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A HIGH–ORDER PERTURBATION OF ENVELOPES (HOPE) METHOD FOR SCATTERING BY PERIODIC INHOMOGENEOUS MEDIA

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Abstract. The interaction of linear waves with periodic structures arises in a broad range of scientific and engineering applications. For such problems it is often mandatory that numerical simulations be rapid, robust, and highly accurate. With such qualities in mind High–Order Spectral methods are often utilized, and in this paper we describe and test a perturbative method which fits into this class. Here we view the inhomogeneous (but laterally periodic) permittivity as a perturbation of a constant value and pursue (regular) perturbation theory. We demonstrate that not only does this lead to a fast and accurate numerical method, but also that the expansion of the field in this geometric parameter is valid for large deformations (up to topological obstruction). Finally, we show that, if the permittivity deformation is spatially analytic, then so is the field scattered by it.

1. Introduction. The interaction of linear waves with periodic structures arises in applications from across the engineering and physical sciences. Examples can readily be found in acoustics (e.g., underwater acoustics [9], remote sensing [49], and nondestructive testing [47]), electromagnetics (e.g., surface enhanced spectroscopy [32], extraordinary optical transmission [14], cancer therapy [15], and surface plasmon resonance (SPR) biosensing [23, 26, 30, 39]), and elastodynamics (e.g., hazard assessment [20] and full waveform inversion [50]).

Due to the technological importance of these models, all of the classical numerical algorithms have been used to simulate solutions of the governing partial differential equations. This includes the Finite Difference [48, 29], Finite Element [25, 24], Discontinuous Galerkin [22], Spectral Element [11], and Spectral [21, 45, 46] methods. While these are compelling choices, due to their fully volumetric character they feature a large number of unknowns ($N = N_x N_y N_z$ for a three–dimensional simulation) and the need to invert

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enormous, non–symmetric positive definite (SPD) matrices (of dimension $N \times N$). Such characteristics are still challenging the most sophisticated research groups; see, e.g., the discussion in [16, 31].

Turning to SPR sensors, their utility stems from two characteristics of an SPR, namely (i.) its extremely strong response and (ii.) its quite sensitive nature. Indeed, over the range of 10–50 nanometers in incident wavelength the reflected energy can fall from nearly 100 % to 10 % (or even 1 %) before returning to almost 100 %. Clearly, to simulate such configurations with fidelity a numerical algorithm should be not only extremely accurate, but also robust and rapid. For this reason we will focus upon High–Order Spectral (HOS) methods [21, 45, 46] which can deliver precisely this behavior.

For the problem of scattering by homogeneous layers it is clearly wasteful to discretize the full bulk of each layer and sophisticated solvers settle for interfacial unknowns with the knowledge that information inside the layers can readily be computed from appropriate integral formulas. Boundary element (BEM) [44] and boundary integral (BIM) [10, 27] methods are foremost among such methodologies and can produce spectrally accurate solutions in a fraction of the time of their volumetric competitors.

The author has investigated a related class of algorithms ("High–Order Perturbation of Surfaces"–HOPS) where the (periodic) layer interfaces, $\{z = a_m + g_m(x, z)\}$, are viewed as perturbations, $g_m(x, y) = \varepsilon f_m(x, y)$, of flat interfaces, $\{z = a_m\}$, and the governing equations are treated by (regular) perturbation theory. This viewpoint has the advantage that the (single) dense, non–SPD BEM/BIM solve (requiring sophisticated quadrature rules, singularity treatment, and Green function quasiperiodization) is replaced by a sequence of trivial flat–interface solves. In addition, once the perturbation calculation is completed, the scattering of waves by a *family* of structures, parameterized by ε_m, can be rapidly computed by simple summation.

However, such surface approaches are not applicable for structures with more general permittivities, $\epsilon(x, y, z)$, which do not have layered structure. In this work we follow the approach of Feng, Lin, and Lorton [18, 19] and adopt a perturbative philosophy akin to that of the HOPS algorithm in that we consider such a permittivity as a perturbation of a trivial one, e.g.,

$$\epsilon(x, y, z) = \bar{\epsilon} + \tilde{\delta} E(x, y, z), \quad \bar{\epsilon} \in \mathbf{R}, \quad E(x + d_x, y + d_y, z) = E(x, y, z),$$

where E is a permittivity "envelope," and again conduct (regular) perturbation theory. With this point of view we denote the resulting algorithm a "High–Order Perturbation of Envelopes" (HOPE) scheme. Feng, Lin, and Lorton focused upon strongly elliptic equations [18] and the Helmholtz problem in Transverse Electric (TE) polarization [19], each with stochastic perturbations, E. In contrast, we consider both TE and TM (Transverse Magnetic) polarization with *deterministic* envelopes in order to provide a novel methodology which should have computational advantages over general–purpose volumetric solvers in certain configurations, e.g., where the support of E is small or where the set on which E significantly changes is small. One choice which we pursue in this work is an approximate indicator function which is nearly zero/unity to denote the absence/presence of a material. For brevity and clarity of presentation, we focus upon the two–dimensional setting of TE or TM polarization governed by the Helmholtz equation.

We leave the nontrivial details of extending our approach to the fully three–dimensional setting governed by the Maxwell equations for future investigations.

The contribution of the current work is not only a detailed description of the algorithm for both TE and TM polarization supplemented with illuminating computations (very much in the spirit of [18, 19]), but also a new, extensive, and rigorous analysis which justifies the implementation we employ. More specifically, we prove not only that the domain of analyticity of the scattered field in δ can be extended to a neighborhood of the *entire* real axis (up to topological obstruction), but also that this field is *jointly* analytic in parametric and spatial variables provided that $E(x, y, z)$ is spatially analytic.

The rest of the paper is organized as follows. In § 2 we recall the governing equations complete with a discussion of transparent boundary conditions in § 3. We describe the HOPE algorithm in § 4 and begin our theoretical developments with a description of the relevant function spaces in § 5. We state and prove our analytic continuation results in § 6 and our joint analyticity results in § 7. Finally, we describe numerical results in § 8, complete with implementation details in § 8.1 and results for layered media scattering in § 8.2. In Appendix A we record the proof of an involved joint analyticity result, while in Appendix B we give the proof of an intricate elliptic estimate.

2. Governing Equations. We assume a constant permeability equal to that of the vacuum $\mu = \mu_0$ and that there are no currents or sources so that the time–harmonic Maxwell equations become

$$\operatorname{curl}[E] - i\omega\mu_0 H = 0, \quad \operatorname{curl}[H] + i\omega\epsilon E = 0, \tag{2.1}$$

where (E, H) are the electric and magnetic field vectors, respectively, and time dependence of the form $\exp(-i\omega t)$ has been factored out [43, 4]. The d–periodic permittivity is specified as

$$\epsilon = \epsilon(x, z) = \begin{cases} \epsilon^{(u)}, & z > h, \\ \epsilon^{(v)}(x, z), & -h < z < h, \\ \epsilon^{(w)}, & z < -h, \end{cases}$$

$\epsilon^{(u)}, \epsilon^{(w)} \in \mathbf{R}$, and $\epsilon^{(v)}(x + d, z) = \epsilon^{(v)}(x, z)$. We further specify that

$$\lim_{z \to h-} \epsilon^{(v)}(x, z) = \epsilon^{(u)}, \quad \lim_{z \to (-h)+} \epsilon^{(v)}(x, z) = \epsilon^{(w)},$$

and typically $\epsilon^{(u)} = \epsilon^{(w)}$. With the permittivity of the vacuum ϵ_0 we can define

$$k_0^2 = \omega^2 \epsilon_0 \mu_0 = \omega^2 / c_0^2, \quad (k^{(m)})^2 = \epsilon^{(m)} k_0^2, \quad m \in \{u, v, w\},$$

which also introduces the speed of light, $c_0 = 1/\sqrt{\epsilon_0 \mu_0}$.

This structure is illuminated from above by y–independent plane–wave incident radiation of the form

$$E^{\text{inc}}(x, z) = A \exp(i(\alpha x - \gamma^{(u)} z)), \quad H^{\text{inc}}(x, z) = B \exp(i(\alpha x - \gamma^{(u)} z)),$$
$$\alpha = k^{(u)} \sin(\theta), \quad \gamma^{(u)} = k^{(u)} \cos(\theta), \tag{2.2}$$

where $|A| = |B| = 1$. If this is incident upon a y–invariant structure and the radiation is appropriately polarized, then the fully vectorial Maxwell equations (2.1) can be reduced to one of two scalar, two–dimensional Helmholtz problems. For instance, if

$$A = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad B = \frac{1}{i\omega\mu_0} \begin{pmatrix} i\gamma^{(u)} \\ 0 \\ i\alpha \end{pmatrix},$$

then the transverse component $v = v(x,z)$ of the electric field satisfies the Transverse Electric (TE) Helmholtz equation

$$\frac{1}{\epsilon} \mathrm{div}\left[\nabla v\right] + k_0^2 v = 0.$$

By contrast, if

$$A = -\frac{1}{i\omega\epsilon} \begin{pmatrix} i\gamma^{(u)} \\ 0 \\ i\alpha \end{pmatrix}, \quad B = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix},$$

then the transverse component $v = v(x,z)$ of the magnetic field satisfies the Transverse Magnetic (TM) Helmholtz equation

$$\mathrm{div}\left[\frac{1}{\epsilon}\nabla v\right] + k_0^2 v = 0.$$

In each case we will seek quasiperiodic solutions satisfying [51]

$$v(x+d, z) = \exp(i\alpha d) v(x,z).$$

3. Transparent Boundary Conditions. We now seek to not only rigorously specify the appropriate boundary conditions on solutions in the far–field, but also reduce the infinite domain to one of finite extent. Happily, both can be accomplished with the same formalism [5, 6]. In the upper domain $\{z > h\}$ we ask for solutions which are the sum of the incident radiation and an upward propagating (reflected) component, e.g.,

$$\begin{aligned} v &= v^{\mathrm{inc}} + v^{\mathrm{refl}} \\ &= \exp(i\alpha x - i\gamma^{(u)} z) + c_0 \exp(i\alpha x + i\gamma^{(u)}(z-h)) + \sum_{p \neq 0} \hat{u}_p \exp(i\alpha_p x + i\gamma_p^{(u)}(z-h)), \end{aligned}$$

[43, 51] where

$$\alpha_p = \alpha + (2\pi/d)p, \quad \gamma_p^{(m)} = \sqrt{\epsilon^{(m)} k_0^2 - \alpha_p^2}, \quad \mathrm{Im}\{\gamma_p^{(m)}\} \geq 0, \quad m \in \{u, w\}.$$

If we set $c_0 = \hat{u}_0 - \exp(-i\gamma^{(u)} h)$, implying $\hat{u}_0 = c_0 + \exp(-i\gamma^{(u)} h)$, then

$$v = \exp(i\alpha x - i\gamma^{(u)} z) - \exp(i\alpha x + i\gamma^{(u)}(z - 2h)) + \sum_{p=-\infty}^{\infty} \hat{u}_p \exp(i\alpha_p x + i\gamma_p^{(u)}(z-h)),$$

and $v(x,h) = u(x)$. It is a simple matter to show that

$$\begin{aligned} \partial_z v = (-i\gamma^{(u)}) \exp(i\alpha x - i\gamma^{(u)} z) - (i\gamma^{(u)}) \exp(i\alpha x + i\gamma^{(u)}(z - 2h)) \\ + \sum_{p=-\infty}^{\infty} (i\gamma_p^{(u)}) \hat{u}_p \exp(i\alpha_p x + i\gamma_p^{(u)}(z-h)), \end{aligned}$$

so that

$$-\partial_z v(x,h) = (i\gamma^{(u)})\exp(i\alpha x - i\gamma^{(u)}h) + (i\gamma^{(u)})\exp(i\alpha x + i\gamma^{(u)}(-h)) + \sum_{p=-\infty}^{\infty}(-i\gamma_p^{(u)})\hat{u}_p\exp(i\alpha_p x).$$

If we define the function

$$\phi(x) := \left(2i\gamma^{(u)}\exp(-i\gamma^{(u)}h)\right)\exp(i\alpha x), \tag{3.1}$$

and the order–one Fourier multiplier (the externally directed Dirichlet–Neumann operator for the Helmholtz equation on $\{z > h\}$)

$$T_u[\psi] := \sum_{p=-\infty}^{\infty}(-i\gamma_p^{(u)})\hat{\psi}_p\exp(i\alpha_p x),$$

then we see that we can express the Upward Propagating Condition (UPC) [1] exactly with the boundary condition

$$-\partial_z v(x,h) - T_u[v(x,h)] = \phi(x).$$

By contrast, in the domain $\{z < -h\}$ we seek a solution which is purely downward propagating (transmitted)

$$v = v^{\text{trans}} = \sum_{p=-\infty}^{\infty}\hat{w}_p\exp(i\alpha_p x - i\gamma_p^{(w)}(z+h)),$$

