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Asymptotic Formula for Scattering Problems Related to Thin Metasurfaces

Zachary Jermain
Louisiana State University and Agricultural and Mechanical College

ASYMPTOTIC FORMULA FOR SCATTERING PROBLEMS RELATED TO THIN METASURFACES

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This thesis is dedicated to Marylin Jermain and Lori Bray.

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Abstract

The goal of this work is to develop an asymptotic formula for the behavior of a scattered electromagnetic field in the presence of a thin metamaterial known as a metasurface. By using a carefully chosen Green's function and the single and double layer potentials we analyze the perturbed scattering problem in the presence of the metamaterial and a background scattering problem. By using Lippman-Schwinger type representation formulas for the two fields we develop the asymptotic formula for the perturbed field. From here we prove the asymptotic formula holds up to a specific error term based on the size of the particles comprising the metasurface. Arising from this asymptotic formula is the polarization tensor which describes how the metasurface interacts with light based on the component particles' dielectric permittivity and geometry. We then use the polarization tensor to derive key optical constants for the metasurface such as the reflection and transmission coefficients for normal incidence.

Chapter 1. Introduction

Metamaterials have been an active area of research for some time, with various applications in acoustics, infrared and microwave technology, and other engineering endeavors. The intrigue surrounding metamaterials stems from their novel properties, which are not found in naturally occurring materials. Examples dealing with electromagnetic radiation include waveguides, negative index materials, and plasmon resonances [6], [25]. Metamaterials also present a unique framework for new mathematics in scattering problems, homogenization, and numerical techniques such as finite element methods. Mathematics offers a unique perspective on the problem, often handling scattering problems by describing the metamaterial as an effective medium or effective material parameter that approximates the real problem up to a rigorously proved error estimate which tends to zero as the size of particles go to zero.

The focus of this work lies in the intersection of the physical need to model and construct new optical metamaterials and the rigorous mathematical framework for scattering problems involving small particles and metamaterials. As new fabrication techniques have arisen, nano-scale geometry of the small particles of a metamaterial allows novel interaction and control of electromagentic radiation in the optical range [6], [7]. In addition, new materials such as noble metals (gold, silver, etc.) are being investegated. The challenge of modeling nano-scale geometries with materials such as noble metals is two-fold. Firstly, the small geometry requires extremely fine meshing for traditional finite element methods and Maxwell solvers, causing these methods to become more computationally expensive. Secondly, noble metals are dispersive in optical wavelengths and can possess a negative real part of the dielectric permittivity. For dispersive materials, a range of incident wavelengths must be modeled, and where the permittivity becomes negative in the real part, we lose ellipticity of the governing partial differential equations. Here traditional solvers such as RCWA require a large number of Fourier modes to converge, and in some cases convergence is lost all together [15]. In this work, we present a first step towards a mathematical solution to some of the above problems encountered in modeling these optical metamaterials. We develop an asymptotic formula for the scattered magnetic field from a periodic arrangement of inhomogenities which approximates the actual solution up to certain error estimates. The asymptotic formula depends on the the polarization tensor denoted by M, which is determined by solving a simpler partial differential equation (PDE).

The polarization tensor is well studied and describes how waves behave in the presence of an inhomogeneous material, in this case small periodic particles [14], [20]. Because the PDE for the polarization tensor is easier to solve, by using the asymptotic formula the computational cost is reduced making it easier to inform design of new systems. Furthermore, by using techniques such as topology optimization and machine-learning techniques one can predict the optical control over an entire design space [24], [26]. Using M we are able to treat the metasurface as a scattering problem with an impedance surface similar to the work in [1]. This formulation also allows us to represent the original scattering problem as scattering by an open waveguide. Lastly, we are able to derive approximations for the radiating far-field reflection and transmission coefficients. Using approximate optical constants or material parameters, we are able to aid in the design and inverse design of new metasurfaces [24].

We start by considering a thin metamaterial consisting of a single layer with periodically spaced particles with period d and dielectric permittivity ε_m. The height of the particles is of order δ with $d > \delta$ and the width is similar scale with $w = a\delta$. Thin metamaterials such as these are also known as metasurfaces. The periodicity of the particles lies in the x_1 direction and the particles are centered on the x_2 axis. The particles are uniform in the x_3 direction, so we can simplify the geometry to the 2D case. We denote each individual particle as B_j and the collection of particles which make up the metasurface as

$$\mathcal{B}_{meta} = \cup_{j=1}^{n}(d + \mathcal{B}_j) \tag{1.1}$$

One key distinction for the metasurface of interest is the period, d, is not assumed to be significantly smaller than the incident wavelength. Instead the height of the particles is assumed to be small compared to the period as stated above. This allows the analysis to hold for a wider range of incident wavelengths compared to traditional homogenization techniques. With this in mind we shift from homogenization techniques seen in similar problems [8], [21], and instead proceed with our formulation which is similar to works in [3], [9], [17], [18], [23].

For now, we simply embed the metasurface in a domain denoted Ω_R, where R is some positive number which represents the distance the region Ω_R extends to the right and left of the metasurface respectively. The domain Ω_R consists of a homogeneous medium which we take to be air, so $\varepsilon_0 = 1$ (see Figure 1.1). In this work, we only consider materials with a positive real part of their permittivity ($Real(\varepsilon_m) > 0$), but otherwise the permittivity can be complex-valued. Materials with negative real permittivity can also be handled, but require careful treatment for existence proofs, so they will be handled in future work.

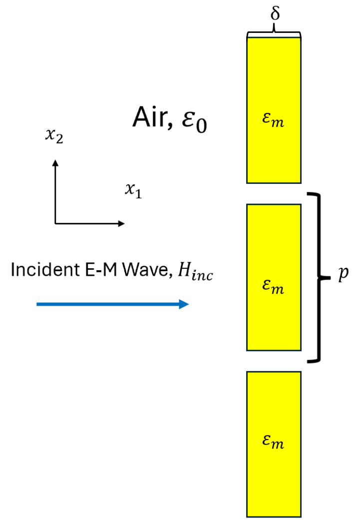

Figure 1.1. Material Geometry

The metasurface interacts with an incident electromagnetic wave propagating from negative infinity in the x_1 direction. The governing equations for the system are the classic time-harmonic Maxwell equations with no source charges or current in the presence of an inhomogeneous material [4], [16]. Here $\mathbf{E}$ will denote the electric field and $\mathbf{H}$ will denote the magnetic field. The material is assumed nonmagnetic, i.e., $\mu = \mu_0$, and $\varepsilon = \varepsilon_0\varepsilon_\delta$ where the relative dielectric constant ε_δ can depend upon x.

$$\nabla \times \mathbf{E} = i\omega\mu_0\mathbf{H} \qquad \nabla \times \mathbf{H} = -i\omega\epsilon_0\varepsilon_\delta\mathbf{E}$$
$$\nabla \cdot \varepsilon\mathbf{E} = 0 \qquad \nabla \cdot \mathbf{H} = 0 \tag{1.2}$$

We are interested in the case of Transverse Magnetic (TM) polarization which gives

$$\begin{gathered}\mathbf{E} = E_1(x_1, x_2)e^{i(kx-\omega t)}\vec{e_1} + E_2e^{i(kx-\omega t)}\vec{e_2} \\ \mathbf{H} = H_3e^{i(kx-\omega t)}\vec{e_3}\end{gathered} \tag{1.3}$$

By using the TM polarization we ensure the electric field has a component which is parallel to the direction of periodicity which provides the potential for plasmonic behavior and resonance in the metasurface [6]. We note that with the TM polarization we can write the curl equation to give the relationship between H_3 and the electric field components E_1 and E_2

$$\partial x_1 H_3 = -i\frac{\omega}{c}E_2 \qquad \partial x_2 H_3 = i\frac{\omega}{c}E_1 \tag{1.4}$$

This allow us to solve for the magnetic field and then find the electric field using the curl equation above.

The piece wise constant dielectric permittivity ε_δ describing the metasurface is defined by

$$\varepsilon_\delta = \begin{cases} 1 & x \in \Omega_R \setminus \mathcal{B} \\ \varepsilon_m & x \in \mathcal{B}. \end{cases} \tag{1.5}$$

Recall $\mu_0\varepsilon_0 = c^2$ and set $k = \omega/c$. Using the assumptions of TM polarization and some vector identities we reduce the Maxwell system to the scalar Helmholtz equation in terms of the magnetic field, H_3. For notation, we will denote this field H_δ as it represents the magnetic field in the presence of the metasurface, which we will also call the "perturbed" field. The incident magnetic field is H_{inc} and $H_\delta = H_{inc} + H_\delta^s$ where H_δ^s is the "scattered" magnetic field. H_δ is the solution of the Helmholtz equation

$$\nabla \cdot \left(\frac{1}{\varepsilon_\delta}\nabla H_\delta\right) + k^2 H_\delta = 0, \tag{1.6}$$

where H_δ^s satisfies the out going radiation conditions given by: There exists an $R > 0$ for which

$$H_\delta^s = \sum_{m=0}^{\infty} r_m e^{ikg_m x_1} e^{i\beta_m x_2}, x_1 < -R. \tag{1.7}$$

and

$$H_\delta^s = \sum_{m=0}^{\infty} t_m e^{-ikg_m x_1} e^{i\beta_m x_2}, x_1 > R, \tag{1.8}$$

where r_m and t_m are reflection and transmission coefficents. We also define the "background" magnetic field, H_0 which solves the Helmholtz equation in the absence of the metasurface,

$$\Delta H_0 + k^2 H_0 = 0 \tag{1.9}$$

In the absence of the metasurface we just have the homogeneous region Ω_R, so in this case H_0 is simply just the incident field H_{inc}.

Chapter 2. Preliminaries

2.1. Weak Formulation and Quasi-Periodic Green's Function

In the first step of our analysis we utilize the periodic geometry of the domain and simplify the problem to a single particle on an infinite strip with $-\infty < x_1 < \infty$, $-d/2 < x_2 < d/2$ and quasi-periodic boundary conditions in the x_1 coordinate. The periodic domain has width d with a single particle, B, centered at $(x_1, x_2) = (0, 0)$. We denote the truncated domain by Ω_R, which extends to a distance R above and below the particle in the x_2 direction. We denote the periodic strip with width d which contains Ω_R and the particle as $R^2_{\#}$. We recall that the height of the particle is denoted by δ and here we will also take the width to be δ.

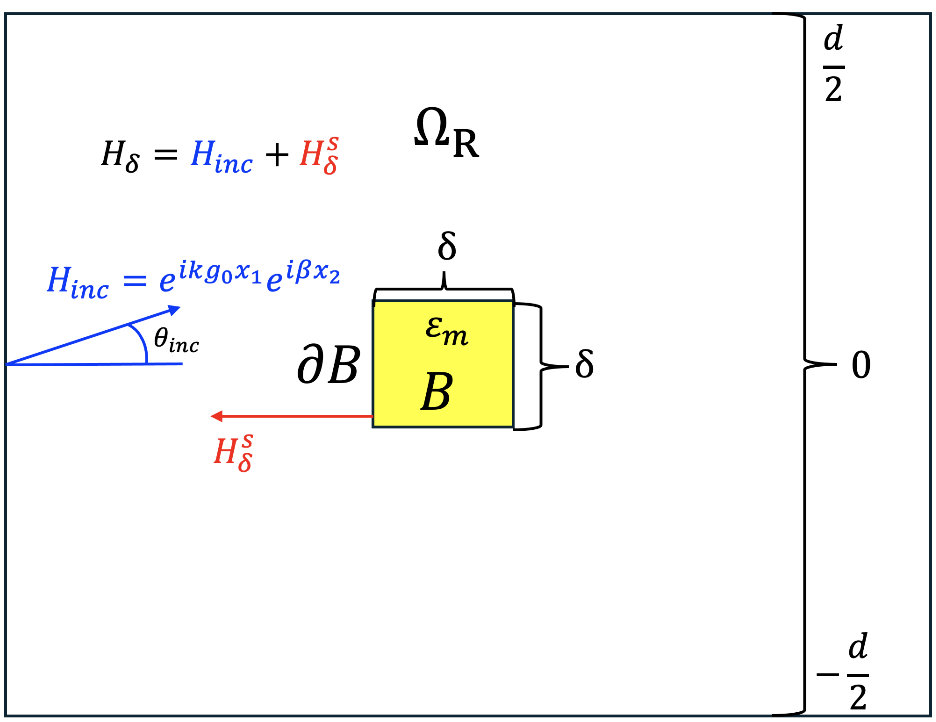

Figure 2.1. Periodic Domain

We define $\beta = k\sin(\theta_{inc})$ as the incident wavenumber for a prescribed incoming wave with angle of incidence θ_{inc}. The incoming wave is from the left and is of the form $H_{inc} = e^{ikg_0 x_1} e^{i\beta x_2}$ where $g_0 = \left[1 - \left(\frac{\beta}{k}\right)^2\right]^{1/2}$. The solution of the scattering problem is written as H_δ. The variational form of the scattering problem (1.6)-(1.8) is given by

$$\int_{\mathbb{R}^2_\#} \varepsilon_\delta^{-1} \nabla H_\delta(y) \cdot \nabla v(y) + k^2 H_\delta(y) v(y) dy = 0 \tag{2.1}$$

where the solution H_δ belongs to $H^1_\#(\beta, \mathbb{R}^2_\#)$ which is the Hilbert space given by

$$H^1_\#(\beta, \mathbb{R}^2_\#) = \{v \in H^1_{loc}(\mathbb{R}^2) : v \text{ is } \beta \text{ quasi-periodic}\} \tag{2.2}$$

and v is any function in the space $C^\infty_{0,\beta}(\mathbb{R}^2_\#)$ of infinitely differentiable functions with compact support on the closure of $\mathbb{R}^2_\#$ and that satisfy the same quasiperiodic constraint as functions in $H^1_\#(\beta, \mathbb{R}^2_\#)$. We set $p = 2\pi/d$ and define $\beta_m = \beta + mp$ for $m \in \mathbb{Z}$. The solution is of the form $H_\delta = H_{inc} + H^s_\delta$ where H^s_δ satisfies the out going radiation conditions given by: There exists an $R > 0$ for which

$$H^s_\delta = \sum_{m=0}^{\infty} r_m e^{ikg_m x_1} e^{i\beta_m x_2}, x_1 < -R. \tag{2.3}$$

and

$$H^s_\delta = \sum_{m=0}^{\infty} t_m e^{-ikg_m x_1} e^{i\beta_m x_2}, x_1 > R, \tag{2.4}$$

where r_m and t_m are reflection and transmission coefficients. Here

$$g_m = \left[1 - \left(\frac{\beta_m}{k}\right)^2\right]^{1/2} \tag{2.5}$$

and g_0 is associated with the incident wave and $g_0 = \left[1 - \left(\frac{\beta}{k}\right)^2\right]^{1/2}$. Existence of unique solutions for all wave numbers k with the exception of a countable set for the scattering problem are proved in [5], [25].

