Simulation of Localized Surface Plasmon Resonances in Two Dimensions via Impedance–Impedance Operators

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July 15, 2019

Abstract

It is critically important that engineers be able to numerically simulate the scattering of electromagnetic radiation by bounded obstacles. Additionally, that these simulations be robust and highly accurate is necessitated by many applications of great interest. High–Order Spectral algorithms applied to interfacial formulations can rapidly deliver high fidelity approximations with a modest number of degrees of freedom. The class of High–Order Perturbation of Surfaces methods have proven to be particularly appropriate for these simulations and in this contribution we consider questions of both practical implementation and rigorous analysis. For the former we generalize our recent results to utilize the uniformly well–defined Impedance–Impedance Operators rather than the Dirichlet–Neumann Operators which occasionally encounter unphysical singularities. For the latter we utilize this new formulation to establish the existence, uniqueness, and analyticity of solutions in non–resonant configurations. We also include results of numerical simulations based on an implementation of our new formulation which demonstrates its noteworthy accuracy and robustness.

Keywords: High–Order Spectral Methods, Linear Wave Scattering, Bounded Obstacles, High–Order Perturbation of Surfaces Methods
Mathematics Subject Classification: 65N35; 65N12; 78A45; 78M22; 35Q60; 35J05

1 Introduction

It is critically important that engineers be able to numerically simulate the scattering of electromagnetic radiation by bounded obstacles. Applications abound, and solely in the field of plasmonics [Rae88, Mai07, NH12, EB12] one find surface enhanced Raman scattering (SERS) biosensing [XBKB99], imaging [LLH$^+$05, LLH$^+$05], and cancer therapy [LLH$^+$05, ESHES06]. For more details please see one of the many surveys on the topic, e.g., the volume [Mai07] (Chapters 5, 9, and 10), the article [MCAPS$^+$08], and the publications considering gold nanoparticles [MRFPS$^+$08, LGSLG07]. For many reasons, these simulations must be robust and highly accurate, e.g., due to the very strong plasmonic effect (the field enhancement can be several orders of magnitude) and its quite sensitive nature (the enhancement is only seen over a range of tens of nanometers in incident radiation for gold and silver particles).

As in our previous contribution [NT18], we focus on Localized Surface Plasmon Resonances (LSPRs) which can be induced in metal (e.g., gold or silver) nanorods with radiation in the visible range. In particular how these change as the shape of the cross–section of the rod is varied from perfectly cylindrical. More specifically, consider a rod with cross–section shaped by $\{r = \bar{g}\}$, composed of a noble metal with a wavelength–dependent permittivity, $\epsilon_m = \epsilon_m(\lambda)$, mounted in a dielectric with constant permittivity, ϵ_d. If $\bar{g}$ is sufficiently small an LSPR is excited with incident radiation of wavelength, λ_F, that (nearly) satisfies the two–dimensional "Fröhlich condition" [Mai07]

$$\mathrm{Re}\left[\epsilon_m(\lambda)\right] = -\epsilon_d. \tag{1.1}$$

It is clear, however, that if the cross–section of the rod is specified by

$$r = \bar{g} + \varepsilon f(\theta),$$

for some smooth function f and ε sufficiently small, then the value $\lambda_F = \lambda_F(\varepsilon)$ will change. The method we advocate here is well–suited to study the evolution in ε.

Due to the importance of these models, it is not surprising that the full range of modern numerical methods have been brought to bear upon this problem, including Finite Difference Methods [Str04, LeV07], Finite Element Methods [Joh87, Ihl98], Discontinous Galerkin Methods [HW08], Spectral Element Methods [DFM02], and Spectral Methods [GO77, CHQZ88, Boy01]. We have recently argued [Nic15, NOJR16, NT18] that such *volumetric* approaches are greatly disadvantaged with an unnecessarily large number of unknowns for the piecewise homogeneous problems of relevance here. Interfacial methods based upon Integral Equations (IEs) [CK13] deliver a compelling class of algorithms but, as we have pointed out, these also face difficulties. Most of these have been addressed in recent years through the use of sophisticated quadrature rules to deliver High–Order Spectral accuracy, and the design of preconditioned iterative solvers with suitable acceleration [GR87]. Consequently, they specify a method which deserves serious consideration (see, e.g., the survey article of [RT04] for more details), however, two properties render them non–competitive for the *parameterized* problems we consider compared to the methods we outline here:

1. We parameterize our geometry by the real value ε (the deviation of the nanorod cross–section from cylindrical), and an IE solver will compute the scattering data only for one value of ε at a time. If this value is changed then the solver must be run again.

2. The dense, non–symmetric positive definite systems of linear equations which must be inverted with each simulation.

As we have previously shown [NT18], a "High–Order Perturbation of Surfaces" (HOPS) approach can mollify these concerns. In particular, we investigated an implementation of the method of Field Expansions (FE) originating in the low–order calculations of Rayleigh [Ray07] and Rice [Ric51]. The high–order implementation was developed by Bruno & Reitich [BR93a, BR93b, BR93c, BR98] and later enhanced and stabilized by the first author and Reitich [NR04a, NR04b], the first author and Nigam [NN04], and the first author and Shen [NS06], resulting in the Method of Transformed Field Expansions (TFE). These algorithms retain the advantageous properties of classical IE methods (e.g., surface formulation and exact enforcement of far–field conditions) while avoiding the shortcomings listed above:

1. Since HOPS algorithms are built upon expansions in the parameter, ε, once the Taylor coefficients are known for the scattering quantities, it is simply a matter of summing these (rather than beginning a new simulation) for any given choice of ε to recover the returns.

2. At every Taylor order, the method need only invert a single, sparse operator corresponding to the cylindrical–interface, order–zero approximation of the problem.

In this contribution we build upon the work of the authors in [NT18] by devising, implementing, and testing a HOPS scheme based, not upon Dirichlet–Neumann Operators (DNOs), but rather upon Impedance–Impedance Operators (IIOs). We do this for several reasons, principally that our new approach does not suffer from the artificial "Dirichlet eigenvalues" which plague the relevant DNOs while requiring no increase in computational effort. In addition, we supply for the first time a rigorous analysis of the existence, uniqueness, and analyticity of solutions to the problem of scattering of linear waves by an object of bounded cross–section. While the technique of proof is well–established [NR01a, NR03, NR04b, Nic17, Nic18], the technical details are rather involved, c.f. [NN06], and somewhat limited by the complication of *rigorously* establishing that physical configurations are "non–resonant." Finally, with an implementation of this algorithm we display the efficiency, robustness, and high–order accuracy one can achieve.

The paper is organized as follows: In § 2 we outline the governing equations for linear waves reflected and transmitted by a cylindrical obstacle, with transparent boundary conditions described in § 2.1. We give a boundary formulation of the resulting problem in § 3, together with a HOPS algorithm in § 3.1 and a study of the classical problem of scattering by a rod in § 3.2. For use with our rigorous analysis we define our function spaces in § 4, and we deliver our proof of analyticity of solutions in § 5. The fundamental results required in the proof are the analyticity of the IIOs proven in § 6. Finally, in § 7 we present numerical results followed by concluding remarks in § 8.

2 Governing Equations

We consider a y–invariant obstacle of bounded cross–section as displayed in Figure 1. Materials of refractive index n^u and n^w fill the (unbounded) exterior and (bounded) interior, respectively. The interface between the two domains is described in polar coordinates, $\{x = r\cos(\theta), z = r\sin(\theta)\}$, by the graph $r = \bar{g} + g(\theta)$ so that the exterior and interior domains are specified by

$$S^u := \{r > \bar{g} + g(\theta)\}, \quad S^w := \{r < \bar{g} + g(\theta)\},$$

respectively. The superscripts are chosen to conform to the notation of previous work by the authors [NOJR16, Nic12, NT18]. The cylindrical geometry demands that the interface be 2π–periodic, $g(\theta + 2\pi) = g(\theta)$. We consider monochromatic plane–wave illumination by incident radiation of frequency ω and wavenumber $k^u = n^u\omega/c_0 = \omega/c^u$ (c_0 is the speed of light) aligned with the corrugations of the obstacle. We denote the reduced illuminating fields of incidence angle ϕ

$$\mathbf{E}^{\text{inc}} = \mathbf{A}e^{i\alpha x - i\gamma^u z}, \quad \mathbf{H}^{\text{inc}}(x,z) = \mathbf{B}e^{i\alpha x - i\gamma^u z},$$
$$\alpha = k^u\sin(\phi), \quad \gamma^u = k^u\cos(\phi), \quad |\mathbf{A}| = |\mathbf{B}| = 1;$$

we have factored out time dependence of the form $\exp(-i\omega t)$, and we can write these as

$$\mathbf{E}^{\text{inc}} = \mathbf{A}e^{ik^u r\sin(\phi-\theta)}, \quad \mathbf{H}^{\text{inc}} = \mathbf{B}e^{ik^u r\sin(\phi-\theta)}.$$

The geometry demands that the reduced electric and magnetic fields, $\{\mathbf{E}, \mathbf{H}\}$, be 2π–periodic in θ, and the scattered radiation is "outgoing" in S^u and bounded in S^w.

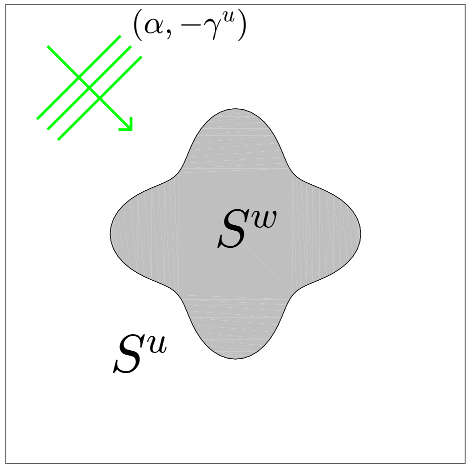


Figure 1: Plot of the cross–section of a nanorod (occupying S^w) shaped by $r = \bar{g} + \varepsilon \cos(4\theta)$ ($\varepsilon = \bar{g}/5$) housed in a dielectric (occupying S^u) under plane–wave illumination with wavenumber $(\alpha, -\gamma^u)$.

In this two–dimensional setting the time–harmonic Maxwell equations decouple into two scalar Helmholtz problems which govern the transverse electric (TE) and transverse magnetic (TM) polarizations [Pet80]. The invariant (y) directions of the scattered (electric or magnetic) fields are denoted by $\{u(r,\theta), w(r,\theta)\}$ in S^u and S^w, respectively, and the incident radiation in the outer domain by $u^{\text{inc}}(r,\theta)$.

All of these developments lead us to seek outgoing/bounded, 2π–periodic solutions of

$$\Delta u + (k^u)^2 u = 0, \qquad r > \bar{g} + g(\theta), \tag{2.1a}$$

$$\Delta w + (k^w)^2 w = 0, \qquad r < \bar{g} + g(\theta), \tag{2.1b}$$

$$u - w = \xi, \qquad r = \bar{g} + g(\theta), \tag{2.1c}$$

$$\tau^u \partial_N u - \tau^w \partial_N w = \tau^u \nu, \qquad r = \bar{g} + g(\theta), \tag{2.1d}$$

where the Dirichlet data is

$$\xi(\theta) := \left[-u^{\text{inc}}\right]_{r=\bar{g}+g(\theta)} = -e^{ik^u(\bar{g}+g(\theta))\sin(\phi-\theta)}, \tag{2.1e}$$

and the Neumann data is

$$\nu(\theta) := \left[-\partial_N u^{\text{inc}}\right]_{r=\bar{g}+g(\theta)} = \left\{(\bar{g}+g(\theta)) i k^u \sin(\phi-\theta) + \left(\frac{g'(\theta)}{\bar{g}+g(\theta)}\right)\cos(\phi-\theta)\right\}\xi(\theta). \tag{2.1f}$$

In these

$$\partial_N = \hat{r}(\bar{g}+g)\partial_r - \hat{\theta}\left(\frac{g'}{\bar{g}+g}\right)\partial_\theta,$$

for unit vectors in the radial ($\hat{r}$) and angular ($\hat{\theta}$) directions, and

$$\tau^m = \begin{cases} 1, & \text{TE}, \\ 1/\epsilon^{(m)}, & \text{TM}, \end{cases} \qquad m \in \{u, w\},$$

where $\gamma^w = k^w \cos(\phi)$. The case of TM polarization is of fundamental importance in the study of Localized Surface Plasmon Resonances (LSPRs) [Rae88] and thus we concentrate our attention on the TM case from here.

2.1 Transparent Boundary Conditions

Regarding the Outgoing Wave Condition (OWC), commonly known as the Sommerfeld Radiation Condition [CK13], and Boundedness Boundary Condition (BBC), we introduce the circles $\{r = R^o\}$ and $\{r = R_i\}$, where

$$R^o > \bar{g} + |g|_{L^\infty}, \quad 0 < R_i < \bar{g} - |g|_{L^\infty},$$

define the domains

$$S^o := \{r > R^o\}, \quad S_i := \{r < R_i\},$$

and note that we can find periodic solutions of the relevant Helmholtz problems on these domains given generic Dirichlet data, say $\underline{u}(\theta)$ and $\underline{w}(\theta)$. These read [CK13]

$$u(r,\theta) = \sum_{p=-\infty}^{\infty} \hat{\underline{u}}_p \frac{H_p(k^u r)}{H_p(k^u R^o)} e^{ip\theta}, \quad w(r,\theta) = \sum_{p=-\infty}^{\infty} \hat{\underline{w}}_p \frac{J_p(k^w r)}{J_p(k^w R_i)} e^{ip\theta}, \tag{2.2}$$

where, J_p is the p–th Bessel function of the first kind and H_p is the p–th Hankel function of the first kind. We note that

$$u(R^o,\theta) = \sum_{p=-\infty}^{\infty} \hat{\underline{u}}_p e^{ip\theta}, \quad w(R_i,\theta) = \sum_{p=-\infty}^{\infty} \hat{\underline{w}}_p e^{ip\theta}.$$

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

$$\begin{aligned}
-\partial_r u(R^o,\theta) &= \sum_{p=-\infty}^{\infty} \left(-k^u \frac{H_p'(k^u R^o)}{H_p(k^u R^o)} \right) \hat{\underline{u}}_p e^{ip\theta} =: T^{(u)}\left[\underline{u}(\theta)\right], \\
\partial_r w(R_i,\theta) &= \sum_{p=-\infty}^{\infty} \left(k^w \frac{J_p'(k^w R_i)}{J_p(k^w R_i)} \right) \hat{\underline{w}}_p e^{ip\theta} =: T^{(w)}\left[\underline{w}(\theta)\right].
\end{aligned}$$

These define the order–one Fourier multipliers $\{T^{(u)}, T^{(w)}\}$.

With the operator $T^{(u)}$ it is not difficult to see that periodic, outward propagating solutions to the Helmholtz equation

$$\Delta u + (k^u)^2 u = 0, \quad r > \bar{g} + g(\theta),$$

equivalently solve

$$\begin{aligned}
&\Delta u + (k^u)^2 u = 0, && \bar{g} + g(\theta) < r < R^o, \\
&\partial_r u + T^{(u)}[u] = 0, && r = R^o.
\end{aligned}$$

Similarly, one can show that periodic, bounded solutions to the Helmholtz equation

$$\Delta w + (k^w)^2 w = 0, \quad r < \bar{g} + g(\theta),$$

equivalently solve

$$\begin{aligned}
&\Delta w + (k^w)^2 w = 0, && R_i < r < \bar{g} + g(\theta), \\
&\partial_r w - T^{(w)}[w] = 0, && r = R_i.
\end{aligned}$$

3 Boundary Formulation

At this point we follow the philosophy of [Nic12, Nic17, NT18] and reduce our degrees of freedom to surface unknowns. However, rather than select the Dirichlet and Neumann traces utilized in these papers, we choose impedance traces. To motivate our particular choices we focus upon the boundary conditions (2.1c) and (2.1d) and operate upon this pair by the linear operator

$$P = \begin{pmatrix} Y & -I \\ Z & -I \end{pmatrix},$$

where I is the identity, and Y and Z are unequal operators to be specified. In the work of Despres [Des91b, Des91a] these were chosen to be $\pm i\eta$ for a constant $\eta \in \mathbf{R}^+$, however, other choices are also possible. The resulting boundary conditions are

$$\begin{aligned} [-\tau^u \partial_N u + Yu] + [\tau^w \partial_N w - Yw] &= [-\tau^u \nu + Y\xi], \\ [-\tau^u \partial_N u + Zu] + [\tau^w \partial_N w - Zw] &= [-\tau^u \nu + Z\xi], \end{aligned}$$

which inspire the following definitions for impedances

$$U := [-\tau^u \partial_N u + Yu]_{r=\bar{g}+g}, \quad W := [\tau^w \partial_N w - Zw]_{r=\bar{g}+g},$$

their "conjugates"

$$\tilde{U} := [-\tau^u \partial_N u + Zu]_{r=\bar{g}+g}, \quad \tilde{W} := [\tau^w \partial_N w - Yw]_{r=\bar{g}+g},$$

and the interfacial data

$$\zeta := [-\tau^u \nu + Y\xi], \quad \psi := [-\tau^u \nu + Z\xi].$$

Via an integral formula these quantities can deliver the scattered field at *any* point [Eva10, CK13], thus, the governing equations reduce to the boundary conditions

$$U + \tilde{W} = \zeta, \quad \tilde{U} + W = \psi. \tag{3.1}$$

Now, we have two equations for four unknowns, however, the pairs $\{U, \tilde{U}\}$ and $\{W, \tilde{W}\}$ are not independent and we make this explicit through the introduction of Impedance–Impedance operators (IIOs). However, care is required as a poor choice of the operator Y or Z may induce a lack of uniqueness in the governing Helmholtz equation, i.e., k^u or k^w may be an eigenvalue of the Laplacian (with the impedance boundary conditions) on the domain in question.

