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Gang Bao
Major Professor's Signature

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STUDIES OF NONLINEAR PROBLEMS FOR MAXWELL'S EQUATIONS

By

Ying Li

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ABSTRACT

STUDIES OF NONLINEAR PROBLEMS FOR MAXWELL'S EQUATIONS

By

Ying Li

Consider the electromagnetic field scattered by a nonlinear optical medium. Because of inhomogeneity of the medium, the governing equations are Maxwell's equation with jump coefficients and a source term. By using the Sommerfeld radiation condition, the model scattering problem may be truncated into a bounded domain. In this paper, L^p estimates for Maxwell's equation are established. The solution of Maxwell's equation is represented by spherical harmonics. L^p estimate is for the Maxwell equations with jump coefficients. An application of our L^p estimates gives rise to the wellposedness of a linearized model.

In part two, an adaptive finite element method is developed for solving Maxwell's equations in a nonlinear periodic structure. The medium or computational domain is truncated by a perfect matched layer (PML) technique. Error estimates are established. Numerical examples are provided, which illustrate the efficiency of the method.

In part three, an inverse scattering problem is formulated for breast cancer detection. A recursive linearization algorithm is used to solve the inverse scattering problem. We employed the idea of finite element boundary integral method and added suitable boundary conditions on the surface of the breast and an artificial boundary which encloses the tumor. Finite element method is used for the interior domain containing inhomogeneity. Nyström method is used for the integral equations and exterior domain. Numerical examples are presented.

To my beloved grandma and grandpa.

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Introduction

This research focuses on mathematical and computational studies of second harmonic generation in electromagnetism and optics. Second harmonic generation arises from the nonlinearity of optical materials. When a plane wave with frequency ω is incident on a nonlinear structure, the nonlinearity of the structure gives rise to the scattered waves at both frequency ω and 2ω. This important phenomenon is known as Second Harmonic Generation (SHG) in nonlinear optics. A significant application of SHG is to obtain coherent beams of light in parts of the spectrum at which lasers cannot be made and to construct optoelectronic devices based on nonlinear effects in waveguides and optical fibers.

In chapter one, we established the uniqueness and existence of the solution of Maxwell's equations in a bounded domain containing a nonlinear medium. Consider the electromagnetic field scattered by the nonlinear medium. Because of inhomogeneity of the medium, the governing equations are Maxwell's equation with jump coefficients and a source term. By using the Sommerfeld radiation condition, the model scattering problem may be truncated into a bounded domain. The solution of Maxwell's equation is represented by spherical harmonics. L^p estimate for the equations are established, which gives rise to the wellposedness of a linearized model.

In practice, the SHG optical effects are often too weak to be observed. Therefore, modeling and enhancement of SHG are of great interest to potential real applications. It is pointed out that the SHG can be greatly enhanced in periodic structures.

In chapter two, questions on the existence and uniqueness have been studied. We have developed an adaptive finite element method for solving the model scattering problem. The medium or computational domain is truncated by a perfect matched layer (PML) technique. Error estimates are established. Numerical examples are provided, which illustrate the efficiency of the method. Numerical solution of the nonlinear model problem in three dimensions is completely open, which will be one of my future projects.

In chapter three, we consider the inverse scattering problem arising from breast cancer detection. The problem is to determine the dielectric property of the tissues from the measurements of electromagnetic field on the surface, given the incident field. In addition to the ill-posedness and nonlinearity of the inverse scattering problem, one major difficulty lies in the multiple scales of the problem. The tumor is comparably small in the computational domain, which makes the computation challenging. Another difficulty is due to the dispersive nature of the human body. Maxwell's equations in dispersive media must be studied. A continuation method is developed for this problem. The algorithm needs multi-frequency Dirichlet and Neumann data on the surface. The initial guess comes from Born approximation. The dielectric constant is updated by using higher and higher wavenumber k.

CHAPTER 1

L^p estimate of Maxwell's equations in a bounded domain

1.1 Introduction

Second harmonic generation (SHG) is a well known nonlinear optical effect. It was first demonstrated by P. A. Franken, A. E. Hill, C. W. Peters, and G. Weinreich [33] in 1961. The demonstration was made possible by the invention of laser in 1960, which created the required high intensity monochromatic light. In the experiment, they focused a ruby laser with a wavelength of 694 nm into a quartz sample. They sent the output light through a spectrometer, recording the spectrum on photographic paper, which indicated the production of light at 347 nm. The physical mechanism behind SHG can be understood as follows. Due to the nonlinearity, the incident (pump) wave generates a nonlinear polarization which oscillates with twice the fundamental frequency. According to Maxwell's equations, this nonlinear polarization radiates an electromagnetic field with this doubled frequency. The latter also interacts with the fundamental wave, so that the pump wave can be attenuated (pump depletion) when the second harmonic intensity develops. Energy is transferred from the pump wave to the second harmonic wave. It is a very important nonlinear optical effect because theoretically coherent beams of light can be obtained in parts of the spectrum at which lasers cannot be made and optoelectronic devices based on nonlinear effects in waveguides and optical fibres can be constructed. The reader is referred to [52] for detailed descriptions of nonlinear optics.

A PDE model was introduced in [48], [49] and [50] to describe nonlinear SHG in periodic structures. In Bao, Minut and Zhou [18], the regularity is studied for the solutions of Maxwell's equations with source term in a domain with jump dielectric coefficients. These L^p estimates are further employed to solve the linearized SHG problem in a periodic structure. In this paper, we study the regularity of Maxwell's equations for the scattering by a bounded domain of a nonlinear medium. Although the interior estimate is the same as in [18], the boundary estimate requires a new technique. A striking difference is due to the decay rate of the fields away from the medium. In the periodic case [18], the fields decay exponentially, which makes the L^∞ norm estimate easier. For the scattering from a bounded medium, because of the slow decay of the fields away from the medium, we must use fine properties of the Hankel functions and spherical harmonics.

For simplicity we assume the medium is nonmagnetic ($\mu \equiv \mu_0$) and no external current or charge is present in the field. The following Maxwell's equations hold:

$$-\frac{\partial \vec{B}}{\partial t} = \nabla \times \vec{E},$$
$$\frac{\partial \vec{D}}{\partial t} = \nabla \times \vec{H},$$

where $\vec{E}$ is the electric field, $\vec{H}$ is the magnetic field, $\vec{B}$ is the magnetic induction, and $\vec{D}$ is the electric induction. The constitutive equations are:

$$\vec{B} = \mu_0 \vec{H},$$
$$\vec{D} = \epsilon_0 \vec{E} + \vec{P},$$

where μ_0 is the constant magnetic permeability, ϵ_0 is the dielectric permittivity in vacuum. $\vec{P}$ is the polarization.

The time harmonic solutions of Maxwell equations, also called **plane waves**, are complex-valued fields:

$$\vec{E}(x,t) = \Re(\vec{E}(x)e^{(-i\omega t)}),$$
$$\vec{H}(x,t) = \Re(\vec{H}(x)e^{(-i\omega t)}),$$

that satisfy the system of **time-harmonic Maxwell equations**:

$$\nabla \times \vec{E} = -i\omega\mu\vec{H},$$
$$\nabla \times \vec{H} = i\omega\epsilon\vec{E},$$

where ω stands for the frequency of the electromagnetic waves.

In the linear case, the polarization is induced linearly by the electric field:

$$\vec{P} = \chi^{(1)}\vec{E},$$

where $\chi^{(1)}$ is called the linear susceptibility tensor. Thus, if a beam of angular frequency ω is passing through the medium, a polarization oscillating at ω is produced which in turn serves as a source for the further propagation of the original wave at ω.