For completeness, we relate the weak formulation to the classic strong formulation by a proper choice of test functions. By choosing v with support in $\mathbb{R}^2_\# \setminus \mathcal{B}$ and using integration by parts on (2.1) we have

$$\int_{\mathbb{R}^2_\# \setminus \mathcal{B}} \left[\Delta H_\delta(y) + k^2 H_\delta(y)\right] v(y) dy = 0$$

Similarly taking v with support only in the particle $\mathcal{B}$ we have

$$\int_{\mathcal{B}} \left[\varepsilon_m^{-1} \Delta H_\delta(y) + k^2 H_\delta(y)\right] v(y) dy = 0$$

Finally if we take v with support only on the boundary of the particle, $\partial\mathcal{B}$ we have

$$\int_{\partial\mathcal{B}} \varepsilon_m^{-1} \left[\partial_n H_\delta(y)|^- - \partial_n H_\delta(y)|^+\right] v(y) ds_y = 0$$

Combining the above variational forms we have the strong from of the scattering problem on each domain

$$\begin{aligned} \Delta H_\delta(x) + k^2 H_\delta(x) &= 0 \text{ for } x \in \mathbb{R}^2_\# \setminus \mathcal{B} \\ \varepsilon_m^{-1} \Delta H_\delta(x) + k^2 H_\delta(x) &= 0 \text{ for } x \in \mathcal{B} \end{aligned} \tag{2.6}$$

with the flux continuity boundary condition on $\partial\mathcal{B}$

$$\varepsilon_m^{-1} \partial_n H_\delta|^- - \partial_n H_\delta|^+ = 0 \text{ on } \partial\mathcal{B} \tag{2.7}$$

and the continuity of H_δ across $\partial\mathcal{B}$ follows from our choice of weak formulation. Equations (2.1), (2.7) together with the incident wave and outgoing radiation conditions constitute the strong form of the scattering problem.

The main tool of our analysis is the representation of solutions by the Green's function as formulated by Linton [19]. We introduce $X = (x_1 - y_1)$ and $Y = (x_2 - y_2)$ and the quasi-periodic Green's function, G^k_{qp}, satisfies

$$\Delta_y G^k_{qp}(X,Y) + k^2 G^k_{qp}(X,Y) = -\delta(x_1) \sum_{m=-\infty}^{\infty} \delta(x_2 - mp) e^{im\beta d} \text{ in } \Omega_R \tag{2.8}$$

where $y = (y_1, y_2)$. The formula for G^k_{qp} given by,

$$G^k_{qp}(X,Y) = -\frac{1}{2d} \sum_{-\infty}^{\infty} \frac{e^{-\gamma_m |X|} e^{i\beta_m Y}}{\gamma_m} \tag{2.9}$$

where

$$\beta_m = \beta + mp$$

$$\gamma_m = (\beta_m^2 - k^2)^{1/2} = -i(k^2 - \beta_m^2)^{1/2}. \tag{2.10}$$

As before d is the period of the metasurface, and we define $\beta = k \sin(\theta_{inc})$ as the incident wave number for an incoming wave with angle of incidence θ_{inc}. Note if $k^2 < \beta_m^2$ then $\gamma_m = |k^2 - \beta_m^2| > 0$ and the m^{th} order mode decays exponentially in $|X|$. On the other hand for $k^2 > \beta_m^2$ the m^{th} mode is oscillating in $|X|$. The first case corresponds to ($k < \beta < p - k$). The second consideration shows that as $|X| \to \infty$, G^k_{qp} behaves as

$$G^k_{qp} \sim -\frac{i}{2kd} \sum_{-M}^{N} \frac{e^{ikg_m |X|} e^{i\beta_m Y}}{g_m}, \tag{2.11}$$

where M is a non-negative integer such that $\beta_{-M-1} < -k < \beta_{-M}$ and N is a non-negative integer such that $\beta_N < k < \beta_{N+1}$ and g_m is given by (2.5)

The Linton's Green's function is essential to the analysis of the metasurface. The leading order theory is found by relating decay properties of a suitable Dirichlet Green's function and the free space Laplace Green's function to G^k_{qp}. We start with the periodic Green's function given by Linton, G^k_{per}, which can be written as the Green's function for the Helmholtz equation G^k_0 with zero Dirichlet data on the truncated domain Ω_R plus a smooth kernel. Similarly, we can write G^k_0 as the sum of the Green's function for the Laplacian, G^0, plus another smooth kernel. The use of successive Green's functions delivers explicit formulas for the leading order theory and bounds on the higher order error that are valid when the scatter dimensions lie below the period length.

The Green's function for the Helmhotz equation with zero Dirichlet boundary data. For any $x \in \Omega_R$

$$\begin{aligned} \Delta G^k_0(x,\cdot) + k^2 G^k_0(x,\cdot) &= -\delta_x \text{ in } \Omega_R \\ G^k_0(x,\cdot) &= 0 \text{ on } \partial\Omega_R \end{aligned} \tag{2.12}$$

We note here that G^k_0 is symmetric for all $x, y \in \Omega_R$ with $x \neq y$, as well as the following relation between G^k_{qp} and G^k_0

$$G^k_0(x,y) = G^k_{qp}(x,y) + K_1(x,y) \tag{2.13}$$

where $K_1(\cdot,\cdot)$ is a smooth kernel belonging to $C^\infty(\Omega_R \times \Omega_R)$. We also can express G^k_0 in terms of the free space Green's function for the Laplacian, G^0, by

$$G^k_0(x,y) = G^0(x,y) + K_2(x,y) \tag{2.14}$$

where

$$G^0(x,y) = -\frac{1}{2\pi}\log|x-y| \tag{2.15}$$

Again $K_2(x,y)$ is a smooth kernel for $x \neq y$, belonging to $C^\infty\left(\Omega_R \times \Omega_R \setminus \{(x,y) : x = y\}\right)$, where for fixed $x \in \Omega_R$, K_2 satisfies

$$\Delta K_2(x,\cdot) = \Delta G_0^k(x,\cdot) - \Delta G^0(x,\cdot) = -k^2 G_0^k(x,\cdot) \tag{2.16}$$

Lastly, we can relate the Linton Green's function to the Green's function for the Laplacian by

$$G_{qp}^k(x,y) = G^0(x,y) + K_3(x,y) \tag{2.17}$$

Due to the definition of G_{qp}^k and the fact that K_3 is uniformly bounded on any compact set [27], we have that $G_0^k(x,\cdot)$ is in $L^p(\Omega_R)$ for $p < \infty$. Also since $K_2 \in C^\infty(\Omega_R \times \Omega_R)$ for $x \neq y$ we have $K_2(x,\cdot)$ is in $W^{2,p}$ for any $p < \infty$. Therefore $\|K_2(x,\cdot)\|_{W^{2,p}}$ is uniformly bounded for any x in a compact subset of Ω_R. Now by Sobolev's Imbedding Theorem [11],[13] for any compact set $\mathcal{K} \subset \Omega_R$ there exists a constant C such that

$$\|K_2(x,\cdot)\|_{L^\infty(\Omega_R)} + \|\nabla_y K_2(x,\cdot)\|_{L^\infty(\Omega_R)} \leq C \text{ for all } x \in \mathcal{K} \tag{2.18}$$

Here we note that H_0 belongs to $C^\infty(\Omega_R)$ and H_δ belongs to $C^{0,\beta}$ for some $\beta > 0$ due to elliptic regularity estimates [13]. We also have that H_δ is C^∞ in each domain separately, i.e. $H_\delta \in C^\infty(\overline{\mathcal{B}})$, and $H_\delta \in C^\infty(\Omega_R \setminus \mathcal{B})$ with the normal derivative of H_δ having the jump relation across $\partial\mathcal{B}$ given by (2.7)

2.2. Polarization Tensor

Here we introduce the well-known polarization tensor which describes how the particle interacts with the incident electromagnetic wave [14] [20]. First, we define the vector-valued potential $\phi = \phi_1 e_1 + \phi_2 e_2$ which solves the following equation. We note $\{e_1, e_2\}$ is the standard basis in $\mathbb{R}^2$

$$\begin{cases} \Delta\phi = 0 \text{ in } \mathcal{B} \text{ and } \mathbb{R}^2_{\#} \setminus \overline{\mathcal{B}} \\ \phi^+ = \phi^- \text{ across } \partial\mathcal{B} \\ \varepsilon_m \frac{\partial\phi}{\partial n}|^+ - \frac{\partial\phi}{\partial n}|^- = -n \\ \lim_{|z\to\infty|} |\phi(z)| = 0 \end{cases} \tag{2.19}$$

The existence and uniqueness of ϕ is established using single layer potentials with appropriate densities [14]. The polarization tensor, M, for the inclusion $\mathcal{B}$ is now given by

$$M(\varepsilon_m) = |\mathcal{B}|I + (\varepsilon_m - 1)\int_{\partial\mathcal{B}} n(y)\phi(y)ds_y \tag{2.20}$$

We can see for a given inclusion, the polarization tensor is dependent upon the ratio of the dielectric permittivity of the particle and the surrounding medium, in this case just ε_m since the background medium is air. In general M is a 2x2 matrix given by

$$M = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} \tag{2.21}$$

Furthermore M is a symmetric and positive definite [14]. As we shall see in chapter 3 we derive an asymptotic formula for the magnetic field with the only unknown being the polarization tensor. Therefore we just have to solve the simplified PDE (2.19) to find the scattered field seen in chapter 4.

2.3. Well-Posedness of first and second order corrector problems

We begin by asserting the well-posedness of two auxiliary problems posed over the truncated domain Ω_R. The first problem is standard and is the Helmholtz problem over a domain with dielectric constant $\varepsilon_0 = 1$. The second problem is a Helmholtz equation for a domain with dielectric constant one containing an inclusion of dielectric constant ε_m. For each of the two problems well-posedness for the problem with nonzero right hand side and zero Dirichlet data on the boundary is asserted. From there the well-posedness on the truncated domain with zero right hand side and non-zero boundary data follows as a corollary.

Define the background field u_0 to be the solution to the following Helmholtz problem

$$\begin{cases} \Delta u_0 + k^2 u_0 = F \text{ in } \Omega_R \\ u = 0 \text{ on } \partial\Omega_R \end{cases} \tag{2.22}$$

In order to assure well-posedness we assume

$$-k^2 \text{ is not an eigenvalue for the operator } \Delta \text{ with Dirichlet boundary conditions} \tag{2.23}$$

With the assumption (2.23) it follows from standard elliptic PDE methods [11],[13],[22] we have that (2.22) is well-posed, i.e. for any $F \in H^{-1}(\Omega_R)$ there exists a unique solution and a constant C such that $\|u_0\|_{H^1(\Omega_R)} \leq C\|F\|_{H^{-1}(\Omega)}$. Now we perturb the background problem by adding an inclusion of dimension $\delta < k$. The field u_δ is the solution of the perturbed problem

$$\begin{cases} \nabla \cdot \left(\frac{1}{\varepsilon_\delta} \nabla u_\delta\right) + k^2 u_\delta - F \text{ in } \Omega_R \\ u_\delta = 0 \text{ on } \partial\Omega_R \end{cases} \tag{2.24}$$

We state the well-posedness for this Dirichlet problem when δ is small relative to p which is given in [27]

Proposition 2.3.1. *Suppose condition (*2.23*) is satisfied. Then there exists constants* $\delta_0 > 0$ *and* C *such that for any* $0 < \delta < \delta_0$ *and any* $F \in H^{-1}(\Omega_R)$*, (*2.24*) has a unique variational solution,* $u_\delta \in H^1_0(\Omega_R)$*. Furthermore,* u_δ *satisfies*

$$\|u_\delta\|_{H^1(\Omega_R)} \leq C\|F\|_{H^{-1}(\Omega_R)} \tag{2.25}$$

To extend the well-posedness for the background problem to the scattering problem in the presence of the metasurface for given Dirichlet data f we apply the corollary of Proposition 2.3.1 which is also given in [27]

Corollary 2.3.1. *Suppose condition (*2.23*) is satisfied. Then there exists constants* $\delta_0 > 0$ *and* C *such that for any* $0 < \delta < \delta_0$ *and any* $f \in H^{1/2}(\Omega_R)$ *the problem*

$$\begin{cases} \nabla \cdot \left(\frac{1}{\varepsilon_\delta}\nabla u_\delta\right) + k^2 u_\delta = 0 \;\; in \;\Omega_R \\ \\ u_\delta = f \;\; on \;\partial\Omega_R \end{cases} \tag{2.26}$$

as long as δ *is sufficiently small has a unique variational solution,* $u_\delta \in H^1(\Omega_R)$*. Furthermore,* u_δ *satisfies*

$$\|u_\delta\|_{H^1(\Omega_R)} \leq C\|f\|_{H^{1/2}(\Omega_R)} \tag{2.27}$$

With the well-posedness in hand we now obtain the leading order terms and bound the error for inclusions of size $\delta/p < 1$. This is done in the following sections.

2.4. Use of single and double layer potentials

The leading order theory and error bounds follow from integral representations of the solution to the scattering problem using boundary layer potentials [2], [10]. The single layer potential S acts on an element ψ belonging to the Hilbert space, $H^{-1/2}(\partial\Omega_R)$ and sends it to an element of the Hilbert space $H^{1/2}(\partial\Omega_R)$, i.e.

$$S : H^{-1/2}(\partial\Omega_R) \to H^{1/2}(\partial\Omega_R) \tag{2.28}$$

The single layer potential is defined as

$$S : \psi \to \int_{\partial\Omega_R} G_{qp}^k(x,y)\psi(y)ds_y \tag{2.29}$$

The double layer potential operator,D, is given by

$$D : H^{1/2}(\partial\Omega_R) \to H^{1/2}(\partial\Omega_R) \tag{2.30}$$

where D is defined as

$$D : \varphi \to \int_{\partial\Omega_R} \frac{\partial G_{qp}^k(x,y)}{\partial n(y)}\varphi(y)ds_y \tag{2.31}$$

Here we also note the boundary relations for the single and double layer potentials [10].

