Q & (I+G) + \tilde{G}S \end{pmatrix} \begin{pmatrix} U \\ W \end{pmatrix} = \begin{pmatrix} \zeta \\ \psi \end{pmatrix},$$

where

$$U = U^{(0),\ell}, \quad W = U^{(1),u}, \quad \zeta = \zeta^{(1)}, \quad \psi = \psi^{(1)},$$
$$F = F^{(1)}, \quad \tilde{F} = \tilde{F}^{(1)}, \quad G = G^{(1)}, \quad \tilde{G} = \tilde{G}^{(1)},$$

$$Y = Y^{(1)}, \quad Z = Z^{(1)}, \quad \tau^{(u)} = \tau^{(0)}, \quad \tau^{(w)} = \tau^{(1)}.$$

Following the guidance of Remarks A1 and A2, we choose $Z = \tau^{(u)}(i\gamma_D^{(u)})$ and $Y = \tau^{(w)}(i\gamma_D^{(w)})$, where

$$\gamma_D^{(u)} = \gamma_D^{(0)}, \quad \gamma_D^{(w)} = \gamma_D^{(1)},$$

so that $Q(0) \equiv S(0) \equiv 0$. With this choice

$$Y_p + Z_p = \tau^{(w)}(i\gamma_p^{(w)}) + \tau^{(u)}(i\gamma_p^{(u)}),$$

and, as this is never zero, Hypothesis 2 is satisfied. We can also see that

$$\Delta_p^{(u)} = -\tau^{(u)}(i\gamma_p^{(u)}) - Y_p = -\tau^{(u)}(i\gamma_p^{(u)}) - \tau^{(w)}(i\gamma_p^{(w)}) = -(Z_p + Y_p),$$

and

$$\Delta_p^{(w)} = \tau^{(w)}(-i\gamma_p^{(w)}) - Z_p = \tau^{(w)}(-i\gamma_p^{(w)}) - \tau^{(u)}(i\gamma_p^{(u)}) = -(Y_p + Z_p),$$

and, since these are also nonzero, Hypothesis 3 is also true. Meanwhile, Hypothesis 4 is vacuous and thus unnecessary. Finally, Hypothesis 5 requires investigation of the condition that $(I + G_0)$ be invertible. In the absence of a current this is always true as $G_0 \equiv 0$. For a nonzero current, this can be accomplished by studying the symbol of $(I + G_0)$ in Fourier space and demanding

$$(Y_p + Z_p) + Z_p\left[p^{(1)}Y_p + s^{(1)}\right] \neq 0,$$

since $Y_p + Z_p \neq 0$. This formula is quite complicated even with the simple Drude model we have selected, (4), and we leave this as a constraint to be verified on a case by case basis. Thus, if we simply choose the interface $f(x) \in C^{s+r+3/2+\delta}$ we will satisfy Hypothesis 1 and Theorem 2 assures us a unique solution which depends analytically upon ε. In the presence of a two-dimensional material, this is a novel result.

We can pursue these calculations further by noting that in the flat-interface case ($g \equiv 0$ and $\partial_N = \partial_z$), the governing equations become

$$\begin{pmatrix} I & F \\ 0 & I + G \end{pmatrix} \begin{pmatrix} U \\ W \end{pmatrix} = \begin{pmatrix} \zeta \\ \psi \end{pmatrix}.$$

In this simplified case, we know that

$$u(x,z) = R e^{i\alpha x + i\gamma^{(u)} z}, \quad w(x,z) = T e^{i\alpha x - i\gamma^{(w)} z}, \tag{E1}$$

so that, since

$$Y e^{i\alpha x} = \tau^{(w)}(i\gamma^{(w)}) e^{i\alpha x}, \quad Z e^{i\alpha x} = \tau^{(u)}(i\gamma^{(u)}) e^{i\alpha x},$$

we have

$$u(x,0) = Re^{i\alpha x}, \quad \partial_z u(x,0) = (i\gamma^{(u)})Re^{i\alpha x},$$

$$w(x,0) = Te^{i\alpha x}, \quad \partial_z w(x,0) = (-i\gamma^{(w)})Te^{i\alpha x},$$

$$\xi(x) = -e^{i\alpha x}, \quad \nu(x) = (i\gamma^{(u)})e^{i\alpha x},$$

$$Y\xi = \tau^{(w)}(i\gamma^{(w)})(-e^{i\alpha x}), \quad Z\xi = \tau^{(u)}(i\gamma^{(u)})(-e^{i\alpha x}).$$