In order to avoid this problem we fix some $\delta > 0$ and, in Appendix B, define the notion of δ–permissibility, (B.5). In addition, in order to simplify the proofs we present in Appendix B, we make the further restriction that we are δ–permissible in the $k = 0$ case, (B.13). While this latter restriction can be omitted, we find it convenient and not overly burdensome.

The details of these definitions can be found in Appendix B, but, in brief, a configuration is a quintuple of wavenumber (k), inner and outer domain radius (a and b), and inner and outer operators (A and B). A configuration is δ–permissible if a certain determinant function is bounded from below by $\delta > 0$ ensuring unique solvability. With our perturbative philosophy in mind we specify this bound in the zero–deformation case knowing that violations may occur when ε becomes too large. On some level is this inconvenient, however, we point out that the $\varepsilon = 0$ conditions can, in theory, be *explicitly* computed so that particular choices of Y and Z can be evaluated.

Definition 3.1. Given a δ–permissible configuration

$$(k^u, \bar{g}, R^o, Y/(\tau^u \bar{g}), -T^{(u)}) \in \mathcal{C}_\delta(k^u, \bar{g}, R^o, Y/(\tau^u \bar{g}), -T^{(u)}), \tag{3.2a}$$
$$(0, \bar{g}, R^o, Y/(\tau^u \bar{g}), -T^{(u)}) \in \mathcal{C}_\delta(0, \bar{g}, R^o, Y/(\tau^u \bar{g}), -T^{(u)}), \tag{3.2b}$$

and a sufficiently smooth and small deformation $g(\theta)$, the unique periodic solution of

$$\Delta u + (k^u)^2 u = 0, \qquad \bar{g} + g(\theta) < r < R^o, \tag{3.3a}$$
$$-\tau^u \partial_N u + Y u = U, \qquad r = \bar{g} + g(\theta), \tag{3.3b}$$
$$\partial_r u + T^{(u)}[u] = 0, \qquad r = R^o, \tag{3.3c}$$

defines the Impedance–Impedance Operator

$$Q[U] = Q(R^o, \bar{g}, g)[U] := \tilde{U}. \tag{3.4}$$

Definition 3.2. Given a δ–permissible configuration

$$(k^w, R_i, \bar{g}, T^{(w)}, Z/(\tau^w \bar{g})) \in \mathcal{C}_\delta(k^w, R_i, \bar{g}, T^{(w)}, Z/(\tau^w \bar{g})), \tag{3.5a}$$
$$(0, R_i, \bar{g}, T^{(w)}, Z/(\tau^w \bar{g})) \in \mathcal{C}_\delta(0, R_i, \bar{g}, T^{(w)}, Z/(\tau^w \bar{g})), \tag{3.5b}$$

and a sufficiently smooth and small deformation $g(\theta)$, the unique periodic solution of

$$\Delta w + (k^w)^2 w = 0, \qquad R_i < r < \bar{g} + g(\theta), \tag{3.6a}$$
$$\tau^w \partial_N w - Z w = W, \qquad r = \bar{g} + g(\theta), \tag{3.6b}$$
$$\partial_r w - T^{(w)}[w] = 0, \qquad r = R_i, \tag{3.6c}$$

defines the Impedance–Impedance Operator

$$S[W] = S(R_i, \bar{g}, g)[W] := \tilde{W}. \tag{3.7}$$

In terms of these operators the boundary conditions, (3.1), become

$$U + S[W] = \zeta, \quad Q[U] + W = \psi,$$

or

$$\begin{pmatrix} I & S \\ Q & I \end{pmatrix} \begin{pmatrix} U \\ W \end{pmatrix} = \begin{pmatrix} \zeta \\ \psi \end{pmatrix}. \tag{3.8}$$

For later use, we write this more compactly as

$$\mathbf{A}\mathbf{V} = \mathbf{R}, \tag{3.9}$$

where

$$\mathbf{A} = \begin{pmatrix} I & S \\ Q & I \end{pmatrix}, \quad \mathbf{V} = \begin{pmatrix} U \\ W \end{pmatrix}, \quad \mathbf{R} = \begin{pmatrix} \zeta \\ \psi \end{pmatrix}. \tag{3.10}$$

3.1 A High–Order Perturbation of Surfaces Method

Our approach to simulating solutions to (3.9) is perturbative in nature and based upon the assumption that $g(\theta) = \varepsilon f(\theta)$ where ε is sufficiently small. As we shall show in Section 6, provided that f is sufficiently smooth (which we shall make more precise later), then the IIOs, Q and S, are analytic in the perturbation parameter ε so that the following expansions are strongly convergent in an appropriate Sobolev space

$$Q(\varepsilon f) = \sum_{n=0}^{\infty} Q_n(f)\varepsilon^n, \tag{3.11a}$$

$$S(\varepsilon f) = \sum_{n=0}^{\infty} S_n(f)\varepsilon^n. \tag{3.11b}$$

Clearly, if this is the case then the operator $\mathbf{A}$ will also be analytic, as will $\mathbf{R}$ so that

$$\{\mathbf{A}(\varepsilon f), \mathbf{R}(\varepsilon f)\} = \sum_{n=0}^{\infty} \{\mathbf{A}_n(f), \mathbf{R}_n(f)\}\varepsilon^n. \tag{3.12}$$

We will shortly show that, under certain circumstances, there will be a unique solution, $\mathbf{V}$, of (3.9) which is also analytic in ε

$$\mathbf{V}(\varepsilon f) = \sum_{n=0}^{\infty} \mathbf{V}_n(f)\varepsilon^n. \tag{3.13}$$

Furthermore, it is clear that the $\mathbf{V}_n$ must satisfy

$$\mathbf{V}_n = \mathbf{A}_0^{-1} \left\{ \mathbf{R}_0 - \sum_{\ell=0}^{n-1} \mathbf{A}_{n-\ell} \mathbf{V}_\ell \right\}, \tag{3.14}$$

and one key in the analysis is the invertibility of the operator $\mathbf{A}_0$ which we now investigate.

3.2 The Trivial Configuration: LSPR Condition

To investigate this invertibility question we show how our formulation delivers the classical solution for plane wave scattering by a cylindrical obstacle. For this we consider (3.8) in the case $g \equiv 0$,

$$\begin{pmatrix} I & S_0 \\ Q_0 & I \end{pmatrix} \begin{pmatrix} U \\ W \end{pmatrix} = \begin{pmatrix} \zeta_0 \\ \psi_0 \end{pmatrix}. \tag{3.15}$$

In this trivial configuration, the solutions to (3.3) and (3.6) are, (c.f. (2.2)),

$$u(r,\theta) = \sum_{p=-\infty}^{\infty} \frac{\hat{U}_p}{-\tau^u(k^u\bar{g})H_p'(k^u\bar{g}) + \hat{Y}_p H_p(k^u\bar{g})} H_p(k^u r) e^{ip\theta},$$

$$w(r,\theta) = \sum_{p=-\infty}^{\infty} \frac{\hat{W}_p}{\tau^w(k^w\bar{g})J_p'(k^u\bar{g}) - \hat{Z}_p J_p(k^w\bar{g})} J_p(k^w r) e^{ip\theta},$$

respectively. From these we find for (3.4)

$$\begin{aligned} Q_0[U] &= \sum_{p=-\infty}^{\infty} \widehat{(Q_0)}_p \hat{U}_p e^{ip\theta} = \sum_{p=-\infty}^{\infty} \left(\frac{-\tau^u(k^u\bar{g})H_p'(k^u\bar{g}) + \hat{Z}_p H_p(k^u\bar{g})}{-\tau^u(k^u\bar{g})H_p'(k^u\bar{g}) + \hat{Y}_p H_p(k^u\bar{g})} \right) \hat{U}_p e^{ip\theta} \\ &=: \left(\frac{-\tau^u(k^u\bar{g})H_D'(k^u\bar{g}) + Z H_D(k^u\bar{g})}{-\tau^u(k^u\bar{g})H_D'(k^u\bar{g}) + Y H_D(k^u\bar{g})} \right) U, \end{aligned}$$

and for (3.7)

$$S_0[W] = \sum_{p=-\infty}^{\infty} \widehat{(S_0)}_p \hat{W}_p e^{ip\theta} = \sum_{p=-\infty}^{\infty} \left(\frac{\tau^w(k^w\bar{g}) J_p'(k^w\bar{g}) - \hat{Y}_p J_p(k^w\bar{g})}{\tau^w(k^w\bar{g}) J_p'(k^w\bar{g}) - \hat{Z}_p J_p(k^w\bar{g})} \right) \hat{W}_p e^{ip\theta}$$
$$=: \left(\frac{\tau^w(k^w\bar{g}) J_D'(k^w\bar{g}) - Y J_D(k^w\bar{g})}{\tau^w(k^w\bar{g}) J_D'(k^w\bar{g}) - Z J_D(k^w\bar{g})} \right) W,$$

which define the order–one Fourier multipliers

$$Q_0 = \left(\frac{-\tau^u(k^u\bar{g}) H_D'(k^u\bar{g}) + Z H_D(k^u\bar{g})}{-\tau^u(k^u\bar{g}) H_D'(k^u\bar{g}) + Y H_D(k^u\bar{g})} \right), \quad S_0 = \left(\frac{\tau^w(k^w\bar{g}) J_D'(k^w\bar{g}) - Y J_D(k^w\bar{g})}{\tau^w(k^w\bar{g}) J_D'(k^w\bar{g}) - Z J_D(k^w\bar{g})} \right), \tag{3.16}$$

respectively.

Returning to (3.15) we find the solution at each wavenumber is given by

$$\begin{pmatrix} \hat{U}_p \\ \hat{W}_p \end{pmatrix} = \frac{1}{1 - \widehat{(S_0)}_p \widehat{(Q_0)}_p} \begin{pmatrix} 1 & -\widehat{(S_0)}_p \\ -\widehat{(Q_0)}_p & 1 \end{pmatrix} \begin{pmatrix} \widehat{(\zeta_0)}_p \\ \widehat{(\psi_0)}_p \end{pmatrix}, \tag{3.17}$$

and it is clear that unique solvability of this system hinges on the determinant function

$$\Delta_p := 1 - \widehat{(S_0)}_p \widehat{(Q_0)}_p. \tag{3.18}$$

With the notation

$$\mathbf{J} = J_p(k^w\bar{g}), \quad \mathbf{J}' = -\tau^w(k^w\bar{g}) J_p'(k^w\bar{g}), \quad \mathbf{H} = H_p(k^u\bar{g}), \quad \mathbf{H}' = -\tau^u(k^u\bar{g}) H_p'(k^u\bar{g}),$$

we find

$$\begin{aligned} \Delta_p &= 1 - \left(\frac{\mathbf{H}' + Z\mathbf{H}}{\mathbf{H}' + Y\mathbf{H}} \right) \left(\frac{\mathbf{J}' - Y\mathbf{J}}{\mathbf{J}' - Z\mathbf{J}} \right) \\ &= \frac{(\mathbf{H}' + Y\mathbf{H})(\mathbf{J}' - Z\mathbf{J}) - (\mathbf{H}' + Z\mathbf{H})(\mathbf{J}' - Y\mathbf{J})}{(\mathbf{H}' + Y\mathbf{H})(\mathbf{J}' - Z\mathbf{J})} \\ &= \frac{(Y + Z)(\mathbf{J}'\mathbf{H} - \mathbf{J}\mathbf{H}')}{(\mathbf{H}' + Y\mathbf{H})(\mathbf{J}' - Z\mathbf{J})}. \end{aligned} \tag{3.19}$$

The zeros of this function are the same as those we found in [NT18], and thus deliver the same result in the "small radius" (quasistatic) limit [Mai07], $k^u\bar{g} \ll 1$ and $k^w\bar{g} \ll 1$,

$$\epsilon^{(u)} = -\mathrm{Re}\left\{\epsilon^{(w)}\right\} - i\mathrm{Im}\left\{\epsilon^{(w)}\right\}.$$

If the Fröhlich condition, c.f. (1.1),

$$\epsilon^{(u)} = -\mathrm{Re}\left\{\epsilon^{(w)}\right\},$$

is verified then it can "almost" be true. Again, this is *different* from the three dimensional Fröhlich condition for nanoparticles [Mai07]

$$\epsilon^{(u)} = -2\mathrm{Re}\left\{\epsilon^{(w)}\right\}.$$

Remark 3.3. At this point we further restrict our configuration so that the function Δ_p is always non–zero which is equivalent to the invertibility of $\mathbf{A}_0$. More precisely, in addition to conditions (3.2) and (3.5), we also require that the quantities $\{k^u, k^w, R_i, R^o, Y, Z\}$ be such that

$$|\Delta_p| > \delta, \quad \forall p \in \mathbf{Z}. \tag{3.20}$$

To summarize our restrictions:

1. We demand (3.2) to guarantee that $Q(g)$ is well–defined for g sufficiently small.
2. We demand (3.5) to guarantee that $S(g)$ is well–defined for g sufficiently small.
3. We demand (3.20) to guarantee that $\mathbf{A}_0$ is invertible.

4 Interfacial Function Spaces

We begin with a careful mathematical analysis of (3.9) which will help justify the computational results we present in Section 7. Before describing these rigorous results we specify the interfacial function spaces we require. For any real $s \geq 0$ we recall the classical, periodic, L^2–based Sobolev norm [Kre14]

$$\|U\|_{H^s}^2 := \sum_{p=-\infty}^{\infty} \langle p \rangle^{2s} \left|\hat{U}_p\right|^2, \quad \langle p \rangle^2 := 1 + |p|^2, \quad \hat{U}_p := \frac{1}{2\pi} \int_0^{2\pi} U(\theta) e^{i\alpha_p x} \, d\theta, \tag{4.1}$$

which gives rise to the periodic Sobolev space [Kre14]

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

We also require the dual space of $H^s([0, 2\pi])$ which is characterized by Theorem 8.10 of [Kre14] and typically denoted $H^{-s}([0, 2\pi])$. In short, if $U' \in (H^s)' = H^{-s}$ then $\|U'\|_{H^{-s}}$ is defined by (4.1) where $\widehat{U'}_p = U'(\hat{U}_p)$.

With this definition it is a simple matter to prove the following Lemma.

Lemma 4.1. *For any $s \in \mathbf{R}$ there exist constants $C_Q, C_S > 0$ such that*

$$\|Q_0 U\|_{H^s} \leq C_Q \|U\|_{H^s}, \quad \|S_0 W\|_{H^s} \leq C_S \|W\|_{H^s},$$

for any $U, W \in H^s$.

We also recall, for any integer $s \geq 0$, the space of s–times continuously differentiable functions with the Hölder norm

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

For later reference we recall the following classical result.

Lemma 4.2. *For any integer $s \geq 0$, any $\beta > 0$, and any set $U \subset \mathbf{R}^m$, if $f, u, g, \mu : U \to \mathbf{C}$, $f \in C^s(U)$, $u \in H^s(U)$, $g \in C^{s+1/2+\beta}(U)$, $\mu \in H^{s+1/2}(U)$, then*

$$\|fu\|_{H^s} \leq \tilde{M}(m, s, U) \, |f|_{C^s} \, \|u\|_{H^s}, \quad \|g\mu\|_{H^{s+1/2}} \leq \tilde{M}(m, s, U) \, |g|_{C^{s+1/2+\beta}} \, \|\mu\|_{H^{s+1/2}},$$

for some constant $\tilde{M}$.

In addition, we require the analogous result valid for *any* real value of s [Fol76, NN06].

Lemma 4.3. *For any $s \in \mathbf{R}$ and any set $U \subset \mathbf{R}^m$, if $\varphi, \psi : U \to \mathbf{C}$, $\varphi \in H^{|s|+m+2}(U)$ and $\psi \in H^s(U)$, then*

$$\|\varphi\psi\|_{H^s} \leq M(m,s,U) \|\varphi\|_{H^{|s|+m+2}} \|\psi\|_{H^s},$$

for some constant M.