For $x \in \partial\Omega_R$

$$\frac{\partial S_\pm}{\partial n}(x) = \int_{\partial\Omega_R} \psi(y)\frac{\partial G_{qp}^k(x,y)}{\partial n(x)}ds_y \mp \frac{1}{2}\psi(x) \tag{2.32}$$

where the normal derivative is understood as a limiting value approaching the boundary

$$\frac{\partial S_\pm}{\partial n}(x) := \lim_{h\to 0} n(x)\cdot\nabla S(x \pm hn(x)) \tag{2.33}$$

For the double layer potential

$$D_\pm(x) = \int_{\partial\Omega_R} \varphi(y)\frac{\partial G_{qp}^k(x,y)}{\partial n(y)}ds_y \pm \frac{1}{2}\varphi(x) \tag{2.34}$$

where $D_\pm$ is similarly understood as a limiting value approaching the boundary

$$D_\pm(x) := \lim_{h\to 0} D(x \pm hn(x)) \tag{2.35}$$

We also define the Dirichlet to Neumann map

$$N_\delta : H^{1/2}(\partial\Omega_R) \to H^{-1/2}(\partial\Omega_R)$$
$$N_\delta(f) = \frac{\partial u_\delta}{\partial n} \tag{2.36}$$

where u_δ solves

$$\nabla \cdot \left(\frac{1}{\varepsilon_\delta}\nabla u_\delta\right) + k^2 u_\delta = 0 \text{ in } \Omega_R$$
$$u_\delta = f \text{ on } \partial\Omega_R \tag{2.37}$$

We also define the Dirichlet to Neumann map for the background problem

$$N_0 : H^{1/2}(\partial\Omega_R) \to H^{-1/2}(\partial\Omega_R)$$
$$N_0(f) = \frac{\partial u_0}{\partial n} \tag{2.38}$$

Similarly u_0 solves

$$\Delta u_0 + k^2 u_0 = 0 \text{ in } \Omega_R$$
$$u_0 = f \text{ on } \partial\Omega_R \tag{2.39}$$

We note that n will always denote the outward facing normal component on the boundary $\partial\Omega_R$ or ∂B. Without loss of generality we have assumed k^2 is not an eigenvalue of the operator $-\Delta$ in Ω_R with Dirichlet boundary conditions on $\partial\Omega_R$.

Using the operators defined above we can derive the Lippman-Schwinger equation seen in [10] using the variational form (2.1). The Lippman-Schwinger equation recasts our problem in terms of the double and single layer potentials, setting up the framework to derive the asymptotic formula for H_δ in terms of the polarization tensor.

First, we consider (1.6) on $\mathbb{R}^2_{\#} \setminus \Omega_R$ and define the rectangle $\Omega_L \subset \mathbb{R}^2_{\#}$ such that $\Omega_R \subset \Omega_L$ with $L > R$. Here we suppose x lies inside $\Omega_R^c = \Omega_L \setminus \Omega_R$. Using G^k_{qp} as our test function and integrating over Ω_R^c we have

$$\int_{\Omega_R^c} (\Delta H_\delta(y) + k^2 H_\delta(y)) G^k_{qp}(x,y)dy = 0 \tag{2.40}$$

Here we proceed by using integration by parts which gives

$$\begin{aligned}\int_{\Omega_R^c} \nabla H_\delta(y) \cdot \nabla G^k_{qp}(x,y) + k^2 H_\delta(y) G^k_{qp}(x,y)dy \\ - \int_{\partial\Omega_R} \frac{\partial H_\delta(y)}{\partial n} G^k_{qp}(x,y)ds_y + \int_{\partial\Omega_L} \frac{\partial H_\delta(y)}{\partial n} G^k_{qp}(x,y)ds_y = 0\end{aligned} \tag{2.41}$$

We note the boundary integral on the vertical boundaries vanish due to the quasi-periodic boundary conditions. Applying another integration by parts to move the derivatives onto G^k_{qp} gives

$$\begin{aligned}\int_{\Omega_R^c} \left[\Delta G^k_{qp}(x,y) + k^2 G^k_{qp}(x,y)\right] H_\delta(y)dy \\ + \int_{\partial\Omega_R} \left(\frac{\partial G^k_{qp}(x,y)}{\partial n(y)} H_\delta(y) - \frac{\partial H_\delta(y)}{\partial n} G^k_{qp}(x,y) \right) ds_y \\ + \int_{\partial\Omega_L} \left(\frac{\partial H_\delta(y)}{\partial n} G^k_{qp}(x,y) - \frac{\partial G^k_{qp}(x,y)}{\partial n} H_\delta(y) \right) ds_y = 0\end{aligned} \tag{2.42}$$

Using the definition of G^k_{qp} on Ω_R^c gives,

$$\begin{aligned}- H_\delta(x) + \int_{\partial\Omega_R} \left(\frac{\partial G^k_{qp}(x,y)}{\partial n(y)} H_\delta(y) - \frac{\partial H_\delta(y)}{\partial n} G^k_{qp}(x,y) \right) ds_y + \\ + \int_{\partial\Omega_L} \left(\frac{\partial H_\delta(y)}{\partial n} G^k_{qp}(x,y) - \frac{\partial G^k_{qp}(x,y)}{\partial n} H_\delta(y) \right) ds_y = 0.\end{aligned} \tag{2.43}$$

On the other hand choosing Ω_L, $H_0 = H_{inc}$, and $x \in \Omega_R^c$ gives

$$\int_{\Omega_R^c} (\Delta H_0(y) + k^2 H_\delta(y)) G^k_{qp}(x,y)dy = 0, \tag{2.44}$$

and proceeding similarly we obtain

$$-H_0(x)+\int_{\partial\Omega_L}\left(\frac{\partial H_\delta(y)}{\partial n}G^k_{qp}(x,y)-\frac{\partial G^k_{qp}(x,y)}{\partial n}H_\delta(y)\right)ds_y=0. \tag{2.45}$$

Subtracting (2.45) from (2.43) gives

$$\begin{aligned}-H_\delta(x)+H_0(x)+\int_{\partial\Omega_R}\left(\frac{\partial G^k_{qp}(x,y)}{\partial n(y)}H_\delta(y)-\frac{\partial H_\delta(y)}{\partial n}G^k_{qp}(x,y)\right)ds_y+\\+\int_{\partial\Omega_L}\left(\frac{\partial H^s_\delta(y)}{\partial n}G^k_{qp}(x,y)-\frac{\partial G^k_{qp}(x,y)}{\partial n}H^s_\delta(y)\right)ds_y=0.\end{aligned} \tag{2.46}$$

where $H^s_\delta = H_\delta - H_0$ satisfies the out going radiation condition and passing to the limit $L\to\infty$ gives the Lipmann-Schwinger equations for $x\in\mathbb{R}^2_\#\setminus\Omega_R$. The Lippman-Schwinger equations are common integral representation tools seen in [10].

$$H_\delta(x)=H_0(x)+\int_{\partial\Omega_R}\frac{\partial G^k_{qp}(x,y)}{\partial n(y)}H_\delta(y)ds_y-\int_{\partial\Omega_R}\frac{\partial H_\delta(y)}{\partial n}G^k_{qp}(x,y)ds_y \tag{2.47}$$

This integral equation holds for $x\in R^2_\#\setminus\overline{\Omega_R}$ where n is this unit outward normal to $\partial\Omega_R$. We note (2.47) holds up to the boundary of Ω_R, but not for $x\in\partial\Omega_R$. However, we can take the limit as $x\to\partial\Omega_R$ and use the double-layer potential relation (2.34) to give a boundary integral equation for $x\in\partial\Omega_R$

$$\frac{1}{2}H_\delta|_{\partial\Omega_R}=H_0|_{\partial\Omega_R}+\int_{\partial\Omega_R}\frac{\partial G^k_{qp}(x,y)}{\partial n(y)}H_\delta(y)ds_y-\int_{\partial\Omega_R}G^k_{qp}(x,y)\frac{\partial H_\delta(y)}{\partial n}ds_y \tag{2.48}$$

Now we can use the layer potential definitions to recast the boundary integral equation (2.48) in operator notation as,

$$\left(\frac{I}{2}-D+SN_\delta\right)(H_\delta|_{\partial\Omega_R})=H_0|_{\partial\Omega_R} \tag{2.49}$$

Similarly, H_0 satisfies

$$\left(\frac{I}{2}-D+SN_0\right)(H_0|_{\partial\Omega_R})=H_0|\partial\Omega_R \tag{2.50}$$

Using the two operator notation equations we can define two new operators which describe the full scattering problem and background scattering problem in terms of layer potential operators. First we define

$$T_\delta := \frac{I}{2} - D + SN_\delta \tag{2.51}$$

where T_δ sends an element from $H^{1/2}$ on the boundary of Ω_R to the same space, i.e.

$$T_\delta : H^{1/2}(\partial\Omega_R) \to H^{1/2}(\partial\Omega_R)$$

Similarly for the background problem we define

$$T_0 := \frac{I}{2} - D + SN_0 \tag{2.52}$$

where

$$T_0 : H^{1/2}(\partial\Omega_R) \to H^{1/2}(\partial\Omega_R)$$

If we subtract (2.50) from (2.49) we find that

$$T_\delta(H_\delta|_{\partial\Omega_R}) - T_0(H_0|_{\partial\Omega_R}) = 0 \tag{2.53}$$

Furthermore, we have

$$T_\delta((H_\delta - H_0)|_{\partial\Omega_R}) = S(N_0 - N_\delta)(H_0|_{\partial\Omega_R}) \tag{2.54}$$

We now have everything we need to state and prove our main results provided in the next chapter.

Chapter 3. Asymptotic Formula for H_δ

3.1. Asymptotic Formula for H_δ

In this chapter we derive our main result giving the desired asymptotic formula for H_δ. We begin by stating an asymptotic formula in terms of the operators T_δ and T_0.

Proposition 3.1.1. *Let T_δ and and T_0 be defined by (2.51) and (2.52) respectively. Then the following hold:*

(a) T_δ converges to T_0 pointwise

(b) For δ sufficiently small, there exists a constant C that is independent of δ such that for any $f \in H^{1/2}(\partial\Omega), T_\delta^{-1}$ exists and

$$\|T_\delta^{-1} f\|_{H^{1/2}(\partial\Omega)} \leq C\|f\|_{H^{1/2}(\partial\Omega)}$$

(c) The following asymptotic formula holds:

$$\begin{aligned}(T_0 - T_\delta)(H_0|_{\partial\Omega_R}(x) &= S(N_0 - N_\delta)(H_0|_{\partial\Omega}(x) \\ &= \left(1 - \frac{1}{\varepsilon_m}\right) \delta^2 \nabla_y \tilde{G}^k_{per}(x,0) \cdot M(\varepsilon_m)\nabla H_0(0) + O(\delta^{3-\eta})\end{aligned} \tag{3.1}$$

The asymptotic term $O(\delta^{3-\eta})$ is independent of the point $x \in \partial\Omega$

The proof of Proposition (3.1.1) is involved and the full proof is provided in the Appendix.

We define the leading order term in (3.1) as $\delta^2 H^{(1)}$ where

$$H^{(1)}(x) = \left(1 - \frac{1}{\varepsilon_m}\right) \nabla_y \tilde{G}^k_{per}(x,0) \cdot M(\varepsilon_m)\nabla H_0(0) \tag{3.2}$$

Using the above notation we can use (2.54) to restate part (c) in Proposition 3.1.1 as

$$T_\delta((H_\delta - H_0)|_{\partial\Omega_R}) = \delta^2 H^{(1)}|_{\partial\Omega_R} + O(\delta^{3-\eta}). \tag{3.3}$$

Lemma 3.1.1. *Let the correction term $H^{(1)}$ be defined by (3.2). Then the following equation holds*

$$T_0(H^{(1)}|_{\partial\Omega_R}) = H^{(1)}|_{\partial\Omega_R}$$

Proof. Let $u^{(1)}$ be the unique solution to

$$\begin{cases} \Delta u^{(1)} + k^2 u^{(1)} = 0 \text{ in } \Omega_R \\ u^{(1)} = H^{(1)} \text{ on } \partial\Omega_R \end{cases} \tag{3.4}$$

In terms of the Dirichlet to Nuemann map,

$$\frac{\partial u^{(1)}}{\partial n} = N_0(u^{(1)}|_{\partial\Omega_R}) \tag{3.5}$$

Then we have

$$\int_{\Omega_R} G^k_{qp}(x,y)\left(\Delta\, u^{(1)} + k^2 u^{(1)}\right) dy = 0.$$

An integration by parts gives

$$u^{(1)}(x) = -\int_{\partial\Omega_R} \partial_{n(y)} G^k_{qp}(x,y) u^{(1)} ds_y + \int_{\partial\Omega_R} G^k_{qp}(x,y)\partial_{n(y)} u^{(1)} ds_y$$

and sending the sequence $x_n \in \Omega_R$ to any $x \in \partial\Omega_R$ gives the desired result

$$u^{(1)}|_{\partial\Omega_R} = \left(\frac{I}{2} - D + SN_0\right) u^{(1)}|_{\partial\Omega_R}. \tag{3.6}$$

□

Lemma 3.1.2. *The following estimate holds on the space $H^{1/2}$ on the boundary of Ω_R*

$$\|H_\delta - H_0 - \delta^2 H^{(1)}\|_{H^{1/2}(\partial\Omega_R)} = o(\delta^2) \tag{3.7}$$

Proof. From (3.3) it follows that

$$T_\delta((H_\delta - H_0 - \delta^2 H^{(1)})|_{\partial\Omega_R}) = \delta^2 H^{(1)} - \delta^2 T_\delta(H^{(1)}|_{\partial\Omega_R}) + O(\delta^{3-\eta}). \tag{3.8}$$

Lemma 3.1.1 gives

$$T_\delta((H_\delta - H_0 - \delta^2 H^{(1)})|_{\partial\Omega_R}) = \delta^2(T_0 - T_\delta)(H^{(1)}|_{\partial\Omega_R}) + O(\delta^{3-\eta}). \tag{3.9}$$

Since $T_\delta - T_0 \to 0$ pointwise in $H^{1/2}(\partial\Omega_R)$ we can write

$$T_\delta((H_\delta - H_0 - \delta^2 H^{(1)})|_{\partial\Omega_R}) = o(\delta^2), \tag{3.10}$$

and from part (b) of Proposition 3.1.1 we conclude that

$$\|H_\delta - H_0 - \delta^2 H^{(1)}|_{\partial\Omega_R})\|_{H^{1/2}(\delta\Omega_R)} = \|T_\delta^{-1} o(\delta^2)\|_{H1/2(\partial\Omega_R)} \leq C\|o(\delta^2)\|_{\partial\Omega_R)}, \tag{3.11}$$

and the lemma is proved. □

We now arrive at the explicit expansion for the solution H_δ of the scattering problem for points $x \in \mathbb{R}^2_\# \setminus \Omega_R$ bounded away from $\partial\Omega_R$.