From this,

$$U = -\tau^{(u)}(\partial_z u)(x,0) - Yu(x,0) = \left[-\tau^{(u)}(i\gamma^{(u)}) - \tau^{(w)}(i\gamma^{(w)})\right]Re^{i\alpha x},$$

$$W = \tau^{(w)}(\partial_z w)(x,0) - Zw(x,0) = \left[\tau^{(w)}(-i\gamma^{(w)}) - \tau^{(u)}(i\gamma^{(u)})\right]Te^{i\alpha x},$$

$$\zeta = -\tau^{(u)}\nu - Y\xi = \left[-\tau^{(u)}(i\gamma^{(u)}) - \tau^{(w)}(i\gamma^{(w)})(-1)\right]e^{i\alpha x},$$

$$\psi = -\tau^{(u)}\nu + Z\xi = \left[-\tau^{(u)}(i\gamma^{(u)}) + \tau^{(u)}(i\gamma^{(u)})(-1)\right]e^{i\alpha x},$$

so that

$$\begin{pmatrix} 1 & F \\ 0 & (1+G) \end{pmatrix} \begin{pmatrix} \left[-\tau^{(u)}(i\gamma^{(u)}) - \tau^{(w)}(i\gamma^{(w)})\right]R \\ \left[\tau^{(w)}(-i\gamma^{(w)}) - \tau^{(u)}(i\gamma^{(u)})\right]T \end{pmatrix} = \begin{pmatrix} \left[-\tau^{(u)}(i\gamma^{(u)}) - \tau^{(w)}(i\gamma^{(w)})(-1)\right] \\ \left[-\tau^{(u)}(i\gamma^{(u)}) + \tau^{(u)}(i\gamma^{(u)})(-1)\right] \end{pmatrix},$$

or

$$\begin{pmatrix} 1 & F \\ 0 & (1+G) \end{pmatrix} \begin{pmatrix} R \\ T \end{pmatrix} = \frac{1}{\tau^{(u)}\gamma^{(u)} + \tau^{(w)}\gamma^{(w)}} \begin{pmatrix} \tau^{(u)}\gamma^{(u)} - \tau^{(w)}\gamma^{(w)} \\ 2\tau^{(u)}\gamma^{(u)} \end{pmatrix},$$

which, when $F \equiv G \equiv 0$, deliver the Fresnel coefficients

$$R = \frac{\tau^{(u)}\gamma^{(u)} - \tau^{(w)}\gamma^{(w)}}{\tau^{(u)}\gamma^{(u)} + \tau^{(w)}\gamma^{(w)}}, \quad T = \frac{2\tau^{(u)}\gamma^{(u)}}{\tau^{(u)}\gamma^{(u)} + \tau^{(w)}\gamma^{(w)}}.$$

APPENDIX F: THREE LAYERS

We close with the three-layer model ($M = 2$) where the governing equations, (15), reduce to

$$\begin{pmatrix} I & F_u + (I+\tilde{F}_u)R^{uu} & (I+\tilde{F}_u)R^{u\ell} & 0 \\ Q & (I+G_u) + \tilde{G}_u R^{uu} & \tilde{G}_u R^{u\ell} & 0 \\ 0 & 0 & I & F_\ell + (I+\tilde{F}_\ell)S \\ 0 & R^{\ell u} & R^{\ell\ell} & (I+G_\ell) + \tilde{G}_\ell S \end{pmatrix} \begin{pmatrix} U \\ V^u \\ V^\ell \\ W \end{pmatrix} = \begin{pmatrix} \zeta_u \\ \psi_u \\ \zeta_\ell \\ \psi_\ell \end{pmatrix},$$