Remark 4.4. Presently we will be required to estimate terms of the form

$$\|(\partial_\theta f)u\|_{L^2(\Omega)} = \|(\partial_\theta f)u\|_{H^0(\Omega)}, \quad \|(\partial_\theta f)\mu\|_{H^{-1/2}([0,2\pi])},$$

where $\Omega \subset \mathbf{R}^2$, which feature Sobolev norms too weak for the standard algebra estimate, Lemma 4.2. For this reason we have introduced Lemma 4.3 which allows us to compute, for $m = 2$,

$$\begin{aligned}
\|(\partial_\theta f)u\|_{L^2(\Omega)} &= \|(\partial_\theta f)u\|_{H^0(\Omega)} \\
&\leq M \|(\partial_\theta f)\|_{H^{|0|+2+2}([0,2\pi])} \|u\|_{H^0(\Omega)} \\
&\leq M \|f\|_{H^5([0,2\pi])} \|u\|_{H^0(\Omega)},
\end{aligned}$$

while, for $m = 1$,

$$\begin{aligned}
\|(\partial_\theta f)\mu\|_{H^{-1/2}([0,2\pi])} &\leq M \|(\partial_\theta f)\|_{H^{|-1/2|+1+2}([0,2\pi])} \|\mu\|_{H^{-1/2}([0,2\pi])} \\
&\leq M \|f\|_{H^{4+1/2}([0,2\pi])} \|\mu\|_{H^{-1/2}([0,2\pi])}.
\end{aligned}$$

In this way, if we require $f \in H^5([0,2\pi])$ then we can use the algebra property of Lemma 4.3 throughout our developments. We note that, by Sobolev embedding, if $f \in H^5([0,2\pi])$ then $f \in C^4([0,2\pi])$, and if $f \in C^5([0,2\pi])$ then $f \in H^5([0,2\pi])$.

5 Analyticity of Solutions

We can now take up the rigorous analysis of (3.13) for which we utilize the general theory of analyticity of solutions of linear systems of equations. To be more specific, we follow the developments found in [Nic17] for the solution of (3.9). Given the expansions (3.12) we seek the solution of the form (3.13) which satisfy (3.14). We restate the main result here for completeness.

Theorem 5.1 (Nicholls [Nic17])**.** *Given two Banach spaces X and Y, suppose that:*

(H1) $\mathbf{R}_n \in Y$ *for all $n \geq 0$, and there exist constants $C_R > 0$, $B_R > 0$ such that*

$$\|\mathbf{R}_n\|_Y \leq C_R B_R^n, \quad n \geq 0.$$

(H2) $\mathbf{A}_n : X \to Y$ *for all $n \geq 0$, and there exists constants $C_A > 0$, $B_A > 0$ such that*

$$\|\mathbf{A}_n\|_{X \to Y} \leq C_A B_A^n, \quad n \geq 0.$$

(H3) $\mathbf{A}_0^{-1} : Y \to X$*, and there exists a constant $C_e > 0$ such that*

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

Then the equation (3.9) *has a unique solution* (3.13)*, and there exist constants* $C_V > 0$ *and* $B_V > 0$ *such that*

$$\|\mathbf{V}_n\|_X \leq C_V B_V^n, \quad n \geq 0,$$

for any

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

which implies that, for any $0 \leq \rho < 1$, (3.13) *converges for all* ε *such that* $B_V \varepsilon < \rho$*, i.e.,* $\varepsilon < \rho / B_V$.

All that remains is to find the forms (3.12), and establish Hypotheses (H1), (H2), and (H3). For the former it is quite clear from (3.9) that

$$\mathbf{A}_0 = \begin{pmatrix} I & S_0 \\ Q_0 & I \end{pmatrix}, \quad \mathbf{A}_n = \begin{pmatrix} 0 & S_n \\ Q_n & 0 \end{pmatrix}, \quad n \geq 1,$$
$$\mathbf{V}_n = \begin{pmatrix} U_n \\ W_n \end{pmatrix}, \quad \mathbf{R}_n = \begin{pmatrix} \zeta_n \\ \psi_n \end{pmatrix}.$$

For the spaces X and Y, the natural choices for the weak formulation we pursue here are

$$X = Y = H^{-1/2}([0, 2\pi]) \times H^{-1/2}([0, 2\pi]),$$

so that

$$\left\| \begin{pmatrix} U \\ W \end{pmatrix} \right\|_X^2 = \|U\|_{H^{-1/2}}^2 + \|W\|_{H^{-1/2}}^2.$$

Hypothesis (H1): We begin by noting that

$$\zeta_n = \tau^u \nu_n + Y \xi_n, \quad \psi_n = -\tau^u \nu_n + Z \xi_n,$$

where

$$\xi_n = -e^{ik^u \bar{g} \sin(\phi - \theta)} \left[(ik^u) \sin(\phi - \theta) \right]^n F_n, \quad F_n := \frac{f^n}{n!},$$

and

$$\nu_n = \bar{g} \left[(ik^u) \sin(\phi - \theta) \right] \xi_n + (ik^u) \left[f \sin(\phi - \theta) + (\partial_\theta f) \cos(\phi - \theta) \right] \xi_{n-1}.$$

Now, if $Y : H^{1/2} \to H^{-1/2}$ and $Z : H^{1/2} \to H^{-1/2}$, then

$$\|R_n\|_Y^2 = \|\zeta_n\|_{H^{-1/2}}^2 + \|\psi_n\|_{H^{-1/2}}^2 \leq 2 |\tau^u|^2 \|\nu_n\|_{H^{-1/2}}^2 + (C_Y + C_Z) \|\xi_n\|_{H^{1/2}}^2,$$

and, from the explanation given in Remark 4.4, this will be bounded provided that $f \in H^5([0, 2\pi])$.

Hypothesis (H2): The analyticity estimates for the IIOs Q, Theorem 6.6, and S, Theorem 6.1, show rather directly that Hypothesis (H2) is verified provided that our configuration is δ–permissible: (3.2) and (3.5). Indeed, as we have

$$\|Q_n[U]\|_{H^{-1/2}} \leq C_Q B_Q^n, \quad \|S_n[W]\|_{H^{-1/2}} \leq C_S B_S^n,$$

it is a straightforward matter to show that

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

for $C_A = \max\{C_Q, C_S\}$ and $B_A = \max\{B_Q, B_S\}$.

Hypothesis (H3): We now address the existence and invertibility properties of the linearized operator $\mathbf{A}_0$ in the following Lemma.

Lemma 5.2. *If $\zeta, \psi \in H^{-1/2}([0, 2\pi])$ and our configuration is δ–permissible ((3.2), (3.5), and (3.20)) then there exists a unique solution of*

$$\begin{pmatrix} I & S_0 \\ Q_0 & I \end{pmatrix} \begin{pmatrix} U \\ W \end{pmatrix} = \begin{pmatrix} \zeta \\ \psi \end{pmatrix},$$

c.f. (3.15), *satisfying*

$$\|U\|_{H^{-1/2}} \le \tilde{C}_e \left\{ \|\zeta\|_{H^{-1/2}} + \|\psi\|_{H^{-1/2}} \right\},$$
$$\|W\|_{H^{-1/2}} \le \tilde{C}_e \left\{ \|\zeta\|_{H^{-1/2}} + \|\psi\|_{H^{-1/2}} \right\},$$

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

Proof. The bulk of the proof has already been worked out in Section 3.2. If we expand

$$\zeta(\theta) = \sum_{p=-\infty}^{\infty} \hat{\zeta}_p e^{ip\theta}, \quad \psi(\theta) = \sum_{p=-\infty}^{\infty} \hat{\psi}_p e^{ip\theta},$$

then we can find solutions of (3.15)

$$U(\theta) = \sum_{p=-\infty}^{\infty} \hat{U}_p e^{ip\theta}, \quad W(\theta) = \sum_{p=-\infty}^{\infty} \hat{W}_p e^{ip\theta},$$

where

$$\begin{pmatrix} \hat{U}_p \\ \hat{W}_p \end{pmatrix} = \frac{1}{1 - \widehat{(S_0)}_p \widehat{(Q_0)}_p} \begin{pmatrix} 1 & -\widehat{(S_0)}_p \\ -\widehat{(Q_0)}_p & 1 \end{pmatrix} \begin{pmatrix} \widehat{(\zeta_0)}_p \\ \widehat{(\psi_0)}_p \end{pmatrix},$$

c.f. (3.17). The key is the analysis of the operators $\widehat{(S_0)}_p$, $\widehat{(Q_0)}_p$, and the determinant function

$$\Delta_p = 1 - \widehat{(S_0)}_p \widehat{(Q_0)}_p = \frac{(Y + Z)(\mathbf{J}'\mathbf{H} - \mathbf{J}\mathbf{H}')}{(\mathbf{H}' + Y\mathbf{H})(\mathbf{J}' - Z\mathbf{J})},$$

c.f. (3.18) and (3.19). For these it is not difficult to show that, from their asymptotic properties, there exist constants $\tilde{K}_Q, \tilde{K}_S, \tilde{K}_\Delta > 0$ such that

$$\left| \widehat{(Q_0)}_p \right| < \tilde{K}_Q, \quad \left| \widehat{(S_0)}_p \right| < \tilde{K}_S, \quad \frac{1}{|\Delta_p|} < \tilde{K}_\Delta.$$

With these we can estimate

$$\begin{aligned} \|U\|_{H^{-1/2}}^2 &= \sum_{p=-\infty}^{\infty} \langle p \rangle^{-1} \left| \hat{U}_p \right|^2 \\ &< \sum_{p=-\infty}^{\infty} \langle p \rangle^{-1} \tilde{K}_\Delta^2 \left(\left| \hat{\zeta}_p \right|^2 + \tilde{K}_S^2 \left| \hat{\psi}_p \right|^2 \right) \\ &= \tilde{K} \left(\|\zeta\|_{H^{-1/2}}^2 + \|\psi\|_{H^{-1/2}}^2 \right), \end{aligned}$$

for some $\tilde{K} > 0$. Proceeding similarly for W we complete the proof. □

Having established Hypotheses (H1), (H2), and (H3) we can invoke Theorem 5.1 to discover our final result.

Theorem 5.3. *If $f \in H^5([0, 2\pi])$ and the configuration is δ–permissible ((3.2), (3.5), and (3.20)) there exists a unique solution pair,* (3.13), *of the problem,* (3.9), *satisfying*

$$\|U_n\|_{H^{-1/2}} \le C_U D^n, \quad \|W_n\|_{H^{-1/2}} \le C_W D^n, \quad \forall n \ge 0,$$

for any $D > \|f\|_{H^5}$, where C_U and C_W are universal constants.

6 Analyticity of the Impedance–Impedance Operators

At this point the only remaining task is to establish the analyticity of the IIOs, Q and S. In the exterior this has been accomplished for the DNO in [NN06] so we focus on the interior domain. This analysis is quite intricate and to make our developments more transparent we focus on the dielectric case $\epsilon^{(w)} \in \mathbf{R}$ so that $k^w \in \mathbf{R}$. Given this assumption we prove the following result.

Theorem 6.1. *If $f \in H^5([0, 2\pi])$, the configuration is δ–permissible,* (3.5)*, and $W \in H^{-1/2}([0, 2\pi])$ then the series* (3.11b) *converges strongly as an operator from $H^{-1/2}([0, 2\pi])$ to $H^{-1/2}([0, 2\pi])$. In other words there exist constants $K_S > 0$ and $B_S > 0$ such that*

$$\|S_n(f)[W]\|_{H^{-1/2}} \leq K_S B_S^n. \tag{6.1}$$

We establish this result with the method of Transformed Field Expansions (TFE) [NR01a, NR01b, NR03] which has proven quite successful in establishing analyticity of DNOs in similar settings [NN04, NN06, NS09]. The TFE method proceeds by effecting a domain–flattening change of variables prior to perturbation expansion. On the interior domain the relevant change of variables is

$$r' = \frac{(\bar{g} - R_i)r + R_i g(\theta)}{\bar{g} + g(\theta) - R_i}, \quad \theta' = \theta,$$

which maps the perturbed domain $\{R_i < r < \bar{g} + g(\theta)\}$ to the separable one $\Omega_{R_i,\bar{g}} = \{R_i < r' < \bar{g}\}$. This transformation changes the field w to

$$v(r', \theta') := w\left(\frac{(\bar{g} + g(\theta') - R_i)r' - R_i g(\theta')}{\bar{g} - R_i}, \theta'\right),$$

and modifies (3.6) to

$$\begin{aligned}
&\Delta v + (k^w)^2 v = F(r, \theta; g), && R_i < r < \bar{g}, && (6.2a)\\
&\tau^w \partial_N v - Zv = W(\theta) + l(\theta; g), && r = \bar{g}, && (6.2b)\\
&\partial_r v - T^{(w)}[v] = h(\theta; g), && r = R_i, && (6.2c)
\end{aligned}$$

where we have dropped the primed notation for clarity. It is not difficult to see that

$$\begin{aligned}
F &= -\frac{1}{(\bar{g} - R_i)^2}\left[F^{(0)} + \partial_r F^{(r)} + \partial_\theta F^{(\theta)}\right],\\
F^{(0)} &= -(\bar{g} - R_i)g(r - R_i)\partial_r v - (\bar{g} - R_i)gr\partial_r v - g^2(r - R_i)\partial_r v - (\bar{g} - R_i)g'\partial_\theta v\\
&\quad - gg'\partial_\theta v + (g')^2(r - R_i)\partial_r v + g[2(\bar{g} - R_i)r^2 + 2(\bar{g} - R_i)(r - R_i)r](k^w)^2 v\\
&\quad + g^2[r^2 + 4(r - R_i)r + (r - R_i)^2](k^w)^2 v + g^3\frac{2(r - R_i)(2r - R_i)}{(\bar{g} - R_i)}(k^w)^2 v\\
&\quad + g^4\frac{(r - R_i)^2}{(\bar{g} - R_i)^2}(k^w)^2 v,\\
F^{(r)} &= 2(\bar{g} - R_i)gr(r - R_i)\partial_r v + g^2(r - R_i)^2\partial_r v - (\bar{g} - R_i)g'(r - R_i)\partial_\theta v\\
&\quad - gg'(r - R_i)\partial_\theta v + (g')^2(r - R_i)^2\partial_r v,\\
F^{(\theta)} &= 2(\bar{g} - R_i)g\partial_\theta v - (\bar{g} - R_i)g'(r - R_i)\partial_r v + g^2\partial_\theta v - gg'(r - R_i)\partial_r v,
\end{aligned}$$

and

$$\bar{g}(\bar{g}-R_i)l = -\tau^w \left[2(\bar{g}-R_i)\bar{g}g\partial_r v + g^2(\bar{g}-R_i)\partial_r v \right.$$
$$\left. -(g')^2(\bar{g}-R_i)\partial_r v - g'(\bar{g}-R_i)\partial_\theta v - g'g\partial_\theta v\right]$$
$$+ [(\bar{g}-R_i)g + \bar{g}g + g^2]Zv + [(\bar{g}-R_i)g + \bar{g}g + g^2]W,$$

and

$$h = \frac{g}{\bar{g}-R_i} T^{(w)}\left[v\right].$$

Upon setting $g = \varepsilon f$ and expanding

$$v(r,\theta,\varepsilon) = \sum_{n=0}^{\infty} v_n(r,\theta)\varepsilon^n, \tag{6.3}$$

we can show that

$$\Delta v_n + (k^w)^2 v_n = F_n, \qquad R_i < r < \bar{g}, \tag{6.4a}$$

$$\partial_r v_n - \frac{Z}{\tau^w \bar{g}} v_n = \delta_{n,0}\frac{W}{\tau^w \bar{g}} + l_n, \qquad r = \bar{g}, \tag{6.4b}$$

$$\partial_r v_n - T^{(w)}\left[v_n\right] = h_n, \qquad r = R_i, \tag{6.4c}$$

where, $\delta_{n,m}$ is the Kronecker delta, and

$$F_n = -\frac{1}{(\bar{g}-R_i)^2}\left[F_n^{(0)} + \partial_r F_n^{(r)} + \partial_\theta F_n^{(\theta)}\right], \tag{6.5a}$$

$$\begin{aligned} F_n^{(0)} = &-(\bar{g}-R_i)f(r-R_i)\partial_r v_{n-1} - (\bar{g}-R_i)fr\partial_r v_{n-1} - f^2(r-R_i)\partial_r v_{n-2} \\ &- (\bar{g}-R_i)f'\partial_\theta v_{n-1} - ff'\partial_\theta v_{n-2} + (f')^2(r-R_i)\partial_r v_{n-2} \\ &+ f(\bar{g}-R_i)[2r^2 + 2(r-R_i)r](k^w)^2 v_{n-1} \\ &+ f^2[r^2 + 4(r-R_i)r + (r-R_i)^2](k^w)^2 v_{n-2} \\ &+ f^3\frac{2(r-R_i)(2r-R_i)}{(\bar{g}-R_i)}(k^w)^2 v_{n-3} + f^4\frac{(r-R_i)^2}{(\bar{g}-R_i)^2}(k^w)^2 v_{n-4}, \end{aligned} \tag{6.5b}$$

$$\begin{aligned} F_n^{(r)} = &\ 2(\bar{g}-R_i)fr(r-R_i)\partial_r v_{n-1} + f^2(r-R_i)^2\partial_r v_{n-2} \\ &- (\bar{g}-R_i)f'(r-R_i)\partial_\theta v_{n-1} \\ &- ff'(r-R_i)\partial_\theta v_{n-2} + (f')^2(r-R_i)^2\partial_r v_{n-2}, \end{aligned} \tag{6.5c}$$

$$\begin{aligned} F_n^{(\theta)} = &\ 2(\bar{g}-R_i)f\partial_\theta v_{n-1} - (\bar{g}-R_i)f'(r-R_i)\partial_r v_{n-1} + f^2\partial_\theta v_{n-2} \\ &- ff'(r-R_i)\partial_r v_{n-2}, \end{aligned} \tag{6.5d}$$

and

$$\begin{aligned} l_n = &\ \frac{1}{\bar{g}(\bar{g}-R_i)(\tau^w\bar{g})}\Big\{\bar{g}f\delta_{n,1}W + (\bar{g}-R_i)f\delta_{n,1}W + f^2\delta_{n,2}W \\ &- \tau^w\left[2\bar{g}(\bar{g}-R_i)f\partial_r v_{n-1} + (\bar{g}-R_i)f^2\partial_r v_{n-2} + (\bar{g}-R_i)(f')^2\partial_r v_{n-2}\right. \\ &\left.-(\bar{g}-R_i)f'\partial_\theta v_{n-1} - ff'\partial_\theta v_{n-2}\right] + \bar{g}fZv_{n-1} + (\bar{g}-R_i)fZv_{n-1} + f^2Zv_{n-2}\Big\}, \end{aligned} \tag{6.6}$$

and

$$h_n = \frac{f}{\bar{g}-R_i}T^{(w)}\left[v_{n-1}\right].$$

In addition, the IIO S, (3.7), can be stated in transformed coordinates as

$$S[W] = \tau^w \left\{ \frac{\bar{g} - R_i}{\bar{g} - R_i + g} \left[(\bar{g} + g) + \frac{(g')^2}{\bar{g} + g} \right] \partial_r v - \frac{g'}{\bar{g} + g} \partial_\theta v \right\} - Y v.$$