Theorem 3.1.1. *Let H_δ be the solution to* (1.6)*, and let $M(\varepsilon_m)$ be the polarization tensor for the particle B defined by* (2.20)*. Then for $x \in \mathbb{R}^2_\# \setminus \Omega_R$ bounded away from $\partial\Omega_R$, we have the expansion*

$$H_\delta(x) = H_{inc}(x) + \delta^2 \left[\left(1 - \frac{1}{\varepsilon_m}\right) \nabla_y G^k_{qp}(x, 0) \cdot M(\varepsilon_m) \nabla H_{inc}(0)\right] + o(\delta^2). \tag{3.12}$$

where the remainder term $o(\delta^2)$ is independent of x.

Proof. Using Lemma 3.1.2 we have $H_\delta - H_0$ in $\Omega_L \setminus \overline{\Omega}_R$ satisfies

$$\begin{cases} \Delta(H_\delta - H_0) + k^2(H_\delta - H_0) = 0 \text{ in } \Omega_L \setminus \overline{\Omega}_R \\ (H_\delta - H_0) = \delta^2 H^{(1)} + o(\delta^2) \text{ on } \partial\Omega_R \\ \text{ outward radiation conditions (1.7), (1.8)} \end{cases} \tag{3.13}$$

Next we define the outgoing Dirichlet Green function, $\mathcal{G}$, on the domain $\Omega_L \setminus \overline{\Omega}_R$

$$\begin{cases} \Delta\mathcal{G}(x,y) + k^2\mathcal{G}(x,y) = -\delta_x \text{ in } \Omega_L \setminus \overline{\Omega}_R \\ \mathcal{G}(x,y) = 0 \text{ on } \partial\Omega_R \\ \text{outward radiation conditions (1.7), (1.8)} \end{cases} \tag{3.14}$$

Multiplying (3.13) by $\mathcal{G}$, integrating over $\Omega_L \setminus \overline{\Omega}_R$ and using Green's Theorem and sending L to ∞ gives the representation for $H_\delta - H_0$

$$(H_\delta - H_0)(x) = \int_{\partial\Omega_R} \frac{\partial\mathcal{G}}{\partial n(y)}(x,y)(H_\delta - H_0)(y)ds_y \quad \forall x \in \mathbb{R}^2_\# \setminus \overline{\Omega}_R \tag{3.15}$$

Choosing $x \in \mathbb{R}^2_\# \setminus \overline{\Omega}_R$ bounded away from $\partial\Omega_R$ we can apply the boundary estimate from Lemma 3.1.2 on $(H_\delta - H_0)$ inside the integral of equation (3.15)

$$(H_\delta - H_0)(x) = \delta^2 \int_{\partial\Omega_R} \frac{\partial\mathcal{G}}{\partial n(y)}(x,y)H^{(1)}(y)ds_y + o(\delta^2) \tag{3.16}$$

where the error term $o(\delta^2)$ is independent of the point x. We now follow steps identical to identifying (3.15), i.e., integration by parts and the definition of the outgoing Dirichlet Green's function, to derive the following identity for any $x \in \mathbb{R}^2_\# \setminus \overline{\Omega}_R$ and $x' \in \Omega_R$

$$\int_{\partial\Omega_R} \frac{\partial\mathcal{G}}{\partial n(y)}(x,y)\nabla_{x'}G^k_{qp}(y,x')ds_y = \nabla_{x'}G^k_{qp}(x,x') \tag{3.17}$$

Application of this identity to $H^{(1)}$ in equation (3.16) gives desired asymptotic expansion, completing the proof. $\square$

Our last result in this section is to give an energy estimate on the norm of the scattered field $H_\delta - H_0$ in $H^1(\Omega_R)$.

Proposition 3.1.2. *The following energy estimate holds,*

$$\|H_\delta - H_0\|_{L^2(\Omega_R)} + \|\nabla H_\delta - \nabla H_0\|_{L^2(\Omega_R)} = O(\delta). \tag{3.18}$$

Proof. Let u_δ be defined as the unique solution to

$$\begin{cases} \Delta u_\delta + k^2 u_\delta = 0 \text{ in } \Omega_R \\ \\ u_\delta = H_\delta \text{ on } \partial\Omega_R \end{cases} \tag{3.19}$$

Since H_0 also satisfies Helmholtz equation in Ω_R we have

$$\begin{cases} \Delta(u_\delta - H_0) + k^2(u_\delta - H_0) = 0 \text{ in } \Omega_R \\ \\ (u_\delta - H_0) = H_\delta - H_0 \text{ on } \partial\Omega_R, \end{cases} \tag{3.20}$$

which leads to

$$\|u_\delta - H_0\|_{H^1(\Omega_R)} \leq C\|H_\delta - H_0\|_{H^{1/2}\partial(\Omega_R)}. \tag{3.21}$$

Moreover from Proposition (2.3.1) it follows that C is independent of δ for $0 < \delta < \delta_0$. Using Lemma 3.1.2 we see that $H_\delta - H_0$ is of order δ^2 in the $H^{1/2}(\partial\Omega_R)$ norm. Note that $H_\delta - u_\delta$ belong to $H_0^1(\Omega_R)$ and for any $v \in H_0^1(\Omega_R)$ we can write

$$\begin{aligned}
&\int_{\Omega_R} \frac{1}{\varepsilon_\delta} \nabla(H_\delta - u_\delta) \cdot \nabla v dx - k^2 \int_{\Omega_R} (H_\delta - u_\delta) v dx \\
&= \int_{\Omega_R} \frac{1}{\varepsilon_\delta} \nabla H_\delta \cdot \nabla v dx - k^2 \int_{\Omega_R} H_\delta v dx \\
&- \int_{\Omega_R} \nabla u_\delta \cdot \nabla v dx + k^2 \int_{\Omega_R} u_\delta v dx \\
&+ (1 - \frac{1}{\varepsilon_m}) \int_B \nabla u_\delta \cdot \nabla v dx \\
&= (1 - \frac{1}{\varepsilon_m}) \int_B \nabla u_\delta \cdot \nabla v dx.
\end{aligned} \tag{3.22}$$

Now we can bound the last term using the Cauchy-Schwarz inequality giving,

$$\left| \int_B \nabla u_\delta \cdot \nabla v dx \right| \leq \|\nabla u_\delta\|_{L^2(B)} \|\nabla v\|_{L^2(\Omega_R)}. \tag{3.23}$$

Applying the triangle inequality

$$\|\nabla u_\delta\|_{L^2(B)} \leq \|\nabla u_\delta - \nabla H_0\|_{L^2(\Omega_R)} + \|\nabla H_0\|_{L^2(B)}, \tag{3.24}$$

and

$$\|u_\delta\|_{L^2(B)} \leq \|u_\delta - H_0\|_{L^2(\Omega_R)} + \|H_0\|_{L^2(B)}. \tag{3.25}$$

Since

$$\begin{aligned} &\|u_\delta - H_0\|_{H^1(\Omega_R)} = O(\delta^2), \\ &\|H_0\|_{H^1(B)} = O(\delta), \end{aligned} \tag{3.26}$$

we get

$$\|u_\delta\|_{H^1(B)} = O(\delta), \tag{3.27}$$

and

$$\left| \int_{\Omega_R} \frac{1}{\varepsilon_\delta} \nabla (H_\delta - u_\delta) \cdot \nabla v dx - k^2 \int_{\Omega_R} (H_\delta - u_\delta) v dx \right| = O(\delta) \|v\|_{H^!(\Omega_R)}, \tag{3.28}$$

for all $v \in H_0^1(\Omega_R)$. So from Proposition (2.3.1) it follows that

$$\|u_\delta - H_\delta\|_{H^1(\Omega_R)} = O(\delta). \tag{3.29}$$

Collecting results and using the triangle inequality gives

$$\|H_\delta - H_0\|_{H^1(B)} \leq \|H_\delta - u_\delta\|_{H^1(\Omega_R)} + \|u_\delta - H_0\|_{H^1(B)} = O(\delta), \tag{3.30}$$

and the theorem is proved. □

Chapter 4. Far-field Scattering: Reflection and Transmission from an Impedance Surface

4.1. Impedance Formulation for Scattered Field

We reformulate our asymptotic expansion in Chapter 3 as an impedance boundary condition at $x_1 = 0$. We recall from Theorem (3.1.1) that the perturbed field, H_δ is given by

$$H_\delta = H_0 + \delta^2 H^{(1)} + o(\delta^2) \tag{4.1}$$

where $H^{(1)}$ is given by (3.2). We first have that

$$\begin{aligned}
\Delta H^{(1)} &= \left(1 - \frac{1}{\varepsilon_m}\right) \Delta_x \nabla_y G^k_{qp}(x,0) \cdot M(\varepsilon_m) \nabla H_0(0) \\
&= \left(1 - \frac{1}{\varepsilon_m}\right) \nabla_y \Delta_x G^k_{qp}(x,0) \cdot M(\varepsilon_m) \nabla H_0(0) \\
&= -k^2 \left(1 - \frac{1}{\varepsilon_m}\right) \nabla_y G^k_{qp}(x,0) \cdot M(\varepsilon_m) \nabla H_0(0) \\
&= -k^2 H^{(1)}
\end{aligned} \tag{4.2}$$

Therefore $H^{(1)}$ solves Helmholtz equation and since $G^k_{qp}(x,y)$ satisfies the outgoing radiation condition we have

$$\begin{cases} \Delta H^{(1)} + k^2 H^{(1)} = 0 \\ H^{(1)} \text{ satisfies outgoing radiation condition} \end{cases} \tag{4.3}$$

From here we will show $H^{(1)} = H_1^{(1)} + H_2^{(1)}$ where $H_1^{(1)}$ is driven by a source term and $H_2^{(1)}$ is driven by a surface current. We define $H_1^{(1)}$ $H_2^{(2)}$ respectively as follows

$$H_1^{(1)} = \partial_{y_1} G^k_{qp}(x,0) \partial_{y_1} H_0(0) \, (m_{11} + m_{12}) \tag{4.4}$$

$$H_2^{(1)} = \partial_{y_2} G^k_{qp}(x,0) \partial_{y_2} H_0(0) \, (m_{21} + m_{22}) \tag{4.5}$$

We note we can replace the derivatives on $H_0(0)$ with the electric field using the curl equations (1.4), which gives

$$H_1^{(1)} = \partial_{y_1} G_{qp}^k(x,0) \frac{\omega}{c} E_0^2(0) \left(m_{11} + m_{12}\right) \tag{4.6}$$

$$H_2^{(1)} = \partial_{y_2} G_{qp}^k(x,0) \frac{\omega}{c} E_0^1(0) \left(m_{21} + m_{22}\right) \tag{4.7}$$

where E_0^1 is the e_1 component of the background electric field and E_0^2 is the e_2 component of the background electric field. We first set $y_1 = 0$, then by the definition of G_{qp}^k we can write down the y_1 and y_2 derivatives of G_{qp}^k as,

$$\partial_{y_1} G_{qp}^k(x,0) = -\frac{1}{2d} \sum_{-\infty}^{\infty} e^{-\gamma_m x_1} e^{i\beta_m x_2} \text{ for } x_1 \geq 0 \tag{4.8}$$

$$\partial_{y_1} G_{qp}^k(x,0) = \frac{1}{2d} \sum_{-\infty}^{\infty} e^{-\gamma_m x_1} e^{i\beta_m x_2} \text{ for } x_1 \leq 0 \tag{4.9}$$

$$\partial_{y_2} G_{qp}^k(x,0) = \frac{1}{2d} \sum_{-\infty}^{\infty} \frac{e^{-\gamma_m x_1}}{\gamma_m} i\beta_m e^{i\beta_m x_2} \text{ for } x_1 \geq 0 \tag{4.10}$$

$$\partial_{y_2} G_{qp}^k(x,0) = \frac{1}{2d} \sum_{-\infty}^{\infty} \frac{e^{-\gamma_m x_1}}{\gamma_m} i\beta_m e^{i\beta_m x_2} \text{ for } x_1 \leq 0 \tag{4.11}$$

Now if we take the limit as $x_1 \to 0^+$ and $x_1 \to 0^-$ we have the following jump relations for the y_1 and y_2 derivatives of G_{qp}^k respectively

$$\partial_{y_1} G_{qp}^k(0,x_2,0,0)|^+ - \partial_{y_1} G_{qp}^k(0,x_2,0,0)|^- = -\frac{1}{d} \sum_{-\infty}^{\infty} e^{i\beta_m x_2} \tag{4.12}$$

$$\partial_{y_2} G_{qp}^k(0,x_2,0,0)|^+ - \partial_{y_2} G_{qp}^k(0,x_2,0,0)|^- = 0 \tag{4.13}$$

Therefore using the jump relations given by (4.12) and (4.13), we have the jump condition at $x_1 = 0$ for $H_1^{(1)}$ given by

$$H_1^{(1)}|^+ - H_1^{(1)}|^- = -\frac{1}{d} \sum_{-\infty}^{\infty} e^{i\beta_m x_2} \left(m_{11} \partial_{y_1} H_0(0) + m_{12} \partial_{y_1} H_0(0)\right) \tag{4.14}$$

Considering the jump condition for $\partial_{x_1} H_1^{(1)}$ we have

$$\partial_{x_1} H_1^{(1)}|^+ - \partial_{x_1} H_1^{(1)}|^- = 0 \tag{4.15}$$

Therefore we have that $H_1^{(1)}$ solves the following system,

$$\begin{cases} \Delta H_1^{(1)} + k^2 H_1^{(1)} = 0 & x_1 < 0, x_1 > 0 \\ H_1^{(1)}|^+ - H_1^{(1)}|^- = -\frac{1}{d}\sum_{-\infty}^{\infty} e^{i\beta_m x_2} \partial_{y_1} H_0(0)\left(m_{11} + m_{12}\right) & x_1 = 0 \\ \partial_{x_1} H_1^{(1)}|^+ - \partial_{x_1} H_1^{(1)}|^- = 0 & x_1 = 0 \\ H_1^{(1)} \text{ satisfies outgoing radiation condition } (2.3), (2.4) \end{cases} \tag{4.16}$$

