Joint Analyticity of the Transformed Field and Dirichlet–Neumann Operator in Periodic Media

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Joint Analyticity (Thesis Defense)

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- Develop a numerical algorithm to record scattered energy in a two-layer periodic structure.
- Prove a theorem on the existence and uniqueness of solutions to a system of partial differential equations which model the interaction of linear waves in periodic layered media.

Overview

Introduction

- 2 Governing Equations
- Bigh–Order Perturbation of Surfaces
- Wave Scattering
- 5 Joint Analyticity of Solutions

Conclusion

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Maxwell's Equations

As a starting point we consider the time-harmonic Maxwell's equations of electromagnetism in a homogeneous region:

 $\nabla \times \mathbf{E} = i\omega\mu_0 \mathbf{H},$ $\nabla \times \mathbf{H} = -i\omega\epsilon_0\epsilon\mathbf{E},$ $\nabla \cdot \mathbf{E} = 0,$ $\nabla \cdot \mathbf{H} = 0.$

- **E** is the electric field, **H** is the magnetic field.
- ϵ_0 and μ_0 represent the permittivity and permeability in vacuum.
- ϵ is the complex permittivity, ω is the frequency.

Two–Dimensional Simplifications

- We choose an interface shaped by z = g(x, y) where the normal is defined by N := (-∂_xg, -∂_yg, 1)^T.
- To obtain two-dimensional solutions, we assume the grating shape is invariant in the y-direction:

$$z = g(x),$$

which implies that the interfacial normal becomes

$$\mathbf{N} = \begin{pmatrix} -\partial_{\mathsf{x}}g\\ 0\\ 1 \end{pmatrix}$$

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The Geometry



A two-layer structure with a periodic interface, z = g(x), separating two material layers, $S^{(u)}$ and $S^{(w)}$.

- We consider a y-invariant, doubly layered structure. The interface z = g(x) is d-periodic so that g(x + d) = g(x).
- A dielectric (with refractive index n^u) occupies the domain above the interface

 $S^{(u)} := \{z > g(x)\}.$

• A material of refractive index n^w is in the lower layer

$$S^{(w)} := \{z < g(x)\}.$$

Incident Radiation



A two-layer structure with a periodic interface, z = g(x), illuminated by plane-wave incidence.

- The structure is illuminated from above by monochromatic plane–wave incident radiation of frequency ω.
- We consider the reduced incident fields

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

where the time dependence $\exp(-i\omega t)$ is removed.

 The scattered radiation is "outgoing," upward propagating in S^(u) and downward propagating in S^(w).

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Governing Equations for Layered Media

- In this 2D setting the time-harmonic Maxwell equations decouple into two scalar Helmholtz problems: Transverse electric (TE) and transverse magnetic (TM) polarizations.
- We define the invariant (y) directions of the scattered (electric or magnetic) fields by {ũ, w̃} in S^(u) and S^(w) and seek outgoing/bounded, periodic solutions of

$$\begin{split} &\Delta \tilde{u} + (k^u)^2 = 0, & z > g(x), \\ &\Delta \tilde{w} + (k^w)^2 = 0, & z < g(x), \\ &\tilde{u} - \tilde{w} = -\tilde{u}^i, & z = g(x), \\ &\partial_N \tilde{u} - \tau^2 \partial_N \tilde{w} = -\partial_N \tilde{u}^i, & z = g(x). \end{split}$$

g(x) is the grating interface, ũⁱ is the incident radiation.
τ² = 1 in TE, τ² = (k^u/k^w)² in TM.
For q ∈ {u, w}, k^q = ω/c^q is the wavenumber.

Governing Equations Without Phase

• We further factor out the phase $\exp(i\alpha x)$ from the fields \tilde{u} and \tilde{w}

$$u(x,z) = e^{-i\alpha x} \tilde{u}(x,z), \quad w(x,z) = e^{-i\alpha x} \tilde{w}(x,z).$$

 With these, our governing equations consist of outgoing/bounded, periodic solutions of

$$\begin{split} &\Delta u + 2i\alpha \partial_x u + (\gamma^u)^2 u = 0, & z > g(x), \\ &\Delta w + 2i\alpha \partial_x w + (\gamma^w)^2 w = 0, & z < g(x), \\ &u - w = \zeta, & z = g(x), \\ &\partial_N u - i\alpha (\partial_x g) u - \tau^2 \left[\partial_N w - i\alpha (\partial_x g) w \right] = \psi, & z = g(x). \end{split}$$

• $\alpha = k^u \sin(\theta)$, and for $q \in \{u, w\}, \gamma^q = k^q \cos(\theta)$.