[43, 51]. Clearly $v(x,h) = w(x)$ and, with the calculation

$$\partial_z v(x,-h) = \sum_{p=-\infty}^{\infty}(-i\gamma_p^{(w)})\hat{w}_p\exp(i\alpha_p x),$$

and the analogous order–one Fourier multiplier (again, the externally directed Dirichlet–Neumann operator for the Helmholtz equation on $\{z < -h\}$)

$$T_w[\psi] := \sum_{p=-\infty}^{\infty}(-i\gamma_p^{(w)})\hat{\psi}_p\exp(i\alpha_p x),$$

we can state the Downward Propagating Condition (DPC) [1] transparently using

$$\partial_z v(x,-h) - T_w[v(x,-h)] = 0.$$

Summarizing all of our conclusions thus far, we settle upon the following problems to solve. In TE polarization we must find a unique solution of

$$\frac{1}{\epsilon^{(v)}(x,z)}\Delta v + k_0^2 v = 0, \qquad -h < z < h, \tag{3.2a}$$

$$-\partial_z v - T_u[v] = \phi, \qquad z = h, \tag{3.2b}$$

$$\partial_z v - T_w[v] = 0, \qquad z = -h, \tag{3.2c}$$

$$v(x+d,z) = \exp(i\alpha d)v(x,z). \tag{3.2d}$$

In TM polarization we seek a unique solution of

$$\operatorname{div}\left[\frac{1}{\epsilon^{(v)}(x,z)}\nabla v\right] + k_0^2 v = 0, \qquad -h < z < h, \tag{3.3a}$$

$$-\partial_z v - T_u[v] = \phi, \qquad z = h, \tag{3.3b}$$

$$\partial_z v - T_w[v] = 0, \qquad z = -h, \tag{3.3c}$$

$$v(x+d,z) = \exp(i\alpha d) v(x,z). \tag{3.3d}$$

4. A High–Order Perturbation of Envelopes Method. At this point there are many approaches available to us for the numerical simulation of solutions to the TE, (3.2), and TM, (3.3), problems stated above. Among these are the classical Finite Difference [48, 29], Finite Element [25, 13, 5, 6], Spectral Element [11], and Spectral Methods [21, 45, 46]. For more details about these and other approaches one can consult one of the many surveys on the topic, e.g. [3].

Rather than pursue one of these standard volumetric approaches, we follow the lead of Feng, Lin, and Lorton [18, 19] and view the problem perturbatively. More specifically, we think of our configuration as a small deviation from a trivial, constant–permittivity, structure,

$$\epsilon^{(v)} = \bar{\epsilon}\,(1 - \delta E) = \bar{\epsilon} - \delta(\bar{\epsilon}E),$$

where $\bar{\epsilon} \in \mathbf{R}$ is a constant, and $\delta \ll 1$ (initially). For future reference (TM polarization) we note that, in this case,

$$\frac{1}{\epsilon^{(v)}} = \frac{1}{\bar{\epsilon}} \sum_{\ell=0}^{\infty} E^{\ell} \delta^{\ell}.$$

In the case of TE polarization it was shown by Feng, Lin, and Lorton [19] that, provided that $E(x,z)$ is smooth enough, the field $v = v(x,z;\delta)$ depends analytically upon δ so that

$$v = v(x,z;\delta) = \sum_{\ell=0}^{\infty} v_\ell(x,z)\delta^\ell, \tag{4.1}$$

converges strongly in a Sobolev space. It is not difficult to show that, upon multiplication of the Helmholtz equation by $\epsilon^{(v)}$, in TE polarization these v_ℓ satisfy

$$\Delta v_\ell + \bar{\epsilon} k_0^2 v_\ell = F_\ell^{(\mathrm{TE})}, \qquad -h < z < h, \tag{4.2a}$$

$$-\partial_z v_\ell - T_u[v_\ell] = \delta_{\ell,0}\phi, \qquad z = h, \tag{4.2b}$$

$$\partial_z v_\ell - T_w[v_\ell] = 0, \qquad z = -h, \tag{4.2c}$$

$$v_\ell(x+d,z) = \exp(i\alpha d) v_\ell(x,z), \tag{4.2d}$$

where $\delta_{\ell,q}$ is the Kronecker delta function, and

$$F_\ell^{(\mathrm{TE})}(x,z) := \bar{\epsilon} E(x,z) k_0^2 v_{\ell-1}(x,z).$$

The situation is not much more difficult in TM polarization where, using the fact that $\bar{\epsilon}$ is constant, the v_ℓ must verify

$$\Delta v_\ell + \bar{\epsilon} k_0^2 v_\ell = F_\ell^{(\mathrm{TM})}, \qquad -h < z < h, \tag{4.3a}$$
$$-\partial_z v_\ell - T_u[v_\ell] = \delta_{\ell,0}\phi, \qquad z = h, \tag{4.3b}$$
$$\partial_z v_\ell - T_w[v_\ell] = 0, \qquad z = -h, \tag{4.3c}$$
$$v_\ell(x+d, z) = \exp(i\alpha d) v_\ell(x, z), \tag{4.3d}$$

where

$$F_\ell^{(\mathrm{TM})}(x, z) := -\sum_{q=0}^{\ell-1} \operatorname{div}\left[E(x,z)^{\ell-q} \nabla v_q(x,z)\right].$$

It is easy to see [51] that the unique solution at order $\ell = 0$, in either polarization, is

$$v_0(x, z) = \exp(i(\alpha x - \gamma^{(v)} z)),$$

and a "High–Order Perturbation" scheme can be built upon this where we make the approximation

$$v(x, z) \approx v^L(x, z) := \sum_{\ell=0}^{L} v_\ell(x, z) \delta^\ell.$$

This is pursued in detail in Section 8.

In making the *nature* of the perturbation more precise we can formulate the particular algorithm we pursue in this contribution. We consider an envelope function, $E = E(x, z)$, which indicates the support of the domain inside $\{-h < z < h\}$ where the permittivity is not equal to $\bar{\epsilon}$. For instance, we may choose

$$E = E_{a,b}(z) = E_0 \left\{ \frac{\tanh(w(z-a)) - \tanh(w(z-b))}{2} \right\}, \tag{4.4}$$

with transition sharpness parameter w, which is nearly zero for $-h < z < a - \varepsilon$ and $b + \varepsilon < z < h$, but is almost E_0 on the interval $a + \varepsilon < z < b - \varepsilon$. This function and the resulting permittivity are depicted in Figure 1 (left and right, respectively).

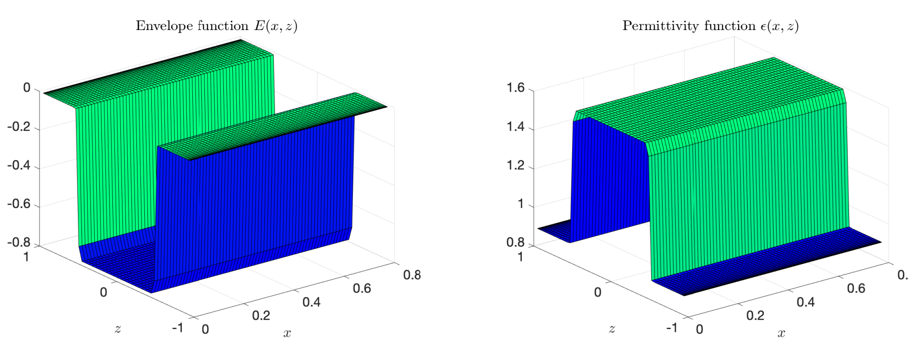

FIG. 1. Plot of $E(x, z)$ (left) and $\epsilon^{(v)}(x, z)$ (right).

With this *form* of perturbation we classify our approach as a "High–Order Perturbation of Envelopes" (HOPE) scheme [33] to distinguish it from the High–Order Perturbation of Surfaces (HOPS) algorithms which the author has advocated in previous work [34, 37, 38, 42, 41].

5. Function Spaces. Before pursuing our theoretical results we specify the function spaces we require for the analysis. For any real $s \geq 0$ we have the classical interfacial quasiperiodic L^2–based Sobolev norm [27]

$$\|U\|_{H^s}^2 := \sum_{p=-\infty}^{\infty} \langle p \rangle^{2s} \left| \hat{U}_p \right|^2, \quad \langle p \rangle^2 := 1 + |p|^2, \quad \hat{U}_p := \frac{1}{d} \int_0^d U(x) e^{i \alpha_p x} \, dx,$$

which gives rise to the quasiperiodic Sobolev space [27]

$$H^s([0,d]) = \left\{ U(x) \in L^2([0,2\pi]) \mid \|U\|_{H^s} < \infty \right\}.$$

The dual of H^s is H^{-s} which can be equivalently defined by the norm above with negative index. We also recall, for any integer $s \geq 0$, the space of s–times continuously differentiable functions with the Hölder norm

$$|f|_{C^s} := \max_{0 \leq \ell \leq s} \left| \partial_x^\ell f \right|_{L^\infty}.$$

We also require, for any integer $s \geq 0$, the volumetric quasiperiodic L^2–based Sobolev norm

$$\|u\|_{H^s}^2 = \sum_{j=0}^{s} \sum_{p=-\infty}^{\infty} \langle p \rangle^{2s-2j} \int_{-h}^{h} \left| \partial_z^j \hat{u}_p(z) \right|^2 \, dz,$$

which defines the quasiperiodic Sobolev class

$$H^s([0,d] \times [-h,h]) = \left\{ u(x,z) \in L^2([0,2\pi] \times [-h,h]) \mid \|U\|_{H^s} < \infty \right\}.$$

As we shall see, the following algebra property will be crucial for our subsequent developments [28, 17, 34].

Lemma 5.1. For any integer $s \geq 0$ and any set $\Omega \subset \mathbf{R}^m$, if $\{f, u\} : \Omega \to \mathbf{C}$, $f \in C^s(\Omega)$, $u \in H^s(\Omega)$, then

$$\|f u\|_{H^s} \leq M(m, s, \Omega) \, |f|_{C^s} \, \|u\|_{H^s},$$

for some universal constant $M(m, s, \Omega)$.

Finally, we will need a particular notion of analytic function.

Definition 5.2. Given an integer $m \geq 0$, the functions $f = f(x)$ and $E = E(x,z)$ are members of the spaces $C_m^\omega([0,d])$ and $C_m^\omega([0,d] \times [-h,h])$, respectively, if they are real analytic and satisfy the estimates

$$\left| \frac{\partial_x^r}{r!} f \right|_{C^m} \leq C_f \frac{A^r}{(r+1)^2}, \quad \left| \frac{\partial_x^r \partial_z^t}{(r+t)!} E \right|_{C^m} \leq C_E \frac{A^r}{(r+1)^2} \frac{D^t}{(t+1)^2}, \quad \forall \, r, t \geq 0,$$

for some $C_f, C_E, A, D > 0$.

The notation C_m^ω defines the space of real analytic functions, C^ω, with radius of analyticity (given by A and D) measured in the C^m norm.

Remark 5.3. Note that the incident radiation function ϕ, (3.1), is clearly real analytic in x and satisfies

$$\left\| \frac{\partial_x^r}{r!} \phi \right\|_{H^{1/2}} \leq C_\phi \frac{A^r}{(r+1)^2}, \quad \forall\, r \geq 0,$$

for some $C_\phi, A > 0$.

Before closing this section we quote an invaluable family of elementary bounds [36, 40].

Lemma 5.4. For any integer $r \geq 0$ there exists a universal constant $S < \infty$ such that the following sums are bounded

$$\sum_{j=0}^{r} \frac{(r+1)^2}{(r-j+1)^2 (j+1)^2} < S, \quad \sum_{j=0}^{r} \sum_{p=0}^{j} \frac{(r+1)^2}{(r-j+1)^2 (j-p+1)^2 (p+1)^2} < S^2.$$

Clearly, changing the entries in the summations by one or two, e.g.,

$$\sum_{j=0}^{r} \frac{r^2}{(r-j+1)^2 (j+1)^2},$$

will not affect the *convergence* of these sums and, among the finite collection of such trivial changes, there is a universal S which works for all.

6. Analytic Continuation. As we mentioned above, in TE polarization the expansion of v in δ, (4.1), was shown to be strongly convergent in an appropriate function space by Feng, Lin, and Lorton [19], provided that $E(x,z)$ is sufficiently smooth. This result justifies our HOPE approach, but only in the case $\delta \ll 1$. The situation of TM polarization or, in either polarization, δ moderate to large is outside the scope of their theory. However, by following the work of the author and Reitich [36] and the author and Taber [40], we can demonstrate the analyticity of the solution for *any* real value of the perturbation parameter (up to topological obstruction). This result is one of analytic continuation and justifies our use of Padé approximation to simulate deformations which are large and/or rough.