If we then expand S in ε, (3.11b), the n–th term in the expansion can be expressed as

$$\begin{aligned} S_n[W] = & -f \left(\frac{1}{\bar{g}} + \frac{1}{\bar{g} - R_i} \right) S_{n-1}[W] - \frac{f^2}{\bar{g}(\bar{g} - R_i)} S_{n-2}[W] \\ & + \tau^w \left\{ \bar{g} \partial_r v_n + 2 f \partial_r v_{n-1} + \frac{f^2 + (f')^2}{\bar{g}} \partial_r v_{n-2} - \frac{f'}{\bar{g}} \partial_\theta v_{n-1} - \frac{f(f')}{\bar{g}(\bar{g} - R_i)} \partial_\theta v_{n-2} \right\} \\ & - Y v_n - f \left(\frac{1}{\bar{g}} + \frac{1}{\bar{g} - R_i} \right) Y v_{n-1} - \frac{f^2}{\bar{g}(\bar{g} - R_i)} Y v_{n-2}, \end{aligned} \tag{6.7}$$

so that, provided with estimates on the $\{v_n\}$, we can control the terms, $\{S_n\}$.

Our main result is the following analyticity theorem.

Theorem 6.2. *If $f \in H^5([0, 2\pi])$, the configuration is δ–permissible,* (3.5), *and $W \in H^{-1/2}([0, 2\pi])$ then the series* (6.3) *converges strongly. In other words there exist constants $K_v > 0$ and $B_S > 0$ such that*

$$\|v_n\|_{H^1} \leq K_v B_S^n. \tag{6.8}$$

The proof of Theorem 6.2 proceeds by applying an elliptic estimate (Lemma 6.3) to (6.4) followed by a recursive result (Lemma 6.5).

Lemma 6.3. *Suppose the configuration is δ–permissible,* (3.5), *$F_n \in (H^1(\Omega_{R_i,\bar{g}}))'$, $W \in H^{-1/2}([0, 2\pi])$, $l_n \in H^{-1/2}([0, 2\pi])$, and $h_n \in H^{-1/2}([0, 2\pi])$. Then there is a unique solution of* (6.4) *satisfying*

$$\|v_n\|_{H^1} \leq C_e \left\{ \|F_n\|_{(H^1)'} + \delta_{n,0} \|W\|_{H^{-1/2}} + \|l_n\|_{H^{-1/2}} + \|h_n\|_{H^{-1/2}} \right\},$$

for some universal constant $C_e > 0$.

Proof. We wish to apply the elliptic estimate Theorem B.2 and for this we only need show

$$\mathrm{Re}\left\{ \widehat{\left(T^{(w)}\right)}_p \right\} \geq 0, \quad \mathrm{Re}\left\{ \frac{\hat{Z}_p}{\tau^w \bar{g}} \right\} \leq 0, \quad \left| \mathrm{Im}\left\{ \widehat{\left(T^{(w)}\right)}_p \right\} \right| < \infty, \quad \left| \mathrm{Im}\left\{ \frac{\hat{Z}_p}{\tau^w \bar{g}} \right\} \right| < \infty, \tag{6.9}$$

for $p \neq 0$. We note that Z is free to be chosen, and in the work of Despres [Des91b, Des91a] it was selected to be $(-i\eta)$ for a constant $\eta \in \mathbf{R}^+$. With this choice the second and fourth conditions in (6.9) are automatically satisfied as we have assumed that k^w, and thus τ^w, is real and positive.

To address the first and third conditions in (6.9) we recall that

$$\widehat{\left(T^{(w)}\right)}_p = k^w \frac{J_p'(k^w R_i)}{J_p(k^w R_i)}.$$

The identity $J_{-n}(z) = (-1)^n J_n(z)$ implies that

$$\widehat{\left(T^{(w)}\right)}_{-p} = k^w \frac{J_{-p}'(k^w R_i)}{J_{-p}(k^w R_i)} = k^w \frac{(-1)^p J_p'(k^w R_i)}{(-1)^p J_p(k^w R_i)} = \widehat{\left(T^{(w)}\right)}_p,$$

hence it suffices to consider $\widehat{\left(T^{(w)}\right)}_p$ for $p > 0$. We notice that both $J_p(k^w R_i)$ and $J_p'(k^w R_i)$ are real–valued for real arguments $k^w R_i$ which implies that

$$\left|\mathrm{Im}\left\{\widehat{\left(T^{(w)}\right)}_p\right\}\right| = \left|\mathrm{Im}\left\{k^w \frac{J_p'(k^w R_i)}{J_p(k^w R_i)}\right\}\right| = 0 < \infty.$$

Let $\{j_p\}_{p=1}^{\infty} = \{j_1, j_2, \dots\}$ be the first (smallest) zeroes of Bessel's functions of order p, $\{J_p(z)\}$, and $\{j_p'\}_{p=1}^{\infty} = \{j_1', j_2', \dots\}$ be the first (smallest) zeroes of the first derivatives of Bessel's functions of order p, $\{J_p'(z)\}$. From [DLMF, Eq. 10.21.3 and Eq. 10.14.2], we have

$$p \leq j_p, \quad \text{and} \quad J_p(p) > 0, \quad \forall p \geq 1.$$

Additionally, we notice that $J_p(0) = 0$ for all $p \geq 1$. Thus, for fixed p, $J_p(z)$ is positive over the interval $(0, j_p)$ which contains $(0, p)$.

Next we apply the Mean Value Theorem over the interval $(0, p)$: There exists an x in $(0, p)$ such that

$$J_p'(x) = \frac{J_p(p) - J_p(0)}{p - 0} = \frac{J_p(p)}{p} > 0.$$

From [DLMF, Eq. 10.21.3] we have $p \leq j_p'$ and $J_p'(0) = 0$ for all $p \geq 1$, thus we can conclude that $J_p'(z)$ is positive over the interval $(0, j_p')$ which contains $(0, p)$.

We finish the proof by considering the interval $(0, 1)$, which is contained in the interval $(0, p)$ for all $p \geq 1$, and choosing R_i such that $0 < k^w R_i < 1$. Then we have

$$\mathrm{Re}\left\{\widehat{\left(T^{(w)}\right)}_p\right\} = \widehat{\left(T^{(w)}\right)}_p = k^w \frac{J_p'(k^w R_i)}{J_p(k^w R_i)} \geq 0$$

and we are done. $\square$

Remark 6.4. Before proceeding we note that the first equation in (6.9) is false at $p = 0$ as $J_0'(z) = -J_1(z)$ which necessitates the condition $p \neq 0$.

To control the right hand side of (6.4) we prove the following.

Lemma 6.5. *Suppose that $f \in H^5([0, 2\pi])$ and the configuration is δ–permissible,* (3.5). *Assume that*

$$\|v_n\|_{H^1(\Omega_{R_i,\bar{g}})} \leq K_v B_S^n, \quad \forall n < N,$$

for constants $K_v > 0$ and $B_S > 0$, then there exists a constant $C_v > 0$ such that

$$\max\left\{\|F_N\|_{(H^1(\Omega_{R_i,\bar{g}}))'}, \|h_N\|_{H^{-1/2}([0,2\pi])}, \|l_N\|_{H^{-1/2}([0,2\pi])}\right\} \\ \leq C_v K_v \left(\|f\|_{H^5} B_S^{N-1} + \|f\|_{H^5}^2 B_S^{N-2}\right).$$

Proof. Note that from (6.5) and Appendix A

$$\|F_N\|_{(H^1)'} \leq \left\|F_N^{(0)}\right\|_{L^2} + \left\|F_N^{(r)}\right\|_{L^2} + \left\|F_N^{(\theta)}\right\|_{L^2},$$

and, for conciseness, we consider only one term from $F_N^{(\theta)}$,

$$\mathcal{F}_N^{(\theta)} := -f f'(r - R_i)\partial_r v_{N-2};$$

the rest can be treated in a similar fashion. For this we estimate, using Lemma 4.3,

$$\begin{aligned}\left\|\mathcal{F}_N^{(\theta)}\right\|_{L^2} &\leq \left\|-ff'(r-R_i)\partial_r v_{N-2}\right\|_{L^2}\\ &\leq M\left\|f\right\|_{H^4} M\left\|f\right\|_{H^5}\mathcal{R}\left\|v_{N-2}\right\|_{H^1}\\ &\leq M^2\left\|f\right\|_{H^5}^2\mathcal{R}K_v B_S^{N-2},\end{aligned}$$

where $\mathcal{R}$ is defined by

$$\left\|(r-R_i)v\right\|_{L^2} \leq \mathcal{R}\left\|v\right\|_{L^2},$$

and we are done if C_v is chosen appropriately.

For h_N we conduct the following sequence of steps

$$\begin{aligned}\left\|h_N\right\|_{H^{-1/2}} &\leq \left\|\frac{f}{\bar{g}-R_i}T^{(w)}\left[v_{N-1}\right]\right\|_{H^{-1/2}}\\ &\leq \frac{M}{\bar{g}-R_i}\left\|f\right\|_{H^{3+1/2}}\left\|T^{(w)}\left[v_{N-1}\right]\right\|_{H^{-1/2}}\\ &\leq \frac{M}{\bar{g}-R_i}\left\|f\right\|_{H^5} C_{T^{(w)}}\left\|v_{N-1}\right\|_{H^{1/2}}\\ &\leq \frac{MC_{T^{(w)}}}{\bar{g}-R_i}\left\|f\right\|_{H^5} C_t\left\|v_{N-1}\right\|_{H^1}\\ &\leq \frac{MC_{T^{(w)}}}{\bar{g}-R_i}\left\|f\right\|_{H^5} C_t K_v B_S^{N-1},\end{aligned}$$

where $C_{T^{(w)}}$ is the bounding constant for the operator $T^{(w)}$, and C_t is the bounding constant for the trace operator

$$\left\|v\right\|_{H^{1/2}([0,2\pi])} \leq C_t\left\|v\right\|_{H^1(\Omega_{R_i,\bar{g}})}.$$

We are done if we select C_v large enough.

Regarding the terms l_N, we once again focus on a single term

$$\mathcal{L}_N := \frac{1}{\bar{g}(\bar{g}-R_i)(\tau^w\bar{g})}\left\{(-\tau^w)(\bar{g}-R_i)(f')^2\partial_r v_{N-2}\right\} = -\frac{1}{\bar{g}^2}(f')^2\partial_r v_{N-2},$$

and make the estimates

$$\begin{aligned}\left\|\mathcal{L}_N\right\|_{H^{-1/2}} &= \left\|-\frac{1}{\bar{g}^2}(f')^2\partial_r v_{N-2}\right\|_{H^{-1/2}}\\ &\leq \frac{M^2}{\bar{g}^2}\left\|f\right\|_{H^{4+1/2}}^2\left\|\partial_r v_{N-2}\right\|_{H^{-1/2}}\\ &\leq \frac{M^2}{\bar{g}^2}\left\|f\right\|_{H^{4+1/2}}^2 C_t\left\|v_{N-2}\right\|_{H^1}\\ &\leq \frac{M^2C_t}{\bar{g}^2}\left\|f\right\|_{H^5}^2 K_v B_S^{N-2},\end{aligned}$$

and we are done if C_v is chosen well. $\square$

We can now present the proof of Theorem 6.2.

Proof. (Theorem 6.2). We work by induction and begin with $n = 0$. The estimate on v_0 follows directly from Lemma 6.3 with F and L identically zero. We now assume that (6.8) holds for all $n < N$ and apply Lemma 6.3 which implies that

$$\|v_N\|_{H^1} \leq C_e \left\{ \|F_N\|_{(H^1)'} + \|l_N\|_{H^{-1/2}} + \|h_N\|_{H^{-1/2}} \right\}.$$

Using Lemma 6.5 we have

$$\|v_N\|_{H^1} \leq C_e 3C_v K_v \left\{ \|f\|_{H^5} B_S^{N-1} + \|f\|_{H^5}^2 B_S^{N-2} \right\} \leq K_v B_S^N,$$

provided that we choose

$$3C_e C_v \|f\|_{H^5} < \frac{1}{2} B_S, \quad 3C_e C_v \|f\|_{H^5}^2 < \frac{1}{2} B_S^2,$$

which can be ensured by demanding

$$B_S > \max\left\{ 6C_e C_v, \sqrt{6C_e C_v} \right\} \|f\|_{H^5}.$$

□

Finally, we are in a position to establish Theorem 6.1.

Proof. (Theorem 6.1). From (6.7) and applying Lemma 6.2, it is straightforward to see that

$$\begin{aligned}
\|S_0(f)[W]\|_{H^{-1/2}} &\leq \|\tau^w \bar{g} \partial_r v_0 - Y v_0\|_{H^{-1/2}} \\
&\leq \|\tau^w \bar{g} \partial_r v_0\|_{H^{-1/2}} + \|Y v_0\|_{H^{-1/2}} \\
&\leq |\tau^w| \, \bar{g} \, \|v_0\|_{H^{1/2}} + C_Y \|v_0\|_{H^{1/2}} \\
&\leq (|\tau^w| \, \bar{g} + C_Y) \, C_t \|v_0\|_{H^1} \\
&\leq (|\tau^w| \, \bar{g} + C_Y) \, C_t K_v \\
&\leq K_S,
\end{aligned}$$

if $K_S > 0$ is chosen appropriately.

Assuming that (6.1) holds for all $n < N$ we now investigate an estimate of S_N. For simplicity we consider the single term

$$\mathcal{S}_N := \tau^w \left(\frac{-ff'}{\bar{g}(\bar{g} - R_i)} \right) \partial_\theta v_{N-2}$$

and we measure

$$\begin{aligned}
\|\mathcal{S}_N\|_{H^{-1/2}} &\leq \left\| \tau^w \left(\frac{-ff'}{\bar{g}(\bar{g} - R_i)} \right) \partial_\theta v_{N-2} \right\|_{H^{-1/2}} \\
&\leq |\tau^w| \frac{M^2}{\bar{g}(\bar{g} - R_i)} \|f\|_{H^{4+1/2}}^2 \|\partial_\theta v_{N-2}\|_{H^{-1/2}} \\
&\leq |\tau^w| \frac{M^2}{\bar{g}(\bar{g} - R_i)} \|f\|_{H^5}^2 C_t \|v_{N-2}\|_{H^1} \\
&\leq |\tau^w| \frac{M^2}{\bar{g}(\bar{g} - R_i)} \|f\|_{H^5}^2 C_t K_v B_S^{N-2}.
\end{aligned}$$

We are done provided that we choose

$$K_S > |\tau^w| \frac{M^2}{\bar{g}(\bar{g} - R_i)} C_t K_v,$$

and $B_S > \|f\|_{H^5}$. $\square$

In an analgous manner, the analyticity of Q can be established.