We note that the term on the right hand side for the jump condition of $H_1^{(1)}$ at $x_1 = 0$ is a source term. Equivalently, we can use the curl equations (1.4) to again replace $\partial_{y_1} H_0(0)$ with the electric field term. This formulation presents the source term as an impedance boundary condition since it relates the magnetic field to the electric field.

$$\begin{cases} \Delta H_1^{(1)} + k^2 H_1^{(1)} = 0 & x_1 < 0, x_1 > 0 \\ H_1^{(1)}|^+ - H_1^{(1)}|^- = \frac{1}{d}\sum_{-\infty}^{\infty} e^{i\beta_m x_2} \left(\frac{i\omega}{c}\right) E_0^2 \left(m_{11} + m_{12}\right) & x_1 = 0 \\ \partial_{x_1} H_1^{(1)}|^+ - \partial_{x_1} H_1^{(1)}|^- = 0 & x_1 = 0 \\ H_1^{(1)} \text{ satisfies outgoing radiation condition } (2.3), (2.4) \end{cases} \tag{4.17}$$

Following the same process as above we can derive the system for $H_2^{(1)}$. The jump conditions for $H_2^{(1)}$ and $\partial_{x_1} H_2^{(1)}$ at $x_1 = 0$ are

$$H_2^{(1)}|^+ - H_2^{(1)}|^- = 0 \tag{4.18}$$

and

$$\partial_{x_1} H_2^{(1)}|^+ - \partial_{x_1} H_2^{(1)}|^- = -\frac{1}{d}\sum_{-\infty}^{\infty} i\beta_m e^{i\beta_m x_2}\left(m_{21}\partial_{y_2} H_0(0) + m_{22}\partial_{y_2} H_0(0)\right) \tag{4.19}$$

Therefore $H_2^{(1)}$ solves the following system,

$$\begin{cases} \Delta H_2^{(1)} + k^2 H_2^{(1)} = 0 & x_1 < 0, x_1 > 0 \\ H_2^{(1)}|^+ - H_2^{(1)}|^- = 0 & x_1 = 0 \\ \partial_{x_1} H_2^{(1)}|^+ - \partial_{x_1} H_2^{(1)}|^- = -\frac{1}{d}\sum_{-\infty}^{\infty} i\beta_m e^{i\beta_m x_2} \partial_{y_2} H_0(0)\,(m_{21} + m_{22}) & x_1 = 0 \\ H_2^{(1)} \text{ satisfies outgoing radiation condition}(2.3), (2.4) \end{cases} \tag{4.20}$$

The term on the right hand side for the jump of $\partial_{x_1} H_2^{(1)}$ is a surface current term. Again using the curl equations (1.4) we can write the surface current term in terms of the electric field E_0^1 which gives us another impedance boundary condition.

$$\begin{cases} \Delta H_2^{(1)} + k^2 H_2^{(1)} = 0 & x_1 < 0, x_1 > 0 \\ H_2^{(1)}|^+ - H_2^{(1)}|^- = 0 & x_1 = 0 \\ \partial_{x_1} H_2^{(1)}|^+ - \partial_{x_1} H_2^{(1)}|^- = \frac{1}{d}\sum_{-\infty}^{\infty} \beta_m e^{i\beta_m x_2} \left(\frac{\omega}{c}\right) E_0^1\,(m_{21} + m_{22}) & x_1 = 0 \\ H_2^{(1)} \text{ satisfies outgoing radiation condition}(2.3), (2.4) \end{cases} \tag{4.21}$$

Using the properties of the Green's function to derive the various jump conditions and with the asymptotic representation of the perturbed magnetic field, we have shown the metasurface can be reformulated as an impedance boundary condition and surface current in terms of the polarization tensor, M, at $x_1 = 0$. Next, for normal incidence we derive the reflection coefficient in terms of the polarization tensor.

4.2. Reflection and Transmission Obtained from Asymptotic Formula

Here we will derive the radiating reflected and transmitted waves up to order δ^2 using the asymptotic formula and the correction term $H^{(1)}$. We note this represents scattering by an open waveguide. In this section we will assume the period is sub-wavelength. With this hypothesis we have only a single diffraction order so the far-field behavior of the scattered field is given in terms of a reflected and transmitted wave i.e. in equations (2.3) and (2.4) we only have m = 1. With this in mind denote the reflection and transmission coefficient of the reflected and transmitted wave as r and t respectively. We also assume that the incoming wave is normally incident upon the particle. We note for normal incidence $H_2^{(1)} = 0$ so we have $H^{(1)} = H_1^{(1)}$ and $H_0 = e^{-ikx_1}$. Therefore, we can write

$$H_\delta = e^{-ikx_1} + \delta^2 H_1^{(1)} + O(\delta^{3-\eta}) \tag{4.22}$$

Motivated by the outgoing radiation conditions for $x_1 > 0$ we set $H_1^{(1)}|^+ = H_r e^{ikx_1}$ where $H_r = r$ and r is the reflection coefficient. For $x_1 < 0$ choose $H_1^{(1)}|^- = H_t e^{-ikx_1}$ where $H_t = t$ and t is the transmission coefficient. Using the jump conditions for $H_1^{(1)}$ at the $x_1 = 0$ boundary we have

$$H_1^{(1)}|^+ - H_1^{(1)}|^- = -\frac{ik}{d}(m_{11} + m_{12}) = -\frac{ik}{d} m_{11} \tag{4.23}$$

since $m_{12} = 0$ for normal incidence. For the second jump condition we have,

$$\partial_{x_1} H_1^{(1)}|^+ = \partial_{x_1} H_1^{(1)}|^-. \tag{4.24}$$

Equation (4.23) gives

$$r = \frac{ik}{d} m_{11} + t. \tag{4.25}$$

Equation (4.24) gives

$$r = -t. \tag{4.26}$$

Plugging this into (4.25) we obtain the formula for the reflection coefficient

$$r = \frac{ik}{2d} m_{11}. \tag{4.27}$$

Since we have the reflection and transmission coefficients we can rewrite the perturbed field in the far field using (2.3) and (2.4) as

$$\begin{cases} H_\delta = e^{-ikx_1} + \frac{ik\delta^2}{2d} m_{11} e^{ikx_1} + o(\delta^2) & x_1 < 0 \\ H_\delta = e^{-ikx_1} - \frac{ik\delta^2}{2d} m_{11} e^{-ikx_1} + o(\delta^2) & x_1 > 0 \end{cases} \tag{4.28}$$

Now we have the behavior of the scattered field in terms of of the reflection and transmission coefficients. So we just need to solve (2.19) numerically to obtain the polarization, m_{11}, for a given metasurface. Thus periodic arrays of particles can be approximated by a metasurface up to error $O(\delta^{3-\eta})$. This provides a rigorous reduced order model for control of light sidestepping the need for more computationally expensive methods. The reduced order model allows one to efficiently explore the universe of particle geometries for development of new materials. Additionally we can handle more complex geometries made with multiple particles in a period cell, by computing just m_{11}.

In future work we wish to show that the mathematical theory holds up for for materials with negative real permittivity so the model can handle noble metals which present intriguing phenomenon such as plasmonic behavior for optical frequencies. Additionally we would like to introduce geometries which include a substrate of a different material underneath the particles or multiple layers. Once we can handle cases like these we can use topology optimization techniques or the physics-guided machine learning techniques seen in [24] to inform the design of novel optical metamaterials.

Appendix. Proof of Proposition 3.1.1

A.1. Setup

We start the appendix by proving part (c) of Proposition (3.1.1). We extend the boundary data f on $\partial\Omega_R$ onto the subdomain Ω_R containing the inclusion $\mathcal{B}$ by the scalar field u_δ which is the soution of

$$\begin{cases} \nabla \cdot \left(\frac{1}{\varepsilon_\delta} \nabla u_\delta \right) + k^2 u_\delta = 0 \text{ in } \Omega_R \\ u_\delta = f \text{ on } \partial\Omega_R \end{cases} \tag{A.1}$$

We then extend the boundary data f on $\partial\Omega_R$ but in the absence of the inclusion $\mathcal{B}$ to arrive at the background scalar field u_0, i.e.,

$$\begin{cases} \Delta u_0 + k^2 u_0 = 0 \text{ in } \Omega_R \\ u_0 = f \text{ on } \partial\Omega_R \end{cases} \tag{A.2}$$

Recall $N_\delta(f) := \frac{\partial u_\delta}{\partial n}$ and $N_0(f) := \frac{\partial u_0}{\partial n}$ and from Section 2.4 we have,

$$(T_\delta - T_0)(H_0)|_{\partial\Omega_R}) = S(N_0 - N_\delta)(H_0|_{\partial\Omega_R}). \tag{A.3}$$

Hence to complete the proof of part (c) of Proposition (3.1.1) we establish the following Theorem

Theorem A.1.1 (First term and error estimate)**.** *For $x \in \partial\Omega_R$ and any boundary data $f \in H^{1/2}(\partial\Omega_R)$,*

$$S\left(N_0 - N_\delta\right)(f) = \left(1 - \frac{1}{\varepsilon_m}\right) \delta^2 \nabla_y G^k_{qp}(x,0) \cdot M(\varepsilon_m) \nabla u_0(0) + O(\delta^{3-\eta}), \tag{A.4}$$

where this expansion holds uniformly for $x \in \partial\Omega_R$.

With Theorem (A.1.1) in hand we may conclude from (A.3) that for $f = H_0$ on $\partial\Omega_R$ that

$$\begin{aligned} &T_\delta((H_\delta - H_0)|_{\partial\Omega_R}) = S(N_0 - N_\delta)(H_0|_{\partial\Omega_R}) = \\ &= \left(1 - \frac{1}{\varepsilon_m}\right)\delta^2\nabla_y G^k_{qp}(x,0)\cdot M(\varepsilon_m)\nabla H_0(0) + O(\delta^{3-\eta}), \end{aligned} \tag{A.5}$$

and part (c) of Proposition (3.1.1) is proved.

We now use part (c) of Proposition (3.1.1) to establish parts (a) and (b) of Proposition (3.1.1). Part (a) follows immediately from part (c) and noting that H_0 can be any entire solution of the Helmholtz equation on $\mathbb{R}^2_\#$. Part (b) follows immediately from part (c) noting that the set of bounded invertible linear transforms over $H^{1/2}(\partial\Omega_R)$ is an open set and T_0 is invertible.

The proof of Theorem (A.1.1) is carried out over the next two sections and is based on an expansion of the difference $u_\delta - u_0$ in δ; first near the inclusion $\mathcal{B}$ in Section A.2 and then extended uniformly to an expansion in the domain $\Omega_R \setminus 2\mathcal{B}$ in Section A.3.

A.2. Asymptotic Behavior of $u_\delta - u_0$ around the inclusion

We find find bounds for $u_\delta - u_0$ in a neighborhood around the small inclusion. This is done using representation formulas for $u_\delta - u_0$ posed in terms of Green's functions. The field u_0 belongs to $C^\infty(\Omega_R)$ and u_δ belong to $C^{0,\beta}$ for $\beta > 0$ from elliptic regularity theory. We also have that u_δ is C^∞ in each domain separately i.e, $u_\delta \in C^\infty(\overline{\mathcal{B}})$, and $u_\delta \in C\infty(\Omega_R \setminus \mathcal{B})$. Here, n represents the outward directed unit normal vector to boundaries $\partial\Omega_R$ and $\partial\mathcal{B}$. On the inclusion the normal derivative of u_δ has the jump relation across $\partial\mathcal{B}$

$$\frac{\partial u_\delta}{\partial n}|^+ = \frac{1}{\varepsilon_m}\frac{\partial u_\delta}{\partial n}|^-.$$

We start by deriving integral representations for u_δ and u_0. In $\Omega_R \setminus \mathcal{B}$ we have

$$\Delta u_\delta(y) + k^2 u_\delta = 0, \tag{A.6}$$

as an identity in $L^2(\Omega_R \setminus B)$. Taking $x \in \Omega_R \setminus \mathcal{B}$, multiplying this equation by G_0^k integrating over $\Omega_R \setminus B$, together with Greens second identity and the definition of G_{qp}^k gives

$$\begin{aligned} u_\delta(x) = &\int_{\partial\Omega_R} \left[-u_\delta(y) \frac{\partial G_0^k(x,y)}{\partial n(y)} + \frac{\partial u_\delta(y)}{\partial n} G_0^k(x,y) \right] ds_y + \\ &+ \int_{\partial\mathcal{B}} \left[u_\delta(y) \frac{\partial G_0^k(x,y)}{\partial n(y)} - \frac{\partial u_\delta(y)}{\partial n}|^+ G_0^k(x,y) \right] ds_y \end{aligned} \tag{A.7}$$

Observing that u_0 satisfies

$$\Delta u_0(y) + k^2 u_0 = 0, \tag{A.8}$$

in Ω_R, taking $x \in \Omega_R \setminus \mathcal{B}$, multiplying this equation by G_0^k integrating over Ω_R and proceeding as before gives

$$u_0(x) = \int_{\partial\Omega_R} \left[-u_0(y) \frac{\partial G_0^k(x,y)}{\partial n(y)} + \frac{\partial u_0(y)}{\partial n} G_0^k(x,y) \right] ds_y \tag{A.9}$$

Noting that $G_0^k(x,y) = 0$ for $y \in \partial\Omega_R$ the representation formulas become

$$\begin{aligned} u_\delta(x) = &- \int_{\partial\Omega_R} u_\delta(y) \frac{\partial G_0^k(x,y)}{\partial n(y)} + \\ &+ \int_{\partial\mathcal{B}} \left[u_\delta(y) \frac{\partial G_0^k(x,y)}{\partial n(y)} - \frac{\partial u_\delta(y)}{\partial n}|^+ G_0^k(x,y) \right] ds_y, \end{aligned} \tag{A.10}$$

and

$$u_0(x) = - \int_{\partial\Omega_R} u_0(y) \frac{\partial G_0^k(x,y)}{\partial n(y)}. \tag{A.11}$$

Taking the difference of equations (A.10) and (A.11) and noting $u_\delta = u_0$ on $\partial\Omega_R$ we have the representation for $u_\delta(x) - u_0(x)$ for $x \in \Omega_R \setminus \mathcal{B}$

$$u_\delta(x) - u_0(x) = \int_{\partial\mathcal{B}} \left[u_\delta(y) \frac{\partial G_0^k(x,y)}{\partial n(y)} - \frac{\partial u_\delta(y)}{\partial n}|^+ G_0^k(x,y) \right] ds_y \tag{A.12}$$

We are now ready to prove the following the lemma

Lemma A.2.1. *For x in the open set $2\mathcal{B} \setminus \overline{\mathcal{B}}$*

$$u_\delta(x) - u_0(x) = \left(1 - \frac{1}{\varepsilon_m}\right) \int_{\partial\mathcal{B}} u_\delta(y) \frac{\partial G_0^k(x,y)}{\partial n(y)} ds_y + O(\delta^2 |\log\delta|) \tag{A.13}$$

The term $O(\delta^2|\log\delta|)$ is bounded by $C\delta^2|\log\delta|$ uniformly in x. The constant C depends on the shape of the particle $\mathcal{B}$, the domain Ω_R, the constant ε_m and the frequency ω.