To demonstrate this we consider the envelope $E(x,z)$ and show that v depends analytically upon $\tilde{\delta} E(x,z)$ for any $\tilde{\delta} \in \mathbf{R}$. To put this into our current framework we consider fixed $\tilde{\delta}_0 \in \mathbf{R}$ and write

$$E_0(x,z) := \tilde{\delta}_0 E(x,z), \quad \delta = \tilde{\delta} - \tilde{\delta}_0,$$

and we must prove analyticity of the field about $\delta = 0$ as

$$\tilde{\delta} E(x,z) = (\tilde{\delta}_0 + \delta) E(x,z) = E_0(x,z) + \delta E(x,z).$$

Thus, we consider

$$\begin{aligned} \epsilon^{(v)}(x,z) &= \bar{\epsilon} \left\{ 1 - \tilde{\delta} E(x,z) \right\} \\ &= \bar{\epsilon} \left\{ 1 - \tilde{\delta}_0 E(x,z) - \delta E(x,z) \right\} \\ &= \bar{\epsilon} \left\{ 1 - E_0(x,z) \right\} - \delta \bar{\epsilon} E(x,z). \end{aligned}$$

We will now demonstrate that the field $v = v(x, z; E_0, \delta)$ is analytic in δ by showing that the expansion

$$v = v(x, z; E_0, \delta) = \sum_{\ell=0}^{\infty} v_\ell(x, z; E_0)\delta^\ell, \tag{6.1}$$

is convergent. In order to give a unified treatment for both polarizations we write (3.2) and (3.3) as

$$\mathcal{L}v = 0, \qquad -h < z < h, \tag{6.2a}$$

$$-\partial_z v - T_u[v] = \phi, \qquad z = h, \tag{6.2b}$$

$$\partial_z v - T_w[v] = 0, \qquad z = -h, \tag{6.2c}$$

$$v(x + d, z) = \exp(i\alpha d)v(x, z), , \tag{6.2d}$$

where

$$\mathcal{L} := \begin{cases} \rho^{(v)}\Delta + k_0^2, & \text{TE polarization,} \\ \operatorname{div}\left[\rho^{(v)}\nabla\right] + k_0^2, & \text{TM polarization,} \end{cases} \tag{6.2e}$$

and

$$\rho^{(v)}(x, z) := \frac{1}{\epsilon^{(v)}(x, z)}. \tag{6.2f}$$

We note that, from the definition of $\epsilon^{(v)}$ above,

$$1 = \rho^{(v)}\epsilon^{(v)} = \rho^{(v)}\left\{\bar{\epsilon}(1 - E_0(x, z)) - \delta\bar{\epsilon}E(x, z)\right\},$$

we can show that

$$\rho^{(v)} = \rho^{(v)}(x, z; \delta) = \sum_{\ell=0}^{\infty} \rho_\ell^{(v)}(x, z)\delta^\ell,$$

where

$$\rho_0^{(v)}(x, z) = \frac{1}{\bar{\epsilon}(1 - E_0(x, z))}, \tag{6.3a}$$

$$\rho_\ell^{(v)}(x, z) = \frac{E(x, z)}{(1 - E_0(x, z))}\rho_{\ell-1}^{(v)}(x, z) = \bar{\epsilon}E(x, z)\rho_0^{(v)}(x, z)\rho_{\ell-1}^{(v)}(x, z), \qquad \ell > 0. \tag{6.3b}$$

In addition, it can also be demonstrated that

$$\mathcal{L} = \mathcal{L}(\delta) = \sum_{\ell=0}^{\infty} \mathcal{L}_\ell \delta^\ell,$$

where

$$\mathcal{L}_\ell = \begin{cases} \rho_\ell^{(v)}\Delta + k_0^2\delta_{\ell,0}, & \text{TE polarization,} \\ \operatorname{div}\left[\rho_\ell^{(v)}\nabla\right] + k_0^2\delta_{\ell,0}, & \text{TM polarization.} \end{cases}$$

Now it is a simple matter to show that the v_ℓ satisfy

$$\mathcal{L}_0 v_\ell = F_\ell := -\sum_{q=0}^{\ell-1} \mathcal{L}_{\ell-q} v_q, \qquad -h < z < h, \tag{6.4a}$$

$$-\partial_z v_\ell - T_u[v_\ell] = \delta_{\ell,0}\phi, \qquad z = h, \tag{6.4b}$$

$$\partial_z v_\ell - T_w[v_\ell] = 0, \qquad z = -h, \tag{6.4c}$$

$$v_\ell(x + d, z) = \exp(i\alpha d)v_\ell(x, z). \tag{6.4d}$$

For this and later results it is convenient to define the extra smoothness parameter we require in TM polarization

$$\sigma := \begin{cases} 0, & \text{TE polarization,} \\ 1, & \text{TM polarization.} \end{cases}$$

To facilitate later results we require the following elementary analyticity estimate.

LEMMA 6.1. Given any integer $s \geq 0$, if $E_0(x,z), E(x,z) \in C^{s+\sigma}([0,d] \times [-h,h])$, and

$$\left| \frac{1}{\bar{\epsilon}(1-E_0)} \right|_{C^{s+\sigma}} < \frac{1}{a},$$

for some $a > 0$ then

$$|\rho_\ell|_{C^{s+\sigma}} \leq C_\rho B_\rho^\ell, \quad \ell \geq 0,$$

for some $C_\rho, B_\rho > 0$.

Proof. We proceed by induction on ℓ and conclude the case $\ell = 0$ by choosing

$$C_\rho := |\rho_0|_{C^{s+\sigma}} = \left| \frac{1}{\bar{\epsilon}(1-E_0)} \right|_{C^{s+\sigma}} < \frac{1}{a}.$$

Now, assuming the estimate for all $\ell < L$ we examine the size of ρ_L,

$$\begin{aligned} |\rho_L|_{C^{s+\sigma}} &= \left| \left(\frac{E}{1-E_0} \right) \rho_{L-1} \right|_{C^{s+\sigma}} \\ &\leq \left| \frac{1}{1-E_0} \right|_{C^{s+\sigma}} |E|_{C^{s+\sigma}} |\rho_{L-1}|_{C^{s+\sigma}} \\ &\leq \frac{1}{a} |E|_{C^{s+\sigma}} C_\rho B_\rho^{L-1}, \end{aligned}$$

and we are done provided that

$$B_\rho > \frac{\bar{\epsilon} |E|_{C^{s+\sigma}}}{a}.$$

□

We now state the elliptic estimate required for our inductive proof, which is proven in [13, 7, 12, 5]. As observed by these authors, the issue of uniqueness of solutions to these Helmholtz problems, e.g.,

$$\mathcal{L}_0 V = 0, \qquad -h < z < h, \tag{6.5a}$$

$$-\partial_z V - T_u[V] = 0, \qquad z = h, \tag{6.5b}$$

$$\partial_z V - T_w[V] = 0, \qquad z = -h, \tag{6.5c}$$

$$V(x+d, z) = \exp(i\alpha d) V(x,z), \tag{6.5d}$$

which should have only the trivial solution $V \equiv 0$, is a subtle one and certain illuminating frequencies ω will induce non–uniqueness in some configurations. Unfortunately a precise characterization of the set of forbidden frequencies is elusive and all that is known is that it is countable and accumulates at infinity [4]. To accommodate this state of affairs we define the set of permissible configurations

$$\mathcal{P} := \{(\omega, \bar{\epsilon}, E_0) \mid V \equiv 0 \text{ is the unique solution of (6.5)}\}. \tag{6.6}$$

With this we can now state the fundamental result.

THEOREM 6.2. For any integer $s \geq 0$, if $(\omega, \bar{\epsilon}, E_0) \in \mathcal{P}$, $E_0 \in C^{s+\sigma}([0,d] \times [-h,h])$, $F \in H^s([0,d] \times [-h,h])$, $Q \in H^{s+1/2}([0,d])$, and $R \in H^{s+1/2}([0,d])$, then there exists a unique solution of

$$\begin{aligned} &\mathcal{L}_0 V = F, && -h < z < h, \\ &-\partial_z V - T_u[V] = Q, && z = h, \\ &\partial_z V - T_w[V] = R, && z = -h, \\ &V(x+d, z) = \exp(i\alpha d) V(x, z), && \end{aligned}$$

satisfying

$$\|V\|_{H^{s+2}} \leq C_e \left\{ \|F\|_{H^s} + \|Q\|_{H^{s+1/2}} + \|R\|_{H^{s+1/2}} \right\},$$

for some universal constant $C_e > 0$.

We are now in a position to establish the recursive estimate required by our analyticity theory.

LEMMA 6.3. Given any integer $s \geq 0$, if $E_0(x,z), E(x,z) \in C^{s+\sigma}([0,d] \times [-h,h])$, and

$$\left| \frac{1}{\bar{\epsilon}(1 - E_0)} \right|_{C^{s+\sigma}} < \frac{1}{a},$$

for some $a > 0$, and

$$\|v_\ell\|_{H^{s+2}} \leq K B^\ell, \quad \ell < L,$$

for constants $K, B > 0$, then the functions F_ℓ in (6.4a) satisfy

$$\|F_L\|_{H^s} \leq \tilde{C} K B_\rho B^{L-1},$$

for some constant $\tilde{C} > 0$.

Proof. The proof depends upon polarization, but the changes are minor so we focus upon TM and leave TE to the reader. Given our hypotheses we can immediately appeal to Lemma 6.1 so that

$$\begin{aligned}
\|F_L\|_{H^s} &= \left\| - \sum_{q=0}^{L-1} \mathcal{L}_{L-q} v_q \right\|_{H^s} \\
&\leq \sum_{q=0}^{L-1} \left\| \operatorname{div}\left[\rho_{L-q}^{(v)} \nabla v_q \right] \right\|_{H^s} \\
&\leq \sum_{q=0}^{L-1} \left\| \rho_{L-q}^{(v)} \nabla v_q \right\|_{H^{s+\sigma}} \\
&\leq \sum_{q=0}^{L-1} M \left| \rho_{L-q}^{(v)} \right|_{C^{s+\sigma}} \|\nabla v_q\|_{H^{s+\sigma}} \\
&\leq \sum_{q=0}^{L-1} M C_\rho B_\rho^{L-q} \|v_q\|_{H^{s+2}} \\
&\leq \sum_{q=0}^{L-1} M C_\rho B_\rho^{L-q} K B^q \\
&\leq K C_\rho M B_\rho B^{L-1} \sum_{q=0}^{L-1} \left(\frac{B_\rho}{B} \right)^{L-1-q} \\
&\leq K C_\rho M B_\rho B^{L-1} \left(\frac{1}{1-\theta} \right),
\end{aligned}$$

where we have defined $\theta := B_\rho / B$ and we select

$$B > B_\rho$$

to ensure $\theta < 1$. We are done provided that we choose

$$\tilde{C} \geq C_\rho M / (1 - \theta).$$

□

With these we can now state and prove our analytic continuation result.

THEOREM 6.4. Given any integer $s \geq 0$, if $(\omega, \bar{\epsilon}, E_0) \in \mathcal{P}$, $E_0(x,z), E(x,z) \in C^{s+\sigma}([0,d] \times [-h,h])$, and

$$\left| \frac{1}{\bar{\epsilon}(1 - E_0)} \right|_{C^{s+\sigma}} < \frac{1}{a},$$

for some $a > 0$, then the series (6.1) converges strongly. More precisely,

$$\|v_\ell\|_{H^{s+2}} \leq K B^\ell, \quad \ell \geq 0, \tag{6.7}$$

for some universal constants $K, B > 0$.

Proof. As before, we proceed inductively. The case $\ell = 0$ is resolved by appealing to Theorem 6.2 with $F \equiv 0$, $Q = \phi$, and $R \equiv 0$, and then setting $K := \|v_0\|_{H^{s+2}}$. Assuming that (6.7) is true for all $\ell < L$ we invoke Theorem 6.2 to deduce that

$$\|v_L\|_{H^{s+2}} \leq C_e \|F_L\|_{H^s}.$$

From Lemma 6.3 we find that

$$\|v_L\|_{H^{s+2}} \leq C_e \tilde{C} K B_\rho B^{L-1},$$

and we are done provided that

$$B > C_e \tilde{C} B_\rho.$$

□

7. Joint Analyticity. To conclude our theoretical developments we produce a joint analyticity result in the spirit of that found in Nicholls and Taber [40], which shows that $v = v(x, z; \delta)$ is analytic in x, z, and δ. For this we will demonstrate that the v_ℓ from (6.1) satisfy the conditions of Definition 5.2. For this we will analyze, quite directly, the equations (6.4), more specifically arbitrary x and z derivatives of these problems.

In order to simplify subsequent developments we require the following analogue of Lemma 6.1 which is established in Appendix A.

LEMMA 7.1. For any integer $m \geq 0$, if $E_0(x,z), E(x,z) \in C^\omega_m([0,d] \times [-h,h])$ so that

$$\left| \frac{\partial_x^r \partial_z^t}{(r+t)!} E_0 \right|_{C^m} \leq C_{E_0} \frac{A_E^r}{(r+1)^2} \frac{D_E^t}{(t+1)^2}, \quad \left| \frac{\partial_x^r \partial_z^t}{(r+t)!} E \right|_{C^m} \leq C_E \frac{A_E^r}{(r+1)^2} \frac{D_E^t}{(t+1)^2},$$

for all $r, t \geq 0$, for some $C_{E_0}, C_E, A_E, D_E > 0$, and

$$\left| \frac{1}{\bar{\epsilon}(1 - E_0)} \right|_{C^m} < \frac{1}{a},$$

for some $a > 0$, then

$$\left| \frac{\partial_x^r \partial_z^t}{(r+t)!} \rho_\ell \right|_{C^m} \leq C_\rho B_\rho^\ell \frac{A^r}{(r+1)^2} \frac{D^t}{(t+1)^2}, \quad \forall\ \ell, r, t \geq 0,$$

for some $C_\rho, B_\rho, A, D > 0$.