and

$$U = U^{(0),\ell}, \quad V^u = U^{(1),u}, \quad V^\ell = U^{(1),\ell}, \quad W = U^{(2),u},$$

$$\zeta_u = \zeta^{(1)}, \quad \psi_u = \psi^{(1)}, \quad \zeta_\ell = \zeta^{(2)}, \quad \psi_\ell = \psi^{(2)},$$

$$F_u = F^{(1)}, \quad \tilde{F}_u = \tilde{F}^{(1)}, \quad F_\ell = F^{(2)}, \quad \tilde{F}_\ell = \tilde{F}^{(2)},$$
$$G_u = G^{(1)}, \quad \tilde{G}_u = \tilde{G}^{(1)}, \quad G_\ell = G^{(2)}, \quad \tilde{G}_\ell = \tilde{G}^{(2)}$$
$$Y^{(u)} = Y^{(1)}, \quad Z^{(u)} = Z^{(1)}, \quad Y^{(\ell)} = Y^{(2)}, \quad Z^{(\ell)} = Z^{(2)},$$
$$\tau^{(u)} = \tau^{(0)}, \quad \tau^{(v)} = \tau^{(1)}, \quad \tau^{(w)} = \tau^{(2)}.$$

Heeding Remarks A1 and A3, we choose $\{Y^{(u)}, Y^{(\ell)}\}$ such that

$$\begin{aligned} Y_p^{(\ell)} &= \tau^{(w)}(i\gamma_p^{(w)}), \\ Y_p^{(u)} &= \frac{-(\tau^{(v)})^2(\gamma_p^{(v)})^2 S(2h) - \tau^{(v)} Y_p^{(\ell)} C(2h)}{-\tau^{(v)} C(2h) + Y_p^{(\ell)} S(2h)} \\ &= \frac{-(\tau^{(v)})^2(\gamma_p^{(v)})^2 T(2h) - \tau^{(v)}\tau^{(w)}(i\gamma_p^{(w)})}{-\tau^{(v)} + \tau^{(w)}(i\gamma_p^{(w)}) T(2h)}, \end{aligned}$$

where

$$\gamma_p^{(u)} = \gamma_p^{(0)}, \quad \gamma_p^{(v)} = \gamma_p^{(1)}, \quad \gamma_p^{(w)} = \gamma_p^{(2)},$$

and

$$T(z) := \frac{S(z)}{C(z)} = \begin{cases} \tan(\gamma_p^{(m)\prime} z)/\gamma_p^{(m)\prime}, & \gamma_p^{(m)\prime\prime} = 0, \\ z, & \gamma_p^{(m)} = 0, \\ \tanh(\gamma_p^{(m)\prime\prime} z)/\gamma_p^{(m)\prime\prime}, & \gamma_p^{(m)\prime} = 0, \end{cases}$$

so that $S(0) \equiv R^{uu}(0) \equiv 0$. With Remarks A2 and A3 in mind, we select $\{Z^{(u)}, Z^{(\ell)}\}$ such that

$$\begin{aligned} Z_p^{(u)} &= \tau^{(u)}(i\gamma_p^{(u)}), \\ Z_p^{(\ell)} &= \frac{-(\tau^{(v)})^2(\gamma_p^{(v)})^2 S(2h) - \tau^{(v)} Z_p^{(u)} C(2h)}{-\tau^{(v)} C(2h) + Z_p^{(u)} S(2h)} \\ &= \frac{-(\tau^{(v)})^2(\gamma_p^{(v)})^2 T(2h) - \tau^{(v)}\tau^{(u)}(i\gamma_p^{(u)})}{-\tau^{(v)} + \tau^{(u)}(i\gamma_p^{(u)}) T(2h)}, \end{aligned}$$

so that $Q(0) \equiv R^{\ell\ell}(0) \equiv 0$.