Proof. Starting with the boundary integral representation for $u_\delta(x) - u_0(x)$ and using the jump condition for u_δ on $\partial\mathcal{B}$ we have,

$$\int_{\partial\mathcal{B}} \frac{\partial u_\delta(y)}{\partial n}|^+ G_0^k(x,y) ds_y = \frac{1}{\varepsilon_m} \int_{\partial\mathcal{B}} \frac{\partial u_\delta(y)}{\partial n}|^- G_0^k(x,y) ds_y$$

Now we use integration by parts to put the derivative back on $G_0^k(x,y)$ in order to obtain the double-layer potential for $u_\delta(y)$ for y on $\partial\Omega_R$

$$\frac{1}{\varepsilon_m} \int_{\partial\mathcal{B}} \frac{\partial u_\delta(y)}{\partial n}|^- G_0^k(x,y) ds_y = \frac{1}{\varepsilon_m} \int_{\partial\mathcal{B}} \nabla u_\delta(y) \cdot \nabla G_0^k(x,y) dy + \int_{\partial\mathcal{B}} \frac{1}{\varepsilon_m} \Delta u_\delta(y) G_0^k(x,y) dy$$

$$= -\int_{\mathcal{B}} \frac{1}{\varepsilon_m} \Delta G_0^k(x,y) u_\delta(y) dy + \int_{\mathcal{B}} \frac{1}{\varepsilon_m} \nabla \cdot \left(\nabla G_0^k(x,y) u_\delta(y)\right) dy - \int_{\mathcal{B}} k_m^2 u_\delta(y) G_0^k(x,y) dy$$

$$= \frac{1}{\varepsilon_m} \int_{\partial\mathcal{B}} u_\delta(y) \frac{\partial G_0^k(x,y)}{\partial n(y)} ds_y + (k^2 - k_m^2) \frac{1}{\varepsilon_m} \int_{\mathcal{B}} u_\delta(y) G_0^k(x,y) dy \tag{A.14}$$

Now we show the second term in (A.14) is $O(\delta^2|\log\delta|)$ for $x \in 2\mathcal{B} \setminus \mathcal{B}$. First we have by using the Cauchy-Schwartz inequality,

$$|\int_{\mathcal{B}} u_\delta(y) G_0^k(x,y) dy| \leq \|u_\delta\|_{L^2(\mathcal{B})} \left(\int_{\mathcal{B}} |G_0^k(x,y)^2| dy\right)^{\frac{1}{2}}$$

From (2.14) and (2.15) and making the change of variables $r = |x-y|$ we have,

$$\|u_\delta\|_{L^2(\mathcal{B})} \left(\int_{\mathcal{B}} |G_0^k(x,y)^2| dy\right)^{\frac{1}{2}} \leq C\|u_\delta\|_{L^2(\mathcal{B}} \left(\int_0^{C\delta} r(\log r)^2 dr\right)^{1/2}$$

$$\leq C\|u_\delta\|_{L^2(\mathcal{B})} \delta |\log\delta| \text{ for } x \in 2\mathcal{B} \setminus \mathcal{B}$$

Now we give a bound for $\|u_\delta\|_{L^2(\mathcal{B})}$. Adding and subtracting u_0 and using the triangle inequality gives

$$\begin{aligned}\|u_\delta\|_{L^2(\mathcal{B})} &\leq \|u_\delta - u_0\|_{L^2(\mathcal{B})} + \|u_0\|_{L^2(\mathcal{B})}\\ &\leq \|u_\delta - u_0\|_{L^2(\Omega)} + C\delta\\ &\leq C\delta\end{aligned}$$

To estimate $\|u_0\|_{L^2(\mathcal{B})}$ we use have used standard interior elliptic regularity first noting that $\|u_0\|_{L^2(\mathcal{B})} \leq C\delta\|u_0\|_{C^\infty(\mathcal{B})} \leq C\delta\|u_0\|_{H^1(\Omega_R)} \leq C\delta\|u_\delta\|_{H^1(\partial\Omega_R)}$. The scattering problem can be viewed as a transmission problem on $\partial\Omega_R$ and one has

$$\|u_\delta\|_{H^{1/2}(\partial\Omega_R)} \leq C\|u^{inc}\|_{H^{1/2}(\partial\Omega_R)}, \tag{A.15}$$

which is bounded and independent of δ. Following the arguments of Propositions 1 and 2 of [27] but using our hypotheses on inclusion geometry allow us to appeal directly to Proposition 2.3.1 and Corollary 2.3.1 and write

$$\|u_\delta - u_0\|_{H^1(\omega_R)} \leq C\delta\|u_\delta\|_{H^{(1+\eta)/2}(\partial\Omega_R)} \leq C\delta\|u^{inc}\|_{H^{1/2}(\partial\Omega_R)}, \tag{A.16}$$

and the Lemma follows. □

Now we would like to replace G_0^k with the simpler Green's Function for the Laplacian, $G^0(x,y)$, see (2.15). For this we have the following Lemma

Lemma A.2.2. *For x in the open set $2\mathcal{B} \setminus \overline{\mathcal{B}}$*

$$u_\delta(x) - u_0(x) = \left(1 - \frac{1}{\varepsilon_m}\right)\int_{\partial\mathcal{B}} u_\delta(y)\frac{\partial G^0(x,y)}{\partial n(y)}ds_y + O(\delta^2|\log\delta|) \tag{A.17}$$

The term $O(\delta^2|\log\delta|)$ is bounded by $C\delta^2|\log\delta|$ uniformly in x. The constant C depends on the shape of the particle $\mathcal{B}$, the domain Ω_R, the constant ε_m and the frequency ω.

Proof. Let $\mathcal{K}$ be a compact subset of Ω_R such that $2\mathcal{B} \setminus \mathcal{B} \subset \mathcal{K}$. First we recall the relation (2.14), and bound on the L^∞ norm of K_2 and ∇K_2. We also have formula (2.16) which simplifies to,

$$\Delta K_2(x,\cdot) = -k^2 G_0^k(x,\cdot) \text{ in } \Omega_R \tag{A.18}$$

Therefore, using the Divergence Theorem we have

$$\begin{aligned} \int_{\partial \mathcal{B}} \frac{\partial K_2(x,y)}{\partial n(y)} ds_y &= \int_{\mathcal{B}} \Delta_y K_2(x,y) dy \\ &= -k^2 \int_{\mathcal{B}} G_0^k(x,y) dy \\ &= O(\delta^2 |\log \delta|) \text{ for } x \in 2\mathcal{B} \setminus \overline{\mathcal{B}} \end{aligned} \tag{A.19}$$

Using (A.19), and by well-posedness of u_0 and (A.15) we have the bound, $\|u_0\|_{L^\infty(2\mathcal{B})} \leq C\|u_0\|_{H^{1/2}(\partial\Omega_R)} \leq C\|u^{inc}\|_{H^{\frac{1}{2}}(\partial\Omega_R)}$ and for $x \in 2\mathcal{B} \setminus \overline{\mathcal{B}}$ we have,

$$\begin{aligned} \int_{\partial \mathcal{B}} u_\delta(y) \frac{\partial K_2(x,y)}{\partial n(y)} ds_y &= \int_{\partial \mathcal{B}} (u_\delta(y) - u_0(x)) \frac{\partial K_2(x,y)}{\partial n(y)} ds_y + O\left(\delta^2 |\log \delta|\right) \\ &= \int_{\partial \mathcal{B}} (u_\delta(y) - u_0(y)) \frac{\partial K_2(x,y)}{\partial n(y)} ds_y \\ &+ \int_{\partial \mathcal{B}} (u_0(y) - u_0(x)) \frac{\partial K_2(x,y)}{\partial n(y)} ds_y + O\left(\delta^2 |\log \delta|\right) \end{aligned} \tag{A.20}$$

The first term is bounded by,

$$\begin{aligned}
|\int_{\partial\mathcal{B}} (u_\delta(y)-u_0(y))\,\frac{\partial K_2(x,y)}{\partial n(y)} ds_y| &\le |-k^2\int_{\mathcal{B}} (u_\delta(y)-u_0(y))\, G_0^k(x,y)dy| \\
&\quad + |\int_{\mathcal{B}} \nabla\,(u_\delta(y)-u_0(y))\,\nabla_y K_2(x,y)dy| \\
&\le C\|u_\delta-u_0\|_{L^2(\mathcal{B})}\left(\int_{\mathcal{B}} |G_0^k(x,y)^2|dy\right)^{\frac{1}{2}} \\
&\quad + \|\nabla\,(u_\delta-u_0)\|_{L^2(\mathcal{B})}\left(\int_{\mathcal{B}} |\nabla_y K_2(x,y)|^2 dy\right)^{\frac{1}{2}} \\
&\le C\delta^2|\log\delta| + C\delta^2 \\
&\le C\delta^2|\log\delta|
\end{aligned} \tag{A.21}$$

Here we used the energy estimates from Proposition 3.1.2 as well as the formulas for G_0^k and K_2. Now we can bound the second term by

$$|\int_{\partial\mathcal{B}} (u_0(y)-u_0(x))\,\frac{\partial K_2(x,y)}{\partial n(y)} ds_y| \le C\delta\|u_0(\cdot)-u_0(x)\|_{L^\infty(\partial\mathcal{B})} \le C\delta^2 \tag{A.22}$$

We can now insert (A.21) and (A.22) into (A.20) to get

$$\int_{\partial\mathcal{B}} u_\delta(y)\frac{\partial K_2(x,y)}{\partial n(y)} ds_y = O\left(\delta^2|\log\delta|\right),\ \text{ for } x\in 2\mathcal{B}\setminus\overline{\mathcal{B}}$$

With this estimate, we plug the relation (2.14) into the result from Lemma (2.1) to obtain our result

$$\begin{aligned}
u_\delta(x)-u_0(x) &= \left(1-\frac{1}{\varepsilon_m}\right)\int_{\partial\mathcal{B}} u_\delta(y)\frac{\partial G_0^k(x,y)}{\partial n(y)} ds_y + O(\delta^2|\log\delta|) \\
&= \left(1-\frac{1}{\varepsilon_m}\right)\int_{\partial\mathcal{B}} \left[u_\delta(y)\frac{\partial G^0(x,y)}{\partial n(y)} + u_\delta(y)\frac{\partial K_2(x,y)}{\partial n(y)}\right] ds_y + O(\delta^2|\log\delta|) \\
&= \left(1-\frac{1}{\varepsilon_m}\right)\int_{\partial\mathcal{B}} u_\delta(y)\frac{\partial G^0(x,y)}{\partial n(y)} ds_y + O(\delta^2|\log\delta|)
\end{aligned}$$

□

Now we consider the behavior of $u_\delta-u_0$ as $x\in 2\mathcal{B}\setminus\mathcal{B}$ tends to the boundary $\partial\mathcal{B}$. Here we take $\lim_{x\to\partial\mathcal{B}}$ and use the jump condition for the double layer potential

$$\lim_{x\to\partial\mathcal{B}}\left(1-\frac{1}{\varepsilon_m}\right)\int_{\partial\mathcal{B}} u_\delta(y)\frac{\partial G^0(x,y)}{\partial n(y)}ds_y$$
$$=\left(1-\frac{1}{\varepsilon_m}\right)\int_{\partial\mathcal{B}} u_\delta(y)\frac{\partial G^0(x,y)}{\partial n(y)}ds_y+\frac{1}{2}\left(1-\frac{1}{\varepsilon_m}\right)u_\delta(x)\text{ for }x\text{ on }\partial\mathcal{B}$$

Therefore for x on $\partial\mathcal{B}$

$$\frac{1}{2}\left(1+\frac{1}{\varepsilon_m}\right)u_\delta(x)-u_0(x)=\left(1-\frac{1}{\varepsilon_m}\right)\int_{\partial\mathcal{B}} u_\delta(y)\frac{\partial G^0(x,y)}{\partial n(y)}ds_y+O(\delta^2|\log\delta|)\qquad\text{(A.23)}$$

We note here that

$$\int_{\partial\mathcal{B}}\frac{\partial G^0(x,y)}{\partial n(y)}ds_y=-\frac{1}{2}$$

So by adding and subtracting by $\int_{\partial\mathcal{B}} u_0(x)\frac{\partial G^0(x,y)}{\partial n(y)}ds_y$ we can rewrite (A.23) as

$$\frac{1}{2}\left(1+\frac{1}{\varepsilon_m}\right)(u_\delta(x)-u_0(x))=$$
$$=\left(1-\frac{1}{\varepsilon_m}\right)\int_{\partial\mathcal{B}}(u_\delta(y)-u_0(x))\frac{\partial G^0(x,y)}{\partial n(y)}ds_y+O(\delta^2|\log\delta|),x\in\partial\mathcal{B}\qquad\text{(A.24)}$$

Here we recall the vector valued function ϕ which corresponds with the polarization tensor. First rescale $z=x/\delta$ so that $\mathcal{B}^*=\delta^{-1}\mathcal{B}$ and $\mathbb{R}^{2*}_\#$ is the strip $-1/2<z_1<1/2$, $-\infty<z_2<\infty$. We have

$$\begin{cases}\Delta\phi=0\text{ in }\mathcal{B}^*\text{ and }\mathbb{R}^{2*}_\#\setminus\overline{\mathcal{B}^*}\\ \phi^+=\phi^-\text{ on }\partial\mathcal{B}^*\\ \frac{\partial\phi}{\partial n}|^+-\frac{1}{\varepsilon_m}\frac{\partial\phi}{\partial n}|^-=-\frac{1}{\varepsilon_m}n\text{ on }\partial\mathcal{B}^*\\ \lim_{|z_2|\to\infty}\phi=0\end{cases}\qquad\text{(A.25)}$$

Using ϕ we can show the asymptotic behavior of $u_\delta-u_0$ on the boundary of the particle

Proposition A.2.1. *For z on $\partial\mathcal{B}$*

$$u_\delta(\delta z) - u_0(\delta z) = \delta\left(\varepsilon_m - 1\right)\phi(z)\cdot\nabla u_0(0) + O(\delta^2|\log\delta|)$$

The term $O(\delta^2|\log\delta|))$ is bounded uniformly in z by $C\delta^2|\log\delta|$. The constant C depends on the shape of the particle $\mathcal{B}$ and the domain Ω_R, the constant ε_δ, and the frequency ω.