Theorem 6.6. *If $f \in H^5([0, 2\pi])$, the configuration is δ–permissible, (3.2), and $U \in H^{-1/2}([0, 2\pi])$ then the series (3.11a) converges strongly as an operator from $H^{-1/2}([0, 2\pi])$ to $H^{-1/2}([0, 2\pi])$. In other words there exist constants $K_Q > 0$ and $B_Q > 0$ such that*

$$\|Q_n(f)[U]\|_{H^{-1/2}} \leq K_Q B_Q^n.$$

Remark 6.7. The proof proceeds in a similar fashion to that of Theorem 6.1. The crucial difference lies in the elliptic estimate, c.f. Lemma 6.3, which in this case requires

$$\mathrm{Re}\left\{\frac{\hat{Y}_p}{\tau^u \bar{g}}\right\} \geq 0, \quad \mathrm{Re}\left\{\widehat{\left(-T^{(u)}\right)}_p\right\} \leq 0, \quad \left|\mathrm{Im}\left\{\frac{\hat{Y}_p}{\tau^u \bar{g}}\right\}\right| < \infty, \quad \left|\mathrm{Im}\left\{\widehat{\left(-T^{(u)}\right)}_p\right\}\right| < \infty. \tag{6.10}$$

As before, the operator Y is free to be chosen and we again follow Despres [Des91b, Des91a] who selected $(i\eta)$ for a constant $\eta \in \mathbf{R}^+$. As k^u, and therefore τ^u, are real and positive, the first and third conditions in (6.10) are satisfied. For the other conditions we note that

$$\widehat{\left(T^{(u)}\right)}_p = -k^u \frac{H_p'(k^u R^o)}{H_p(k^u R^o)}$$

and recall that Shen & Wang [SW07] established

$$0 < \mathrm{Im}\left\{\frac{H_p'(k^u R^o)}{H_p(k^u R^o)}\right\} < 1, \quad p \neq 0,$$

c.f. (2.34a) and (2.34c) in [SW07]. So, for a fixed R^o we have

$$\left|\mathrm{Im}\left\{\widehat{\left(-T^{(u)}\right)}_p\right\}\right| < \infty, \quad \forall p,$$

while (2.34b) of [SW07] delivers

$$\frac{p}{R^o} \geq \mathrm{Re}\left\{-k^u \frac{H_p'(k^u R^o)}{H_p(k^u R^o)}\right\} \geq \frac{1}{2R^o} > 0, \quad p \neq 0.$$

Therefore

$$\mathrm{Re}\left\{\widehat{\left(-T^{(u)}\right)}_p\right\} \leq 0, \quad p \neq 0,$$

and our proof can proceed.

7 Numerical Results

We now present results of simulations of our implementations of the algorithms outlined above. The schemes are essentially High–Order Spectral (HOS) [GO77, CHQZ88, DFM02] with nonlinearities approximated by convolutions implemented with the Fast Fourier Transform algorithm.

7.1 Implementation Details

The numerical approaches we describe in this section utilize either the Dirichlet–Neumann operator (DNO) formulation of the problem [NT18] or its IIO alternative specified in (3.8). The relevant operators (DNO and IIO, respectively) are simulated using the TFE methodology [NR01a, NR03, NR04b]. The TFE method is a Fourier collocation/Taylor method [NR01b, NR04b] enhanced by Padé summation [BGM96]. In more detail, for the IIO S we approximate W by

$$W^{N_\theta,N}(\theta) := \sum_{n=0}^{N} \sum_{p=-N_\theta/2}^{N_\theta/2-1} \hat{W}_{n,p} e^{ip\theta} \varepsilon^n,$$

and insert this into (3.14) for $0 \le n \le N$ to determine approximation $v_n^{N_\theta,N_r,N}(r,\theta)$ which are used in (6.7) to simulate the IIO. As has been pointed out in [NR01b, NN04, NT18], the TFE approach requires an additional discretization in the radial direction which we achieve by a Chebyshev collocation approach. An important consideration is how the Taylor series in ε are summed. The classical numerical analytic continuation technique of Padé approximation [BGM96] has been used very successsfully for HOPS methods (see, e.g., [BR93b, NR03]), and we will use it here.

7.2 The Method of Manufactured Solutions

Before proceeding to our simulation of LSPRs, we begin by demonstrating the validity of our algorithm by conducting experiments using the Method of Manufactured Solutions (MMS) [Bur66, Roa98a, Roa98b, Roa02, KS03, OTH04, Roy05]. To be more specific we consider the 2π–periodic, outgoing solutions of the Helmholtz equation, (2.1a),

$$u^q(r,\theta) = A_u^q H_q(k^u r) e^{iq\theta}, \quad q \in \mathbf{Z}, \quad A_u^q \in \mathbf{C},$$

and their bounded counterparts for (2.1b)

$$w^q(r,\theta) = A_w^q J_q(k^w r) e^{iq\theta}, \quad q \in \mathbf{Z}, \quad A_w^q \in \mathbf{C}.$$

We select an analytic profile

$$g(\theta) = \varepsilon f(\theta) = \varepsilon e^{\cos(\theta)}, \tag{7.1}$$

and define, for any choice of the radius of the interface $\bar{g}$, the Dirichlet and Neumann traces

$$u^{\mathrm{ex}}(\theta) := u(\bar{g} + g(\theta), \theta), \quad \tilde{u}^{\mathrm{ex}}(\theta) := (-\partial_N u^{\mathrm{ex}})(\bar{g} + g(\theta), \theta),$$

and

$$w^{\mathrm{ex}}(\theta) := w(\bar{g} + g(\theta), \theta), \quad \tilde{w}^{\mathrm{ex}}(\theta) := (\partial_N w^{\mathrm{ex}})(\bar{g} + g(\theta), \theta).$$

From these we define, for any real $\eta > 0$, the impedances

$$U^{\mathrm{ex}}(\theta) := \tau^u \tilde{u}^{\mathrm{ex}} + i\eta u^{\mathrm{ex}}, \quad \tilde{U}^{\mathrm{ex}}(\theta) := \tau^u \tilde{u}^{\mathrm{ex}} - i\eta u^{\mathrm{ex}},$$

and

$$W^{\mathrm{ex}}(\theta) := \tau^w \tilde{w}^{\mathrm{ex}} + i\eta w^{\mathrm{ex}}, \quad \tilde{W}^{\mathrm{ex}}(\theta) := \tau^w \tilde{w}^{\mathrm{ex}} - i\eta w^{\mathrm{ex}}.$$

(In this case $Y = i\eta$ and $Z = -i\eta$.) We select the following physical parameters

$$q = 2, \quad A_u^q = 2, \quad A_w^q = 1, \quad \eta = 3.4, \quad \lambda = 0.45, \quad k^u = 13.9626, \quad k^w = 5.13562230, \tag{7.2}$$

and numerical parameter choices

$$N_\theta = 64, \quad N = 16, \quad N_r = 32. \tag{7.3}$$

To demonstrate the behavior of our scheme we studied four choices of $\varepsilon = 0.005, 0.01, 0.05, 0.1$. For this we supplied $\{u^{\text{ex}}, w^{\text{ex}}\}$ to our HOPS algorithm to simulate DNOs producing, $\{\tilde{u}^{\text{approx}}, \tilde{w}^{\text{approx}}\}$, and computed the relative error

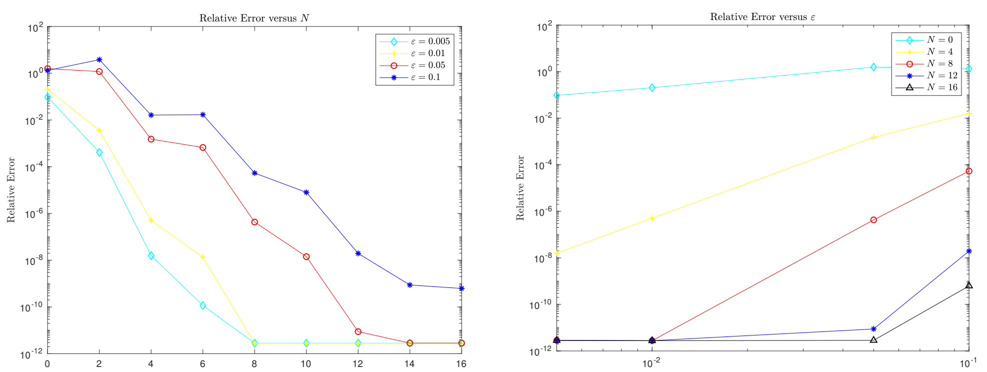
$$\text{Error}_{\text{rel}}^{\text{DNO}} = \frac{\left| \tilde{w}^{\text{ex}} - \tilde{w}_{N_\theta,N}^{\text{approx}} \right|_{L^\infty}}{\left| \tilde{w}^{\text{ex}} \right|_{L^\infty}}.$$

In a similar way, we passed $\{U^{\text{ex}}, W^{\text{ex}}\}$ to our HOPS algorithm to approximate IIOs giving, $\{\tilde{U}^{\text{approx}}, \tilde{W}^{\text{approx}}\}$, and computed the relative error

$$\text{Error}_{\text{rel}}^{\text{IIO}} = \frac{\left| \tilde{W}^{\text{ex}} - \tilde{W}_{N_\theta,N}^{\text{approx}} \right|_{L^\infty}}{\left| \tilde{W}^{\text{ex}} \right|_{L^\infty}}.$$

7.3 Robust Computation: DNOs versus IIOs

To begin our study, we chose $\bar{g} = 0.5$, carried out the MMS simulations with our IIO method, (3.8), and report our results in Figures 2(a) and 2(b). We repeated this with our DNO approach [NT18] and display the outcomes in Figures 3(a) and 3(b). We see in this generic, non–resonant, configuration that both algorithms display a spectral rate of convergence as N is refined (up to the conditioning of the algorithm) which improves as ε is decreased.



(a) Error in IIO formulation versus perturbation order, N.

(b) Error in IIO formulation versus perturbation sizer, ε.

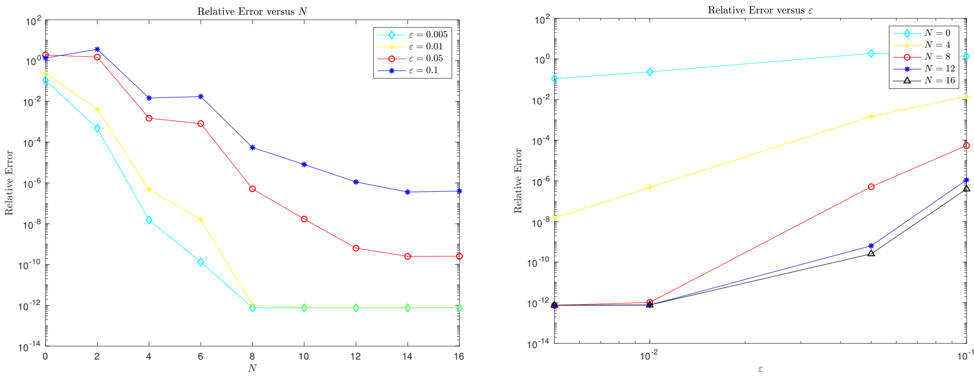
Figure 2: Plot of relative error with five choices of $N = 0, 4, 8, 12, 16$ for a non–resonant configuration using the IIO formulation.

Before proceeding, we note that the choice of radius

$$\bar{g} = 1,$$

will induce a singularity in the interior DNO resulting in a lack of uniqueness. To test performance of our methods near this scenario we selected

$$\bar{g} = 1 - \tau, \tag{7.4}$$



(a) Error in DNO formulation versus perturbation order, N.

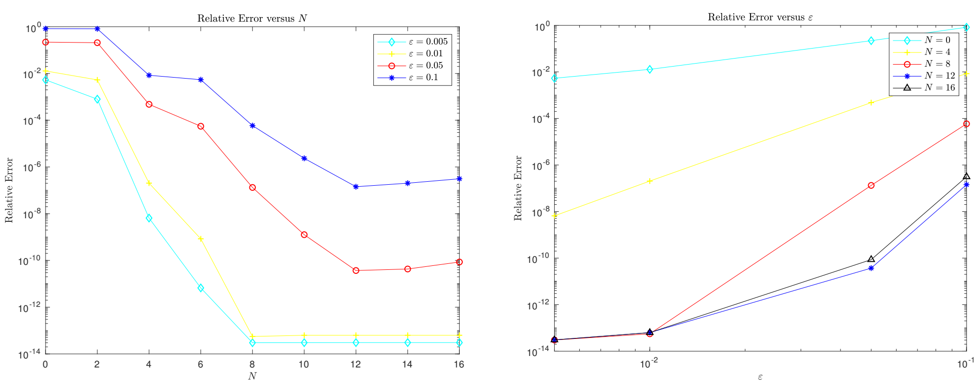
(b) Error in DNO formulation versus perturbation sizer, ε.

Figure 3: Plot of relative error with five choices of $N = 0, 4, 8, 12, 16$ for a non–resonant configuration using the DNO formulation.

for two choices of τ. With the same choices of geometrical, (7.1), physical, (7.2), and numerical, (7.3), parameters as before, we selected $\tau = 10^{-12}$ resulting in

$$\bar{g} = 1 - 10^{-12}.$$

Once again, we conducted simulations with the IIO method, (3.8), and display our results in Figures 4(a) and 4(b). We revisited these computations with our DNO approach [NT18] and show our results in Figures 5(a) and 5(b). We see in this nearly resonant configuration, that while the IIO methodology continues to display a spectral rate of convergence as N is refined (improving as ε is decreased), the DNO approach does *not* provide results of the same quality.



(a) Error in IIO formulation versus perturbation order, N.

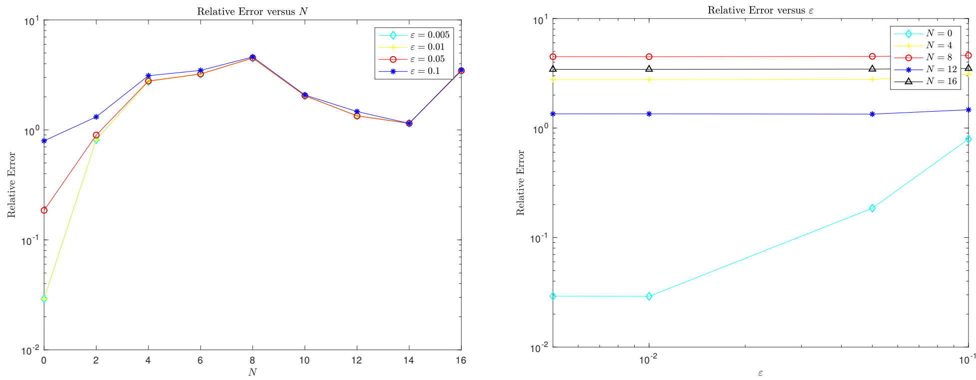
(b) Error in IIO formulation versus perturbation sizer, ε.

Figure 4: Plot of relative error with five choices of $N = 0, 4, 8, 12, 16$ for a nearly resonant configuration using the IIO formulation.

To close, we chose $\tau = 10^{-16}$ in (7.4) resulting in

$$\bar{g} = 1 - 10^{-16}.$$

After running simulations with the IIO method, (3.8), we display our results in Figures 6(a) and 6(b). We revisited these computations with our DNO approach [NT18] and show our

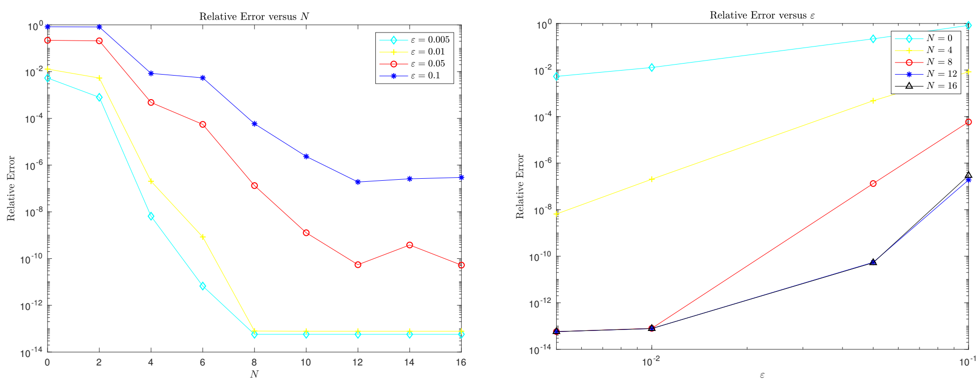


(a) Error in DNO formulation versus perturbation order, N.

(b) Error in DNO formulation versus perturbation sizer, ε.

Figure 5: Plot of relative error with five choices of $N = 0, 4, 8, 12, 16$ for a nearly resonant configuration using the DNO formulation.

results in Figures 7(a) and 7(b). We see in this resonant (to machine precision) configuration, the IIO again displays a spectral rate of convergence as N is refined (improving as ε is decreased), while the DNO approach delivers completely unacceptable results.