If the light intensity is high (as lasers), the nonlinear effect will play a role and the polarization will depend nonlinearly on the electric field [52]:

$$\vec{P} = \chi^{(1)}\vec{E} + \chi^{(2)}\vec{E}^2 + \chi^{(3)}\vec{E}^3 + ...$$

where $\chi^{(i)}$ is the i-th order susceptibility tensor. Throughout, we restrict our attention to the 2nd order susceptibility by ignoring the higher order terms. Hence

$$\vec{P} = \sum_{j=1,2,3} \chi^{(1)}_{\cdot j} E_j + \sum_{j,k=1,2,3} \chi^{(2)}_{\cdot jk} E_j E_k,$$

where E_i is the i-th component of $\vec{E}$. It is clear that the second term in the polarization may generate fields of frequency 2ω. Let

$$\vec{E}^{(j\omega)} = \vec{E}_0^{(j\omega)}(x)e^{-ij\omega t} + \overrightarrow{\bar{E}_0}^{(j\omega)}(x)e^{ij\omega t}.$$

We can write the total field as

$$\vec{E} = \vec{E}^{(\omega)} + \vec{E}^{(2\omega)}.$$

Then, by omitting $e^{\pm i3\omega t}$ terms,

$$\begin{aligned}
E_j E_k = &(E_{0j}^{(\omega)}(x)e^{-i\omega t} + \bar{E}_{0j}^{(\omega)}(x)e^{i\omega t} + E_{0j}^{(2\omega)}(x)e^{-i2\omega t} + \bar{E}_{0j}^{(2\omega)}(x)e^{i2\omega t})\cdot \\
&(E_{0k}^{(\omega)}(x)e^{-i\omega t} + \bar{E}_{0k}^{(\omega)}(x)e^{i\omega t} + E_{0k}^{(2\omega)}(x)e^{-i2\omega t} + \bar{E}_{0k}^{(2\omega)}(x)e^{i2\omega t}) \\
= &E_{0j}^{(\omega)}E_{0k}^{(\omega)}e^{-i2\omega t} + E_{0j}^{(\omega)}\bar{E}_{0k}^{(2\omega)}e^{i\omega t} + \bar{E}_{0j}^{(\omega)}\bar{E}_{0k}^{(\omega)}e^{i2\omega t} \\
&+ \bar{E}_{0j}^{(\omega)}E_{0k}^{(2\omega)}e^{-i\omega t} + E_{0j}^{(2\omega)}\bar{E}_{0k}^{(\omega)}e^{-i\omega t} + \bar{E}_{0j}^{(2\omega)}E_{0k}^{(\omega)}e^{i\omega t}.
\end{aligned}$$

It follows that

$$\begin{aligned}
P_l = &\sum_j \chi_{lj}^{(1)}(E_{0j}^{(\omega)}e^{-i\omega t} + \bar{E}_{0j}^{(\omega)}e^{i\omega t} + E_{0j}^{(2\omega)}e^{-i2\omega t} + \bar{E}_{0j}^{(2\omega)}e^{i2\omega t}) \\
&+ \sum_{j,k} \chi_{ljk}^{(2)}(E_{0j}^{(\omega)}E_{0k}^{(\omega)}e^{-i2\omega t} + E_{0j}^{(\omega)}\bar{E}_{0k}^{(2\omega)}e^{i\omega t} + \bar{E}_{0j}^{(\omega)}\bar{E}_{0k}^{(\omega)}e^{i2\omega t} \\
&+ \bar{E}_{0j}^{(\omega)}E_{0k}^{(2\omega)}e^{-i\omega t} + E_{0j}^{(2\omega)}\bar{E}_{0k}^{(\omega)}e^{-i\omega t} + \bar{E}_{0j}^{(2\omega)}E_{0k}^{(\omega)}e^{i\omega t})
\end{aligned}$$

by ignoring the 3ω and higher order terms. Evidently, the combination of two fields of frequency ω generates the second harmonic field.

The time-harmonic Maxwell's equations become (by dropping subscript 0 to simplify the notation)

$$\begin{aligned}
&\nabla \times \vec{E}^{(\omega)} = -i\omega\mu_0\vec{H}^{(\omega)}, \\
&\nabla \times \vec{H}^{(\omega)} = i\omega\epsilon_0\vec{E}^{(\omega)} + i\omega\sum_{j,k}\chi_{\cdot jk}^{(2)}(\bar{E}_j^{(\omega)}E_k^{(2\omega)} + E_j^{(2\omega)}\bar{E}_k^{(\omega)}),
\end{aligned}$$

$$\nabla \times \vec{E}^{(2\omega)} = -i2\omega\mu_0\vec{H}^{(2\omega)},$$
$$\nabla \times \vec{H}^{(2\omega)} = i2\omega\epsilon_0\vec{E}^{(2\omega)} + i2\omega\sum_{j,k}\chi^{(2)}_{\cdot jk}E^{(\omega)}_j E^{(\omega)}_k.$$

The nonlinear polarization may be treated as a source term in Maxwell's equations. Rewrite the equations as

$$\nabla \times \vec{E} = -i\omega\mu\vec{H},$$
$$\nabla \times \vec{H} = i\omega\epsilon\vec{E} + \vec{g}, \tag{1.1.1}$$

where $\vec{g}$ is the source term.

The rest of this paper is organized as follows. In the next section, spherical harmonics are introduced to represent the magnetic field. The boundary condition is derived on the artificial boundary S_R. Section 3 is devoted to establishing the L^p estimate on S_R. The wellposedness of the model problem is proved in Section 4 and Section 5.

1.2 Spherical Harmonics

Consider a bounded nonlinear medium enclosed by a boundary surface S. Assume that the dielectric coefficient is ϵ_1 inside S; ϵ_0 outside of S. It is assumed to be vacuum outside the medium.

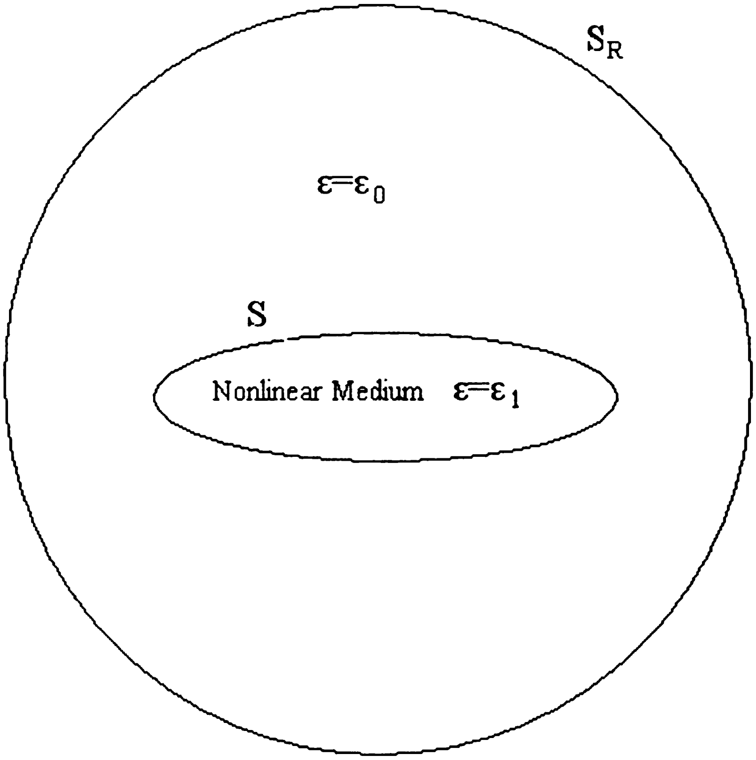
Now let S_R be the sphere of radius R such that S_R encloses the whole nonlinear medium. Outside the medium, the electromagnetic fields satisfy (1.1.1) with $g = 0$. For simplicity, the arrows are omitted throughout this section. Taking curl of the second equation and eliminating the electric field E gives:

$$\nabla \times (\nabla \times H) = -\omega^2\mu\epsilon H.$$

By employing the vector identity:

$$\nabla \times (\nabla \times A) = \nabla(\nabla \cdot A) - (\nabla \cdot \nabla)A,$$

Figure 1.1. Geometry of the scattering problem



and

$$\nabla \cdot (\nabla \times B) = 0,$$

we obtain the Helmholtz equation:

$$\Delta H + k^2 H = 0, \tag{1.2.1}$$

where $k = \omega^2 \epsilon \mu$ is the wave number in vacuum.

To ensure the uniqueness of the solution, the following Sommerfeld's radiation condition is imposed:

$$\lim_{r \to \infty} r(\frac{\partial H}{\partial r} - ikH) = 0.$$

We will now use spherical harmonics to represent the solution of this equation. Spherical harmonics are the angular portion of an orthogonal set of solutions to

Laplace's equation represented in a system of spherical coordinates. The readers are referred to [45] and [1] for detailed discussions of spherical harmonics.

In spherical coordinates, equation (1.2.1) becomes

$$\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial H}{\partial r}) + \frac{1}{r^2}\Delta_{S_U} H + k^2 H = 0,$$

where

$$\Delta_{S_U} = \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta})$$

is the Laplace-Beltrami operator on the unit sphere S_U. The Hermitian product in $L^2(S_U)$ is given by

$$\int_{S_U} u\bar{v}d\sigma = \int_0^{2\pi}\int_0^{\pi} u(\theta,\phi)\bar{v}(\theta,\phi)\sin\theta d\theta d\phi.$$

Let $H^1(S_U)$ be the **Hilbert space**

$$H^1(S) = \{u \in L^2(S_U), \nabla_{S_U} u \in (L^2(S_U))^2\}$$

with its Hermitian product

$$(u,v)_{H^1(S_U)} = \frac{1}{4}\int_S u\bar{v}d\sigma + \int_S(\nabla_S u \, \nabla_S \, \bar{v})d\sigma.$$

The Laplace-Beltrami operator is self-adjoint in the space $L^2(S)$. It admits a family of eigenfunctions which constitutes an orthogonal basis for the space $L^2(S)$. This basis is also orthogonal for the scalar product in $H^1(S)$. These eigenfunctions are called **spherical harmonics**.