As before, we now consider the elliptic estimate necessary for our proof. We state it here but establish it in Appendix B to maintain the flow of our developments.

THEOREM 7.2. Given any integer $m \geq 1 + \sigma$, if $(\omega, \bar{\epsilon}, E_0) \in \mathcal{P}$, $E_0 \in C^\omega_m([0,d] \times [-h,h])$ so that

$$\left| \frac{\partial_x^r \partial_z^t}{(r+t)!} E_0 \right|_{C^m} \leq C_{E_0} \frac{A_E^r}{(r+1)^2} \frac{D_E^t}{(t+1)^2}, \quad \forall\ r, t \geq 0,$$

for some $C_{E_0}, A_E, D_E > 0$, and

$$\left| \frac{1}{\bar{\epsilon}(1 - E_0)} \right|_{C^m} < \frac{1}{a},$$

for some $a > 0$, and $F \in C^\omega([0,d] \times [-h,h])$ satisfying

$$\left\| \frac{\partial_x^r \partial_z^t}{(r+t)!} F \right\|_{H^0} \leq C_F \frac{A^r}{(r+1)^2} \frac{D^t}{(t+1)^2}, \quad \forall\ r, t \geq 0,$$

for the $A, D > 0$ from Lemma 7.1 and some $C_F > 0$, and $Q, R \in C^\omega([0,d])$ satisfying

$$\left\| \frac{\partial_x^r}{r!} Q \right\|_{H^{1/2}} \leq C_Q \frac{A^r}{(r+1)^2}, \quad \left\| \frac{\partial_x^r}{r!} R \right\|_{H^{1/2}} \leq C_R \frac{A^r}{(r+1)^2}, \quad \forall\ r \geq 0,$$

for some $C_Q, C_R > 0$, then there is a unique solution $V \in C^\omega([0,d] \times [-h,h])$ of

$$\mathcal{L}_0 V = F, \qquad -h < z < h, \tag{7.1a}$$
$$-\partial_z V - T_u[V] = Q, \qquad z = h, \tag{7.1b}$$
$$\partial_z V - T_w[V] = R, \qquad z = -h, \tag{7.1c}$$
$$V(x+d,z) = \exp(i\alpha d) V(x,z), \tag{7.1d}$$

satisfying

$$\left\| \frac{\partial_x^r \partial_z^t}{(r+t)!} V \right\|_{H^2} \leq \underline{C}_e \frac{A^r}{(r+1)^2} \frac{D^t}{(t+1)^2}, \quad \forall\, r,t \geq 0, \tag{7.2}$$

where

$$\underline{C}_e := \kappa(h) \left(C_F + C_Q + C_R \right),$$

for some universal constant $\kappa(h) > 0$.

With this we can now state and prove the recursive estimate we require.

Lemma 7.3. For any integer $m \geq \sigma$, if $E_0(x,z), E(x,z) \in C_m^\omega([0,d] \times [-h,h])$ so that

$$\left| \frac{\partial_x^r \partial_z^t}{(r+t)!} E_0 \right|_{C^m} \leq C_{E_0} \frac{A_E^r}{(r+1)^2} \frac{D_E^t}{(t+1)^2}, \quad \left| \frac{\partial_x^r \partial_z^t}{(r+t)!} E \right|_{C^m} \leq C_E \frac{A_E^r}{(r+1)^2} \frac{D_E^t}{(t+1)^2},$$

for all $r, t \geq 0$, for some $C_{E_0}, C_E, A_E, D_E > 0$, and

$$\left| \frac{1}{\bar{\epsilon}(1-E_0)} \right|_{C^m} < \frac{1}{a},$$

for some $a > 0$, and

$$\left\| \frac{\partial_x^r \partial_z^t}{(r+t)!} v_\ell \right\|_{H^2} \leq \underline{K} B^\ell \frac{A^r}{(r+1)^2} \frac{D^t}{(t+1)^2}, \quad \forall\, \ell < L, \quad \forall\, r,t \geq 0,$$

for the $A, D > 0$ from Lemma 7.1 and some $\underline{K}, B > 0$, then

$$\left\| \frac{\partial_x^r \partial_z^t}{(r+t)!} F_L \right\|_{H^0} \leq \underline{\tilde{C} K} B_\rho B^{L-1} \frac{A^r}{(r+1)^2} \frac{D^t}{(t+1)^2}, \quad \forall\, r,t \geq 0,$$

for some $\underline{\tilde{C}} > 0$.

Proof. The cases of TE and TM polarization are similar so we only present the latter for simplicity. We recall that, in this case,

$$F_L = -\sum_{q=0}^{L-1} \mathcal{L}_{L-q} v_q = -\sum_{q=0}^{L-1} \operatorname{div}\left[\rho_{L-q}^{(v)} \nabla v_q \right],$$

so that

$$\frac{\partial_x^r \partial_z^t}{(r+t)!} F_L = -\frac{r!t!}{(r+t)!} \sum_{q=0}^{L-1} \sum_{j=0}^{r} \sum_{k=0}^{t} \operatorname{div}\left[\left(\frac{\partial_x^{r-j}}{(r-j)!} \frac{\partial_z^{t-k}}{(k-r)!} \rho_{L-q}^{(v)} \right) \left(\nabla \frac{\partial_x^j}{j!} \frac{\partial_z^k}{k!} v_q \right) \right].$$

Using Lemma 6.1 and the inequality $(r!t!) \leq (r+t)!$ we have

$$\begin{aligned}
\left\| \frac{\partial_x^r \partial_z^t}{(r+t)!} F_L \right\|_{H^0} &\leq \frac{r!t!}{(r+t)!} \sum_{q=0}^{L-1} \sum_{j=0}^{r} \sum_{k=0}^{t} \left\| \left(\frac{\partial_x^{r-j}}{(r-j)!} \frac{\partial_z^{t-k}}{(k-r)!} \rho_{L-q}^{(v)} \right) \left(\nabla \frac{\partial_x^j}{j!} \frac{\partial_z^k}{k!} v_q \right) \right\|_{H^\sigma} \\
&\leq \frac{r!t!}{(r+t)!} \sum_{q=0}^{L-1} \sum_{j=0}^{r} \sum_{k=0}^{t} M \left| \frac{\partial_x^{r-j}}{(r-j)!} \frac{\partial_z^{t-k}}{(k-r)!} \rho_{L-q}^{(v)} \right|_{C^\sigma} \left\| \frac{\partial_x^j}{j!} \frac{\partial_z^k}{k!} v_q \right\|_{H^2} \\
&\leq \sum_{q=0}^{L-1} \sum_{j=0}^{r} \sum_{k=0}^{t} M C_\rho B_\rho^{L-q} \frac{A^{r-j}}{(r-j+1)^2} \frac{D^{t-k}}{(t-k+1)^2} \underline{K} B^q \frac{A^j}{(j+1)^2} \frac{D^k}{(k+1)^2} \\
&\leq \underline{K} C_\rho M B_\rho B^{L-1} \frac{A^r}{(r+1)^2} \frac{D^t}{(t+1)^2} \sum_{q=0}^{L-1} \left(\frac{B_\rho}{B} \right)^{L-1-q} \\
&\quad \times \sum_{j=0}^{r} \frac{(r+1)^2}{(r-j+1)^2 (j+1)^2} \sum_{k=0}^{t} \frac{(t+1)^2}{(t-k+1)^2 (k+1)^2} \\
&\leq \underline{K} C_\rho M S^2 \left(\frac{1}{1-\theta} \right) B_\rho B^{L-1} \frac{A^r}{(r+1)^2} \frac{D^t}{(t+1)^2},
\end{aligned}$$

provided $\theta = B_\rho / B < 1$. Thus we are done if we choose

$$\underline{\tilde{C}} \geq C_\rho M S^2 / (1-\theta).$$

□

We are now in a position to state and prove our joint analyticity result.

THEOREM 7.4. Given any integer $m \geq 1 + \sigma$, if $(\omega, \bar{\epsilon}, E_0) \in \mathcal{P}$, $E_0 \in C_m^\omega([0,d] \times [-h,h])$ so that

$$\left| \frac{\partial_x^r \partial_z^t}{(r+t)!} E_0 \right|_{C^m} \leq C_{E_0} \frac{A_E^r}{(r+1)^2} \frac{D_E^t}{(t+1)^2}, \quad \forall\, r,t \geq 0,$$

for some $C_{E_0}, A_E, D_E > 0$, and

$$\left| \frac{1}{\bar{\epsilon}(1-E_0)} \right|_{C^m} < \frac{1}{a},$$

for some $a > 0$, then the series (6.1) converges strongly. Furthermore, the solution $v(x,z)$ satisfies the joint analyticity estimate

$$\left\| \frac{\partial_x^r \partial_z^t}{(r+t)!} v_\ell \right\|_{H^2} \leq \underline{K} B^\ell \frac{A^r}{(r+1)^2} \frac{D^t}{(t+1)^2}, \quad \forall\, \ell, r, t \geq 0, \tag{7.3}$$

for the $A, D > 0$ from Lemma 7.1 and some universal constants $\underline{K}, B > 0$.

Proof. Once again we proceed inductively. The case $\ell = 0$ is resolved by appealing to Theorem 7.2 with $F \equiv 0$, $Q = \phi$, and $R \equiv 0$, which delivers the estimate

$$\left\| \frac{\partial_x^r \partial_z^t}{(r+t)!} v_0 \right\|_{H^2} \leq \kappa(h) C_\phi \frac{A^r}{(r+1)^2} \frac{D^t}{(t+1)^2}, \quad \forall\, r,t \geq 0,$$

and we are done if we set $\underline{K} = \kappa(h) C_\phi$. We now assume that (7.3) is true for all $\ell < L$ and, from Lemma 7.3, we know that Theorem 7.2 can be invoked with

$$C_F = \underline{\tilde{C}} \underline{K} B_\rho B^{L-1}, \quad C_Q = C_R = 0.$$

This implies that

$$\left\| \frac{\partial_x^r \partial_z^t}{(r+t)!} v_L \right\|_{H^2} \leq \kappa(h) \tilde{C} \underline{K} B_\rho B^{L-1} \frac{A^r}{(r+1)^2} \frac{D^t}{(t+1)^2}, \quad \forall\, r,t \geq 0.$$

We are done provided that

$$B > \kappa(h) \underline{\tilde{C}} B_\rho.$$

□

8. Numerical Results. We are now in a position to demonstrate the utility and robustness of the HOPE algorithm we have discussed above. After we describe our implementation of the method, we illuminate its usefulness by comparing it to a classical exact solution for multiply layered media with flat interfaces. With this simple configuration we can make several statements regarding the advantages and limitations of this HOPE approach.

8.1. *Implementation.* A practical implementation of the HOPE algorithm involves discretizing the problems (4.2) and (4.3) for TE and TM polarizations, respectively. To start, we truncate the HOPE expansion (4.1) after a finite number of Taylor orders

$$v \approx v^L(x,z;\delta) := \sum_{\ell=0}^{L} v_\ell(x,z) \delta^\ell, \tag{8.1}$$

which should satisfy (4.2) or (4.3) up to perturbation order L. To accomplish this we adopt a High–Order Spectral (HOS) philosophy [21, 45, 46] and, with the quasiperiodic boundary conditions in mind, utilize a spectral Fourier–Chebyshev methodology. For this we approximate

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

where T_q is the q–th Chebyshev polynomial. To discover the Fourier–Chebyshev coefficients, $\{\hat{v}_{\ell,p,q}\}$, we take a collocation approach and simply demand that the equations (4.2) and (4.3) be true at the gridpoints

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

The resulting system of equations can be efficiently and robustly solved by repeated use of the fast Fourier and Chebyshev transforms as outlined in [21, 45, 46].

As with the HOPS schemes we have advocated in the past [36, 38], the current HOPE approach requires careful thought regarding the summation of the Taylor series appearing in (8.1). The natural, direct (Taylor), summation of this quantity is limited to the *disk* in δ of analyticity centered at the *origin* in the complex plane. However, long experience has demonstrated that the true domain of analyticity is typically much larger than this, and the point of our theoretical developments in Section 6 was to demonstrate that this is the case in the current setting. The conclusion that we can reach from Theorem 6.4 is that this domain includes a (small) disk about *any* $\tilde{\delta}_0 \in \mathbf{R}$ such that

$$\left| \frac{1}{\bar{\epsilon}(1 - \tilde{\delta}_0 E)} \right|_{C^{s+\sigma}} < \frac{1}{a},$$

or

$$\frac{a}{|\bar{\epsilon}|} < \left|1 - \tilde{\delta}_0 E\right|_{C^{s+\sigma}}.$$

An effective and efficient algorithm to access this larger region of analyticity is Padé approximation [2] which we have used with great success in the past [35, 36, 42, 33]. In summary, Padé approximation estimates the truncated Taylor series

$$f(\delta) = \sum_{\ell=0}^{L} f_\ell \delta^\ell,$$

by the rational function

$$\left[\frac{M}{N}\right](\delta) := \frac{a^M(\delta)}{b^N(\delta)} = \frac{\sum_{m=0}^{M} a_m \delta^m}{\sum_{n=0}^{N} b_n \delta^n}, \quad M + N = L,$$

where

$$\left[\frac{M}{N}\right](\delta) = f(\delta) + \mathcal{O}(\delta^{M+N+1}).$$

Classical formulas exist for the coefficients $\{a_m, b_n\}$ [2], and these Padé approximants have remarkable properties of convergence enhancement. We refer the interested reader to § 2.2 of [2] and § 8.3 of [8] for a full discussion.