Artificial Boundaries

• To truncate the bi-infinite problem domain to one of finite size we choose values *a* and *b* such that

$$a>\left|g\right|_{\infty},\quad -b<-\left|g\right|_{\infty},$$

and define the artificial boundaries $\{z = a\}$ and $\{z = -b\}$.

 In {z > a} the Rayleigh expansions tell us that upward propagating solutions of the Helmholtz equation are

$$u(x,z) = \sum_{p=-\infty}^{\infty} \hat{a}_p e^{i\tilde{p}x+i\gamma_p^u z}.$$

• With this we can define the Transparent Boundary Conditions in the following way: we rewrite the solution in the upper layer as

$$u(x,z) = \sum_{p=-\infty}^{\infty} \left(\hat{a}_p e^{j\gamma_p^u a}\right) e^{j\tilde{p}x + i\gamma_p^u (z-a)} = \sum_{p=-\infty}^{\infty} \hat{\xi}_p e^{j\tilde{p}x + i\gamma_p^u (z-a)}.$$

Transparent Boundary Conditions

We then observe that

$$\partial_z u(x,a) = \sum_{p=-\infty}^{\infty} (i\gamma_p^u) \hat{\xi}_p e^{i\tilde{p}x} =: T^u[\xi(x)],$$

which defines the order-one Fourier multiplier T^{u} .

• A similar procedure in the lower layer shows that we can write

$$\partial_z w(x,-b) = \sum_{p=-\infty}^{\infty} (-i\gamma_p^w) \hat{\psi}_p e^{i\tilde{p}x} =: T^w[\psi(x)],$$

for the order–one Fourier multiplier T^w .

Upward and Downward Propagating Solutions

• From these we state that upward-propagating solutions of the upper layer satisfy the Transparent Boundary Condition at *z* = *a*

$$\partial_z u(x,a) - T^u[u(x,a)] = 0, \quad z = a.$$

• Similarly, downward-propagating solutions in the lower layer satisfy the Transparent Boundary Condition at z = -b

$$\partial_z w(x,-b) - T^w[w(x,-b)] = 0, \quad z = -b.$$

Full Governing Equations

With these we now state the full set of governing equations as

$$\begin{split} &\Delta u + 2i\alpha\partial_{x}u + (\gamma^{u})^{2}u = 0, & z > g(x), \\ &\Delta w + 2i\alpha\partial_{x}w + (\gamma^{w})^{2}w = 0, & z < g(x), \\ &u - w = \zeta, & z = g(x), \\ &\partial_{N}u - i\alpha(\partial_{x}g)u - \tau^{2}[\partial_{N}w - i\alpha(\partial_{x}g)w] = \psi, & z = g(x), \\ &\partial_{z}u(x,a) - T^{u}[u(x,a)] = 0, & z = a, \\ &\partial_{z}w(x,-b) - T^{w}[w(x,-b)] = 0, & z = -b, \\ &u(x+d,z) = u(x,z), & w(x+d,z) = w(x,z). \end{split}$$

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Domain Decomposition Method

• We now write our governing equations in terms of surface quantities. For this we define the Dirichlet traces and their (outward) Neumann counterparts

$$U(x) := u(x, g(x)), \quad \tilde{U}(x) := -\partial_N u(x, g(x)),$$

$$W(x) := w(x, g(x)), \quad \tilde{W}(x) := \partial_N w(x, g(x)),$$

• In terms of these our full governing equations are equivalent to the pair of boundary conditions,

$$\begin{aligned} & U - W = \zeta, \\ & -\tilde{U} - (i\alpha)(\partial_{x}g)U - \tau^{2}\left[\tilde{W} - (i\alpha)(\partial_{x}g)W\right] = \psi. \end{aligned}$$