Denote by $\mathcal{Y}_l$ the space of homogeneous polynomials of degree l that are harmonic, with restrictions to the unit sphere. We list the following theorem from [45] without proof:

Theorem 1.2.1. *Let Y_l^m, $-l \leq m \leq l$, denote an orthonormal basis of $\mathcal{Y}_l$ for the hermitian product of $L^2(S)$. The functions Y_l^m, for $l \geq 0$ and $-l \leq m \leq l$, constitute an orthogonal basis in $L^2(S)$, which is also orthogonal in $H^1(S)$. Moreover, $\mathcal{Y}_l$*

coincides with the subspace spanned by the eigenfunctions of the Laplace-Beltrami operator associated with the eigenvalue $-l(l+1)$*, i.e.,*

$$\Delta_S Y_l^m + l(l+1)Y_l^m = 0,$$

and the eigenvalue $-l(l+1)$ *has multiplicity* $2l+1$*.*

The spherical harmonics of order l are the $2l+1$ functions of the form:

$$Y_l^m(\theta,\phi) = (-1)^m\left[\frac{l+\frac{1}{2}}{2\pi}\frac{(l-m)!}{(l+m)!}\right]^{\frac{1}{2}} e^{im\phi}\mathbb{P}_l^m(\cos(\theta)),$$

where $\mathbb{P}_l^m(\cos(\theta))$ are **associated Legendre functions**. They have the following properties:

$$\mathbb{P}_l^{-m} = (-1)^m\frac{(l-m)!}{(l+m)!}\mathbb{P}_l^m,$$
$$Y_l^{m*}(\theta,\phi) = (-1)^m Y_l^{-m}(\theta,\phi),$$

where the superscript * denotes complex conjugation. The spherical harmonics form a complete set of orthonormal functions and thus form a vector space analogous to unit basis vectors. On the unit sphere, any square integrable function can thus be expanded as a linear combination of these:

$$f(\theta,\phi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} f_l^m Y_l^m(\theta,\phi).$$

The expansion coefficients can be obtained by:

$$f_l^m = \int_\Omega f(\theta,\phi)Y_l^{m*}(\theta,\phi)d\Omega = \int_0^{2\pi} d\phi\int_0^{\pi} d\theta\sin\theta f(\theta,\phi)Y_l^{m*}(\theta,\phi).$$

We now expand the magnetic field by spherical harmonics. Let

$$H(r,\theta,\phi) = \sum_{l=0}^{\infty} H_l(r)\sum_{m=-l}^{l} h_l^m Y_l^m(\theta,\phi).$$

Suppose that on the boundary S_R:

$$H(R,\theta,\phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} u_l^m Y_l^m(\theta,\phi)$$

for some constants u_l^m. Substituting this solution into the Helmholtz equation, we have

$$\frac{d^2 H_l}{dr^2} + \frac{2}{r}\frac{dH_l}{dr} + (k^2 - \frac{l(l+1)}{r^2})H_l = 0,$$

i.e., the spherical Bessel equation. It can be transformed by rescaling to

$$\frac{d^2 H_l}{dr^2} + \frac{2}{r}\frac{dH_l}{dr} + (1 - \frac{l(l+1)}{r^2})H_l = 0. \tag{1.2.2}$$

A useful Lemma from [45] about the spherical Bessel equation is stated here without proof.

Lemma 1.2.1. *The spherical Bessel equation* (1.2.2) *admits two families of solutions, known as spherical Hankel functions, which satisfy the recursion formulas*

$$\frac{d}{dr}H_l = \frac{l}{r}H_l - H_{l+1} = -\frac{l+1}{r}H_l + H_{l-1},$$
$$H_{l+1} + H_{l-1} = \frac{2l+1}{r}H_l.$$

The spherical Hankel functions are given by the expressions

$$h_l^{(1)}(r) = (-r)^l(\frac{1}{r}\frac{d}{dr})^l(\frac{e^{ir}}{r}),$$
$$h_l^{(2)}(r) = (-r)^l(\frac{1}{r}\frac{d}{dr})^l(\frac{e^{-ir}}{r});$$

more specifically by

$$h_l^{(1)}(r) = (-i)^l\frac{e^{ir}}{r}(\beta_0^l + i\beta_1^l\frac{1}{r} + \ldots + (i)^l\beta_l^l(\frac{1}{r})^l),$$
$$h_l^{(2)}(r) = \overline{h_l^{(1)}(r)};$$
$$\beta_m^l = \frac{(m+l)!}{m!(l-m)!2^m}.$$

The function

$$z_l(r) = r\frac{\frac{d}{dr}h_l^{(1)}(r)}{h_l^{(1)}(r)}$$

satisfies the recursion formula

$$(z_{l-1} - (l-1))(z_l + l + 1) = -r^2.$$

Moreover,

$$1 + \alpha_1^l \frac{1}{r^2} + \ldots + \alpha_l^l \frac{1}{r^{2l}} = r^2 |h_l^{(1)}(r)|^2, \tag{1.2.3}$$
$$\alpha_m^l = \beta_m^l \beta_m^m.$$

In addition

$$1 \leq -\Re(z_l(r)) \leq l + 1,$$
$$0 \leq \Im(z_l(r)) \leq r.$$

Writing the solution as:

$$H_l(r) = \gamma_l^1 h_l^{(1)}(kr) + \gamma_l^2 h_l^{(2)}(kr).$$

By looking at the explicit forms of spherical Hankel functions:

$$h_l^{(1)}(r) = (-i)^l \frac{e^{ir}}{r}(\beta_0^l + i\beta_1^l \frac{1}{r} + \ldots + (i)^l \beta_l^l (\frac{1}{r})^l),$$
$$h_l^{(2)}(r) = \overline{h_l^{(1)}(r)},$$

we obtain:

$$\frac{\partial H}{\partial r} - ikH = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} [k\gamma_l^1 h_l^m (\frac{d}{dr} h_l^{(1)}(kr) - ih_l^{(1)}(kr)),$$
$$+ k\gamma_l^2 h_l^m (\frac{d}{dr} h_l^{(2)}(kr) - ih_l^{(2)}(kr))] Y_l^m(\theta, \phi).$$

From Theorem 1.2.1, we know that

$$\frac{d}{dr}h_l^{(1)}(kr) - ih_l^{(1)}(kr) \sim \beta_0^l((-i)^l \frac{ike^{ikr}r - e^{ikr}}{k^2r^2} - i(-i)^l \frac{e^{ikr}}{r})$$
$$= \beta_0^l(-(-i)^l \frac{e^{ikr}}{k^2r^2}),$$
$$\frac{d}{dr}h_l^{(2)}(kr) - ih_l^{(2)}(kr) \sim \beta_0^l((i)^l \frac{-ike^{-ikr}r - e^{-ikr}}{k^2r^2} - i(i)^l \frac{e^{-ikr}}{r})$$
$$= \beta_0^l(-2(i)^{l+1} \frac{e^{-ikr}}{kr} - i^l \frac{e^{-ikr}}{k^2r^2}).$$

But by the Sommerfeld's radiation condition, we need $r(\frac{\partial H}{\partial r} - ikH) \to 0$ as $r \to \infty$, which concludes that $\gamma_l^2 = 0$.

Plugging in the boundary condition, the solution becomes

$$H(r, \theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{h_l^{(1)}(kr)}{h_l^{(1)}(kR)} u_l^m Y_l^m(\theta, \phi). \tag{1.2.4}$$

On S_R, we have

$$\frac{\partial H}{\partial n}|_{S_R} = T_R H = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{1}{R} z_l(kR) u_l^m Y_l^m(\theta, \phi). \tag{1.2.5}$$

It follows that the problem may be truncated into a bounded domain with the boundary S_R and a boundary condition (1.2.5) on S_R.

1.3 Boundary Estimate

Our goal is to establish global estimates for the solutions of the scattering problem. We first present a local estimate from [18] which provides the L^p estimate inside the dielectric and on the interface. Throughout the paper, C stands for a positive generic constant whose value may vary step by step but should always be clear from the context.

Let $1 < p < \infty$, let B be an open ball in $\mathbb{R}^3$ and let $\vec{g} \in L^p(B)$. Let $\vec{E} \in L^p(B)$ and $\vec{H} \in W^{1,p}(B)$ be a solution of (1.1.1).