8.2. *Layered Media Scattering.* In order to provide a brief demonstration of the convergence properties of our algorithm, we considered the scattering of linear waves by a layered medium. More specifically, we focused on simulating solutions of the Maxwell equations, (2.1), with piecewise constant permittivity

$$\epsilon = \epsilon(z) = \begin{cases} \bar{\epsilon}, & t < z < h, \\ \epsilon', & -t < z < t, \\ \bar{\epsilon}, & -h < z < -t, \end{cases}$$

for $0 < t < h$ and real $\epsilon' > \bar{\epsilon} > 0$, with incident radiation of the form (2.2). It is easy to see that the unique solution to this problem can be written down in terms of a system of linear equations which, in the three–layer case, is not difficult to solve [51] and we used them as exact solutions against which we compared our numerical simulations.

To specify our test more precisely, we selected the following geometric parameters

$$d = 0.8, \quad h = 0.95, \quad t = 0.500,$$

and the following electromagnetic constants

$$\bar{\epsilon} = 0.9, \quad \lambda = 0.7, \quad \theta = 30^\circ.$$

We considered two configurations: (i.) a small deviation from the trivial, constant–permittivity case, specified by $\epsilon' = 1.1$, and (ii.) a large deviation characterized by $\epsilon' = 1.6$. In the small deviation case we required

$$16 \le N_x \le 32, \quad 2 \le L \le 16,$$

while for the large deviation we demanded

$$16 \le N_x \le 64, \quad 2 \le L \le 32,$$

and in each case $N_z = N_x$. We measured convergence in the L^∞ norm and computed

$$\text{Error}^{N_x,N_z,L} := \left| v^{N_x,N_z,L} - v^{\text{Exact}} \right|_{L^\infty}.$$

8.3. *Small Deviation.* We summarize the results of our experiments in the case of a small deviation, $\epsilon' = 1.1$, in Figures 2 & 3. More specifically, we examined the convergence in $N_x = N_z$ in Figure 2 while we studied L convergence in Figure 3.

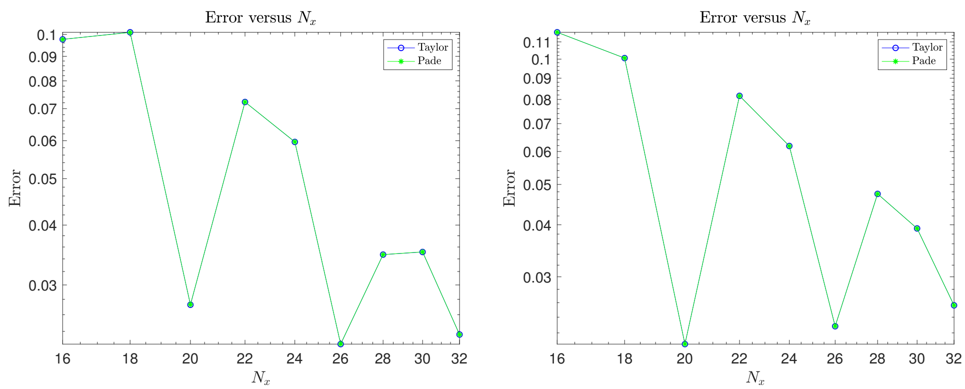

FIG. 2. Error versus N_x for $\epsilon' = 1.1$ (Left: TE, Right: TM).

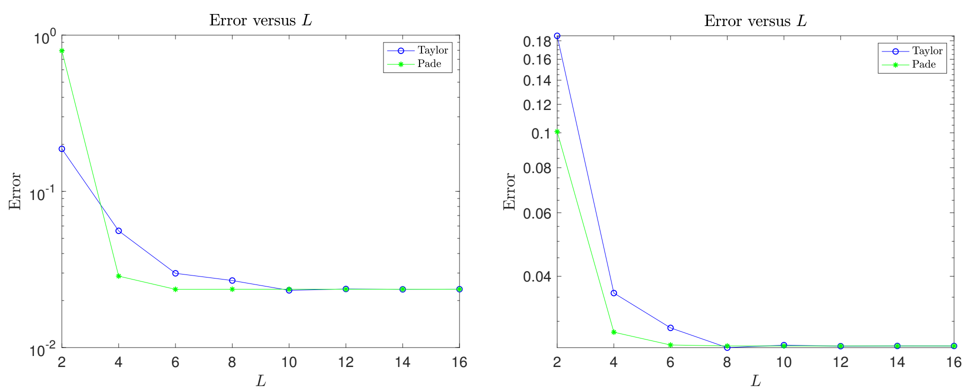

FIG. 3. Error versus L for $\epsilon' = 1.1$ (Left: TE, Right: TM).

While we were pleased that our method showed convergence as all discretization parameters were refined, the results were rather disappointing. We employed not only a HOS Fourier–Chebyshev approach to solve the Helmholtz problems, (4.2) and (4.3), but also utilized a High–Order Perturbation scheme for the deformation variable, δ. We expected that our convergence rates would be *exponential.* However, a quick inspection of the exact solution, which is only in H^2 for TE polarization and merely H^1 for TM polarization, explains that, in the absence of sophisticated mesh refinement strategies (which is an object of current research), one can only expect rather low rates of convergence. In the experiments above we noticed an experimental rate of convergence of 1.87 for TE and 1.60 for TM polarization as $N_x = N_z$ was refined, while the convergence rate in L was difficult to characterize with the spatial resolution of such modest quality.

In order to further validate our code we conducted another convergence study against a different "exact solution" obtained by numerically simulating solutions of (3.2) and (3.3) with our *smooth* permittivity profile, (4.4) ($w = 100$), and a HOS Fourier–Chebyshev approach. Reconsidering the calculations above yielded the results depicted in Figures 4 & 5 for $N_x = N_z$ and L convergence, respectively. Here we saw the behavior we expected, namely exponential rates of convergence in both $N_x = N_z$ and L down to machine precision (to the conditioning of our algorithm). This exhibits a well–known limitation of HOS methods, that high–order rates of convergence are limited by the smoothness of the underlying exact solution [21, 45, 46].

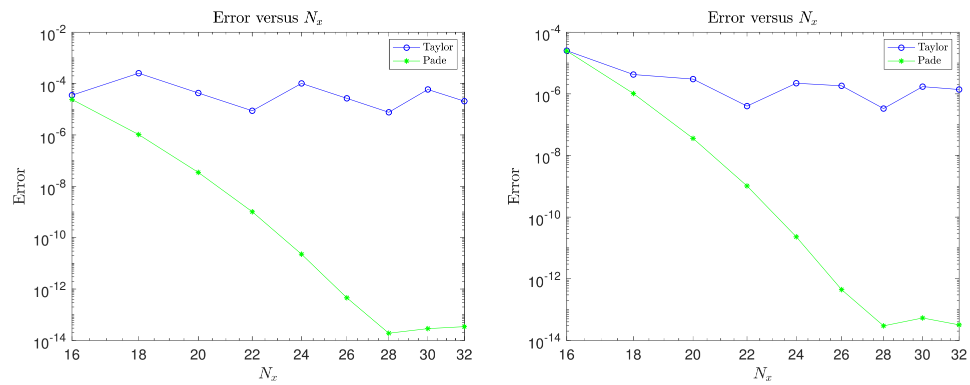

Fig. 4. Error versus N_x for $\epsilon' = 1.1$ with smoothed exact solution (Left: TE, Right: TM).

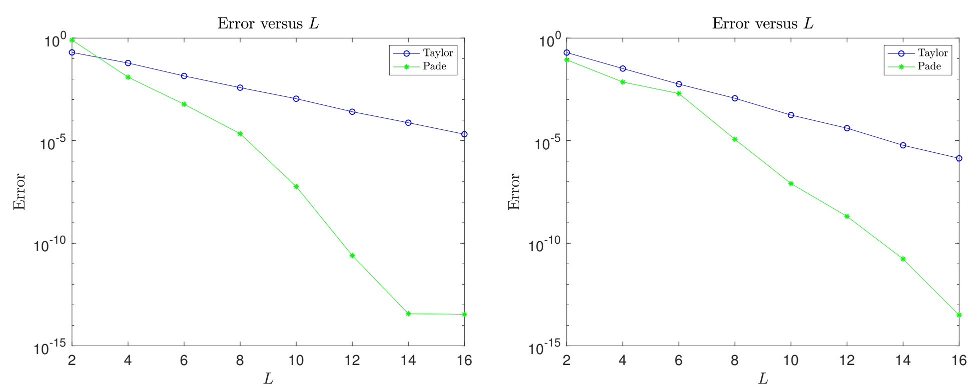

Fig. 5. Error versus L for $\epsilon' = 1.1$ with smoothed exact solution (Left: TE, Right: TM).

Before leaving this simulation we point out, in this latter case of a smoothed solution, the extremely beneficial effect of Padé summation. This approach delivered solutions with *ten* extra digits of accuracy compared to straightforward Taylor summation.

8.4. *Large Deviation.* We repeated these small deformation simulations in the case of a large deviation characterized by $\epsilon' = 1.6$. We display the results of these experiments in comparison to the exact solution in Figures 6 and Figures 7 for N_x and L refinement, respectively. Here we noticed not only the very poor performance of our algorithm with Padé approximation, but also the complete inapplicability of Taylor summation.

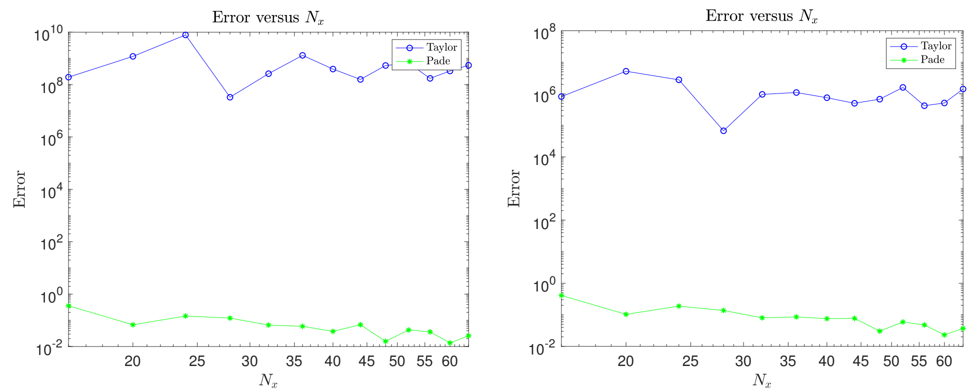

FIG. 6. Error versus N_x for $\epsilon' = 1.6$ (Left: TE, Right: TM).

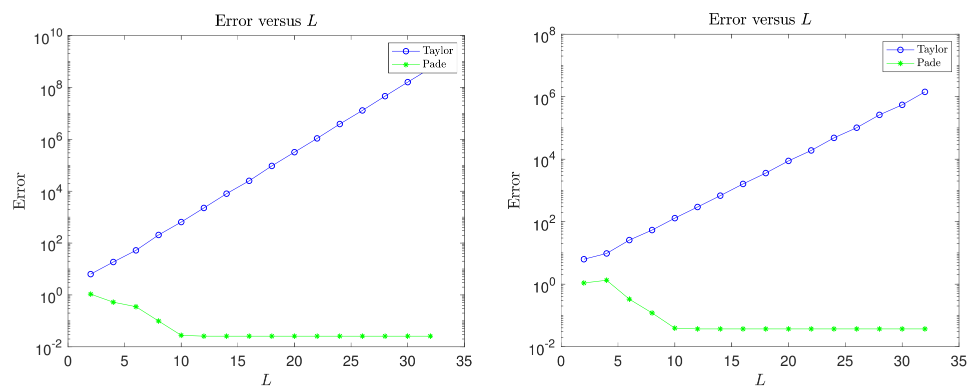

FIG. 7. Error versus L for $\epsilon' = 1.6$ (Left: TE, Right: TM).

As before, by replacing the exact solution with a numerical solution of the smoothed problem with E given by (4.4) ($w = 100$), we obtained the results in Figures 8 and 9 for $N_x = N_z$ and L refinement. Once again we noticed the greatly enhanced performance of our algorithm with Padé approximation in this setting, though Taylor summation was completely unusable.