We now need to verify the hypotheses of Theorem 2:

1. The first, Hypothesis 1, can be satisfied by simply assuming that the interface deformations, $f^{(u)}$ and $f^{(\ell)}$, are sufficiently smooth.

2. The second requires that we determine the invertibility of $(Y^{(u)} + Z^{(u)})$ and $(Y^{(\ell)} + Z^{(\ell)})$. For this, we require

$$Y_p^{(u)} + Z_p^{(u)} = \frac{-(\tau^{(v)})^2(\gamma_p^{(v)})^2 T(2h) - \tau^{(v)}\tau^{(w)}(i\gamma_p^{(w)})}{-\tau^{(v)} + \tau^{(w)}(i\gamma_p^{(w)})T(2h)} + \tau^{(u)}(i\gamma_p^{(u)}) \neq 0, \tag{F1a}$$

$$Y_p^{(\ell)} + Z_p^{(\ell)} = \tau^{(w)}(i\gamma_p^{(w)}) + \frac{-(\tau^{(v)})^2(\gamma_p^{(v)})^2 T(2h) - \tau^{(v)}\tau^{(u)}(i\gamma_p^{(u)})}{-\tau^{(v)} + \tau^{(u)}(i\gamma_p^{(u)})T(2h)} \neq 0. \tag{F1b}$$

3. The third mandates an investigation of

$$\Delta_p^{(u)} = -\tau^{(u)}(i\gamma_p^{(u)}) - Y_p^{(u)} \neq 0, \tag{F2a}$$

$$\Delta_p^{(w)} = \tau^{(w)}(-i\gamma_p^{(w)}) - Z_p^{(\ell)} \neq 0, \tag{F2b}$$

$$\Delta_p^{(v)} = \left((\tau^{(v)})^2(\gamma_p^{(v)})^2 - Z_p^{(u)}Y_p^{(\ell)}\right)S(2h) + \tau^{(v)}\left(Z_p^{(u)} + Y_p^{(\ell)}\right)C(2h) \neq 0. \tag{F2c}$$

4. The fourth hypothesis asks that we verify that the choices for $Y^{(u)}$ and $Z^{(\ell)}$ can be made. These require that, for all $p \in \mathbf{Z}$,

$$Y_p^{(\ell)} S(2h) \neq \tau^{(v)} C(2h), \tag{F3a}$$

$$Z_p^{(u)} S(2h) \neq \tau^{(v)} C(2h). \tag{F3b}$$

5. Finally, Hypothesis 5 requires that both $(I + G_u)$ and $(I + G_\ell)$ be invertible. In the absence of a current, each of these is trivially invertible as they become the identity. In the presence of a current, these can be guaranteed by demanding that

$$(Y_p^{(u)} + Z_p^{(u)}) + Z_p^{(u)}\left[p^{(u)}Y_p^{(u)} + s^{(u)}\right] \neq 0, \tag{F4a}$$

$$(Y_p^{(\ell)} + Z_p^{(\ell)}) + Z_p^{(\ell)}\left[p^{(\ell)}Y_p^{(\ell)} + s^{(\ell)}\right] \neq 0. \tag{F4b}$$

These are quite intricate formulas even with the simple Drude model we have selected, (4), and we leave these as a constraints to be verified based upon the configuration at hand.

Remark F1. Unfortunately, these four sets of constraints, (F1), (F2), (F3), and (F4), are demands upon the grating structure (layer thickness, h, infinitesimal period, d, permittivities, $\epsilon^{(m)}$, and currents, $\hat{\sigma}^{(m)}$) and the illumination (expressed in $\gamma^{(m)}$) that mandate complicated transcendental functions be nonzero on the integer lattice; an unfathomable labyrinth for even the most gifted Number Theorist. While this state of affairs is not ideal, these do present only nine explicitly verifiable conditions which one could readily check once the physical specifications of the problem are made. It is obvious that this extends rather readily to the $(M + 1)$-layer case save that the number of equations grows linearly in M. Of course, any well-posedness results established for the governing equations as a system of Partial Differential Equations[77] or Integral Equations[65] could also be used to verify these conditions.