Let S be a $\mathcal{C}^2$ surface embedded in $\mathbb{R}^3$ such that S divides B into two connected components B^+ and B^-. Assume the electric permittivity ϵ is defined by

$$\epsilon = \begin{cases} \epsilon^+ & \text{in } B^+, \\ \epsilon^- & \text{in } B^-. \end{cases}$$

Theorem 1.3.1. *(Local estimate) For any B' with $\bar{B}' \subset B$,*

$$\|\vec{E}\|_{L^p(B')} + \|\vec{H}\|_{W^{1,p}(B')} \leq C(\|\vec{H}\|_{L^p(B)} + \|\vec{g}\|_{L^p(B)} + \|\vec{E}\|_{W^{-1,p}(B)}),$$

where C is a constant depending only on p, B' and B.

Therefore, in order to establish global estimates, it suffices now to obtain L^p estimates for the solutions of Maxwell's equations on S_R. Our main result in this paper is:

Theorem 1.3.2. *Let $\Omega = \{x | R - \delta < |x| \leq R\}$, $1 < p < \infty$. Assume that $\vec{H} \in W^{1,p}(\Omega)$, $\vec{E} \in L^p(\Omega)$ in Ω satisfy:*

$$\nabla \times \vec{E} = -i\omega\mu\vec{H},$$
$$\nabla \times \vec{H} = i\omega\epsilon\vec{E}.$$

Then

$$\|\vec{H}\|_{W^{1,p}(\Omega')} \leq C\|\vec{H}\|_{L^p(\Omega)}$$

for any $\Omega' = \{x | R - \delta < R' < |x| < R\} \subset \Omega$.

Remark 1.3.3. In fact since no forcing term is present, Theorem 2.5.2 holds also for $p = 1, \infty$.

Let $\Omega_i = \Omega$ and $\Omega_e = \{x | R < |x| < R + \delta\}$, and $\Omega_2 = \{x | R - \delta < |x| < R + \delta\}$. Thus in Ω_2, the Helmholtz equation (1.2.1) holds. We have

$$\|H\|_{W^{1,p}(\Omega_1)} \leq C\|H\|_{L^p(\Omega_2)},$$

for any $\Omega_1 \subset \Omega_2$ from standard interior elliptic estimates [34]. Let $\Omega_1' = \Omega_i \bigcap \Omega_1$. Then

$$\begin{aligned}\|H\|_{W^{1,p}(\Omega_1')} & \leq C\|H\|_{W^{1,p}(\Omega_1)} \leq C\|H\|_{L^p(\Omega_2)} \\ \leq C(\|H\|_{L^p(\Omega_i)} + \|H\|_{L^p(\Omega_e)}).\end{aligned}$$

In order to prove the theorem, we need to estimate $\|H\|_{L^p(\Omega_e)}$ by $\|H\|_{L^p(\Omega_i)}$.

Claim: $\|H\|_{L^p(\Omega_e)} \leq C\|H\|_{L^p(S_R)}$.

If the claim is true, then we have

$$\|H\|_{W^{1,p}(\Omega_1')} \leq C(\|H\|_{L^p(\Omega_i)} + \|H\|_{L^p(S_R)}).$$

The trace theorem and Nirenberg-Gagliardo inequality [2] imply that

$$\begin{aligned}\|H\|_{L^p(S_R)} \leq C\|H\|_{W^{\frac{1}{2}+\zeta,p}(\Omega_1')} & \leq C\|H\|^a_{W^{1,p}(\Omega_1')}\|H\|^{1-a}_{L^p(\Omega_1')} \\ & \leq \eta\|H\|_{W^{1,p}(\Omega_1')} + C_\eta\|H\|_{L^p(\Omega_1')},\end{aligned}$$

where $0 < \zeta < \frac{1}{2}$, $0 < a < 1$, η is any positive constant, and C_η depends on the choice of η. Thus

$$\|H\|_{W^{1,p}(\Omega_1')} \leq C\|H\|_{L^p(\Omega_i)}.$$

Proof of the claim. We prove the result by examining each of the three possible cases.

Case 1: $p = 2$. Note that

$$\begin{aligned}\|H\|^2_{L^2(S_R)} &= \int_0^{2\pi} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} u_l^m Y_l^m(\theta,\phi) \cdot \\ & \quad \cdot \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \bar{u}_l^m \bar{Y}_l^m(\theta,\phi) R^2 \sin\theta d\theta d\phi \\ &= \sum_{l=0}^{\infty} \sum_{m=-l}^{l} |u_l^m|^2 R^2\end{aligned}$$

by the orthonormality of spherical harmonics. It follows from (1.2.3) that

$$
\begin{aligned}
\|H\|^2_{L^2(\Omega_e)} &= \int_R^{R+\delta}\int_0^{2\pi}\sum_{l=0}^{\infty}\sum_{m=-l}^{l} u_l^m \frac{h_l^{(1)}(kr)}{h_l^{(1)}(kR)} Y_l^m(\theta,\phi)\cdot \\
&\quad \cdot \sum_{l=0}^{\infty}\sum_{m=-l}^{l} \bar{u}_l^m \frac{\bar{h}_l^{(1)}(kr)}{\bar{h}_l^{(1)}(kR)} \bar{Y}_l^m(\theta,\phi) r^2 \sin\theta d\theta d\phi \\
&= \sum_{l=0}^{\infty}\sum_{m=-l}^{l} |u_l^m|^2 \int_R^{R+\delta} \left|\frac{h_l^{(1)}(kr)}{h_l^{(1)}(kR)}\right|^2 r^2 dr \\
&= \sum_{l=0}^{\infty}\sum_{m=-l}^{l} |u_l^m|^2 R^2 \int_R^{R+\delta} \left|\frac{h_l^{(1)}(kr)}{h_l^{(1)}(kR)}\right|^2 \frac{r^2}{R^2} dr \\
&= \sum_{l=0}^{\infty}\sum_{m=-l}^{l} |u_l^m|^2 R^2 \int_R^{R+\delta} \frac{r^2}{R^2} \frac{\dfrac{1+\alpha_1^l \frac{1}{k^2r^2}+\dots+\alpha_l^l \frac{1}{k^{2l}r^{2l}}}{k^2r^2}}{\dfrac{1+\alpha_1^l \frac{1}{k^2R^2}+\dots+\alpha_l^l \frac{1}{k^{2l}R^{2l}}}{k^2R^2}} dr \\
&= \sum_{l=0}^{\infty}\sum_{m=-l}^{l} |u_l^m|^2 R^2 \int_R^{R+\delta} \frac{1+\alpha_1^l \frac{1}{k^2r^2}+\dots+\alpha_l^l \frac{1}{k^{2l}r^{2l}}}{1+\alpha_1^l \frac{1}{k^2R^2}+\dots+\alpha_l^l \frac{1}{k^{2l}R^{2l}}} dr \\
&\le \delta \sum_{l=0}^{\infty}\sum_{m=-l}^{l} |u_l^m|^2 R^2 \\
&\le C\|H\|^2_{L^2(S_R)}.
\end{aligned}
$$

It is worthwhile to note that from the computation above

$$\|H\|_{L^2(S_r)} \le \|H\|_{L^2(S_R)} \quad \text{for all } r \ge R.$$

Case 2: $2 < p \le \infty$.

We only need to consider the case $p = \infty$, the rest follows from Riesz convexity theorem. The idea here is that we show first that for small enough $\delta > 0$, there is a positive function $f(r)$ on $[R, R+\delta]$ such that the maximum of $f(r)|H|$ on Ω_e is on $\partial\Omega_e$, i.e., we have the maximum principle for $f(r)H$ on the domain Ω_e. Remember that this $f(r)$ is needed since H itself can not have the maximum principle. After this modified maximum principle is established, we only need to show that $\|H\|_{L^\infty(S_{R+\delta})} \leq C\|H\|_{L^\infty(S_R)}$.