• The set of two equations and four unknowns can be closed by noting that the pairs $\{U, \tilde{U}\}$ and $\{W, \tilde{W}\}$ are connected, e.g., by DNOs

$$G: U o ilde{U}, \quad J: W o ilde{W}.$$

Interfacial Reformulation

The interfacial reformulation of our governing equations becomes

AV = R,

where

$$\mathbf{A} = \begin{pmatrix} I & -I \\ G + (\partial_{x}g)(i\alpha) & \tau^{2}J - \tau^{2}(\partial_{x}g)(i\alpha) \end{pmatrix},$$
$$\mathbf{V} = \begin{pmatrix} U \\ W \end{pmatrix}, \quad \mathbf{R} = \begin{pmatrix} \zeta \\ -\psi \end{pmatrix}.$$

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Numerical Methods

- A variety of numerical algorithms have been devised for the simulation of these problems including Finite Difference, Finite Element, and Spectral Element methods.
- These methods suffer from the requirement that they discretize the full volume of the problem domain.
- We advocate the use of surface methods, especially the High–Order Perturbation of Surfaces (HOPS) methods:
 - provide the solution at the interface.
 - only discretize the layer interfaces.
 - are highly accurate, rapid, and robust.
- The HOPS methods are based on the foundational contributions of
 - Field Expansion (FE) method: Bruno & Reitich (1993).
 - Transformed Field Expansion (TFE) method: Nicholls & Reitich (1999).

Boundary and Frequency Perturbations

- We take a perturbative approach which makes two smallness assumptions:
 - **1** Boundary Perturbation: $g(x) = \varepsilon f(x), \ \varepsilon \in \mathbf{R}, \ \varepsilon \ll 1$,
 - 2 Frequency Perturbation: $\omega = (1 + \delta)\underline{\omega}, \delta \in \mathbf{R}, \delta \ll 1$.

The second of these assumptions has the following important consequences

$$k^q = (1+\delta)\underline{k}^q, \quad \alpha = (1+\delta)\underline{\alpha}, \quad \gamma^q = (1+\delta)\underline{\gamma}^q,$$

for $q \in \{u, w\}$.

Transformed Field Expansions Method

- The method of Transformed Field Expansions (TFE) proceeds a domain-flattening change of variables prior to perturbation expansion.
- Focusing on the upper layer, the change of variable is

$$x' = x$$
, $z' = a\left(rac{z-g(x)}{a-g(x)}
ight)$,

which maps the perturbed domain $\{g(x) < z < a\}$ to the separable domain $\{0 < z' < a\}$.

 A similar transformation occurs in the lower layer where the perturbed domain $\{-b < z < g(x)\}$ becomes $\{-b < z' < 0\}$.

Perturbation Expansions

- Provided f is sufficiently smooth, we will later show we will show the joint analytic dependence of $\mathbf{A} = \mathbf{A}(\varepsilon, \delta)$ and $\mathbf{R} = \mathbf{R}(\varepsilon, \delta)$ upon ε and δ , will induce a jointly analytic solution, $\mathbf{V} = \mathbf{V}(\varepsilon, \delta)$.
- In this case we may expand

$$\{\mathbf{A},\mathbf{V},\mathbf{R}\}(\varepsilon,\delta)=\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\{\mathbf{A}_{n,m},\mathbf{V}_{n,m},\mathbf{R}_{n,m}\}\varepsilon^{n}\delta^{m},$$

and a calculation reveals that at every perturbation order (n, m), we can find the $\mathbf{V}_{n,m}$ by solving

$$\mathbf{A}_{0,0}\mathbf{V}_{n,m} = \mathbf{R}_{n,m} - \sum_{\ell=0}^{n-1} \mathbf{A}_{n-\ell,0}\mathbf{V}_{\ell,m} - \sum_{r=0}^{m-1} \mathbf{A}_{0,m-r}\mathbf{V}_{n,r} - \sum_{\ell=0}^{n-1} \sum_{r=0}^{m-1} \mathbf{A}_{n-\ell,m-r}\mathbf{V}_{\ell,r}.$$

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Order (n, m)