Proof. Using the explicit formula for $G^0(x,y)$ we know,

$$\frac{\partial G^0(x,y)}{\partial n(y)} = -\frac{1}{2\pi}\frac{y-x}{|y-x|^2}\cdot n(y)$$

Rewriting $u_\delta(y) - u_0(x)$ as $(u_\delta(y) - u_0(y)) + (u_0(y) - u_0(x))$ and using the above two equations in (A.24) we have

$$\begin{aligned}\frac{1}{2}\left(1+\frac{1}{\varepsilon_m}\right)(u_\delta(x) - u_0(x)) = &-\frac{1}{2\pi}\left(1-\frac{1}{\varepsilon_m}\right)\int_{\partial\mathcal{B}}(u_\delta(y) - u_0(y))\frac{(y-x)\cdot n(y)}{|y-x|^2}ds_y \\ &-\frac{1}{2\pi}\left(1-\frac{1}{\varepsilon_m}\right)\int_{\partial\mathcal{B}}(u_0(y) - u_0(x))\frac{(y-x)\cdot n(y)}{|y-x|^2}ds_y \\ &+O(\delta^2|\log\delta|) \text{ for } x\in\partial\mathcal{B}\end{aligned} \tag{A.26}$$

We now introduce the re-scaling $z = \frac{x}{\delta}$, $\tilde{y} = \frac{y}{\delta}$ and $\mathcal{B}^* = \frac{1}{\delta}\mathcal{B}$. From (A.26) we immediately have,

$$\begin{aligned}\frac{1}{2}\left(1+\frac{1}{\varepsilon_m}\right)(u_\delta(\delta z) - u_0(\delta z)) = &-\frac{1}{2\pi}\left(1-\frac{1}{\varepsilon_m}\right)\int_{\partial\mathcal{B}^*}(u_\delta(\delta\tilde{y}) - u_0(\delta\tilde{y}))\frac{(\tilde{y}-z)\cdot n(\tilde{y})}{|\tilde{y}-z|^2}ds_{\tilde{y}} \\ &-\frac{1}{2\pi}\left(1-\frac{1}{\varepsilon_m}\right)\int_{\partial\mathcal{B}^*}(u_0(\delta\tilde{y}) - u_0(\delta z))\frac{(\tilde{y}-z)\cdot n(\tilde{y})}{|\tilde{y}-z|^2}ds_{\tilde{y}} \\ &+O(\delta^2|\log\delta|) \text{ for } z\in\partial\mathcal{B}^*\end{aligned} \tag{A.27}$$

From the regularity of u_0 we know u_0 is C^2 in a neighborhood of $\mathcal{B}$ with norm bounded by $C\|f\|_{H^{1/2}(\Omega_R)}$. Taylor Series expansion for $(u_0(\delta\tilde{y}) - u_0(\delta z))$ gives

$$|u_0(\delta\tilde{y} - u_0(\delta z) - \delta\nabla u_0(0)\cdot(\tilde{y}-z)| \le C\left(\delta^2|\tilde{y}-z|^2 + \delta^2|z||\tilde{y}-z|\right)$$

Inserting the Taylor Series expansion into the second term from (A.27), we have

$$\begin{aligned}\frac{1}{2}\left(1+\frac{1}{\varepsilon_m}\right)(u_\delta(\delta z)-u_0(\delta z)) = &-\frac{1}{2\pi}\left(1-\frac{1}{\varepsilon_m}\right)\int_{\partial\mathcal{B}^*}(u_\delta(\delta\tilde{y})-u_0(\delta\tilde{y}))\frac{(\tilde{y}-z)\cdot n(\tilde{y})}{|\tilde{y}-z|^2}ds_{\tilde{y}}\\ &-\frac{\delta}{2\pi}\left(1-\frac{1}{\varepsilon_m}\right)\nabla u_0(0)\cdot\int_{\partial\mathcal{B}^*}(\tilde{y}-z)\frac{(\tilde{y}-z)\cdot n(\tilde{y})}{|\tilde{y}-z|^2}ds_{\tilde{y}}\\ &+O(\delta^2|\log\delta|),\ \text{for } z\in\partial\mathcal{B}^*\end{aligned} \tag{A.28}$$

Examining the second term we have,

$$\begin{aligned}-\frac{1}{2\pi}\int_{\partial\mathcal{B}^*}(\tilde{y}-z)\frac{(\tilde{y}-z)\cdot n(\tilde{y})}{|\tilde{y}-z|^2}ds_{\tilde{y}} &= \int_{\partial\mathcal{B}^*}(\tilde{y}-z)\frac{\partial G^0(z,\tilde{y})}{\partial n(\tilde{y})}ds_{\tilde{y}}\\ &= \int_{\mathcal{B}^*}\nabla_{\tilde{y}}(\tilde{y}-z)\cdot\nabla_{\tilde{y}}G^0(z,\tilde{y})d\tilde{y}\\ &= \int_{\partial\mathcal{B}^*}n(\tilde{y})G^0(z,\tilde{y})ds_{\tilde{y}}\\ &= -\frac{1}{2\pi}\int_{\partial\mathcal{B}^*}n(\tilde{y})\log|z-\tilde{y}|ds_{\tilde{y}}\end{aligned}$$

so we can rewrite (A.28) as

$$\begin{aligned}\frac{1}{2}\left(1+\frac{1}{\varepsilon_m}\right)(u_\delta(\delta z)-u_0(\delta z)) = &-\frac{1}{2\pi}\left(1-\frac{1}{\varepsilon_m}\right)\int_{\partial\mathcal{B}^*}(u_\delta(\delta\tilde{y})-u_0(\delta\tilde{y}))\frac{(\tilde{y}-z)\cdot n(\tilde{y})}{|\tilde{y}-z|^2}ds_{\tilde{y}}\\ &-\frac{\delta}{2\pi}\left(1-\frac{1}{\varepsilon_m}\right)\nabla u_0(0)\cdot\int_{\partial\mathcal{B}^*}n(\tilde{y})\log|z-\tilde{y}|ds_{\tilde{y}}\\ &+O(\delta^2|\log\delta|),\ \text{for } z\in\partial\mathcal{B}^*\end{aligned} \tag{A.29}$$

We have for the ϕ solution of (A.25) on $\partial\mathcal{B}^*$

$$\begin{aligned}\frac{1}{2}\left(1+\frac{1}{\varepsilon_m}\right)\phi(z) = &-\frac{1}{2\pi}\left(1-\frac{1}{\varepsilon_m}\right)\int_{\partial\mathcal{B}^*}\phi(\tilde{y})\frac{(\tilde{y}-z)\cdot n(\tilde{y})}{|\tilde{y}-z|^2}ds_{\tilde{y}}\\ &-\frac{1}{2\pi}\frac{1}{\varepsilon_m}\int_{\partial\mathcal{B}^*}n(\tilde{y})\log|z-\tilde{y}|ds_{\tilde{y}}\ \text{for } z\in\partial\mathcal{B}^*\end{aligned} \tag{A.30}$$

We know that ϕ is the unique solution to (A.25), therefore $\phi|_{\partial\mathcal{B}^*}\in C^0(\partial\mathcal{B}^*)$ is the unique solution to the above integral equation. The Fedholm Theory ([12] Chapter 3) now implies that the bounded linear operator $\psi \ni C^0(\partial\mathcal{B}^*) \to (c+L)\psi \in C^0(\partial\mathcal{B}^*)$, given by

$$(c+L)(\psi)(z) = \frac{1}{2}\left(1+\frac{1}{\varepsilon_m}\right)\psi(z) + \frac{1}{2\pi}\left(1-\frac{1}{\varepsilon_m}\right)\int_{\partial\mathcal{B}^*}\psi(\tilde{y})\frac{(\tilde{y}-z)\cdot n(\tilde{y})}{|\tilde{y}-z|^2}ds_{\tilde{y}}$$

maps $C^0(\partial\mathcal{B}^*)$ onto $C^0(\partial\mathcal{B}^*)$ so has a bounded inverse. Now multiplying (A.30) by $\delta\varepsilon_m\left(1-\frac{1}{\varepsilon_m}\right)\nabla u_0(0)$ and subtracting this from (A.29) gives the following equation for $\psi^*(z) = u_\delta(\delta z) - u_0(\delta z) - \delta\varepsilon_m\left(1-\frac{1}{\varepsilon_m}\right)\nabla u_0(0)\cdot\phi(z)$,

$$\begin{aligned}(c+L)(\psi^*)(z) &= \frac{1}{2}\left(1+\frac{1}{\varepsilon_m}\right)\psi^*(z) + \frac{1}{2\pi}\left(1-\frac{1}{\varepsilon_m}\right)\int_{\partial\mathcal{B}^*}\psi^*(\tilde{y})\frac{(\tilde{y}-z)\cdot n(\tilde{y})}{|\tilde{y}-z|^2}ds_{\tilde{y}} \\ &= O(\delta^2|\log\delta|)\end{aligned}$$

Since $c+L$ is a bounded linear operator which is onto, we have a bounded inverse for $c+L$, thus

$$\begin{aligned}\|u_\delta(\delta\cdot) - u_0(\delta\cdot) - \delta\varepsilon_m\left(1-\frac{1}{\varepsilon_m}\right)\nabla u_0(0)\cdot\phi(\cdot)\|_{C^0(\partial\mathcal{B}^*)} &= \|\psi^*\|_{C^0(\partial\mathcal{B}^*)} \\ &= \|(c+L)^{-1}O(\delta^{1+\eta})\|_{C^0(\partial\mathcal{B}^*)} \\ &\le O(\delta^2|\log\delta|)\end{aligned}$$

This inequality gives us the result of the lemma. □

A.3. Uniform asymptotic behavior of $u_\delta - u_0$ in $\Omega_R \setminus 2\mathcal{B}$

Here we derive the asymptotic behavior of $u_\delta - u_0$ "sufficiently" far from the particle using the Linton Green's function, $G^k_{qp}(x,y)$. Using the same methods as the previous section we can derive the integral representations for u_δ and u_0 for any $x \in \Omega_R \setminus \overline{\mathcal{B}}$

$$\begin{aligned}u_\delta(x) = &\int_{\partial\Omega_R}\left[\frac{\partial u_\delta(y)}{\partial n}G^k_{qp}(x,y) - u_\delta(y)\frac{\partial G^k_{qp}(x,y)}{\partial n(y)}\right]ds_y \\ &+ \int_{\partial\mathcal{B}}\left[u_\delta(y)\frac{\partial G^k_{qp}(x,y)}{\partial n(y)} - \frac{\partial u_\delta(y)}{\partial n}|^+ G^k_{qp}(x,y)\right]ds_y\end{aligned} \tag{A.31}$$

$$u_0(x) = \int_{\partial\Omega_R}\left[\frac{\partial u_0(y)}{\partial n}G^k_{qp}(x,y) - u_0(y)\frac{\partial G^k_{qp}(x,y)}{\partial n(y)}\right]ds_y \tag{A.32}$$

Subtracting (A.32) from (A.31), we have

$$
\begin{aligned}
u_\delta(x) - u_0(x) = &\int_{\partial\Omega_R} \left(\frac{u_\delta(y)}{\partial n} - \frac{\partial u_0(y)}{\partial n} \right) G^k_{qp}(x,y) ds_y \\
&+ \int_{\partial\mathcal{B}} \left[u_\delta(y) \frac{\partial G^k_{qp}(x,y)}{\partial n(y)} - \frac{\partial u_\delta(y)}{\partial n}|^+ G^k_{qp}(x,y) \right] ds_y
\end{aligned}
\tag{A.33}
$$

Here we note the boundary integrals on $\partial\Omega$ involving $G^k_{qp}(x,y)$ do not vanish as in the previous section since $G^k_{qp}(x,y)$ does not satisfy the zero Dirichlet boundary condition $G^k_0(x,y)$ satisfies. As before, we rewrite the last term involving the boundary integral on $\partial\mathcal{B}$ in terms of the double layer potential for u_δ. Using the jump condition $\frac{\partial u_\delta(y)}{\partial n}|^+ = \frac{1}{\varepsilon_m}\frac{\partial u_\delta(y)}{\partial n}|^-$ for $y \in \partial\mathcal{B}$ and integration by parts we have,

$$
\begin{aligned}
\int_{\partial\mathcal{B}} \frac{\partial u_\delta(y)}{\partial n}|^+ G^k_{qp}(x,y) ds_y = &\frac{1}{\varepsilon_m} \int_{\partial\mathcal{B}} \frac{\partial u_\delta(y)}{\partial n}|^- G^k_{qp}(x,y) ds_y \\
&+ \frac{1}{\varepsilon_m} \int_{\partial\mathcal{B}} u_\delta(y) \frac{\partial G^k_{qp}(x,y)}{\partial n(y)} ds_y + (k^2 - k_m^2) \frac{1}{\varepsilon_m} \int_{\mathcal{B}} u_\delta(y) G^k_{qp}(x,y) dy
\end{aligned}
$$

As before $k_m^2 = \varepsilon_m \omega^2$. Substituting the above expression into (A.33), for $x \in \Omega_R \setminus \overline{\mathcal{B}}$

$$
\begin{aligned}
u_\delta(x) - u_0(x) = &\int_{\partial\Omega_R} \left(\frac{u_\delta(y)}{\partial n} - \frac{\partial u_0(y)}{\partial n} \right) G^k_{qp}(x,y) ds_y \\
&+ \left(1 - \frac{1}{\varepsilon_m}\right) \int_{\partial\mathcal{B}} u_\delta(y) \frac{\partial G^k_{qp}(x,y)}{\partial n(y)} ds_y \\
&- (k^2 - k_m^2) \frac{1}{\varepsilon_m} \int_{\mathcal{B}} u_\delta(y) G^k_{qp}(x,y) dy
\end{aligned}
\tag{A.34}
$$

Now we can use Proposition 2.1 to derive the asymptotic behavior of the integral on the boundary of $\mathcal{B}$ and the integral in the volume of $\mathcal{B}$.