To construct the function $f(r)$, set $V = f(r)H$. We have

$$\begin{aligned}
\Delta V &= \left(\frac{1}{r^2}\left(\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\right) + \frac{1}{r^2}\Delta_S\right)V \\
&= \frac{\partial^2 H}{\partial r^2}f(r) + 2\frac{\partial H}{\partial r}f'(r) + f''(r)H + \frac{2}{r}\frac{\partial H}{\partial r}f(r) + \frac{2}{r}Hf'(r) + \frac{1}{r^2}\Delta_S Hf(r) \\
&= -k^2Hf(r) + 2\frac{\partial H}{\partial r}f'(r) + f''(r)H + \frac{2}{r}Hf'(r) \\
&= -k^2V + 2\frac{\partial\frac{V}{f}}{\partial r}f' + \frac{f''}{f}V + \frac{2}{r}V\frac{f'}{f} \\
&= -k^2V + 2f'\frac{V'f - Vf'}{f^2} + \frac{f''}{f}V + \frac{2}{r}V\frac{f'}{f} \\
&= [-k^2 - 2(\frac{f'}{f})^2 + \frac{f''}{f} + \frac{2}{r}\frac{f'}{f}]V + \frac{2ff'}{f^2}V_r.
\end{aligned}$$

In order to use maximum principle of elliptic differential equations, we need to find a function f such that

$$k^2 + 2(\frac{f'}{f})^2 - \frac{f''}{f} - \frac{2}{r}\frac{f'}{f} \leq 0.$$

Let $\frac{f'}{f} = y$. Then the equation becomes

$$k^2 + y^2 - y' - \frac{2y}{r} \leq 0.$$

Now set $y = k\ tan(k(r-R))$, $\delta < \frac{\pi}{4k}$. Then $y' = k^2(1+tan^2(k(r-R))) = k^2+y^2$, and $y \geq 0$ on $[R, R+\delta]$. Consequently, $k^2 + y^2 - y' - \frac{2y}{r} \leq 0$ on $[R, R+\delta]$.

It is easy to verify that

$$f = \frac{1}{cosk(r-R)}$$

is a solution for $y = k\ tan(k(r-R))$. Therefore $1 \leq f \leq \sqrt{2}$ on $[R, R+\delta]$ for any $\delta \leq \frac{\pi}{4k}$. When $r \in [R, R+\delta]$, the function $|V|$ achieves its maximum value on the boundary.

Next, we will show that

$$\|H\|_{L^\infty(S_{R+\delta})} \le C\|H\|_{L^\infty(S_R)}.$$

From the arguments for $p = 2$, we know that

$$\|H\|_{L^2(R<r<R+2\delta)} \le C\|H\|_{L^2(S_R)} \le C\|H\|_{L^\infty(S_R)}.$$

The standard elliptical theory concludes that

$$\|H\|_{W^{2,2}(R+\delta/2<r<R+3\delta/2)} \le C\|H\|_{L^2(R<r<R+2\delta)}.$$

The Sobolev embedding theorem implies that

$$\|H\|_{L^\infty(S_{R+\delta})} \le C\|H\|_{W^{2,2}(R+\delta/2<r<R+3\delta/2)}.$$

Combing these estimates yields

$$\|H\|_{L^\infty(S_{R+\delta})} \le C\|H\|_{L^\infty(S_R)}.$$

Case 3: $1 \le p < 2$.

Consider a sequence of smooth function $\{H_n\}$ on S_R, such that $\|H_n - H\|_{L^1(S_R)} \to 0$ as $n \to \infty$. Write H_n in spherical harmonics: $H_n(R,\theta,\phi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} h_{nl}^m Y_l^m(\theta,\phi)$. Define $TH_n(R,\theta,\phi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} \frac{h_l^{(1)}(kr)}{h_l^{(1)}(kR)} h_{nl}^m Y_l^m(\theta,\phi)$. There exists $g(r,\theta,\phi) \in L^\infty(\Omega_e)$ and $g(r,\theta,\phi) = \sum_{k=1}^{N} g_k(\theta,\phi)\chi_{I_k}$, where χ_{I_k} is the characteristic function on I_k, $\bigcup_{k=1}^{N} I_k = \bigcup_{k=1}^{N} [r_k, r_{k+1}] = [R, R+\delta]$, and $\|g_k(\theta,\phi)\|_{L^\infty(\Omega_k)} \le 2$, where $\Omega_k = \{(r,\theta,\phi) | r \in I_k\}$, such that

$$\|Hn\|_{L^1(\Omega_e)} = \|THn(R,\theta,\phi)\|_{L^1(\Omega_e)}$$
$$= |\int_{\Omega_e} THn(R,\theta,\phi)g(r,\theta,\phi)dV|$$
$$= |\sum_{k=1}^{N} \int_{\Omega_e} THn(R,\theta,\phi)g_k(\theta,\phi)\chi_{I_k} dV|$$
$$= |\sum_{k=1}^{N} \int_{\Omega_k} THn(R,\theta,\phi)g_k(\theta,\phi)dV| = I$$

Write $g_k(\theta,\phi)$ in expansion of spherical harmonics:

$$g_k(\theta,\phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \eta_{kl}^m Y_l^m(\theta,\phi),$$

$$I = |\sum_{k=1}^{N} \int_{r_k}^{r_{k+1}} \int_0^{2\pi} \int_0^{\pi} TH(R,\theta,\phi) \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \eta_{kl}^m Y_l^m(\theta,\phi) r^2 \sin\theta d\theta d\phi dr|$$
$$= |\sum_{k=1}^{N} \int_{r_k}^{r_{k+1}} \int_0^{2\pi} \int_0^{\pi} H(R,\theta,\phi)\cdot$$
$$\cdot \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{h_l^{(1)}(kr)}{h_l^{(1)}(kR)} \eta_{kl}^m Y_l^m(\theta,\phi) r^2 \sin\theta d\theta d\phi dr|$$

From Case 2, we know that $\|Tg_k(\theta,\phi)\|_{L^\infty(\Omega_e)} \leq C\| \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \eta_{kl}^m Y_l^m(\theta,\phi)\|_{L^\infty(S_R)}$. Therefore

$$I \leq C\|H\|_{L^1(S_R)} \sum_{k=1}^{N} \|Tg_k\|_{L^\infty(\Omega_e)} |I_k| \leq C\|H\|_{L^1(S_R)}.$$

By the density of $C^\infty(S_R)$ in $L^1(S_R)$, we proved the conclusion for $p = 1$. Again from the Reisz Convexity Theorem, we get

$$\|H\|_{L^p(\Omega_e)} \leq C\|H\|_{L^p(S_R)}$$

for $1 \leq p \leq 2$. □

1.4 Existence and Uniqueness

In this section, we establish the existence and uniqueness of solutions for the linearized SHG problem. By linearization, we mean the following equations:

$$\nabla \times \vec{E}^{(\omega)} = -i\omega\mu_0\vec{H}^{(\omega)},$$
$$\nabla \times \vec{H}^{(\omega)} = i\omega\epsilon_0\vec{E}^{(\omega)}$$

and

$$\nabla \times \vec{E}^{(2\omega)} = -i2\omega\mu_0\vec{H}^{(2\omega)},$$
$$\nabla \times \vec{H}^{(2\omega)} = i2\omega\epsilon_0\vec{E}^{(2\omega)} + i2\omega\sum_{j,k}\chi^{(2)}_{\cdot jk}E^{(\omega)}_j E^{(\omega)}_k.$$

This approximation assumes that the electric field of the incident and diffracted waves at the initial frequency ω inside the nonlinear medium acts as a source for field generation at 2ω. In addition, the SHG is assumed to be so weak that its influence on the field at the initial frequency is negligible.

From the regularity result proved in this paper, we obtain the following well-posedness result.

Theorem 1.4.1. *Let* $S_R = \{x \mid |x| = R\}$, $B_R = \{x \mid |x| < R\}$ *and* $\Omega \subset B_R$. *Suppose* $\chi^{(2)}_{\cdot jk} \in L^\infty(\Omega)$, $\chi^{(2)}_{\cdot jk} = 0$ *in* $B_R \setminus \bar{\Omega}$, *supp*$(m) \subset B_r \setminus \bar{\Omega}$ *for some* $r < R$, *and* $m \in L^\infty(\Omega)$. *Let*

$$\epsilon = \begin{cases} \epsilon_0 & in\ B_R \setminus \bar{\Omega}, \\ \epsilon_1 & in\ \Omega. \end{cases}$$

Then the linearized SHG model problem

$$\nabla \times \vec{E}^{(\omega)} = -i\omega\mu\vec{H}^{(\omega)},$$
$$\nabla \times \vec{H}^{(\omega)} = i\omega\epsilon\vec{E}^{(\omega)} + \vec{m},$$

$$
\begin{aligned}
&\nabla \times \vec{E}^{(2\omega)} = -i2\omega\mu\vec{H}^{(2\omega)}, \\
&\nabla \times \vec{H}^{(2\omega)} = i2\omega\epsilon\vec{E}^{(2\omega)} + i2\omega\sum_{j,k}\chi^{(2)}_{\cdot jk}E^{(\omega)}_j E^{(\omega)}_k \qquad \text{in } B_R, \\
&\frac{\partial \vec{H}}{\partial \vec{n}}|_{S_R} = T_R\vec{H} \qquad \text{on } S_R
\end{aligned}
$$

has a unique solution $(\vec{H}^{(\omega)}, \vec{H}^{(2\omega)}) \in W^{1,p}$ *and* $(\vec{E}^{(\omega)}, \vec{E}^{(2\omega)}) \in L^p$ *for any* $1 < p < \infty$.