• A brief inspection of the formulas for **A** and **R**, reveals that

$$\begin{split} \mathbf{A}_{0,0} &= \begin{pmatrix} I & -I \\ G_{0,0} & \tau^2 J_{0,0} \end{pmatrix}, \\ \mathbf{A}_{n,m} &= \begin{pmatrix} 0 & 0 \\ G_{n,m} & \tau^2 J_{n,m} \end{pmatrix} \\ &+ \delta_{n,1} \left\{ 1 + \delta_{m,1} \right\} (\partial_x f) (i\underline{\alpha}) \begin{pmatrix} 0 & 0 \\ 1 & -\tau^2 \end{pmatrix}, \quad n \neq 0 \text{ or } m \neq 0, \\ \mathbf{R}_{n,m} &= \begin{pmatrix} \zeta_{n,m} \\ -\psi_{n,m} \end{pmatrix}. \end{split}$$

• $\delta_{n,m}$ is the Kronecker delta function and the forms for $\zeta_{n,m}$ and $\psi_{n,m}$ are known.

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Numerical Approximation

• In our approximation we begin by truncating the Taylor series

$$\{\mathbf{A}, \mathbf{V}, \mathbf{R}\}(\varepsilon, \delta) \approx \{\mathbf{A}^{N,M}, \mathbf{V}^{N,M}, \mathbf{R}^{N,M}\}(\varepsilon, \delta)$$
$$:= \sum_{n=0}^{N} \sum_{m=0}^{M} \{\mathbf{A}_{n,m}, \mathbf{V}_{n,m}, \mathbf{R}_{n,m}\} \varepsilon^{n} \delta^{m},$$

where we must specify (i.) how the forms $\mathbf{A}_{n,m}$ are simulated, and (ii.) how the operator $\mathbf{A}_{0,0}$ is to be inverted.

- Regarding the forms A_{n,m}, these boil down to the (n, m)-th corrections of the DNOs G and J, respectively, in a Taylor series expansion of each jointly in ε and δ. We will simulate these numerically.
- The inversion of **A**_{0,0} will follow from the proof of existence and uniqueness.

A Fourier/Chebyshev Collocation Discretization

• To show how we simulate **A**_{*n*,*m*}, we will focus on the upper layer DNO, *G*. We begin by approximating

$$u(x,z;\varepsilon,\delta) \approx u^{N,M}(x,z;\varepsilon,\delta) := \sum_{n=0}^{N} \sum_{m=0}^{M} u_{n,m}(x,z)\varepsilon^{n}\delta^{m}.$$

• Each of these $u_{n,m}(x, z)$ are then simulated by a Fourier–Chebyshev approach which posits the form

$$u_{n,m}(x,z) pprox u_{n,m}^{N_x,N_z}(x,z) := \sum_{p=-N_x/2}^{N_x/2-1} \sum_{\ell=0}^{N_z} \hat{u}_{n,m,p,\ell} e^{i\tilde{p}x} T_\ell\left(\frac{2z-a}{a}\right),$$

where T_{ℓ} is the ℓ -th Cheybshev polynomial. The unknowns $\hat{u}_{n,m,p,\ell}$ are recovered by the collocation approach.

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Equispaced Grid Points / Collocation Points

As mentioned previously, the Fourier–Chebyshev approach posits the form

$$u_{n,m}(x,z) \approx u_{n,m}^{N_x,N_z}(x,z) := \sum_{p=-N_x/2}^{N_x/2-1} \sum_{\ell=0}^{N_z} \hat{u}_{n,m,p,\ell} e^{i\tilde{p}x} T_\ell\left(\frac{2z-a}{a}\right)$$

- More specifically, our HOPS/AWE algorithm requires $N_x \times N_z$ unknowns at every perturbation order, (n, m).
- As our problem is *d*-periodic in the lateral direction, we will expand using a Fourier spectral method where we require *N*_x equally-spaced gridpoints.
- However, our problem is not z-periodic, so our strategy is to use a Chebyshev spectral method in the vertical direction. For this, we select $N_z + 1$ collocation points.

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Simulation of DNOs

• With this we can simulate the upper layer DNO through

$$G(x;\varepsilon,\delta) \approx G^{N,M}(x;\varepsilon,\delta) := \sum_{n=0}^{N} \sum_{m=0}^{M} G_{n,m}(x)\varepsilon^{n}\delta^{m}.$$

Here

$$G_{n,m}(x) pprox G_{n,m}^{N_x}(x) := \sum_{p=-N_x/2}^{N_x/2-1} \hat{G}_{n,m,p} e^{i\tilde{p}x},$$

and the $\hat{G}_{n,m,p}$ are recovered from the $\hat{u}_{n,m,p,\ell}$.