Lemma A.3.1. *For any fixed $x \in \Omega_R \setminus 2\overline{\mathcal{B}}$, with $0 < \eta < 1$,*

$$
\int_{\mathcal{B}} u_\delta(y) G^k_{qp}(x,y) dy = \delta^2 G^k_{qp}(x,0) |\mathcal{B}^*| u_0(0) + O(\delta^{3-\eta})
$$

and

$$\int_{\partial\mathcal{B}} u_\delta(y)\frac{\partial G^k_{qp}(x,y)}{\partial n(y)}ds_y = \delta^2\nabla_y G^k_{qp}(x,0)\cdot M(\varepsilon_m)\nabla u_0(0)$$

$$-\delta^2 k^2 G^k_{qp}(x,0)|\mathcal{B}^*|u_0(0) + O(\delta^{3-\eta})$$

Recall the impedance tensor (or equivalently the polarization) tensor is defined as,

$$M(\varepsilon_m) = |\mathcal{B}^*|I + (\varepsilon_m - 1)\int_{\partial\mathcal{B}^*} n(y)(\phi(y))^T ds_y.$$

There exits a constant C such that the remainder terms and their derivatives are bounded by $C\delta^{3-\eta}$ uniformly with respect to $x \in \Omega_R \setminus 2\overline{\mathcal{B}}$. The constant depends the shape of the particle, the dielectric constant ε_m, the frequency ω, d, and u^{inc}.

Proof. Since Ω_R is a bounded, Lipshitz domain in $\mathbb{R}^2$ it follows from Sobolev's Imbedding Theorem [11], [13] that

$$\|u_\delta - u_0\|_{L^p(\Omega_R)} \le C\|u_\delta - u_0\|_{H^1(\Omega_R)} \text{ for all } 1 \le p < \infty$$

Using the energy estimate for $u_\delta - u_0$ gives,

$$\|u_\delta - u_0\|_{L^p(\Omega_R)} \le C\delta$$

Using the Holder inequality we now have for any $x \in \mathbb{R}^2_\# \setminus \overline{\mathcal{B}}$

$$\begin{aligned}
|\int_{\mathcal{B}}(u_\delta(y) - u_0(y))G^k_{qp}(x,y)dy| &\le C\|u_\delta - u_0\|_{L^p(\Omega_R)}\left(\int_{\mathcal{B}}|G^k_{qp}(x,y)|^{p'}dy\right)^{\frac{1}{p'}} \\
&\le C\|u_\delta - u_0\|_{L^p(\Omega_R)}(\delta^2)^{\frac{1}{p'}} \\
&\le C\delta(\delta^2)^{\frac{1}{p'}}
\end{aligned}$$

By Sobolev's Imbedding Theorem we are free to choose any $p < \infty$, so for $0 < \eta < 1$ we choose $p = \frac{1}{\eta}$, which gives $\frac{1}{p'} = 1 - \frac{\eta}{2}$. Therefore we have the estimate,

$$|\int_{\mathcal{B}}(u_\delta(y) - u_0(y))G^k_{qp}(x,y)dy| \le C\delta^{3-\eta} \tag{A.35}$$

Using the fact that $u_0(\cdot)$ is and $G^k_{qp}(x,\cdot)$ is smooth in Ω_R for x outside of $\overline{\mathcal{B}}$ we expand in Taylor Series expansion for u_0 and G^k_{qp} about the point $y=0$ to get

$$\int_{\mathcal{B}} u_0(y)G^k_{qp}(x,y)dy = \delta^2|\mathcal{B}^*|u_0(0)G^k_{qp}(x,0) + O(\delta^3) \tag{A.36}$$

Using (A.35) and (A.36) together with the triangle inequality we obtain the first result of the lemma

$$\int_{\mathcal{B}} u_\delta(y)G^k_{qp}(x,y)dy = \delta^2|\mathcal{B}^*|u_0(0)\tilde{G}^k_{per}(x,0) + O(\delta^{3-\delta})$$

For $x \in \Omega_R \setminus \mathcal{B}$ the divergence theorem gives

$$\begin{aligned}\int_{\partial\mathcal{B}} u_0(y)\frac{\partial G^k_{qp}(x,y)}{\partial n(y)}ds_y &= \int_{\mathcal{B}} \nabla\cdot(\nabla G^k_{qp}(x,y)u_0(y))dy\\ &= \int_{\mathcal{B}} \nabla u_0(y)\cdot\nabla_y G^k_{qp}(x,y)ds_y + \int_{\mathcal{B}} u_0(y)\Delta G^k_{qp}(x,y)dy\\ &= \int_{\mathcal{B}} \nabla u_0(y)\cdot\nabla_y G^k_{qp}(x,y)ds_y - k^2\int_{\mathcal{B}} u_0(y)G^k_{qp}(x,y)dy\end{aligned}$$

Since x is outside the particle u_0 and G^k_{qp} are C^2 in y for a neighborhood of $\mathcal{B}$, we use Taylor Series expansion about the point $y=0$ to obtain,

$$\int_{\partial\mathcal{B}} u_0(y)\frac{\partial G^k_{qp}}{\partial n(y)} = \delta^2|\mathcal{B}^*|\nabla_y G^k_{qp}(x,0)\cdot\nabla u_0(0) - \delta^2|\mathcal{B}^*|k^2 G^k_{qp}(x,0)u_0(0) + O(\delta^3)$$

Now we can give a bound for $\int_{\partial\mathcal{B}} u_\delta(y)\frac{\partial G^k_{qp}(x,y)}{\partial n(y)}ds_y$ by adding and subtracting $\int_{\partial\mathcal{B}} u_0(y)\frac{\partial G^k_{qp}(x,y)}{\partial n(y)}ds_y$

$$\begin{aligned}\int_{\partial\mathcal{B}} u_\delta(y)\frac{\partial G^k_{qp}(x,y)}{\partial n(y)}ds_y &= \int_{\partial\mathcal{B}} (u_\delta(y)-u_0(y))\frac{\partial G^k_{qp}(x,y)}{\partial n(y)}ds_y + \int_{\partial\mathcal{B}} u_0(y)\frac{\partial G^k_{qp}(x,y)}{\partial n(y)}ds_y\\ &= \int_{\partial\mathcal{B}} (u_\delta(y)-u_0(y))\frac{\partial G^k_{qp}(x,y)}{\partial n(y)}ds_y + \delta^2\nabla_y G^k_{qp}(x,0)\cdot|\mathcal{B}^*|\nabla u_0(0)\\ &- \delta^2|\mathcal{B}^*|k^2 G^k_{qp}(x,0)u_0(0) + O(\delta^3)\end{aligned} \tag{A.37}$$

By Proposition 2.1 and re-scaling, for any $x \in \Omega_R \setminus 2\overline{\mathcal{B}}$

$$\begin{aligned}
\int_{\partial\mathcal{B}} (u_\delta(y) - u_0(y)) \frac{\partial G^k_{qp}(x,y)}{\partial n(y)} ds_y &= \delta \int_{\partial\mathcal{B}^*} (u_\delta(\delta\tilde{y}) - u_0(\delta\tilde{y})) \nabla_y G^k_{qp}(x, \delta\tilde{y}) \cdot n(\tilde{y}) ds_{\tilde{y}} \\
&= \delta^2 \int_{\partial\mathcal{B}^*} (\varepsilon_m - 1)\, \phi(\tilde{y}) \cdot \nabla u_0(0) \nabla_y G^k_{qp}(x, \delta\tilde{y}) \cdot n(\tilde{y}) ds_{\tilde{y}} \\
&+ \delta \int_{\mathcal{B}^*} O(\delta^2 |\log \delta|) \nabla_y G^k_{qp}(x, \delta\tilde{y}) \cdot n(\tilde{y}) ds_{\tilde{y}} \\
&= \delta^2 \int_{\partial\mathcal{B}^*} (\varepsilon_m - 1)\, \phi(\tilde{y}) \cdot \nabla u_0(0) \nabla_y G^k_{qp}(x, \delta\tilde{y}) \cdot n(\tilde{y}) ds_{\tilde{y}} \\
&+ O(\delta^3 |\log \delta|)
\end{aligned} \tag{A.38}$$

Using a Taylor Expansion for G^k_{qp} about zero, for $x \in \Omega_R \setminus 2\overline{\mathcal{B}}$ we also have

$$\nabla_y G^k_{qp}(x, \delta\tilde{y}) = \nabla_y G^k_{qp}(x, 0) + O(\delta) \text{ for } \tilde{y} \in \partial\mathcal{B}^*$$

Using this expression with (A.38) gives

$$\int_{\partial\mathcal{B}} (u_\delta(y) - u_0(y)) \frac{\partial G^k_{qp}(x,y)}{\partial n(y)} ds_y = \delta^2 (\varepsilon_m - 1) \nabla_y G^k_{qp}(x, 0) \cdot \left[\int_{\partial\mathcal{B}^*} n(y) (\phi(y))^T ds_y \right] \nabla u_0(0) + O(\delta^{3-\eta})$$

Applying the definition of the Polarization Tensor M in (A.37) gives

$$\begin{aligned}
\int_{\partial\mathcal{B}} u_\delta(y) \frac{\partial G^k_{qp}(x,y)}{\partial n(y)} ds_y &= \delta^2 (\varepsilon_m - 1) \nabla_y G^k_{qp}(x, 0) \cdot \left[\int_{\partial\mathcal{B}^*} n(y) (\phi(y))^T ds_y \right] \nabla u_0(0) \\
&+ \delta^2 \nabla_y G^k_{qp}(x, 0) \cdot |\mathcal{B}^*| \nabla u_0(0) - \delta k^2 G^k_{qp}(x, 0) |\mathcal{B}^*| u_0(0) + O(\delta^{3-\eta}) \\
&= \delta^2 \nabla_y G^k_{qp}(x, 0) \cdot \left[|\mathcal{B}^*| I + (\varepsilon_m - 1) \int_{\partial\mathcal{B}^*} n(y) (\phi(y))^T ds_y \right] \nabla u_0(0) \\
&- \delta^2 k^2 G^k_{qp}(x, 0) |\mathcal{B}^*| u_0(0) + O(\delta^{3-\eta}) \\
&= \delta^2 \nabla_y G^k_{qp}(x, 0) \cdot M(\varepsilon_m) \nabla u_0(0) - \delta^2 k^2 \tilde{G}^k_{per}(x, 0) |\mathcal{B}^*| u_0(0) + O(\delta^{3-\eta})
\end{aligned}$$

which gives the second result of the the lemma. □

Using the result of Lemma 3.1 in equation (A.34) we arrive at the desired result, giving the field u_δ in terms of the polarization tensor and the double layer potential applied to $u_\delta - u_0$.

$$
\begin{aligned}
u_\delta(x) - u_0(x) = &\int_{\partial\Omega_R} \left(\frac{u_\delta(y)}{\partial n} - \frac{\partial u_0(y)}{\partial n} \right) G^k_{qp}(x,y) ds_y \\
&+ \left(1 - \frac{1}{\varepsilon_m}\right) [\delta^2 \nabla_y G^k_{qp}(x,0) \cdot M(\varepsilon_m) \nabla u_0(0) - \delta^2 k^2 G^k_{qp}(x,0) |\mathcal{B}^*| u_0(0)] + O(\delta^{3-\eta}) \\
&- \frac{1}{\varepsilon_m}(k^2 - k_m^2) \delta^2 G^k_{qp}(x,0) |\mathcal{B}^*| u_0(0) + O(\delta^{3-\eta})
\end{aligned}
$$

Combining like terms we have

$$
\begin{aligned}
u_\delta(x) - u_0(x) = &\int_{\partial\Omega_R} \left(\frac{u_\delta(y)}{\partial n} - \frac{\partial u_0(y)}{\partial n} \right) G^k_{qp}(x,y) ds_y \\
&+ \left(1 - \frac{1}{\varepsilon_m}\right) \delta^2 \nabla_y \tilde{G}^k_{per}(x,0) \cdot M(\varepsilon_m) \nabla u_0(0) + O(\delta^{3-\eta})
\end{aligned}
\tag{A.39}
$$

We can now recast equation $(A.39)$ in terms of the boundary integral operators and the Dirichlet to Neumann map. Since $u_\delta = u_0 = f$ on $\partial\Omega_R$ taking the limit as $x \to \partial\Omega_R$ gives

$$
0 = \int_{\partial\Omega_R} \left(\frac{u_\delta(y)}{\partial n} - \frac{\partial u_0(y)}{\partial n} \right) G^k_{qp}(x,y) ds_y + \tag{A.40}
$$

$$
+ \left(1 - \frac{1}{\varepsilon_m}\right) \delta^2 \nabla_y G^k_{qp}(x,0) \cdot M(\varepsilon_m) \nabla u_0(0) + O(\delta^{3-\eta}), \tag{A.41}
$$

and we arrive at the desired formula,

$$
S\left(N_0 - N_\delta\right)(f) = \left(1 - \frac{1}{\varepsilon_m}\right) \delta^2 \nabla_y G^k_{qp}(x,0) \cdot M(\varepsilon_m) \nabla u_0(0) + O(\delta^{3-\eta}) \tag{A.42}
$$

and this proves Theorem (A.1.1).

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Vita

Zach Jermain was born in Missouri and raised in the small town of Conception Junction. He earned his dual Bachelor of Science degrees in Physics and Mathematics from the University of Missouri in 2017. Zach first came to Lousiana State Univeristy in 2018 where he served as a graduate assistant for the LSU softball program while working towards his Master of Science in Mathematics which he earned in May of 2020. The following fall he started his doctoral work under the advisement of Robert Lipton. He plans to receive his Doctorate in August 2024, after which he will serve as the Director of Player Performance and Analytics with the LSU softball program.