Proof. By [1], we know that there is a unique solution $\vec{H}^{(\omega)} \in W^{1,2}(\Omega)$ and $\vec{E}^{(\omega)} \in L^2(\Omega)$.

From the regularity result Theorem 2.5.2, $\vec{H}^{(\omega)} \in W^{1,p}(\Omega)$ and $\vec{E}^{(\omega)} \in L^p(\Omega)$. Hence $\vec{g} = i2\omega\sum_{j,k}\chi^{(2)}_{\cdot jk}E^{(\omega)}_j E^{(\omega)}_k \in L^{p/2}(\Omega)$, for $1 < p < \infty$.

It follows that there exists a unique solution $\vec{H}^{(2\omega)} \in W^{1,p}(\Omega)$ and consequently $\vec{E}^{(2\omega)} \in L^p(\Omega)$ by a similar argument. □

Remark 1.4.2. If in addition, $\chi^{(2)}_{\cdot jk} \in C^\alpha(\Omega)$ and $m \in C^\alpha(\Omega)$, we have $\vec{H}^{(2\omega)} \in W^{1,p}(\Omega)\bigcap C^{1,\alpha}(\Omega)$ and $\vec{E}^{(2\omega)} \in L^p(\Omega)\bigcap C^\alpha(\Omega)$ by the following argument.

According to the standard elliptic regularity theory in [34], $H \in C^\beta(\Omega')$ for some $0 < \beta < 1$ and $\|H\|_{C^\beta(\Omega')} \le C$ with $\Omega' \subset \Omega$.

The standard elliptic regularity results indicate the $C^{1,\alpha}$ regularity of H away from a tubular neighborhood of S and near the boundary S_R.

For any fixed $x^0 \in S$ and $r > 0$, denote

$$
Q_r = \{x| \quad |x_1 - x^0_1| < r, |x_2 - x^0_2| < r, |x_3 - x^0_3| < r\}.
$$

One may choose R such that $Q_R \subset \Omega$. Using a transformation, Q_R is mapped into a set containing a neighborhood Q_{R_0} of the origin. Without loss of generality, the preimage of Q_{R_0} is assumed to contain $Q_{R/2}$. For simplicity, we shall omit the primes and set (in the new coordinate system)

$$Q^+_{R_0} = Q_{R_0} \bigcap \{x_3 > 0\}, Q^-_{R_0} = Q_{R_0} \bigcap \{x_3 < 0\}.$$

Consider a more general model problem in Q_{R_0}

$$\frac{\partial}{\partial x_i}(a_{ij}\frac{\partial u}{\partial x_j}) + \frac{\partial}{\partial x_j}(b_j)u + c_j\frac{\partial u}{\partial x_j} + du + f = 0. \tag{1.4.1}$$

Suppose that $u \in C^\gamma(Q_{R_0}) \bigcap H^1(Q_{R_0})$. Suppose also that the coefficients a_{ij}, $b_j \in C^\gamma(Q^\pm_{R_0})$ and c_j, d, $f \in C(Q^\pm_{R_0})$ have a jump at $x_3 = 0$, b_j, and the principle part of the operator is elliptic in Q_{R_0}, i.e., there is a constant c_0 such that

$$|\sum a_{ij}\xi_i\bar{\xi_j}| \geq c_0|\xi|^2.$$

The $C^{1,\alpha}$ regularity of H near the boundary S can be obtained by the following theorem. See [8] for a proof.

Theorem 1.4.3. *Under the above assumptions, the solution of (1.4.1) satisfies*

$$u \in C^{1,\alpha}(Q^\pm_{R_0/4})$$

for some $0 < \alpha < 1$.

CHAPTER 2

Numerical Solution of Nonlinear Diffraction Problems

2.1 Introduction

Consider a plane wave with frequency ω which is incident on a nonlinear periodic structure (grating). The nonlinearity of the structure gives rise to the diffracted waves at both frequency ω and 2ω. This important phenomenon is known as Second Harmonic Generation (SHG) in nonlinear optics. A significant application of SHG is to obtain coherent beams of light in parts of the spectrum at which lasers cannot be made and to construct optoelectronic devices based on nonlinear effects in waveguides and optical fibers. We refer to [52] for a detailed description of nonlinear optics.

In practice, however, the SHG optical effects are often too weak to be observed. Therefore, modeling and enhancement of SHG are of great interest to potential real applications. Recently, a PDE model was introduced in [48], [49] and [50] to describe nonlinear SHG in diffractive gratings. It is also pointed out in [49] and [50] that the SHG can be greatly enhanced in periodic structures. Questions on the existence and uniqueness have been studied in [8]. We also refer to [12] for more recent results on the optimal design of nonlinear gratings.

To solve the model scattering problem, the first difficulty is to truncate the domain into a bounded computational domain. In [7] and [11] the authors used finite element method based on variational formulation in the bounded domain containing the medium, with periodic condition in x_1 direction and transparent boundary condition on the top and bottom boundaries. The derived transparent boundary condition is represented by a quasi-differential operator and is nonlocal. In practical computations, the infinite series in the definition of the quasi-differential operator have to be truncated. Here we apply the perfectly matched layer (PML) technique to truncate the unbounded domain. PML was first introduced by Berenger in [21]. It provides a reflectionless interface between the region of interest and the PML layers at all incident angles. The layers themselves are lossy, so that after a few layers the wave is significantly attenuated. The main advantage of a perfectly matched layer as a boundary condition is that it provides a reflectionless interface for the outgoing wave at all incident angles. Another advantage is that it preserves the sparse nature of the FEM matrix, so that the matrix system can be solved easily. We refer to [54] for a review on PML methods. In practical applications involving the PML method, there is a judicial compromise between a thin layer, which requires a rapid variation of the artificial material property, and a thick layer, which requires more grid points and hence more computer time and more storage (See [25]). In this paper, we use an a posteriori error estimate to determine the PML parameters. Moreover, the derived a posteriori error estimate shows exponential decay in terms of the distance to the computational domain. This property leads to coarse mesh size away from the computational domain and thus makes the total computational cost insensitive to the thickness of the PML absorbing layer.

Moreover, since the grating surface is usually piecewise smooth, and across the surface the dielectric coefficient is discontinuous, the solution of the scattering problem will have singularities which slow down the finite element convergence when using uniform mesh refinements. The a posteriori estimate adaptively determines the finite element mesh size which overcomes this difficulty.

We refer the readers to [10],[11], and [47] for a general review of the modeling and computation of the grating problem. An introduction of PML and adaptive finite element method applied to linear grating problems may be found in [22].

2.2 Modeling of the Nonlinear Grating Problem

Assume the medium is nonmagnetic ($\mu \equiv \mu_0$) and no external current or charge is present in the field. For convenience, the magnetic permeability is assumed to be unity everywhere. The following time harmonic Maxwell's equations (time dependence $e^{-i\omega t}$) hold:

$$\nabla \times \vec{E} = \frac{i\omega}{c}\vec{H} \qquad \nabla \cdot \vec{H} = 0, \tag{2.2.1}$$

$$\nabla \times \vec{H} = -\frac{i\omega}{c}\vec{D} \qquad \nabla \cdot \vec{D} = 0, \tag{2.2.2}$$

where $\vec{E}$ is the electric field, $\vec{H}$ is the magnetic field, $\vec{D}$ is the electric induction, and c is speed of the light. The constitutive equation is:

$$\vec{D} = \epsilon\vec{E} + 4\pi\chi^{(2)}(x,\omega) : \vec{E}\vec{E},$$

where ϵ is the dielectric permittivity, ω is angular frequency, and $\chi^{(2)}$ is the second order nonlinear susceptibility tensor of third rank, i.e., $\chi^{(2)} : \vec{E}\vec{E}$ is a vector whose jth component is $\sum_{k,l=1}^{3} \chi^{(2)}_{jkl} E_k E_l$, $j = 1, 2, 3$. The medium is said to be linear if $\vec{D} = \epsilon\vec{E}$ or $\chi^{(2)}$ vanishes. In principle, essentially all optical media are nonlinear, i.e., $\vec{D}$ is a nonlinear function of $\vec{E}$.