(a) Error in IIO formulation versus perturbation order, N.

(b) Error in IIO formulation versus perturbation sizer, ε.

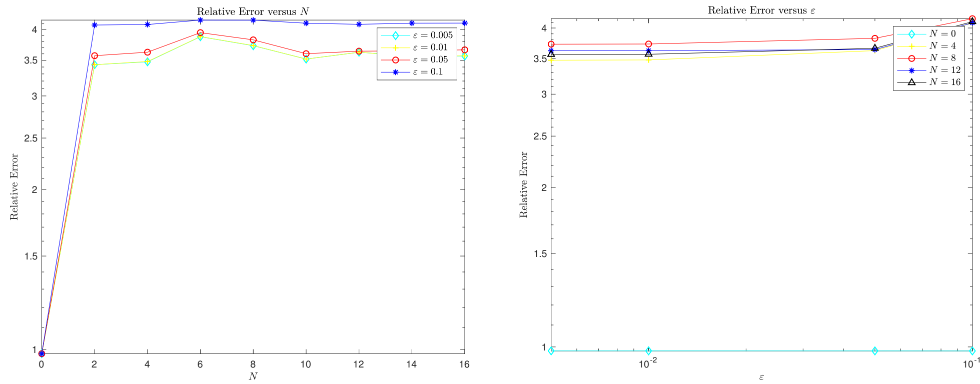
Figure 6: Plot of relative error with five choices of $N = 0, 4, 8, 12, 16$ for a resonant configuration using the IIO formulation.

7.4 Simulation of Nanorods

We close by returning to the problem of scattering of plane–wave incident radiation $u^{\text{inc}} = \exp(i\alpha x - i\gamma^u z)$ by a nanorod (which demands the Dirichlet and Neumann conditions, (2.1c) and (2.1d), respectively). More specifically, we considered metallic nanorods housed in a dielectric with outer interface shaped by

$$r = \bar{g} + g(\theta) = \bar{g} + \varepsilon f(\theta).$$

We illuminated this structure over a range of incident wavelengths $\lambda_{\min} \leq \lambda \leq \lambda_{\max}$ and perturbation sizes $\varepsilon_{\min} \leq \varepsilon \leq \varepsilon_{\max}$, and computed the magnitudes of the reflected and



(a) Error in DNO formulation versus perturbation order, N.

(b) Error in DNO formulation versus perturbation sizer, ε.

Figure 7: Plot of relative error with five choices of $N = 0, 4, 8, 12, 16$ for a resonant configuration using the DNO formulation.

transmitted surface currents, $\tilde{u}$ and $\tilde{w}$. These we term the "Reflection Map" (RM) and "Transmission Map" (TM) in analogy with similar quantities of interest in the study of metallic gratings [Pet80, Rae88, Mai07, NH12, EB12]. Our study of the Fröhlich condition, (1.1), indicates that there should be a sizable enhancement in each at an LSPR. In the case of a nanorod with a perfectly circular cross–section we computed the value as the λ_F satisfying (1.1), and in subsequent plots this is depicted by a dashed red line.

Using the TFE approach to compute the IIOs, we studied the periodic sinusoidal profile

$$f(\theta) = \cos(4\theta), \tag{7.5}$$

see Figure 8. With this we considered the following physical configuration

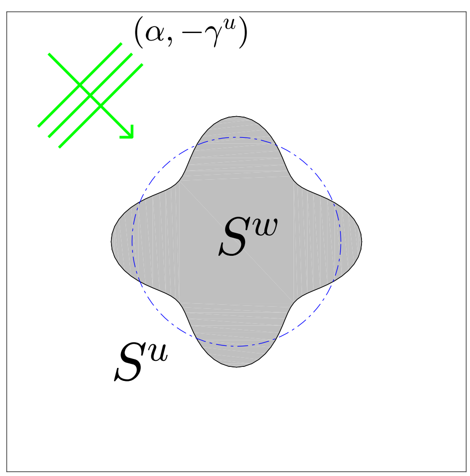


Figure 8: Plot of the cross–section of a metallic nanorod (occupying S^w) shaped by $r = \bar{g} + \varepsilon \cos(4\theta)$ ($\varepsilon = \bar{g}/5$) housed in a dielectric (occupying S^u) under plane–wave illumination with wavenumber $(\alpha, -\gamma^u)$. The dash–dot blue line depicts the unperturbed geometry, the circle $r = \bar{g}$.

$$\bar{g} = 0.025, \quad n^u = n^{\text{Vacuum}}, \quad n^w = n^{\text{Ag}},$$
$$\lambda_{\text{min}} = 0.300, \quad \lambda_{\text{max}} = 0.800, \quad \varepsilon_{\text{min}} = 0, \quad \varepsilon_{\text{max}} = \bar{g}/5,$$

so that a silver (Ag) nanorod sits in vacuum, with numerical parameters

$$N_\lambda = 201, \quad N_\varepsilon = 201, \quad N_\theta = 32, \quad N_r = 16, \quad N = 8.$$

Plots of the RM and TM are displayed in Figure 9. In Figure 10 we show the final slice ($\varepsilon = \varepsilon_{\text{max}}$) of each of these, together with the Fröhlich value of the LSPR, (1.1), as a dashed red line. Here we see how even a relatively moderate value of the deformation parameter

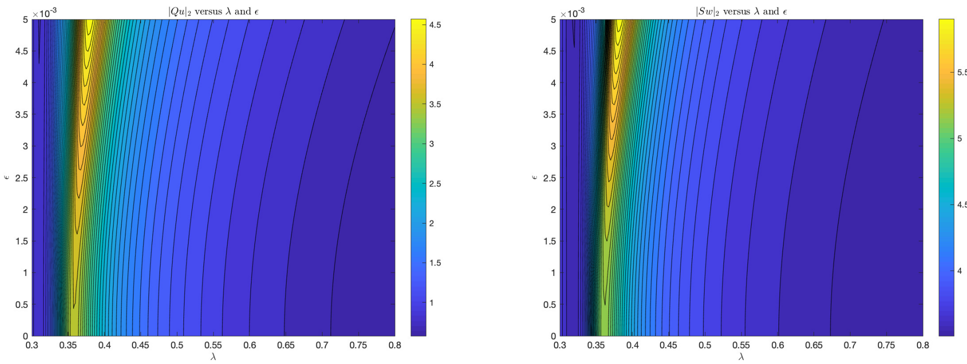


Figure 9: Reflection Map and Transmission Map for a silver nanorod shaped by the sinusoidal profile, (7.5), in vacuum. Here $\varepsilon_{max} = \bar{g}/5$, $\bar{g} = 0.025$, $\lambda_{min} = 0.300$, and $\lambda_{max} = 0.800$.

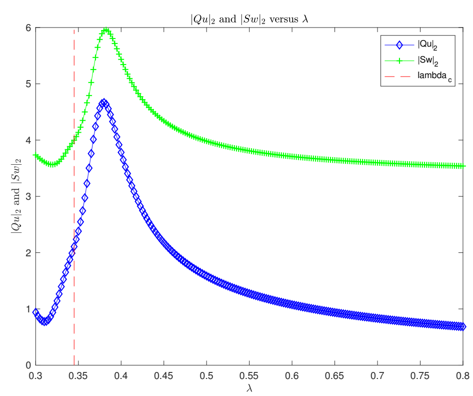


Figure 10: Final Slice of Reflection and Transmission Maps at $\varepsilon = \varepsilon_{max}$ for a silver nanorod shaped by the analytic profile, (7.5), in vacuum.

(one fifth of the rod radius) can produce a sizable shift in the LSPR location which our novel approach can accurately capture.

8 Conclusion

In this paper we have investigated a High–Order Perturbation of Surfaces (HOPS) algorithm for the numerical simulation of a novel formulation of the problem of scattering of linear waves by a nanorod in terms of Impedance–Impedance Operators (IIOs). Not only does our new methodology enjoy the same advantages of our previous implementation in terms of Dirichlet–Neumann Operators (e.g., surface formulation, exact enforcement of Sommerfeld radiation conditions, High–Order Spectral accuracy), but it is also immune to the Dirichlet eigenvalues which cause artificial singularities in our previous approach. In addition, our new formulation enables us to establish the existence, uniqueness, and analyticity of solutions to this problem, which we have taken pains to deliver. Finally, we have given a detailed description of our algorithm, and not only validated it but also demonstrated its efficiency, fidelity, and high–order accuracy.

Acknowledgements

D.P.N. gratefully acknowledges support from the National Science Foundation through grants No. DMS–1522548 and No. DMS–1813033.

A Volumetric Function Spaces

With the goal of establishing the analyticity results of Section 6 we discuss necessary volumetric function spaces in addition to the interfacial spaces we described in Section 4. For this we consider the domain $\Omega := \{a < r < b\}$ with inner and outer boundaries $\Gamma_a := \{r = a\}$ and $\Gamma_b := \{r = b\}$, respectively. For clarity of presentation we use the following notation for the classical θ–periodic volumetric and surface Sobolev spaces

$$V := H^1(\Omega), \quad W_m := H^{1/2}(\Gamma_m), \quad m \in \{a, b\}.$$

The precise nature of the spaces W_m has already been presented, and the details of the space V can be made clear by considerations akin to those for the quasiperiodic functions featured in the Habilitationsschrift of Arens [Are09]. Informally, if $v \in V$ then

$$v(r, \theta) = \sum_{p=-\infty}^{\infty} \hat{v}_p(r) e^{ip\theta}, \quad \hat{v}_p(r) = \frac{1}{2\pi} \int_0^{2\pi} v(r, \theta) e^{-ip\theta} \, d\theta,$$

and $\|v\|_V < \infty$ where

$$\|v\|_V^2 := \sum_{p=-\infty}^{\infty} \left(\langle p \rangle^2 \|\hat{v}_p\|_{L^2(dr)}^2 + \|\partial_r \hat{v}_p\|_{L^2(dr)}^2 \right), \quad \|\hat{v}_p\|_{L^2(dr)}^2 := \int_a^b |\hat{v}_p(r)|^2 \, r \, dr.$$

The existence, uniqueness, and elliptic regularity results we are about to establish demand an understanding of the duals of both V and W_m. As we have seen, the latter are simply the spaces $H^{-1/2}(\Gamma_m)$. However, the former require a little more work to characterize. Following Evans [Eva10] (Section 5.9.1) we use the Riesz Representation Theorem to identify any $F \in V'$ with an element $u_F \in V$ such that

$$\langle F, v \rangle = (u_F, v)_V, \quad \forall v \in V,$$

where $\langle \cdot, \cdot \rangle$ is the duality pairing between V and V', and $(\cdot, \cdot)_V$ is the V inner product

$$(u, v)_V = \int_\Omega \nabla u \cdot \overline{\nabla v} + u \bar{v} \, dV.$$

As $u_F \in V$ we can identify $F^0, F^r, F^\theta \in L^2(\Omega)$ such that, in the weak sense,

$$F = F^0 + (\partial_r F^r)\hat{r} + \frac{(\partial_\theta F^\theta)}{r}\hat{\theta},$$

and

$$\|F\|_{V'}^2 = \left\|F^0\right\|_{L^2(\Omega)}^2 + \|F^r\|_{L^2(\Omega)}^2 + \left\|\frac{F^\theta}{r}\right\|_{L^2(\Omega)}^2$$

gives the norm of V'. We note that since $0 < a < b < \infty$ this is equivalent to

$$\left\|F^0\right\|_{L^2(\Omega)}^2 + \|F^r\|_{L^2(\Omega)}^2 + \left\|F^\theta\right\|_{L^2(\Omega)}^2.$$

Remark A.1. We note, for later use, the important fact that V embeds *compactly* into $L^2(\Omega)$ while W_m embed *compactly* into $L^2(\Gamma_m)$ [SS11].

B The Elliptic Estimate

We now present the fundamental result which enables the proof of our analyticity theorems. For this we consider the generic Helmholtz problem

$$\Delta v + k^2 v = F, \qquad \text{in } \Omega, \tag{B.1a}$$

$$\partial_r v - Av = K, \qquad \text{at } \Gamma_a, \tag{B.1b}$$

$$\partial_r v - Bv = L, \qquad \text{at } \Gamma_b, \tag{B.1c}$$

where A and B can be order–one Fourier multipliers

$$A : W_a \to W_a', \quad B : W_b \to W_b',$$

though they can also be constants, e.g., the choice of Despres [Des91b, Des91a] $A = i\eta_a$, $B = i\eta_b$, where $\eta_m \in \mathbf{R}$.

B.1 Uniqueness

We can decide decisively upon uniqueness of solutions to (B.1) by considering this problem with $F \equiv K \equiv L \equiv 0$ and writing the exact solution via separation of variables. The solution of (B.1a) with $F \equiv 0$ is

$$v(r, \theta) = \sum_{p=-\infty}^{\infty} \{c_p J_p(kr) + d_p Y_p(kr)\} e^{ip\theta}, \tag{B.2}$$

where $Y_p(z)$ is the order p second kind Bessel function, with derivative

$$\partial_r v(r, \theta) = \sum_{p=-\infty}^{\infty} \left\{c_p k J_p'(kr) + d_p k Y_p'(kr)\right\} e^{ip\theta}, \tag{B.3}$$

while the boundary conditions, (B.1b)–(B.1c), in the case $K \equiv L \equiv 0$ deliver

$$\begin{pmatrix} kJ_p'(ka) - \hat{A}_p J_p(ka) & kY_p'(ka) - \hat{A}_p Y_p(ka) \\ kJ_p'(kb) - \hat{B}_p J_p(kb) & kY_p'(kb) - \hat{B}_p Y_p(kb) \end{pmatrix} \begin{pmatrix} c_p \\ d_p \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{B.4}$$

Clearly, this has only the zero solution provided that the determinant function is non–zero

$$\Lambda_p(k,a,b,\hat{A}_p,\hat{B}_p) := \left(kJ_p'(ka) - \hat{A}_p J_p(ka)\right)\left(kY_p'(kb) - \hat{B}_p Y_p(kb)\right) \\ - \left(kY_p'(ka) - \hat{A}_p Y_p(ka)\right)\left(kJ_p'(kb) - \hat{B}_p J_p(kb)\right).$$

If we define a "configuration" (k,a,b,A,B) then we can specify a δ–permissible configuration set

$$\mathcal{C}_\delta(k,a,b,A,B) := \left\{(k,a,b,A,B) \mid \left|\Lambda_p(k,a,b,\hat{A}_p,\hat{B}_p)\right|^2 > \delta^2, \forall p \in \mathbf{Z}\right\}, \tag{B.5}$$

From here we only consider δ–permissible configurations for some $\delta > 0$.

For later reference we explicitly mention the case $k = 0$ which corresponds to Laplace's equation:

$$\begin{aligned} \Delta v &= F, && \text{in } \Omega, && \text{(B.6a)} \\ \partial_r v - Av &= K, && \text{at } \Gamma_a, && \text{(B.6b)} \\ \partial_r v - Bv &= L, && \text{at } \Gamma_b. && \text{(B.6c)} \end{aligned}$$

The exact solution of (B.6a) is, in the case $F \equiv 0$,

$$v(r,\theta) = c_0 \log(r) + d_0 + \sum_{|p|=1}^{\infty} \left\{ c_p \left(\frac{r}{b}\right)^{|p|} + d_p \left(\frac{r}{a}\right)^{-|p|} \right\} e^{ip\theta}, \tag{B.7}$$

with derivative

$$\partial_r v(r,\theta) = \frac{c_0}{r} + \sum_{|p|=1}^{\infty} |p| \left\{ \frac{c_p}{b}\left(\frac{r}{b}\right)^{|p|-1} - \frac{d_p}{a}\left(\frac{r}{a}\right)^{-|p|-1} \right\} e^{ip\theta}. \tag{B.8}$$

The boundary conditions (B.6b)–(B.6c), for $K \equiv L \equiv 0$, demand, for $p \neq 0$,

$$\begin{pmatrix} q^{|p|}\left(|p|/(bq) - \hat{A}_p\right) & \left(-|p|/a - \hat{A}_p\right) \\ \left(|p|/b - \hat{B}_p\right) & q^{|p|}\left(-(|p|\,q)/a - \hat{B}_p\right) \end{pmatrix} \begin{pmatrix} c_p \\ d_p \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \tag{B.9}$$

where $q := a/b$ (note that $0 < q < 1$), and, for $p = 0$,

$$\begin{pmatrix} 1/a - \hat{A}_0 \log(a) & -\hat{A}_0 \\ 1/b - \hat{B}_0 \log(b) & -\hat{B}_0 \end{pmatrix} \begin{pmatrix} c_0 \\ d_0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{B.10}$$

Once again, the uniqueness of solutions to this problem is determined by the vanishing of a determinant function

$$\Lambda_p(0,a,b,\hat{A}_p,\hat{B}_p) = \left(\frac{|p|}{a} + \hat{A}_p\right)\left(\frac{|p|}{b} - \hat{B}_p\right) - q^{2|p|}\left(\frac{|p|}{bq} - \hat{A}_p\right)\left(\frac{|p|\,q}{a} + \hat{B}_p\right), \tag{B.11}$$

for $p \neq 0$, and

$$\Lambda_0(0,a,b,\hat{A}_0,\hat{B}_0) = \frac{a\hat{A}_0 - b\hat{B}_0}{ab} + \hat{A}_0\hat{B}_0 \log(q), \tag{B.12}$$

for $p = 0$. Again, we specify a δ–permissible configuration set

$$\mathcal{C}_\delta(0,a,b,A,B) := \left\{(0,a,b,A,B) \mid \left|\Lambda_p(0,a,b,\hat{A}_p,\hat{B}_p)\right|^2 > \delta^2, \forall p \in \mathbf{Z}\right\}. \tag{B.13}$$

As before, from here we only consider δ–permissible configurations for some $\delta > 0$.