• We apply the same procedure to the lower layer DNO, J.

The Rayleigh Expansions

• Previously, we observed that solutions to the Helmholtz problem in the upper layer can be expressed in terms of Rayleigh expansions

$$u(x,z) = \sum_{p=-\infty}^{\infty} \hat{a}_p e^{i\tilde{p}x+i\gamma_p^u z}.$$

• For $p \in \mathbf{Z}$ we define

$$\tilde{p} := \frac{2\pi p}{d}, \quad \alpha_p := \alpha + \tilde{p}, \quad \gamma_p^u := \begin{cases} \sqrt{(k^u)^2 - \alpha_p^2}, & p \in \mathcal{U}^u, \\ i\sqrt{\alpha_p^2 - (k^u)^2}, & p \notin \mathcal{U}^u. \end{cases}$$

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Propagating Modes

We have

$$\gamma_p^u := \begin{cases} \sqrt{(k^u)^2 - \alpha_p^2}, & p \in \mathcal{U}^u, \\ i \sqrt{\alpha_p^2 - (k^u)^2}, & p \notin \mathcal{U}^u, \end{cases} \quad \mathcal{U}^u := \left\{ p \in \mathbf{Z} \mid \alpha_p^2 < (k^u)^2 \right\}.$$

- Components of u(x, z) corresponding to p ∈ U^u propagate away from the layer interface, while those not in this set decay exponentially from z = g(x).
- The latter are called evanescent waves while the former are propagating (defining the set of propagating modes U^u) and carry energy away from the grating.

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The Reflectivity Map

• With this in mind one defines the efficiencies

$$e^u_p := \left(\gamma^u_p/\gamma^u
ight) \left|\hat{a}_p
ight|^2, \quad p \in \mathcal{U}^u,$$

• and the Reflectivity Map as the sum of efficiencies in the upper layer

$$R:=\sum_{p\in\mathcal{U}^u}e_p^u.$$

• Similar quantities can be defined in the lower layer, and with these the principle of conservation of energy can be stated for structures composed entirely of dielectrics

$$\sum_{m{p}\in\mathcal{U}^u}e^u_{m{p}}+ au^2\sum_{m{p}\in\mathcal{U}^w}e^w_{m{p}}=1.$$

Energy Defect

• In this situation a useful diagnostic of convergence for a numerical scheme is the "Energy Defect"

$$D := 1 - \sum_{p \in \mathcal{U}^u} e^u_p - \tau^2 \sum_{p \in \mathcal{U}^w} e^w_p,$$

which should be zero for a purely dielectric structure.

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Rayleigh Singularities (Wood's Anomalies)

• The Taylor series expansion for γ_{P}^{q} , $q \in \{u, w\}$, is

$$\gamma_p^q = \gamma_p^q(\delta) = \sum_{m=0}^{\infty} \gamma_{p,m}^q \delta^m.$$

• Recalling $\gamma_p^q = (1 + \delta) \underline{\gamma}_p^q$, $k^q = (1 + \delta) \underline{k}^q$ one finds

$$\underline{\alpha}_{p}^{2} + (\underline{\gamma}_{p}^{q})^{2} = (\underline{k}^{q})^{2}.$$

- When $\underline{\gamma}_{p}^{q} = 0$, the Taylor series expansion of $\gamma_{p}^{q}(\delta)$ is invalid. A Rayleigh singularity (or Wood's anamoly) occurs when $\underline{\alpha}_{p}^{2} = (\underline{k}^{q})^{2}$.
- Therefore, the permissible values of δ are constrained by this.

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The Domain of Analyticity

- To guide our computations we explore this restriction on δ .
- In the upper layer, Rayleigh singularities occur when $\underline{\alpha}_p^2 = (\underline{k}^u)^2$ which implies

$$\underline{\omega} = \pm \frac{c_0}{n^u} \left\{ \underline{\alpha} + \frac{2\pi p}{d} \right\}, \quad \text{for any } p \in \mathbf{Z}.$$

In the interest of maximizing our choice of δ we select a "mid-point" value of <u>ω</u> which is as far away as possible from consecutive Rayleigh singularities

$$\underline{\omega}_q := rac{c_0}{n^u} \left\{ \underline{lpha} + rac{2\pi(q+1/2)}{d}
ight\}.$$

• Our algorithm will expand in δ at the "mid-points" away from Rayleigh singularities.