In this paper, we only consider the 1-D grating problem by assuming that all fields are constant in the x_3 direction. The medium is determined by the dielectric coefficient $\epsilon(x,\omega) = \epsilon(x_1, x_2, \omega)$. Assume that the dielectric coefficient is periodic in x_1 direction with period L:

$$\epsilon(x_1 + nL, x_2, \omega) = \epsilon(x_1, x_2, \omega), \quad \forall x_1, x_2 \in R, \quad n \text{ integer}.$$

Assume that the nonlinear medium is contained in the region

$$\Omega = \{(x_1, x_2)\colon\ 0 < x_1 < L \text{ and } b_2 < x_2 < b_1\}$$

for some positive constants b_1 and b_2.

Assume that ϵ is constant away from a region Ω, *i.e.*, there exist constants ϵ_1 and ϵ_2, such that:

$$\epsilon(x_1, x_2, \omega) = \epsilon_1(\omega) \text{ in } \Omega_1 = \{(x_1, x_2) : x_2 \geq b_1\},$$
$$\epsilon(x_1, x_2, \omega) = \epsilon_2(\omega) \text{ in } \Omega_2 = \{(x_1, x_2) : x_2 \leq b_2\},$$

and ϵ is piecewise constant in Ω with jumps at certain interfaces. Assume further that Ω_1, Ω_2 are linear media.

The assumption on the piecewise linear medium is technical which is needed to assure proper regularity of the solution. The main theoretical results (Theorem 2.4.1, Theorem 2.5.2) remain valid in the case of an inhomogeneous medium with sufficient smooth ϵ and interfaces by the regularity result in [8].

The electric field of the incident and diffracted waves at the fundamental frequency ω_1 inside the nonlinear medium acts as a source for the field generation at the second harmonic frequency $2\omega_1$, and it is assumed that the SHG is so weak that its influence on the field at the fundamental frequency is negligible. This is the well known undepleted pump approximation in the literature. See [49] and [50]. Under

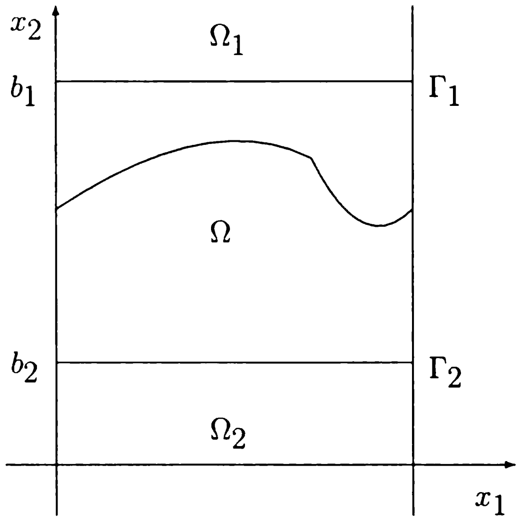


Figure 2.1. Geometry of the grating problem

this assumption, the electric induction $\vec{D}$ may be written as:

$$\vec{D}(x,\omega_1) = \epsilon(x,\omega_1)\vec{E}(x,\omega_1),$$
$$\vec{D}(x,\omega_2) = \epsilon(x,\omega_2)\vec{E}(x,\omega_2) + 4\pi\chi^{(2)}(x,\omega_2) : \vec{E}(x,\omega_1)\vec{E}(x,\omega_1),$$

where $\omega_2 = 2\omega_1$.

In the linear case, TE polarization means the electric field is transversal to (x_1, x_2) plane. TM polarization means the magnetic field is transversal to (x_1, x_2) plane. In the nonlinear case, however, the polarization is determined by group symmetry properties of $\chi^{(2)}$. Here we assume that the electromagnetic fields are TM polarized at the frequency ω_1 and TE polarized at the frequency ω_2. This polarization assumption is known to support a large class of nonlinear optical materials, for example, crystals with cubic symmetry structures. See [12] for detailed information. Therefore

$$\vec{H}(x,\omega_1) = H(x,\omega_1)\vec{x_3},$$
$$\vec{E}(x,\omega_2) = E(x,\omega_2)\vec{x_3}.$$

Define for convenience

$$k_j(x) = \frac{\omega_j}{c}\sqrt{\epsilon(x,\omega_j)}, \quad \text{in } \Omega,$$
$$k_{jl} = \frac{\omega_j}{c}\sqrt{\epsilon_l(\omega_j)}, \quad j,l = 1,2.$$

From equation (2.2.2), we deduce that

$$(\frac{\partial H(x,\omega_1)}{\partial x_2}, -\frac{\partial H(x,\omega_1)}{\partial x_1}, 0) = -\frac{i\omega_1}{c}\epsilon(x,\omega_1)\cdot(E_1(x,\omega_1), E_2(x,\omega_1), E_3(x,\omega_1)).$$

So

$$\frac{\partial H(x,\omega_1)}{\partial x_2} = -\frac{i\omega_1}{c}\epsilon(x,\omega_1)E_1(x,\omega_1),$$
$$\frac{\partial H(x,\omega_1)}{\partial x_1} = -\frac{i\omega_1}{c}\epsilon(x,\omega_1)E_2(x,\omega_1).$$

Also from equation (2.2.1),

$$(\frac{\partial E_3}{\partial x_2} - \frac{\partial E_2}{\partial x_3}, \frac{\partial E_1}{\partial x_3} - \frac{\partial E_3}{\partial x_1}, \frac{\partial E_2}{\partial x_1} - \frac{\partial E_1}{\partial x_2}) = \frac{i\omega_1}{c}(0,0,H),$$

where for simplicity, we omitted the variables. Hence

$$\frac{i\omega_1}{c}H = \frac{\partial E_2}{\partial x_1} - \frac{\partial E_1}{\partial x_2}.$$

It follows that

$$\nabla\cdot(\frac{1}{k_1^2}\nabla H) = \nabla\cdot(\frac{c^2}{\omega_1^2\epsilon}(\frac{\partial H}{\partial x_1}, \frac{\partial H}{\partial x_1}, 0)) = \frac{c^2}{\omega_1^2\epsilon}(\frac{\partial^2 H}{\partial x_1^2} + \frac{\partial^2 H}{\partial x_2^2}),$$
$$H = \frac{c}{i\omega_1}(\frac{\partial E_2}{\partial x_1} - \frac{\partial E_1}{\partial x_2}) = -\frac{c^2}{\omega_1^2\epsilon}(\frac{\partial^2 H}{\partial x_1^2} + \frac{\partial^2 H}{\partial x_2^2}).$$

Therefore we get the equation at frequency ω_1:

$$\nabla\cdot(\frac{1}{k_1^2}\nabla H) + H = 0.$$

By a similar derivation, the equation at frequency ω_2 can be obtained:

$$(\triangle + k_2^2)E = -\frac{4\pi\omega_2^2}{c^2}\sum_{j,l=1,2,3}\chi^{(2)}_{3jl}(x,\omega_2)(\mathbf{E}(x,\omega_1))_j(\mathbf{E}(x,\omega_1))_l$$
$$= \sum_{j,l=1,2}\rho_{j,l}\partial x_j H \partial x_l H,$$

where $\rho_{jl} = (-1)^{j+l}(\frac{16\pi}{(\epsilon(x,\omega_1))^2})\chi^{(2)}_{3jl}$.

Throughout, we assume that $k_{1j} > 0$, $\Re k_{2j} > 0$, $\Im k_{2j} \geq 0$, $\Re k_1(x) > 0$, $\Im k_1(x) \geq 0$.

2.3 Variational Formulation

Let $u_I = e^{i\alpha_1 x_1 - i\beta_1 x_2}$ be the incoming incident plane wave upon the grating surface from the top, where $\alpha_1 = k_{11}\sin\theta$, $\beta_1 = k_{11}\cos\theta$, and $-\frac{\pi}{2} < \theta < \frac{\pi}{2}$ is the angle of the incident. We are interested in the "quasiperiodic" solutions, i.e., solutions $(H,\ E)$, such that $u = He^{-i\alpha_1 x_1}$ and $v = Ee^{-i\alpha_2 x_1}$ ($\alpha_2 = k_{21}\sin\theta$) are periodic in x_1 with period L.