Dedication. I would like to dedicate this work to the memory of my wife's mother, Caryl Steimel. Caryl was a kind woman of strong faith who always put her own needs behind those of others, particularly her family. I knew her for nearly thirty years and

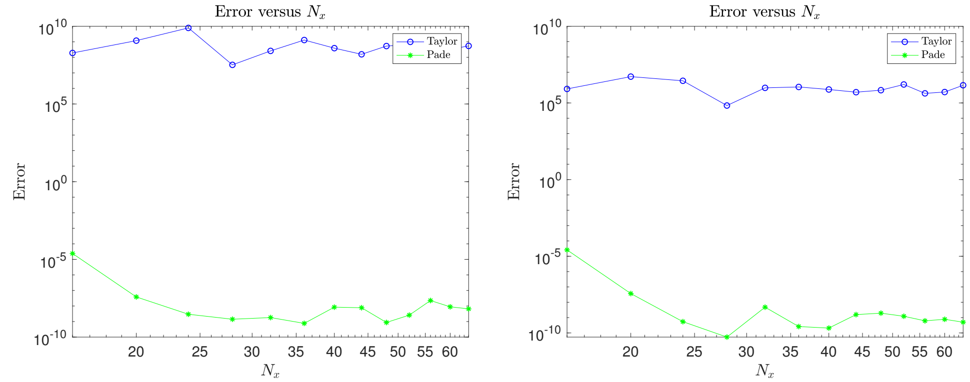

FIG. 8. Error versus N_x for $\epsilon' = 1.6$ with smoothed exact solution (Left: TE, Right: TM).

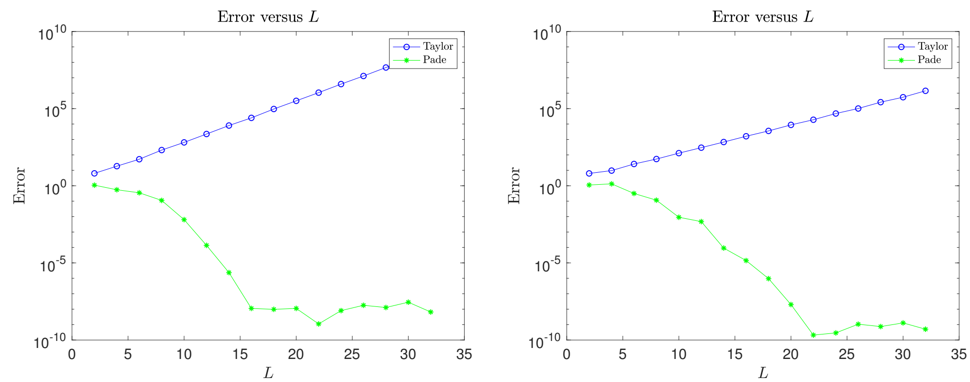

FIG. 9. Error versus L for $\epsilon' = 1.6$ with smoothed exact solution (Left: TE, Right: TM).

was always inspired by the time and talent she spent on her husband, her children (including my wife Kristy), and her grandchildren (particularly my daughter Emma). Her example of patience and selflessness is a model for all who knew her. She is sorely missed. Somehow the natural acronym for the algorithm described in this paper ("HOPE") is singularly appropriate for Caryl as her outlook on life was always full of "hope." Quoting the motto of my Alma Mater: *In Deo Speramus!*

Acknowledgments. D.P.N. gratefully acknowledges support from the National Science Foundation through grant No. DMS–1813033.

Appendix A. Analyticity of the Reciprocal Permittivity. For the proof of Lemma 7.1 we use induction on ℓ, beginning with $\ell = 0$. To accomplish this we induct on t, beginning with $t = 0$. Finally, we establish this via induction on r, beginning with $r = 0$. So, we begin by setting

$$C_\rho = \left| \rho_0^{(v)} \right|_{C^m},$$

which resolves $r = 0$. Now we assume that

$$\left| \frac{\partial_x^r}{r!} \rho_0^{(v)} \right|_{C^m} \leq C_\rho \frac{A^r}{(r+1)^2}, \quad \forall\, r < \bar{r},$$

and note that $\partial_x^r / r!$ applied to

$$\bar{\epsilon}(1 - E_0(x,z)) \rho_0^{(v)} = 1,$$

c.f. (6.3), gives

$$\frac{\partial_x^r}{r!} \rho_0 = -\frac{1}{\bar{\epsilon}(1 - E_0(x,z))} \sum_{j=0}^{r-1} \left(\frac{\partial_x^{r-j}}{(r-j)!} \left[\bar{\epsilon}(1 - E_0(x,z)) \right] \right) \left(\frac{\partial_x^j}{j!} \rho_0 \right).$$

From this we estimate

$$\begin{aligned}
\left| \frac{\partial_x^{\bar{r}}}{\bar{r}!} \rho_0 \right|_{C^m} &\leq \left| \frac{1}{\bar{\epsilon}(1 - E_0(x,z))} \right|_{C^m} \sum_{j=0}^{\bar{r}-1} \left| \frac{\partial_x^{\bar{r}-j}}{(\bar{r}-j)!} \left[\bar{\epsilon}(1 - E_0(x,z)) \right] \right|_{C^m} \left| \frac{\partial_x^j}{j!} \rho_0 \right|_{C^m} \\
&\leq \frac{|\bar{\epsilon}|}{a} \sum_{j=0}^{\bar{r}-1} C_E \frac{A_E^{\bar{r}-j}}{(r-j+1)^2} C_\rho \frac{A^j}{(j+1)^2} \\
&\leq \frac{|\bar{\epsilon}|}{a} C_E C_\rho A_E \frac{A^{\bar{r}-1}}{(\bar{r}+1)^2} \sum_{j=0}^{\bar{r}-1} \frac{(\bar{r}+1)^2}{(\bar{r}-j+1)^2 (j+1)^2} \left(\frac{A_E}{A} \right)^{\bar{r}-j-1} \\
&\leq \frac{|\bar{\epsilon}|}{a} C_E C_\rho A_E \frac{A^{\bar{r}-1}}{(\bar{r}+1)^2} S,
\end{aligned}$$

if A_E/A is chosen less than one. Thus we are done with our induction on r provided that

$$A > \max \left\{ 1, C_E \frac{|\bar{\epsilon}|}{a} S \right\} A_E.$$

Conveniently this result resolves our base induction on t at $t = 0$. So, we proceed by assuming that

$$\left| \frac{\partial_x^r \partial_z^t}{(r+t)!} \rho_0^{(v)} \right|_{C^m} \leq C_\rho \frac{A^r}{(r+1)^2} \frac{D^t}{(t+1)^2}, \quad \forall\, r \geq 0, \quad \forall\, t < \bar{t},$$

and note that $(\partial_x^r \partial_z^t)/(r+t)!$ applied to

$$\bar{\epsilon}(1 - E_0(x,z)) \rho_0^{(v)} = 1,$$

c.f. (6.3), gives

$$
\begin{aligned}
\frac{\partial_x^r \partial_z^t}{(r+t)!} \rho_0^{(v)} = & -\frac{1}{\bar{\epsilon}(1 - E_0(x,z))} \frac{r! t!}{(r+t)!} \\
& \times \left\{ \sum_{j=0}^{r-1} \sum_{k=0}^{t-1} \left(\frac{\partial_x^{r-j}}{(r-j)!} \frac{\partial_z^{t-k}}{(t-k)!} \left[\bar{\epsilon}(1 - E_0(x,z)) \right] \right) \left(\frac{\partial_x^j}{j!} \frac{\partial_z^k}{k!} \rho_0^{(v)} \right) \right. \\
& - \sum_{j=0}^{r-1} \left(\frac{\partial_x^{r-j}}{(r-j)!} \left[\bar{\epsilon}(1 - E_0(x,z)) \right] \right) \left(\frac{\partial_x^j}{j!} \frac{\partial_z^t}{t!} \rho_0^{(v)} \right) \\
& \left. - \sum_{k=0}^{t-1} \left(\frac{\partial_z^{t-k}}{(t-k)!} \left[\bar{\epsilon}(1 - E_0(x,z)) \right] \right) \left(\frac{\partial_x^r}{r!} \frac{\partial_z^k}{k!} \rho_0^{(v)} \right) \right\}.
\end{aligned}
$$

With this and the fact that $(r!t!) \leq (r+t)!$ we estimate

$$
\begin{aligned}
\left| \frac{\partial_x^r \partial_z^{\bar{t}}}{(r+\bar{t})!} \rho_0^{(v)} \right|_{C^m} \leq & \left| \frac{1}{\bar{\epsilon}(1 - E_0(x,z))} \right|_{C^m} \\
& \times \left\{ \sum_{j=0}^{r-1} \sum_{k=0}^{\bar{t}-1} \left| \frac{\partial_x^{r-j}}{(r-j)!} \frac{\partial_z^{\bar{t}-k}}{(\bar{t}-k)!} \left[\bar{\epsilon}(1 - E_0(x,z)) \right] \right|_{C^m} \left| \frac{\partial_x^j}{j!} \frac{\partial_z^k}{k!} \rho_0^{(v)} \right|_{C^m} \right. \\
& + \sum_{j=0}^{r-1} \left| \frac{\partial_x^{r-j}}{(r-j)!} \left[\bar{\epsilon}(1 - E_0(x,z)) \right] \right|_{C^m} \left| \frac{\partial_x^j}{j!} \frac{\partial_z^{\bar{t}}}{\bar{t}!} \rho_0^{(v)} \right|_{C^m} \\
& \left. + \sum_{k=0}^{\bar{t}-1} \left| \frac{\partial_z^{\bar{t}-k}}{(\bar{t}-k)!} \left[\bar{\epsilon}(1 - E_0(x,z)) \right] \right|_{C^m} \left| \frac{\partial_x^r}{r!} \frac{\partial_z^k}{k!} \rho_0^{(v)} \right|_{C^m} \right\},
\end{aligned}
$$

and continue

$$
\begin{aligned}
\left| \frac{\partial_x^r \partial_z^{\bar{t}}}{(r+\bar{t})!} \rho_0^{(v)} \right|_{C^m} \leq \frac{|\bar{\epsilon}|}{a} & \left\{ \sum_{j=0}^{r-1} \sum_{k=0}^{\bar{t}-1} C_E \frac{A_E^{r-j}}{(r-j+1)^2} \frac{D_E^{\bar{t}-k}}{(\bar{t}-k+1)^2} C_\rho \frac{A^j}{(j+1)^2} \frac{D^k}{(k+1)^2} \right. \\
& + \sum_{j=0}^{r-1} C_E \frac{A_E^{r-j}}{(r-j+1)^2} C_\rho \frac{A^j}{(j+1)^2} \frac{D^{\bar{t}}}{(\bar{t}+1)^2} \\
& \left. + \sum_{k=0}^{\bar{t}-1} C_E \frac{D_E^{\bar{t}-k}}{(\bar{t}-k+1)^2} C_\rho \frac{A^r}{(r+1)^2} \frac{D^k}{(k+1)^2} \right\}.
\end{aligned}
$$

We now have

$$\left| \frac{\partial_x^r \partial_z^{\bar{t}}}{(r+\bar{t})!} \rho_0^{(v)} \right|_{C^m} \leq \frac{|\bar{\epsilon}|}{a} \left\{ C_E C_\rho A_E D_E \frac{A^{r-1}}{(r+1)^2} \frac{D^{\bar{t}-1}}{(\bar{t}+1)^2} \right.$$
$$\times \sum_{j=0}^{r-1} \sum_{k=0}^{\bar{t}-1} \frac{(r+1)^2}{(r-j+1)^2 (j+1)^2} \left(\frac{A_E}{A} \right)^{r-j-1} \frac{(\bar{t}+1)^2}{(\bar{t}-k+1)^2 (k+1)^2} \left(\frac{D_E}{D} \right)^{\bar{t}-k-1}$$
$$+ C_E C_\rho A_E \frac{A^{r-1}}{(r+1)^2} \frac{D^{\bar{t}}}{(\bar{t}+1)^2} \sum_{j=0}^{r-1} \frac{(r+1)^2}{(r-j+1)^2 (j+1)^2} \left(\frac{A_E}{A} \right)^{r-j-1}$$
$$\left. + C_E C_\rho D_E \frac{A^r}{(r+1)^2} \frac{D^{\bar{t}-1}}{(\bar{t}+1)^2} \sum_{k=0}^{\bar{t}-1} \frac{(\bar{t}+1)^2}{(\bar{t}-k+1)^2 (k+1)^2} \left(\frac{D_E}{D} \right)^{\bar{t}-k-1} \right\},$$

upon choosing $A > A_E$ and $D > D_E$ we find

$$\left| \frac{\partial_x^r \partial_z^{\bar{t}}}{(r+\bar{t})!} \rho_0^{(v)} \right|_{C^m} \leq \frac{|\bar{\epsilon}|}{a} C_E C_\rho \left\{ A_E D_E \frac{A^{r-1}}{(r+1)^2} \frac{D^{\bar{t}-1}}{(\bar{t}+1)^2} S^2 \right.$$
$$\left. + A_E \frac{A^{r-1}}{(r+1)^2} \frac{D^{\bar{t}}}{(\bar{t}+1)^2} S + D_E \frac{A^r}{(r+1)^2} \frac{D^{\bar{t}-1}}{(\bar{t}+1)^2} S \right\},$$

and are finished provided that

$$A > A_E, \quad D > D_E, \quad A > 3 \frac{|\bar{\epsilon}|}{a} S C_E A_E, \quad D > 3 \frac{|\bar{\epsilon}|}{a} S C_E D_E, \quad AD > 3 \frac{|\bar{\epsilon}|}{a} S^2 C_E A_E D_E.$$