Remark B.1. Regarding the possibility of Λ_p being zero, general statements are difficult to make. However, if, for instance, we make the choice of Despres [Des91b, Des91a], $\hat{A}_p = \hat{B}_p = i\eta$, then

$$\Lambda_p = \left(1 - q^{2|p|}\right)\left(|p|^2 + \eta^2\right) + i\,|p|\,q^{2|p|}\eta\,(q - 1/q) = \mathcal{O}(p^2),$$

and both the real and imaginary parts of Λ_p are non–zero [Mar06, Mar18].

B.2 Existence

We are now in a good position to establish existence of solutions and estimates on these in permissible configurations satisfying (B.5) and (B.13) which, by defintion, are unique.

Theorem B.2. *If $F \in V'$, $K \in W_a'$, $L \in W_b'$, the configurations satisfy*

$$(k, a, b, A, B) \in \mathcal{C}_\delta(k, a, b, A, B), \quad (0, a, b, A, B) \in \mathcal{C}_\delta(0, a, b, A, B),$$

for some $\delta > 0$, and the Fourier multiplier operators satisfy the conditions

$$\operatorname{Re}\left\{\hat{A}_p\right\} \geq 0, \quad \operatorname{Re}\left\{\hat{B}_p\right\} \leq 0, \quad \left|\operatorname{Im}\left\{\hat{A}_p\right\}\right| < \infty, \quad \left|\operatorname{Im}\left\{\hat{B}_p\right\}\right| < \infty, \quad p \neq 0, \tag{B.14}$$

then there exists a unique solution of the Helmholtz problem, (B.1)*, which satisfies the estimate*

$$\|v\|_V \leq C_e \left\{\|F\|_{V'} + \|K\|_{W_a'} + \|L\|_{W_b'}\right\}, \tag{B.15}$$

for some universal constant $C_e > 0$.

Remark B.3. We only demand (B.14) for $p \neq 0$ as in several cases of interest these conditions are violated only at $p = 0$ which, as we will show, does not affect the results.

Proof. To establish this result we write the solution $v = v_0 + v_1$ where the first function satisfies (B.1) with homogeneous boundary conditions and slightly modified inhomogeneity

$$\begin{aligned}
\Delta v_0 + k^2 v_0 &= G, && \text{in } \Omega, && \text{(B.16a)}\\
\partial_r v_0 - A v_0 &= 0, && \text{at } \Gamma_a, && \text{(B.16b)}\\
\partial_r v_0 - B v_0 &= 0, && \text{at } \Gamma_b, && \text{(B.16c)}
\end{aligned}$$

and the second resolves the boundary conditions

$$\begin{aligned}
\partial_r v_1 - A v_1 &= K, && \text{at } \Gamma_a, && \text{(B.17a)}\\
\partial_r v_1 - B v_1 &= L, && \text{at } \Gamma_b. && \text{(B.17b)}
\end{aligned}$$

We produce a choice of v_1 which, for convenience, is harmonic

$$\Delta v_1 = 0, \quad \text{in } \Omega, \tag{B.17c}$$

though this is not necessary. Since the configuration is in the set $\mathcal{C}_\delta(k, a, b, A, B)$, we will show in Theorem B.4 that (B.16) has a unique solution satisfying the estimate

$$\|v_0\|_V \leq C_0 \|G\|_{V'}, \tag{B.18}$$

and, since the configuration is in the set $\mathcal{C}_\delta(0, a, b, A, B)$, we will show in Theorem B.5 that (B.17) has a unique solution such that

$$\|v_1\|_V \leq C_1 \left\{ \|K\|_{W_a'} + \|L\|_{W_b'} \right\}. \tag{B.19}$$

Inserting $v = v_0 + v_1$ into (B.1) we find that v_0 satisfies (B.16) with $G = F - k^2 v_1$ so that

$$\begin{aligned}
\|v\|_V &\leq \|v_0\|_V + \|v_1\|_V \\
&\leq C_0 \left\| F - k^2 v_1 \right\|_V + \|v_1\|_V \\
&\leq C_0 \left\{ \|F\|_{V'} + k^2 \|v_1\|_{V'} \right\} + \|v_1\|_V \\
&\leq C_0 \left\{ \|F\|_{V'} + k^2 \|v_1\|_V \right\} + \|v_1\|_V \\
&\leq C_0 \|F\|_{V'} + (C_0 k^2 + 1) C_1 \left\{ \|K\|_{W_a'} + \|L\|_{W_b'} \right\},
\end{aligned}$$

and we are done provided

$$C_e = \max \left\{ 2C_0, 2C_1(C_0 k^2 + 1) \right\}.$$

□

We begin with the estimate for v_0.

Theorem B.4. *If $G \in V'$, the configuration $\{k, a, b, A, B\} \in \mathcal{C}_\delta$ for some $\delta > 0$, and the Fourier multiplier operators satisfy the conditions* (B.14)*, then there exists a unique solution of the Helmholtz problem,* (B.16)*, which satisfies the estimate* (B.18) *for some universal constant $C_0 > 0$.*

Proof. We follow very closely the work of Harari and Hughes [HH92] and Demkowicz and Ihlenburg [DI01], which was later enhanced by the author and Nigam [NN06] for use on domains with perturbed interface shape. Here, once again, we modify this approach to address a related but significantly different problem.

To begin, we define the zero–mode Fourier multiplier operators A_0 and B_0 by

$$A_0[\psi(\theta)] := \sum_{p=-\infty}^{\infty} \hat{A}_p \hat{\psi}_p e^{ip\theta} \delta_{p,0} = \hat{A}_0 \hat{\psi}_0, \quad B_0[\psi(\theta)] := \sum_{p=-\infty}^{\infty} \hat{B}_p \hat{\psi}_p e^{ip\theta} \delta_{p,0} = \hat{B}_0 \hat{\psi}_0.$$

It is easy to show that A_0 and B_0 each map $L^2(\Gamma_m)$ to $L^2(\Gamma_m)$. With this, a weak formulation of (B.16) is:

$$\text{Find } v_0 \in V \text{ such that } \mathcal{A}(v_0, \phi) + \mathcal{D}_1(v_0, \phi) + \mathcal{D}_2(v_0, \phi) = \mathcal{L}(\phi), \quad \forall \phi \in V,$$

where

$$\begin{aligned}
\mathcal{A}(v,\phi) &:= \int_\Omega \nabla v \cdot \overline{\nabla \phi}\, dV + \int_\Omega v\overline{\phi}\, dV \\
&\quad + \operatorname{Re}\left\{ \int_{\Gamma_a} ((A-A_0)v)\overline{\phi}\, ds \right\} - \operatorname{Re}\left\{ \int_{\Gamma_b} ((B-B_0)v)\overline{\phi}\, ds \right\}, \\
\mathcal{D}_1(v,\phi) &:= -(k^2+1) \int_\Omega v\overline{\phi}\, dV, \\
\mathcal{D}_2(v,\phi) &:= \operatorname{Im}\left\{ \int_{\Gamma_a} ((A-A_0)v)\overline{\phi}\, ds \right\} - \operatorname{Im}\left\{ \int_{\Gamma_b} ((B-B_0)v)\overline{\phi}\, ds \right\} \\
&\quad + \int_{\Gamma_a} (A_0 v)\overline{\phi}\, ds - \int_{\Gamma_b} (B_0 v)\overline{\phi}\, ds, \\
\mathcal{L}(\phi) &:= -\int_\Omega G\overline{\phi}\, dV.
\end{aligned}$$

Following [HH92, DI01, NN06] it is not difficult to show that $\mathcal{A}$ is a continuous, sesquilinear form from $V \times V$ to $\mathbf{C}$ which induces a bounded operator $\mathbf{A} : V \to V'$ (see Lemma 2.1.38 of [SS11]). The first two terms are "standard" while the latter two require that A and B be at most order–one Fourier multipliers. For instance

$$\left| \operatorname{Re}\left\{ \int_{\Gamma_a} A[v_{r=a}]\overline{\phi_{r=a}}\, ds \right\} \right| \leq |\langle A[v_{r=a}], \phi_{r=a} \rangle| \leq \|A[v_{r=a}]\|_{W_a'} \|\phi_{r=a}\|_{W_a},$$

which is bounded as $v, \phi \in V$, the trace operator maps each to W_a, and $A : W_a \to W_a'$.

Furthermore, $\mathcal{A}$ is V–elliptic [SS11], i.e., there is a $\gamma > 0$ such that

$$\operatorname{Re}\{\mathcal{A}(v,v)\} \geq \gamma \|v\|_V^2 .$$

Again, the first two terms do not cause any problem as they are the V–norm, however the second two must be handled by estimates such as

$$\operatorname{Re}\left\{ \int_{\Gamma_a} (A-A_0)[v_{r=a}]\overline{v_{r=a}}\, ds \right\} = \sum_{p=-\infty, p\neq 0}^{\infty} \operatorname{Re}\left\{ \hat{A}_p \right\} |\hat{v}_p(a)|^2 \geq \sum_{p=-\infty, p\neq 0}^{\infty} |\hat{v}_p(a)|^2 \geq 0,$$

and

$$\begin{aligned}
-\operatorname{Re}\left\{ \int_{\Gamma_b} (B-B_0)[v_{r=a}]\overline{v_{r=b}}\, ds \right\} &= \sum_{p=-\infty, p\neq 0}^{\infty} \operatorname{Re}\left\{ -\hat{B}_p \right\} |\hat{v}_p(b)|^2 \\
&\geq \sum_{p=-\infty, p\neq 0}^{\infty} |\hat{v}_p(b)|^2 \geq 0.
\end{aligned}$$

By the Lax–Milgram Lemma (see Lemma 2.1.51 of [SS11]) the operator $\mathbf{A}$ satisfies

$$\left\| \mathbf{A}^{-1} \right\|_{V \leftarrow V'} \leq \frac{1}{\gamma}$$

(see Theorem 2.1.44 of [SS11]).

Again, as shown in [HH92, DI01, NN06] it is not hard to show that $\mathcal{D}_1$ is a continuous sesquilinear form from $L^2(\Omega) \times L^2(\Omega)$ to $\mathbf{C}$ which induces another bounded operator $\mathbf{D}_1$:

$L^2(\Omega) \to L^2(\Omega)$. Since V embeds compactly into $L^2(\Omega)$ we have that $\mathbf{D}_1$ is a compact operator.

It is a little more difficult to show that $\mathcal{D}_2$ is a continuous sesquilinear form mapping $L^2(\Gamma_m) \times L^2(\Gamma_m)$ to $\mathbf{C}$. For instance, of special note is the calculation

$$\operatorname{Im}\left\{\int_{\Gamma_a} (A - A_0)[v_{r=a}]\overline{\phi_{r=a}}\, ds\right\} = \sum_{p=-\infty, p\neq 0}^{\infty} \operatorname{Im}\left\{\hat{A}_p \hat{v}_p(a)\overline{\hat{\phi}_p(a)}\right\},$$

which is bounded by the boundedness of $\operatorname{Im}\left\{\hat{A}_p\right\}$ and the Cauchy–Schwartz inequality. In addition $A_0 : L^2(\Gamma_a) \to L^2(\Gamma_a)$ so

$$\int_{\Gamma_a} A_0[v_{r=a}]\overline{\phi_{r=a}}\, ds \leq \|A_0[v_{r=a}]\|_{L^2(\Gamma_a)} \|\phi_{r=a}\|_{L^2(\Gamma_a)}.$$

So, since W_m embeds compactly into $L^2(\Gamma_m)$ we have that the induced operator $\mathbf{D}_2$ is a compact operator.

Thus, the governing equations can be written as

$$(\mathbf{A} + \mathbf{D}_1 + \mathbf{D}_2)v_0 = G \quad \Longrightarrow \quad (I + \mathbf{A}^{-1}(\mathbf{D}_1 + \mathbf{D}_2))v_0 = \mathbf{A}^{-1}G,$$

where $\mathbf{A}^{-1}(\mathbf{D}_1 + \mathbf{D}_2)$ is a compact map from V to V. Thus, by Fredholm's theory [HH92, DI01, NN06], provided that the null space of $(\mathbf{A} + \mathbf{D}_1 + \mathbf{D}_2)$ is trivial (which we are guaranteed by our choice of configuration), there exists a (unique) solution satisfying

$$\|v_0\|_V \leq \left\|(I + \mathbf{A}^{-1}(\mathbf{D}_1 + \mathbf{D}_2))\mathbf{A}^{-1}G\right\|_V \leq \left\|I + \mathbf{A}^{-1}(\mathbf{D}_1 + \mathbf{D}_2)\right\|_{V\leftarrow V} \left\|\mathbf{A}^{-1}\right\|_{V\leftarrow V'} \|G\|_{V'},$$

and we are done. □

We close with the estimate for v_1.

Theorem B.5. *If $K \in W_a'$, $L \in W_b'$, the configuration $(k = 0, a, b, A, B) \in \mathcal{C}_\delta$ for some $\delta > 0$, then there exists a harmonic function satisfying* (B.17) *which verifies the estimate* (B.19).

Proof. The solution of (B.17c) is given by (B.7) with r–derivative specified in (B.8). To satisify the boundary conditions we use the Fourier series representations

$$K(\theta) = \sum_{p=-\infty}^{\infty} \hat{K}_p e^{ip\theta}, \quad L(\theta) = \sum_{p=-\infty}^{\infty} \hat{L}_p e^{ip\theta},$$

and generate (B.9) and (B.10) with right–hand–side $(\hat{K}_p, \hat{L}_p)^T$. More specifically, for $p \neq 0$,

$$\begin{pmatrix} q^{|p|}\left(|p|/(bq) - \hat{A}_p\right) & \left(-|p|/a - \hat{A}_p\right) \\ \left(|p|/b - \hat{B}_p\right) & q^{|p|}\left(-(|p|\, q)/a - \hat{B}_p\right) \end{pmatrix} \begin{pmatrix} c_p \\ d_p \end{pmatrix} = \begin{pmatrix} \hat{K}_p \\ \hat{L}_p \end{pmatrix},$$

and, for $p = 0$,

$$\begin{pmatrix} 1/a - \hat{A}_0 \log(a) & -\hat{A}_0 \\ 1/b - \hat{B}_0 \log(b) & -\hat{B}_0 \end{pmatrix} \begin{pmatrix} c_0 \\ d_0 \end{pmatrix} = \begin{pmatrix} \hat{K}_0 \\ \hat{L}_0 \end{pmatrix}.$$

We recall the definition of the determinant function, (B.11),

$$\Lambda_p(0,a,b,\hat{A}_p,\hat{B}_p) = \left(\frac{|p|}{a}+\hat{A}_p\right)\left(\frac{|p|}{b}-\hat{B}_p\right) - q^{2|p|}\left(\frac{|p|}{bq}-\hat{A}_p\right)\left(\frac{|p|\,q}{a}+\hat{B}_p\right),$$

for $p \neq 0$, and, (B.12),

$$\Lambda_0(0,a,b,\hat{A}_0,\hat{B}_0) = \frac{a\hat{A}_0 - b\hat{B}_0}{ab} + \hat{A}_0\hat{B}_0\log(q).$$

With this we can write the solution as

$$\begin{pmatrix} c_p \\ d_p \end{pmatrix} = \frac{1}{\Lambda_p}\left\{ \begin{pmatrix} \left(|p|/a+\hat{A}_p\right)\hat{L}_p \\ \left(-|p|/b+\hat{B}_p\right)\hat{K}_p \end{pmatrix} + q^{|p|}\begin{pmatrix} \left(-(|p|\,q)/a-\hat{B}_p\right)\hat{K}_p \\ \left(|p|/(bq)-\hat{A}_p\right)\hat{L}_p \end{pmatrix}\right\},$$

for $p \neq 0$, and

$$\begin{pmatrix} c_0 \\ d_0 \end{pmatrix} = \frac{1}{\Lambda_0}\begin{pmatrix} -\hat{B}_0\hat{K}_0 + \hat{A}_0\hat{L}_0 \\ \left(-1/b+\hat{B}_0\log(b)\right)\hat{K}_0 + \left(1/a-\hat{A}_0\log(a)\right)\hat{L}_0 \end{pmatrix}.$$

We have already assumed that we are in a δ–permissible configuration so we know that $\Lambda_p > \delta$ and all of these solutions are well–defined. To study the regularity results which we claim, we must investigate the asymptotics of (B.11). This is a little difficult as this form is quite complicated, however, as $0 < q < 1$ we can see that

$$\Lambda_p(0,a,b,\hat{A}_p,\hat{B}_p) \sim \left(\frac{|p|}{a}+\hat{A}_p\right)\left(\frac{|p|}{b}-\hat{B}_p\right).$$

Since A and B are at most order–one Fourier multipliers, i.e., there exist $\tilde{C}_A > 0$ and $\tilde{C}_B > 0$ such that

$$\left|\hat{A}_p\right| < \tilde{C}_A\langle p\rangle, \quad \left|\hat{B}_p\right| < \tilde{C}_B\langle p\rangle,$$

it is clear that there is a constant $\tilde{C}_\Lambda > 0$, such that

$$\frac{1}{\tilde{C}_\Lambda} < \frac{|\Lambda_p|}{\langle p\rangle^2} < \tilde{C}_\Lambda.$$

Thus, we find, as $p \to \infty$,

$$c_p \sim \left(\frac{|p|/a+\hat{A}_p}{\Lambda_p}\right)\hat{K}_p, \quad d_p \sim \left(\frac{-|p|/b+\hat{B}_p}{\Lambda_p}\right)\hat{L}_p,$$

so that

$$|c_p|^2 \leq C_c\langle p\rangle^{-2}\left|\hat{K}_p\right|^2, \quad |d_p|^2 \leq C_d\langle p\rangle^{-2}\left|\hat{L}_p\right|^2,$$

for constants $C_c, C_d > 0$.