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Simulation: Reflectivity Map for Vacuum over Dielectric



Figure 1: The Reflectivity Map, $R(\varepsilon, \delta)$, and energy defect D computed with our HOPS/AWE algorithm with Taylor summation. We set N = M = 16 and the parameter choices were $\alpha = 0$, $n^u = 1$, and $n^w = 1.1$.

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Simulation: Reflectivity Map for Vacuum over Silver and Gold



Figure 2: The Reflectivity Map, $R(\varepsilon, \delta)$, for silver (left) and gold (right) with Padé summation. We set N = M = 15 and parameter choices were $\alpha = 0$, $n^{u} = 1$, $n^{w} = 0.05 + 2.275i$ (left) and $n^{w} = 1.48 + 1.883i$ (right).

 The interfacial reformulation of our governing equations is AV = R and the formulas for A and R at order (n, m) are

$$\begin{split} \mathbf{A}_{0,0} &= \begin{pmatrix} I & -I \\ G_{0,0} & \tau^2 J_{0,0} \end{pmatrix}, \\ \mathbf{A}_{n,m} &= \begin{pmatrix} 0 & 0 \\ G_{n,m} & \tau^2 J_{n,m} \end{pmatrix} \\ &+ \delta_{n,1} \left\{ 1 + \delta_{m,1} \right\} (\partial_x f) (i\underline{\alpha}) \begin{pmatrix} 0 & 0 \\ 1 & -\tau^2 \end{pmatrix}, \quad n \neq 0 \text{ or } m \neq 0, \\ \mathbf{R}_{n,m} &= \begin{pmatrix} \zeta_{n,m} \\ -\psi_{n,m} \end{pmatrix}. \end{split}$$

- We will now establish the existence, uniqueness, and analyticity of solutions to **AV** = **R**.
- To accomplish this we will show the joint analytic dependence of A = A(ε, δ) and R = R(ε, δ) upon ε and δ, will induce a jointly analytic solution, V = V(ε, δ).

Theorem: Analyticity of Solutions [Kehoe, Nicholls 22]

Theorem

Given two Banach spaces X and Y, suppose that

H1 $\mathbf{R}_{n,m} \in Y$ for all $n, m \ge 0$, and there exists constants $B_R > 0, C_{R,N} > 0, C_{R,M} > 0, D_R > 0$ such that

 $\|\mathbf{R}_{n,m}\|_{Y} \leq C_{R,N}C_{R,M}B_{R}^{n}D_{R}^{m},$

H2 $\mathbf{A}_{n,m}$: $X \to Y$ for all $n, m \ge 0$, and there exists constants $B_A > 0, C_{A,N} > 0, C_{A,M} > 0, D_A > 0$ such that

$$\|\mathbf{A}_{n,m}\|_{X\to Y} \leq C_{A,N}C_{A,M}B_A^n D_A^m,$$

H3 $\mathbf{A}_{0,0}^{-1}$: $Y \to X$ for all $n, m \ge 0$, and there exists a constant $C_e > 0$ such that

$$\|\mathbf{A}_{0,0}^{-1}\|_{Y o X} \leq C_e$$

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Theorem: Analyticity of Solutions (Continued)

Theorem (continued)

Then, given an integer $s \ge 0$, if $f \in C^{s+2}([0, d])$ then the linear system $\mathbf{AV} = \mathbf{R}$ has a unique solution, $\sum_{n,m} \mathbf{V}_{n,m} \varepsilon^n \delta^m$, and there exist constants B, C, D > 0 such that

$$\|\mathbf{V}_{n,m}\|_{X^s} \leq CB^n D^m,$$

for all $n, m \ge 0$. This implies that for any $0 \le \rho, \sigma < 1$, $\sum_{n,m} \mathbf{V}_{n,m} \varepsilon^n \delta^m$ converges for all ε such that $B\varepsilon < \rho$, i.e., $\varepsilon < \rho/B$ and all δ such that $D\delta < \sigma$, i.e., $\delta < \sigma/D$.