This previous result establishes the base of our induction on ℓ at $\ell = 0$. To finish our proof we assume that

$$\left| \frac{\partial_x^r \partial_z^t}{(r+t)!} \rho_\ell \right|_{C^m} \leq C_\rho B_\rho^\ell \frac{A^r}{(r+1)^2} \frac{D^t}{(t+1)^2}, \quad \forall\ \ell < L, \quad \forall\ r, t \geq 0,$$

and recall that, for $\ell > 0$,

$$\rho_\ell^{(v)}(x,z) = \bar{\epsilon} \rho_0^{(v)}(x,z) E(x,z) \rho_{\ell-1}^{(v)}(x,z),$$

c.f. (6.3). From Leibniz's Rule we have

$$\frac{\partial_x^r \partial_z^t}{(r+t)!} \rho_\ell^{(v)} = \bar{\epsilon} \frac{r! t!}{(r+t)!}$$
$$\times \sum_{j=0}^{r} \sum_{k=0}^{t} \sum_{p=0}^{j} \sum_{q=0}^{k} \left(\frac{\partial_x^{r-j}}{(r-j)!} \frac{\partial_z^{t-k}}{(t-k)!} \rho_0^{(v)} \right) \left(\frac{\partial_x^{j-p}}{(j-p)!} \frac{\partial_z^{k-q}}{(k-q)!} E \right) \left(\frac{\partial_x^p}{p!} \frac{\partial_z^q}{q!} \rho_{\ell-1}^{(v)} \right),$$

which, since $(r!t!) \leq (r+t)!$, leads to the estimate

$$\begin{aligned}\left| \frac{\partial_x^r \partial_z^t}{(r+t)!} \rho_L^{(v)} \right|_{C^m} &\leq \bar{\epsilon} C_\rho^2 C_E B_\rho^{L-1} \frac{A^r}{(r+1)^2} \frac{D^t}{(t+1)^2} \\ &\quad \sum_{j=0}^{r} \sum_{p=0}^{j} \frac{(r+1)^2}{(r-j+1)^2 (j-p+1)^2 (p+1)^2} \\ &\quad \sum_{k=0}^{t} \sum_{q=0}^{k} \frac{(t+1)^2}{(t-k+1)^2 (k-q+1)^2 (q+1)^2} \\ &\leq \bar{\epsilon} C_\rho^2 C_E B_\rho^{L-1} S^4 \frac{A^r}{(r+1)^2} \frac{D^t}{(t+1)^2},\end{aligned}$$

provided that, as we have already enforced, $A > A_E$ and $D > D_E$. We are done if we choose

$$B_\rho > \bar{\epsilon} C_\rho C_E S^4.$$

Appendix B. Generalized Elliptic Estimate. In our proof of Theorem 7.2 we focus upon TM polarization for brevity as the case of TE polarization is very similar (and slightly easier). To begin we establish this result in the case of pure x–derivatives, which we now state and prove.

Theorem B.1. Given any integer $m \geq 1 + \sigma$, if $(\omega, \bar{\epsilon}, E_0) \in \mathcal{P}$, $E_0 \in C_m^\omega([0, d] \times [-h, h])$ so that

$$\left| \frac{\partial_x^r}{r!} E_0 \right|_{C^m} \leq C_{E_0} \frac{A_E^r}{(r+1)^2}, \quad \forall\, r \geq 0,$$

for some $C_{E_0}, A_E > 0$, and

$$\left| \frac{1}{\bar{\epsilon}(1 - E_0)} \right|_{C^m} < \frac{1}{a},$$

for some $a > 0$, and $F \in C^\omega([0, d] \times [-h, h])$ satisfying

$$\left\| \frac{\partial_x^r}{r!} F \right\|_{H^0} \leq C_F \frac{A^r}{(r+1)^2}, \quad \forall\, r \geq 0,$$

for the $A > 0$ from Lemma 7.1 and some $C_F > 0$, and $Q, R \in C^\omega([0, d])$ satisfying

$$\left\| \frac{\partial_x^r}{r!} Q \right\|_{H^{1/2}} \leq C_Q \frac{A^r}{(r+1)^2}, \quad \left\| \frac{\partial_x^r}{r!} R \right\|_{H^{1/2}} \leq C_R \frac{A^r}{(r+1)^2}, \quad \forall\, r \geq 0,$$

for some $C_Q, C_R > 0$, then there is a unique solution $V \in C^\omega([0, d] \times [-h, h])$ of

$$\mathcal{L}_0 V = F, \qquad -h < z < h, \tag{B.1a}$$

$$-\partial_z V - T_u[V] = Q, \qquad z = h, \tag{B.1b}$$

$$\partial_z V - T_w[V] = R, \qquad z = -h, \tag{B.1c}$$

$$V(x + d, z) = \exp(i\alpha d) V(x, z), \tag{B.1d}$$

satisfying

$$\left\| \frac{\partial_x^r}{r!} V \right\|_{H^2} \leq \underline{C}_e \frac{A^r}{(r+1)^2}, \quad \forall\, r \geq 0, \tag{B.2}$$

where

$$\underline{C}_e := \kappa(h)\left(C_F + C_Q + C_R\right),$$

for some universal constant $\kappa(h) > 0$.

Proof. We work by induction on r and establish the base case, $r = 0$, by using the elliptic estimate, Theorem 6.2, with $s = 0$, and the hypotheses of the theorem,

$$\|V\|_{H^2} \leq C_e \left\{\|F\|_{H^0} + \|Q\|_{H^{1/2}} + \|R\|_{H^{1/2}}\right\} = C_e \left\{C_F + C_Q + C_R\right\},$$

and we choose

$$\underline{C}_e \geq C_e \left\{C_F + C_Q + C_R\right\}.$$

To proceed we study the operator $\partial_x^r/r!$ applied to (B.1) which delivers

$$\mathcal{L}_0\left[\frac{\partial_x^r}{r!}V\right] = \frac{\partial_x^r}{r!}F + \left[\mathcal{L}_0, \frac{\partial_x^r}{r!}\right]V, \qquad -h < z < h, \tag{B.3a}$$

$$-\partial_z\left[\frac{\partial_x^r}{r!}V\right] - T_u\left[\frac{\partial_x^r}{r!}V\right] = \frac{\partial_x^r}{r!}Q, \qquad z = h, \tag{B.3b}$$

$$\partial_z\left[\frac{\partial_x^r}{r!}V\right] - T_w\left[\frac{\partial_x^r}{r!}V\right] = \frac{\partial_x^r}{r!}R, \qquad z = -h, \tag{B.3c}$$

$$\frac{\partial_x^r}{r!}V(x+d,z) = \exp(i\alpha d)\frac{\partial_x^r}{r!}V(x,z), \tag{B.3d}$$

where $[\cdot,\cdot]$ is the commutator

$$[A,B] = AB - BA.$$

We now assume

$$\left\|\frac{\partial_x^r}{r!}V\right\|_{H^2} \leq \underline{C}_e \frac{A^r}{(r+1)^2}, \quad \forall\ r < \bar{r},$$

c.f. (B.2), which, as we shall see in Lemma B.2, implies that

$$\left\|\left[\mathcal{L}_0, \frac{\partial_x^{\bar{r}}}{\bar{r}!}\right]V\right\|_{H^0} \leq \underline{C}_e (MSC_\rho)\frac{A^{\bar{r}-1}}{(\bar{r}+1)^2}.$$

Applying the elliptic estimate, Theorem 6.2, to (B.3) and using the hypotheses on F, Q, and R, we find

$$\begin{aligned}\left\|\frac{\partial_x^{\bar{r}}}{\bar{r}!}V\right\|_{H^2} &\leq C_e\left\{\left\|\frac{\partial_x^{\bar{r}}}{\bar{r}!}F + \left[\mathcal{L}_0, \frac{\partial_x^{\bar{r}}}{\bar{r}!}\right]V\right\|_{H^0} + \left\|\frac{\partial_x^{\bar{r}}}{\bar{r}!}Q\right\|_{H^{1/2}} + \left\|\frac{\partial_x^{\bar{r}}}{\bar{r}!}R\right\|_{H^{1/2}}\right\} \\ &\leq C_e\left\{C_F + C_Q + C_R\right\}\frac{A^{\bar{r}}}{(\bar{r}+1)^2} + \underline{C}_e\left\{MSC_\rho\right\}\frac{A^{\bar{r}-1}}{(\bar{r}+1)^2},\end{aligned}$$

and we are done provided

$$\underline{C}_e \geq 2C_e\left\{C_F + C_Q + C_R\right\}, \quad A \geq 2MSC_\rho.$$

□

We now present the estimate on commutators which we require above.

LEMMA B.2. Given any integer $m \geq 1+\sigma$, if $E_0 \in C_m^\omega([0,d] \times [-h,h])$ so that

$$\left| \frac{\partial_x^r}{r!} E_0 \right|_{C^m} \leq C_{E_0} \frac{A_E^r}{(r+1)^2}, \quad \forall\ r \geq 0,$$

for some $C_{E_0}, A_E > 0$, and

$$\left| \frac{1}{\bar{\epsilon}(1-E_0)} \right|_{C^m} < \frac{1}{a},$$

for some $a > 0$, and

$$\left\| \frac{\partial_x^r}{r!} V \right\|_{H^2} \leq \underline{C}_e \frac{A^r}{(r+1)^2}, \quad \forall\ r < \bar{r},$$

then

$$\left\| \left[\mathcal{L}_0, \frac{\partial_x^{\bar{r}}}{\bar{r}!} \right] V \right\|_{H^0} \leq \underline{C}_e (MSC_\rho) \frac{A^{\bar{r}-1}}{(\bar{r}+1)^2}.$$

Proof. Focusing on TM polarization, we recall that

$$\mathcal{L}_0 = \operatorname{div}\left[\rho_0^{(v)} \nabla\right] + k_0^2,$$

so that

$$\begin{aligned}
\left[\mathcal{L}_0, \frac{\partial_x^r}{r!} \right] V &= \mathcal{L}_0 \left[\frac{\partial_x^r}{r!} V \right] - \frac{\partial_x^r}{r!} \left[\mathcal{L}_0 V \right] \\
&= \operatorname{div}\left[\rho_0^{(v)} \nabla \frac{\partial_x^r}{r!} V \right] + k_0^2 \frac{\partial_x^r}{r!} V - \frac{\partial_x^r}{r!} \left[\operatorname{div}\left[\rho_0^{(v)} \nabla V \right] + k_0^2 V \right] \\
&= \operatorname{div}\left[\rho_0^{(v)} \nabla \frac{\partial_x^r}{r!} V \right] + k_0^2 \frac{\partial_x^r}{r!} V \\
&\quad - \sum_{j=0}^{r} \operatorname{div}\left[\left(\frac{\partial_x^{r-j}}{(r-j)!} \rho_0^{(v)} \right) \nabla \left(\frac{\partial_x^j}{j!} V \right) \right] - k_0^2 \frac{\partial_x^r}{r!} V \\
&= - \sum_{j=0}^{r-1} \operatorname{div}\left[\left(\frac{\partial_x^{r-j}}{(r-j)!} \rho_0^{(v)} \right) \nabla \left(\frac{\partial_x^j}{j!} V \right) \right].
\end{aligned}$$

We can now estimate

$$\begin{aligned}
\left\| \left[\mathcal{L}_0, \frac{\partial_x^{\bar{r}}}{\bar{r}!} \right] V \right\|_{H^0} &\leq \sum_{j=0}^{\bar{r}-1} \left\| \left(\frac{\partial_x^{\bar{r}-j}}{(\bar{r}-j)!} \rho_0^{(v)} \right) \nabla \left(\frac{\partial_x^j}{j!} V \right) \right\|_{H^\sigma} \\
&\leq \sum_{j=0}^{\bar{r}-1} M \left| \frac{\partial_x^{\bar{r}-j}}{(\bar{r}-j)!} \rho_0^{(v)} \right|_{C^\sigma} \left\| \frac{\partial_x^j}{j!} V \right\|_{H^2} \\
&\leq \sum_{j=0}^{\bar{r}-1} M \frac{1}{(\bar{r}-j)} \left| \frac{\partial_x^{\bar{r}-j-1}}{(\bar{r}-j-1)!} \rho_0^{(v)} \right|_{C^{\sigma+1}} \left\| \frac{\partial_x^j}{j!} V \right\|_{H^2} \\
&\leq \sum_{j=0}^{\bar{r}-1} M C_\rho \frac{A^{\bar{r}-j-1}}{(\bar{r}-j-1+1)^2} \underline{C}_e \frac{A^j}{(j+1)^2} \\
&\leq \underline{C}_e \left(MSC_\rho \right) \frac{A^{\bar{r}-1}}{(\bar{r}+1)^2},
\end{aligned}$$

and we are done. ∎

REMARK B.3. We comment here that it is in this final step of the previous proof that the requirement $m \geq 1+\sigma$ is explained. This is necessary in order to reduce the number of derivatives on the function $\rho_0^{(v)}$ by one.