Regarding the V norm of v_1 we note that, from Parseval's relation,

$$\|v_1\|_V^2 = \sum_{p=-\infty}^{\infty}\langle p\rangle^2\left\|\widehat{(v_1)}_p\right\|_{L^2(dr)}^2 + \left\|\partial_r\widehat{(v_1)}_p\right\|_{L^2(dr)}^2.$$

From (B.7) we have

$$\left\|\widehat{(v_1)}_p\right\|^2_{L^2(dr)} \le |c_p|^2 \left\|\left(\frac{r}{b}\right)^{|p|}\right\|^2_{L^2(dr)} + |d_p|^2 \left\|\left(\frac{r}{a}\right)^{-|p|}\right\|^2_{L^2(dr)},$$

and from (B.8)

$$\left\|\partial_r \widehat{(v_1)}_p\right\|^2_{L^2(dr)} \le |p|^2 \left|\frac{c_p}{b}\right|^2 \left\|\left(\frac{r}{b}\right)^{|p|-1}\right\|^2_{L^2(dr)} + |p|^2 \left|\frac{d_p}{a}\right|^2 \left\|\left(\frac{r}{a}\right)^{-|p|-1}\right\|^2_{L^2(dr)}.$$

For $p \neq -1$ it is an elementary Calculus exercise to deduce that

$$\|r^p\|^2_{L^2(dr)} = \int_a^b r^{2p+1}\, dr = \frac{b^{2p+2} - a^{2p+2}}{2p+2} < C\langle p\rangle^{-1},$$

while $\left\|r^{-1}\right\|_{L^2(dr)} = \log(b/a) < \infty$. With this it is not difficult to show that

$$\begin{aligned}
\|v_1\|^2_V &\le C_0 \sum_{p=-\infty}^{\infty} \langle p\rangle^2 \langle p\rangle^{-1} \left(|c_p|^2 + |d_p|^2\right) + C_1 \sum_{p=-\infty}^{\infty} \langle p\rangle^{-1} |p|^2 \left(|c_p|^2 + |d_p|^2\right) \\
&\le C \sum_{p=-\infty}^{\infty} \langle p\rangle^1 \langle p\rangle^{-2} \left(\left|\hat{K}_p\right|^2 + \left|\hat{L}_p\right|^2\right) \\
&\le C \left\{\|K\|_{H^{-1/2}} + \|L\|_{H^{-1/2}}\right\},
\end{aligned}$$

and we are done. □

Remark B.6. The reason we consider the Laplace equation at all is this latter study of the asymptotics of the $\{c_p, d_p\}$ which is greatly simplified in comparison to the analogous forms in terms of Bessel functions.

References

[Are09] Tilo Arens. *Scattering by Biperiodic Layered Media: The Integral Equation Approach.* Habilitationsschrift, Karlsruhe Institute of Technology, 2009.

[BGM96] George A. Baker, Jr. and Peter Graves-Morris. *Padé approximants.* Cambridge University Press, Cambridge, second edition, 1996.

[Boy01] John P. Boyd. *Chebyshev and Fourier spectral methods.* Dover Publications Inc., Mineola, NY, second edition, 2001.

[BR93a] O. Bruno and F. Reitich. Numerical solution of diffraction problems: A method of variation of boundaries. *J. Opt. Soc. Am. A*, 10(6):1168–1175, 1993.

[BR93b] O. Bruno and F. Reitich. Numerical solution of diffraction problems: A method of variation of boundaries. II. Finitely conducting gratings, Padé approximants, and singularities. *J. Opt. Soc. Am. A*, 10(11):2307–2316, 1993.

[BR93c] O. Bruno and F. Reitich. Numerical solution of diffraction problems: A method of variation of boundaries. III. Doubly periodic gratings. *J. Opt. Soc. Am. A*, 10(12):2551–2562, 1993.

[BR98] Oscar P. Bruno and Fernando Reitich. Boundary–variation solutions for bounded–obstacle scattering problems in three dimensions. *J. Acoust. Soc. Am.*, 104(5):2579–2583, 1998.

[Bur66] O. R. Burggraf. Analytical and numerical studies of the structure of steady separated flows. *J. Fluid Mech.*, 24:113–151, 1966.

[CHQZ88] C. Canuto, M. Y. Hussaini, A. Quarteroni, and T. A. Zang. *Spectral methods in fluid dynamics*. Springer-Verlag, New York, 1988.

[CK13] David Colton and Rainer Kress. *Inverse acoustic and electromagnetic scattering theory*, volume 93 of *Applied Mathematical Sciences*. Springer, New York, third edition, 2013.

[Des91a] Bruno Després. Domain decomposition method and the Helmholtz problem. In *Mathematical and numerical aspects of wave propagation phenomena (Strasbourg, 1991)*, pages 44–52. SIAM, Philadelphia, PA, 1991.

[Des91b] Bruno Després. *Méthodes de décomposition de domaine pour les problèmes de propagation d'ondes en régime harmonique. Le théorème de Borg pour l'équation de Hill vectorielle*. Institut National de Recherche en Informatique et en Automatique (INRIA), Rocquencourt, 1991. Thèse, Université de Paris IX (Dauphine), Paris, 1991.

[DFM02] M. O. Deville, P. F. Fischer, and E. H. Mund. *High-order methods for incompressible fluid flow*, volume 9 of *Cambridge Monographs on Applied and Computational Mathematics*. Cambridge University Press, Cambridge, 2002.

[DI01] Leszek Demkowicz and Frank Ihlenburg. Analysis of a coupled finite-infinite element method for exterior Helmholtz problems. *Numer. Math.*, 88(1):43–73, 2001.

[DLMF] *NIST Digital Library of Mathematical Functions*. http://dlmf.nist.gov/, Release 1.0.22 of 2019-03-15. F. W. J. Olver, A. B. Olde Daalhuis, D. W. Lozier, B. I. Schneider, R. F. Boisvert, C. W. Clark, B. R. Miller and B. V. Saunders, eds.

[EB12] S. Enoch and N. Bonod. *Plasmonics: From Basics to Advanced Topics*. Springer Series in Optical Sciences. Springer, New York, 2012.

[ESHES06] I. El-Sayed, X. Huang, and M. El-Sayed. Selective laser photo-thermal therapy of epithelial carcinoma using anti-egfr antibody conjugated gold nanoparticles. *Cancer Lett.*, 239(1):129–135, 2006.

[Eva10] Lawrence C. Evans. *Partial differential equations*. American Mathematical Society, Providence, RI, second edition, 2010.

[Fol76] Gerald B. Folland. *Introduction to partial differential equations*. Princeton University Press, Princeton, N.J., 1976. Preliminary informal notes of university courses and seminars in mathematics, Mathematical Notes.

[GO77] D. Gottlieb and S. A. Orszag. *Numerical analysis of spectral methods: theory and applications*. Society for Industrial and Applied Mathematics, Philadelphia, Pa., 1977. CBMS-NSF Regional Conference Series in Applied Mathematics, No. 26.

[GR87] L. Greengard and V. Rokhlin. A fast algorithm for particle simulations. *J. Comput. Phys.*, 73(2):325–348, 1987.

[HH92] Isaac Harari and Thomas J. R. Hughes. Analysis of continuous formulations underlying the computation of time-harmonic acoustics in exterior domains. *Comput. Methods Appl. Mech. Engrg.*, 97(1):103–124, 1992.

[HW08] Jan S. Hesthaven and Tim Warburton. *Nodal discontinuous Galerkin methods*, volume 54 of *Texts in Applied Mathematics*. Springer, New York, 2008. Algorithms, analysis, and applications.

[Ihl98] Frank Ihlenburg. *Finite element analysis of acoustic scattering*. Springer-Verlag, New York, 1998.

[Joh87] Claes Johnson. *Numerical solution of partial differential equations by the finite element method*. Cambridge University Press, Cambridge, 1987.

[Kre14] Rainer Kress. *Linear integral equations*. Springer-Verlag, New York, third edition, 2014.

[KS03] P. Knupp and K. Salari. *Verification of Computer Codes in Computational Science and Engineering*. Chapman and Hall/CRC, Boca Raton, 2003.

[LeV07] Randall J. LeVeque. *Finite difference methods for ordinary and partial differential equations*. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 2007. Steady-state and time-dependent problems.

[LGSLG07] M. Liu, P. Guyot-Sionnest, T.-W. Lee, and S. Gray. Optical properties of rodlike and bipyramidal gold nanoparticles from three–dimensional computations. *Physical Review B*, 76:235428, 2007.

[LLH$^+$05] C. Loo, A. Lowery, N. Halas, J. West, and R. Drezek. Immunotargeted nanoshells for integrated cancer imaging and therapy. *Nano Letters*, 5(4):709–711, 2005.

[Mai07] S. A. Maier. *Plasmonics: Fundamentals and Applications*. Springer, New York, 2007.

[Mar06] P. A. Martin. *Multiple scattering*, volume 107 of *Encyclopedia of Mathematics and its Applications*. Cambridge University Press, Cambridge, 2006. Interaction of time-harmonic waves with N obstacles.

[Mar18] Paul Martin. Personal Communication, 2018.

[MCAPS$^+$08] V. Myroshnychenko, E. Carbo-Argibay, I. Pastoriza-Santos, J. Perez-Juste, L. Liz-Marzan, and F. Garcia de Abajo. Modeling the optical response of highly faceted metal nanoparticles with a fully 3d boundary element method. *Advanced Materials*, 20:4288–4293, 2008.

[MRFPS+08] V. Myroshnychenko, J. Rodriguez-Fernandez, I. Pastoriza-Santos, A. Funston, C. Novo, P. Mulvaney, L. Liz-Marzan, and J. Garcia de Abajo. Modelling the optical response of gold nanoparticles. *Chemical Society Reviews*, 37:1792–1805, 2008.

[NH12] L. Novotny and B. Hecht. *Principles of Nano–Optics*. Cambridge University Press, Cambridge, second edition, 2012.

[Nic12] D. P. Nicholls. Three–dimensional acoustic scattering by layered media: A novel surface formulation with operator expansions implementation. *Proceedings of the Royal Society of London, A*, 468:731–758, 2012.

[Nic15] D. P. Nicholls. A method of field expansions for vector electromagnetic scattering by layered periodic crossed gratings. *Journal of the Optical Society of America, A*, 32(5):701–709, 2015.

[Nic17] D. P. Nicholls. On analyticity of linear waves scattered by a layered medium. *Journal of Differential Equations*, 263(8):5042–5089, 2017.

[Nic18] D. P. Nicholls. Stable, high–order computation of impedance–impedance operators for three–dimensional layered media simulations. *Proc. Roy. Soc. Lond., A*, 474:20170704, 2018.

[NN04] D. P. Nicholls and N. Nigam. Exact non-reflecting boundary conditions on general domains. *J. Comput. Phys.*, 194(1):278–303, 2004.

[NN06] D. P. Nicholls and N. Nigam. Error analysis of an enhanced DtN–fe method for exterior scattering problems. *Numer. Math.*, 105(2):267–298, 2006.

[NOJR16] D. P. Nicholls, S.-H. Oh, T. W. Johnson, and F. Reitich. Launching surface plasmon waves via vanishingly small periodic gratings. *Journal of Optical Society of America, A*, 33(3):276–285, 2016.

[NR01a] D. P. Nicholls and F. Reitich. A new approach to analyticity of Dirichlet-Neumann operators. *Proc. Roy. Soc. Edinburgh Sect. A*, 131(6):1411–1433, 2001.

[NR01b] D. P. Nicholls and F. Reitich. Stability of high-order perturbative methods for the computation of Dirichlet-Neumann operators. *J. Comput. Phys.*, 170(1):276–298, 2001.

[NR03] D. P. Nicholls and F. Reitich. Analytic continuation of Dirichlet-Neumann operators. *Numer. Math.*, 94(1):107–146, 2003.

[NR04a] D. P. Nicholls and F. Reitich. Shape deformations in rough surface scattering: Cancellations, conditioning, and convergence. *J. Opt. Soc. Am. A*, 21(4):590–605, 2004.

[NR04b] D. P. Nicholls and F. Reitich. Shape deformations in rough surface scattering: Improved algorithms. *J. Opt. Soc. Am. A*, 21(4):606–621, 2004.

[NS06] D. P. Nicholls and J. Shen. A stable, high–order method for two–dimensional bounded–obstacle scattering. *SIAM J. Sci. Comput.*, 28(4):1398–1419, 2006.

[NS09] D. P. Nicholls and J. Shen. A rigorous numerical analysis of the transformed field expansion method. *SIAM Journal on Numerical Analysis*, 47(4):2708–2734, 2009.

[NT18] D. P. Nicholls and X. Tong. A high–order perturbation of surfaces algorithm for the simulation of localized surface plasmon resonances in two dimensions. *J. Sci. Comput.*, 76:1370–1395, 2018.

[OTH04] W. L. Oberkampf, T. G. Trucano, and C. Hirsch. Verification, validation, and predictive capability in computational engineering and physics. *Appl. Mech. Rev.*, 57(5):345–384, 2004.

[Pet80] R. Petit, editor. *Electromagnetic theory of gratings*. Springer-Verlag, Berlin, 1980.

[Rae88] H. Raether. *Surface plasmons on smooth and rough surfaces and on gratings*. Springer, Berlin, 1988.

[Ray07] Lord Rayleigh. On the dynamical theory of gratings. *Proc. Roy. Soc. London*, A79:399–416, 1907.

[Ric51] S. O. Rice. Reflection of electromagnetic waves from slightly rough surfaces. *Comm. Pure Appl. Math.*, 4:351–378, 1951.

[Roa98a] P. J. Roache. *Verification and Validation in Computational Science and Engineering*. Hermosa Publishers, Albuquerque, 1998.

[Roa98b] P. J. Roache. Verification of codes and calculations. *AIAA Journal*, 36(5):696–702, 1998.

[Roa02] P. J. Roache. Code verification by the method of manufactured solutions. *J. Fluids Eng.*, 124(1):4–10, 2002.

[Roy05] C. J. Roy. Review of code and solution verification procedures for computational simulation. *J. Comp. Phys.*, 205(1):131–156, 2005.

[RT04] F. Reitich and K. Tamma. State–of–the–art, trends, and directions in computational electromagnetics. *CMES Comput. Model. Eng. Sci.*, 5(4):287–294, 2004.

[SS11] Stefan A. Sauter and Christoph Schwab. *Boundary element methods*, volume 39 of *Springer Series in Computational Mathematics*. Springer-Verlag, Berlin, 2011. Translated and expanded from the 2004 German original.

[Str04] John C. Strikwerda. *Finite difference schemes and partial differential equations*. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, second edition, 2004.

[SW07] Jie Shen and Li-Lian Wang. Analysis of a spectral-Galerkin approximation to the Helmholtz equation in exterior domains. *SIAM J. Numer. Anal.*, 45(5):1954–1978, 2007.

[XBKB99] H. Xu, E. Bjerneld, M. Käll, and L. Börjesson. Spectroscopy of single hemoglobin molecules by surface enhanced raman scattering. *Phys. Rev. Lett.*, 83:4357–4360, 1999.