Sketch of Proof

• First, we define the vector-valued spaces for $s \ge 0$

$$\begin{split} X^{s} &:= \left\{ \left. \mathbf{V} = \begin{pmatrix} U \\ W \end{pmatrix} \right| U, W \in H^{s+3/2}([0,d]) \right\}, \\ Y^{s} &:= \left\{ \left. \mathbf{R} = \begin{pmatrix} \zeta \\ -\psi \end{pmatrix} \right| \zeta \in H^{s+3/2}([0,d]), \psi \in H^{s+1/2}([0,d]) \right\}. \end{split}$$

• These have the norms

$$\|\mathbf{V}\|_{X^{s}}^{2} = \left\| \begin{pmatrix} U \\ W \end{pmatrix} \right\|_{X^{s}}^{2} := \|U\|_{H^{s+3/2}}^{2} + \|W\|_{H^{s+3/2}}^{2},$$
$$\|\mathbf{R}\|_{Y^{s}}^{2} = \left\| \begin{pmatrix} \zeta \\ -\psi \end{pmatrix} \right\|_{Y^{s}}^{2} := \|\zeta\|_{H^{s+3/2}}^{2} + \|\psi\|_{H^{s+1/2}}^{2}.$$

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Hypothesis H1: Consider the Banach spaces X = X^s and Y = Y^s.
 Our first task is to show that

$$\mathbf{R}_{n,m} = \begin{pmatrix} \zeta_{n,m} \\ -\psi_{n,m} \end{pmatrix},$$

is bounded in Y^s for any $s \ge 0$.

• Upon performing the boundary/frequency perturbations, we define

$$\mathcal{E}(x;\varepsilon,\delta):=e^{-i(1+\delta)\underline{\gamma}^{u}\varepsilon f(x)},$$

so that

$$\begin{split} \zeta(x) &= \zeta(x;\varepsilon,\delta) = -\mathcal{E}(x;\varepsilon,\delta),\\ \psi(x) &= \psi(x;\varepsilon,\delta) = \left\{ i(1+\delta)\underline{\gamma}^u + i(1+\delta)\underline{\alpha}(\varepsilon\partial_x f) \right\} \mathcal{E}(x;\varepsilon,\delta). \end{split}$$

• A joint Taylor expansion followed by an induction argument shows that $\|\zeta_{n,m}\|_{H^{s+3/2}}$ and $\|\psi_{n,m}\|_{H^{s+1/2}}$ are bounded. Therefore, $\|\mathbf{R}_{n,m}\|_{Y^s}$ is bounded.

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• Hypothesis H2: Our next task is to show that the operators $G_{n,m}$ and $J_{n,m}$ in

$$\mathbf{A}_{n,m}^{\prime} = \begin{pmatrix} 0 & 0 \\ G_{n,m} & \tau^2 J_{n,m} \end{pmatrix},$$

for the Taylor series expansions of the DNOs satisfy the appropriate bounds.

- For brevity, we will outline our technique for the Taylor expansion of the upper layer DNO, *G*_{*n*,*m*}.
- Lemma (Algebra Property): Given an integer s ≥ 0, there exists a constant M = M(s) such that if f ∈ C^s([0, d]) and u ∈ H^s([0, d]× [0, a]) then

$$\|fu\|_{H^{s}} \leq \mathcal{M} \|f\|_{C^{s}} \|u\|_{H^{s}}.$$

• The bound on $G_{n,m}$ follows from

Applying the boundary and frequency perturbations followed by the TFE method results in the upper layer DNO problem

$$\begin{split} \Delta u_{n,m} &+ 2i\underline{\alpha}\partial_{x}u_{n,m} + (\underline{\gamma}^{u})^{2}u_{n,m} = F_{n,m}(x,z), & 0 < z < a, \\ u_{n,m}(x,0) &= U_{n,m}(x), & z = 0, \\ \partial_{z}u_{n,m}(x,a) - T^{u}[u_{n,m}(x,a)] &= P_{n,m}(x), & z = a, \end{split}$$

where

$$G_{n,m}(f) = -\partial_z u_{n,m}(x,0) + H_{n,m}(x).$$

- **2** The Algebra Property establishes bounds on the non-homogeneous terms $F_{n,m}$, $P_{n,m}$, and $H_{n,m}$.
- With these, the Elliptic Estimate and an induction argument establishes

$$\|u_{n,m}\|_{H^{s+2}} \leq KB^n D^m,$$

for constants K, B, D > 0. This shows that the transformed upper field is jointly analytic with respect a boundary/frequency perturbation.