Proof. (Theorem 7.2) Once again, we proceed by induction, this time on t. The base case $t = 0$ is resolved by Lemma B.1. We now assume

$$\left\| \frac{\partial_x^r \partial_z^t}{(r+t)!} V \right\|_{H^2} \leq \underline{C}_e \frac{A^r}{(r+1)^2} \frac{D^t}{(t+1)^2}, \quad \forall\, t < \bar{t}, \quad \forall\, r \geq 0,$$

c.f. (7.2), and examine

$$\begin{aligned} \left\| \frac{\partial_x^r \partial_z^{\bar{t}}}{(r+\bar{t})!} V \right\|_{H^2} &= \left\| \frac{\partial_x^r \partial_z^{\bar{t}}}{(r+\bar{t})!} V \right\|_{H^1} + \left\| \frac{\partial_x^r \partial_z^{\bar{t}}}{(r+\bar{t})!} \partial_x V \right\|_{H^1} + \left\| \frac{\partial_x^r \partial_z^{\bar{t}}}{(r+\bar{t})!} \partial_z V \right\|_{H^1} \\ &= \left\| \frac{\partial_x^r \partial_z^{\bar{t}-1}}{(r+\bar{t})!} V \right\|_{H^2} + \left\| \frac{\partial_x^r \partial_z^{\bar{t}-1}}{(r+\bar{t})!} \partial_x V \right\|_{H^2} + \left\| \frac{\partial_x^r \partial_z^{\bar{t}-1}}{(r+\bar{t})!} \partial_z^2 V \right\|_{H^1}. \end{aligned}$$

The first two terms can be addressed with our inductive hypothesis as they involve z derivatives of order $\bar{t}-1$. The third we call Z, which we simplify with the following calculation (remembering that $\epsilon_0^{(v)} = 1/\rho_0^{(v)}$) using the TM Helmholtz equation, (3.3a),

$$\begin{aligned} \partial_z^2 V &= \partial_z \left[\frac{1}{\rho_0^{(v)}} \rho_0^{(v)} \partial_z V \right] = \partial_z \left[\epsilon_0^{(v)} \rho_0^{(v)} \partial_z V \right] \\ &= (\partial_z \epsilon_0) \rho_0^{(v)} \partial_z V + \epsilon_0^{(v)} \partial_z \left[\rho_0^{(v)} \partial_z V \right] \\ &= (\partial_z \epsilon_0^{(v)}) \rho_0^{(v)} \partial_z V - \epsilon_0^{(v)} \partial_x \left[\rho_0^{(v)} \partial_x V \right] - \epsilon_0^{(v)} k_0^2 V. \end{aligned}$$

With this we estimate

$$\begin{aligned} Z &= \left\| \frac{\partial_x^r \partial_z^{\bar{t}-1}}{(r+\bar{t})!} \partial_z^2 V \right\|_{H^1} \\ &= \left\| \frac{\partial_x^r \partial_z^{\bar{t}-1}}{(r+\bar{t})!} \left[(\partial_z \epsilon_0^{(v)}) \rho_0^{(v)} \partial_z V - \epsilon_0^{(v)} \partial_x \left[\rho_0^{(v)} \partial_x V \right] - \epsilon_0^{(v)} k_0^2 V \right] \right\|_{H^1} \\ &\leq \left\| \frac{\partial_x^r \partial_z^{\bar{t}-1}}{(r+\bar{t})!} \left[(\partial_z \epsilon_0^{(v)}) \rho_0^{(v)} \partial_z V \right] \right\|_{H^1} + \left\| \frac{\partial_x^r \partial_z^{\bar{t}-1}}{(r+\bar{t})!} \left[\epsilon_0^{(v)} \partial_x \left[\rho_0^{(v)} \partial_x V \right] \right] \right\|_{H^1} \\ &\quad + \left\| \frac{\partial_x^r \partial_z^{\bar{t}-1}}{(r+\bar{t})!} \left[\epsilon_0^{(v)} k_0^2 V \right] \right\|_{H^1}. \end{aligned}$$

For brevity we focus upon the first and second of these terms

$$\begin{aligned} Z_1 &:= \left\| \frac{\partial_x^r \partial_z^{\bar{t}-1}}{(r+\bar{t})!} \left[(\partial_z \epsilon_0^{(v)}) \rho_0^{(v)} \partial_z V \right] \right\|_{H^1} \\ Z_2 &:= \left\| \frac{\partial_x^r \partial_z^{\bar{t}-1}}{(r+\bar{t})!} \left[\epsilon_0^{(v)} \partial_x \left[\rho_0^{(v)} \partial_x V \right] \right] \right\|_{H^1}. \end{aligned}$$

For the first, with the calculation

$$\frac{\partial_x^r \partial_z^{\bar{t}-1}}{(r+\bar{t})!}\left[(\partial_z \epsilon_0^{(v)})\rho_0^{(v)}\partial_z V\right] = \frac{1}{r+\bar{t}}\frac{r!(\bar{t}-1)!}{(r+\bar{t}-1)!}\sum_{j=0}^{r}\sum_{p=0}^{j}\sum_{k=0}^{\bar{t}-1}\sum_{q=0}^{k}\left(\frac{\partial_x^{r-j}}{(r-j)!}\frac{\partial_z^{\bar{t}-1-k}}{(\bar{t}-1-k)!}\partial_z \epsilon_0^{(v)}\right) \left(\frac{\partial_x^{j-p}}{(j-p)!}\frac{\partial_z^{k-q}}{(k-q)!}\rho_0^{(v)}\right)\left(\frac{\partial_x^p}{p!}\frac{\partial_z^q}{q!}\partial_z V\right),$$

we estimate, since $(r!(t-1)!) \leq (r+t-1)!$,

$$\begin{aligned} Z_1 &\leq \frac{1}{r+\bar{t}}\sum_{j=0}^{r}\sum_{p=0}^{j}\sum_{k=0}^{\bar{t}-1}\sum_{q=0}^{k} M\left|\frac{\partial_x^{r-j}}{(r-j)!}\frac{\partial_z^{\bar{t}-1-k}}{(\bar{t}-1-k)!}\partial_z \epsilon_0^{(v)}\right|_{C^1} \\ &\quad \times M\left|\frac{\partial_x^{j-p}}{(j-p)!}\frac{\partial_z^{k-q}}{(k-q)!}\rho_0^{(v)}\right|_{C^1}\left\|\frac{\partial_x^p}{p!}\frac{\partial_z^q}{q!}\partial_z V\right\|_{H^1} \\ &\leq \frac{1}{r+\bar{t}}\sum_{j=0}^{r}\sum_{p=0}^{j}\sum_{k=0}^{\bar{t}-1}\sum_{q=0}^{k} M\left|\frac{\partial_x^{r-j}}{(r-j)!}\frac{\partial_z^{\bar{t}-1-k}}{(\bar{t}-1-k)!}\epsilon_0^{(v)}\right|_{C^2} \\ &\quad \times M\left|\frac{\partial_x^{j-p}}{(j-p)!}\frac{\partial_z^{k-q}}{(k-q)!}\rho_0^{(v)}\right|_{C^1}\left\|\frac{\partial_x^p}{p!}\frac{\partial_z^q}{q!}V\right\|_{H^2}. \end{aligned}$$

With the inductive hypotheses we continue

$$\begin{aligned} Z_1 &\leq \frac{1}{r+\bar{t}}\sum_{j=0}^{r}\sum_{p=0}^{j}\sum_{k=0}^{\bar{t}-1}\sum_{q=0}^{k} MC_E\frac{A_E^{r-j}}{(r-j+1)^2}\frac{D_E^{\bar{t}-1-k}}{(\bar{t}-1-k+1)^2} \\ &\quad \times MC_\rho\frac{A^{j-p}}{(j-p+1)^2}\frac{D^{k-q}}{(k-q+1)^2}\underline{C}_e\frac{A^p}{(p+1)^2}\frac{D^q}{(q+1)^2} \\ &\leq \underline{C}_e\frac{M^2 C_E C_\rho}{r+\bar{t}}\frac{A^r}{(r+1)^2}\frac{D^{\bar{t}-1}}{(\bar{t}+1)^2}\sum_{j=0}^{r}\sum_{p=0}^{j}\frac{(r+1)^2}{(r-j+1)^2(j-p+1)^2(p+1)^2} \\ &\quad \times \sum_{k=0}^{\bar{t}-1}\sum_{q=0}^{k}\frac{(\bar{t}+1)^2}{(\bar{t}-1-k+1)^2(k-q+1)^2(q+1)^2} \\ &\leq \underline{C}_e\frac{M^2 C_E C_\rho}{r+\bar{t}}S^4\frac{A^r}{(r+1)^2}\frac{D^{\bar{t}-1}}{(\bar{t}+1)^2}, \end{aligned}$$

and this term is addressed provided that

$$\frac{M^2 C_E C_\rho}{r+\bar{t}}S^4 \leq D/3.$$

Regarding the term Z_2, we begin with the computation

$$\frac{\partial_x^r \partial_z^{\bar{t}-1}}{(r+\bar{t})!}\left[\epsilon_0^{(v)}\partial_x\left[\rho_0^{(v)}\partial_x V\right]\right]$$
$$= \frac{1}{r+\bar{t}}\frac{r!(\bar{t}-1)!}{(r+\bar{t}-1)!}\sum_{j=0}^{r}\sum_{p=0}^{j}\sum_{k=0}^{\bar{t}-1}\sum_{q=0}^{k}\left(\frac{\partial_x^{r-j}}{(r-j)!}\frac{\partial_z^{\bar{t}-1-k}}{(\bar{t}-1-k)!}\epsilon_0^{(v)}\right)$$
$$\times\left\{\left(\frac{\partial_x^{j-p+1}}{(j-p)!}\frac{\partial_z^{k-q}}{(k-q)!}\rho_0^{(v)}\right)\left(\frac{\partial_x^p}{p!}\frac{\partial_z^q}{q!}\partial_x V\right)+\left(\frac{\partial_x^{j-p}}{(j-p)!}\frac{\partial_z^{k-q}}{(k-q)!}\rho_0^{(v)}\right)\left(\frac{\partial_x^{p+1}}{p!}\frac{\partial_z^q}{q!}\partial_x V\right)\right\},$$

with which we estimate, since $(r!(t-1)!) \leq (r+t-1)!$,

$$Z_2 \leq \frac{1}{r+\bar{t}}\sum_{j=0}^{r}\sum_{p=0}^{j}\sum_{k=0}^{\bar{t}-1}\sum_{q=0}^{k} M\left|\frac{\partial_x^{r-j}}{(r-j)!}\frac{\partial_z^{\bar{t}-1-k}}{(\bar{t}-1-k)!}\epsilon_0^{(v)}\right|_{C^1}$$
$$\times\left\{M\left|\frac{\partial_x^{j-p+1}}{(j-p)!}\frac{\partial_z^{k-q}}{(k-q)!}\rho_0^{(v)}\right|_{C^1}\left\|\frac{\partial_x^p}{p!}\frac{\partial_z^q}{q!}V\right\|_{H^2}\right.$$
$$\left.+M\left|\frac{\partial_x^{j-p}}{(j-p)!}\frac{\partial_z^{k-q}}{(k-q)!}\rho_0^{(v)}\right|_{C^1}\left\|\frac{\partial_x^{p+1}}{p!}\frac{\partial_z^q}{q!}V\right\|_{H^2}\right\}.$$

With the inductive hypotheses we can estimate

$$Z_2 \leq \frac{1}{r+\bar{t}}\sum_{j=0}^{r}\sum_{p=0}^{j}\sum_{k=0}^{\bar{t}-1}\sum_{q=0}^{k} MC_E\frac{A_E^{r-j}}{(r-j+1)^2}\frac{D_E^{\bar{t}-1-k}}{(\bar{t}-k)^2}$$
$$\times\left\{MC_\rho(j-p+1)\frac{A^{j-p+1}}{(j-p+2)^2}\frac{D^{k-q}}{(k-q+1)^2}\underline{C}_e\frac{A^p}{(p+1)^2}\frac{D^q}{(q+1)^2}\right.$$
$$\left.+MC_\rho\frac{A^{j-p}}{(j-p+1)^2}\frac{D^{k-q}}{(k-q+1)^2}\underline{C}_e(p+1)\frac{A^{p+1}}{(p+2)^2}\frac{D^q}{(q+1)^2}\right\}.$$
$$\leq \underline{C}_e M^2 C_E C_\rho S^4\frac{A^{r+1}}{(r+1)^2}\frac{D^{\bar{t}-1}}{(\bar{t}+1)^2},$$

and this term is appropriately bounded if

$$M^2 C_E C_\rho S^4 A \leq D/3,$$

since $(j-p+1) \leq r+\bar{t}$ and $(p+1) \leq r+\bar{t}$. □

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