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• The bound on $G_{n,m}$ follows from (continued)

The bound on the upper layer DNO

$$G_{n,m}(f) = -\partial_z u_{n,m}(x,0) + H_{n,m}(x),$$

then follows from the joint analyticity of the transformed upper field, $u_{n,m}$, an induction argument, and the fact that $H_{n,m}$ is bounded. One finds

$$\|G_{n,m}\|_{H^{s+1/2}} \leq \tilde{K}\tilde{B}^n\tilde{D}^m,$$

for constants $\tilde{K}, \tilde{B}, \tilde{D} > 0$ which shows that $G_{n,m}$ is bounded. A similar argument works for the lower layer DNO, $J_{n,m}$, so that $\mathbf{A}_{n,m}$ is bounded and **H2** is satisfied.

Hypothesis H3: Our final task is show that A⁻¹_{0,0} exists and the estimates and mapping properties of A⁻¹_{0,0} hold where A_{0,0} is defined by

$$\mathbf{A}_{0,0} = \begin{pmatrix} I & -I \\ G_{0,0} & \tau^2 J_{0,0} \end{pmatrix}$$

We define the operator

$$\Delta := G_{0,0} + \tau^2 J_{0,0} = (-i\gamma_D^u) + \tau^2 (-i\gamma_D^w),$$

so that Δ^{-1} exists and that

$$\Delta: H^{s+3/2} \to H^{s+1/2}, \quad \Delta^{-1}: H^{s+1/2} \to H^{s+3/2},$$

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• Next, we write generic elements of X^s and Y^s as

$$\mathbf{V} = \begin{pmatrix} U \\ W \end{pmatrix} \in X^s, \quad \mathbf{R} = \begin{pmatrix} \zeta \\ -\psi \end{pmatrix} \in Y^s.$$

• Using the definitions of the norms of X^s and Y^s we find

$$\|\mathbf{A}_{0,0}\mathbf{V}\|_{Y^{s}}^{2} \leq C \|\mathbf{V}\|_{X^{s}}^{2},$$

so that $\mathbf{A}_{0,0}$ maps X^s to Y^s . Furthermore,

$$\left\| \mathbf{A}_{0,0}^{-1} \mathbf{R} \right\|_{X^{s}}^{2} \leq C_{\Delta^{-1}} \left\| \mathbf{R} \right\|_{Y^{s}}^{2},$$

which shows that $\mathbf{A}_{0,0}^{-1}$ maps Y^s to X^s .

• Thus, $\|\mathbf{A}_{0,0}^{-1}\|_{Y^s \to X^s}$ is bounded and the mapping properties hold.

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Conclusion

We seek outgoing/bounded, periodic solutions of the scattering problem

$$\Delta u + 2i\alpha \partial_x u + (\gamma^u)^2 u = 0, \qquad z > g(x),$$

$$\Delta w + 2i\alpha \partial_x w + (\gamma^w)^2 w = 0, \qquad z < g(x),$$

$$u-w=\zeta, \qquad \qquad z=g(x),$$

$$\partial_N u - i\alpha(\partial_x g)u - \tau^2 [\partial_N w - i\alpha(\partial_x g)w] = \psi, \qquad z = g(x).$$

Numerical Algorithm

- DNOs, boundary/frequency perturbations, and COV through TFE
- Joint Taylor expansion followed by Fourier/Chebyshev collocation
- Simulated scattered energy through Reflectivity map
- Ø Joint Analyticity of Solutions
 - Reformulate governing equations in terms of a linear system
 - Sobolev space theory: Algebra Property and Elliptic Estimate

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Future Work

- Extend HOPS/AWE algorithm to multilayered surfaces with different material layers. Introduce a new DNO to handle the intermediate layers.
- Implement parallel programming techniques to handle the computation of the intermediate layers.
- Introduce multiple small perturbation parameters outside of an interfacial perturbation and a frequency perturbation. Extend the proof of analyticity to handle any finite number of perturbation parameters.
- Oevelop techniques to expand around Rayleigh singularities where the Taylor series expansion is invalid.

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