For each integer n, let $\alpha^{(n)} = \frac{2\pi n}{L}$. Since u and v are periodic in x_1, they have the following Fourier expansions:

$$u(x_1,x_2) = \sum_{n\in\mathbb{Z}} u^{(n)}(x_2)e^{i\alpha^{(n)}x_1},$$
$$v(x_1,x_2) = \sum_{n\in\mathbb{Z}} v^{(n)}(x_2)e^{i\alpha^{(n)}x_1},$$

where $u^{(n)}(x_2) = \frac{1}{L}\int_0^L ue^{-i\alpha^{(n)}x_1}dx_1$ and $v^{(n)}(x_2) = \frac{1}{L}\int_0^L ve^{-i\alpha^{(n)}x_1}dx_1$. Hence we have the expansion for H and E:

$$H = ue^{i\alpha_1 x_1} = \sum_{n\in\mathbb{Z}} u^{(n)}e^{i\alpha^{(n)}x_1 + i\alpha_1 x_1},$$
$$E = ve^{i\alpha_2 x_1} = \sum_{n\in\mathbb{Z}} v^{(n)}e^{i\alpha^{(n)}x_1 + i\alpha_2 x_1}.$$

Define $\Gamma_j = \{(x_1,x_2) : 0 < x_1 < L, x_2 = b_j\}$, $j = 1,2$. We wish to reduce the problem to the bounded domain Ω. The radiation condition for the diffraction problem insists that (H,E) is composed of bounded outgoing plane waves in Ω_1 and Ω_2, plus the incident wave u_I in Ω_1.

Since H satisfies the Helmholtz equation $\Delta H + k_{11}^2 H = 0$ in Ω_1, we have

$$\sum_{n \in \mathbb{Z}} [k_{11}^2 - (\alpha^{(n)} + \alpha_1)^2 + \frac{d^2}{dx_2^2} u^{(n)}(x_2)] e^{i(\alpha^{(n)} + \alpha_1)x_1} = 0,$$

$$k_{11}^2 - (\alpha^{(n)} + \alpha_1)^2 + \frac{d^2}{dx_2^2} u^{(n)}(x_2) = 0 \quad \text{for } x_2 \geq b_1. \tag{2.3.1}$$

For any integer n, and $j, l = 1, 2$, define β_{jl}^n that satisfies $(\beta_{jl}^n)^2 = k_{jl}^2 - (\alpha^{(n)} + \alpha_j)^2$ and $\Im(\beta_{jl}^n) \geq 0$. One can easily verify that $\beta_{11}^0 = \beta_1$. Solution of (2.3.1) can then be written as

$$u^{(n)}(x_2) = U_1^{(n)} e^{i\beta_{11}^n x_2} + \tilde{U}_1^{(n)} e^{-i\beta_{11}^n x_2}$$

with complex constants $U_1^{(n)}$ and $\tilde{U}_1^{(n)}$. The radiation condition implies $\tilde{U}_1^{(n)} = 0$ in Ω_1 and gives:

$$H = u_I + \sum_{n \in \mathbb{Z}} U_1^{(n)} e^{i(\alpha^{(n)} + \alpha_1)x_1 + i\beta_{11}^n x_2}, \quad x \in \Omega_1.$$

Similarly, we can deduce the following equations:

$$H = \sum_{n \in \mathbb{Z}} U_2^{(n)} e^{i(\alpha^{(n)} + \alpha_1)x_1 - i\beta_{12}^n x_2}, \quad x \in \Omega_2,$$

$$E = \sum_{n \in \mathbb{Z}} V_1^{(n)} e^{i(\alpha^{(n)} + \alpha_2)x_1 + i\beta_{21}^n x_2}, \quad x \in \Omega_1,$$

$$E = \sum_{n \in \mathbb{Z}} V_2^{(n)} e^{i(\alpha^{(n)} + \alpha_2)x_1 - i\beta_{22}^n x_2}, \quad x \in \Omega_2.$$

For any quasiperiodic function at frequency ω_1, $f = \sum_{n \in \mathbb{Z}} f^{(n)} e^{i(\alpha^{(n)} + \alpha_1)x_1}$ or at frequency ω_2, $f = \sum_{n \in \mathbb{Z}} f^{(n)} e^{i(\alpha^{(n)} + \alpha_2)x_1}$, define respectively the Dirichlet to Neumann operator, which is introduced in [11],

$$T_{jl} f = \sum_{n \in \mathbb{Z}} i\beta_{jl}^{(n)} f^{(n)} e^{i(\alpha^{(n)} + \alpha_j)x_1}, \quad 0 < x_1 < L, j, l = 1, 2.$$

The 1-D grating problem can then be formulated as follows:

$$\nabla \cdot (\frac{1}{k_1^2}\nabla H) + H = 0 \qquad \text{in } \Omega,$$

$$(\triangle + k_2^2)E = \sum_{j,l=1,2} \rho_{j,l}\partial x_j H \partial x_l H \qquad \text{in } \Omega,$$

$$\frac{\partial(H-u_I)}{\partial\nu} - T_{11}(H-u_I) = 0 \qquad \text{on } \Gamma_1,$$

$$\frac{\partial H}{\partial\nu} - T_{12}H = 0 \qquad \text{on } \Gamma_2,$$

$$\frac{\partial E}{\partial\nu} - T_{21}E = 0 \qquad \text{on } \Gamma_1,$$

$$\frac{\partial E}{\partial\nu} - T_{22}E = 0 \qquad \text{on } \Gamma_2,$$

where ν is the unit outer normal to $\partial\Omega$. See [8] for the details.

To find the variational form of this problem, we need to use the above transparent boundary conditions and introduce the following subspace of $H^1(\Omega)$:

$$X_j(\Omega) = \{w \in H^1(\Omega)\colon\ w_\alpha = we^{-i\alpha_j x_1} \text{ is periodic in } x_1 \text{ with period } L\}.$$

Define $\mathcal{B}_j$: $X_j(\Omega) \times X_j(\Omega) \mapsto C$:

$$\mathcal{B}_1(\varphi,\psi) = \int_\Omega (\frac{1}{k_1^2}\nabla\varphi\nabla\overline{\psi} - \varphi\overline{\psi})dx - \sum_{j=1}^{2}\int_{\Gamma_j}\frac{1}{k_{1j}^2}(T_{1j}\varphi)\overline{\psi}dx,$$

$$\mathcal{B}_2(\varphi,\psi) = \int_\Omega \nabla\varphi\nabla\overline{\psi} - \int_\Omega k_2^2\varphi\overline{\psi} - \sum_{j=1}^{2}\int_{\Gamma_j} T_{2j}\varphi\overline{\psi}.$$

Note that $\frac{\partial u_I}{\partial\nu} - T_{11}u_I = -2i\beta_1 u_I$; the weak formulation of the nonlinear 1-D grating problem then reads as follows: Given incoming plane wave $u_I = e^{i\alpha_1 x_1 - i\beta_1 x_2}$, find $H \in X_1(\Omega)$ and $E \in X_2(\Omega)$ such that:

$$\mathcal{B}_1(H,\psi) = -\int_{\Gamma_1}\frac{2i\beta_1}{k_{11}^2}u_I\overline{\psi}dx, \quad \forall\psi \in X_1(\Omega),$$

$$\mathcal{B}_2(E,\psi) = -\sum_{j,l=1,2}\rho_{jl}\int_\Omega \frac{\partial H}{\partial x_j}\frac{\partial H}{\partial x_l}\overline{\psi}dx, \quad \forall\psi \in X_2(\Omega).$$

Assume in the following that the variational problem has a unique solution. Then the general theory in [6] implies that there exists constants $\gamma_1 > 0$, $\gamma_2 > 0$, such that:

$$\sup_{0 \neq \psi \in H^1(\Omega)} \frac{|\mathcal{B}_j(\varphi,\psi)|}{\|\psi\|_{H^1(\Omega)}} \geq \gamma_j \|\psi\|_{H^1(\Omega)}, \quad \forall \varphi \in X_j(\Omega).$$

2.4 PML Formulation

Now we introduce the PML layers. We surround our computational domain Ω with two PML layers of thickness δ_1 and δ_2 in Ω_1 and Ω_2, respectively. The specially designed model medium in the PML layers should be chosen such that either the wave never reaches the outside boundary or the reflected wave is so small that it essentially does not affect the solution in Ω. Let $s(x_2) = s_1(x_2) + is_2(x_2)$ be the model medium property which satisfies $s_1, s_2 \in C(\mathbb{R})$, $s_1 \geq 0$, $s_2 \geq 0$, and $s(x_2) = 1$ for $b_2 \leq x_2 \leq b_1$. Introduce the PML regions:

$$\Omega_1^{PML} = \{(x_1, x_2)\colon\ 0 < x_1 < L \text{ and } b_1 < x_2 < b_1 + \delta_1\},$$

$$\Omega_2^{PML} = \{(x_1, x_2)\colon\ 0 < x_1 < L \text{ and } b_2 - \delta_2 < x_2 < b_2\},$$

$$\Gamma_1^{PML} = \{(x_1, x_2)\colon\ 0 < x_1 < L \text{ and } x_2 = b_1 + \delta_1\},$$

$$\Gamma_2^{PML} = \{(x_1, x_2)\colon\ 0 < x_1 < L \text{ and } x_2 = b_2 - \delta_2\}$$

and the PML differential operators:

$$\mathcal{L}_1 = \frac{\partial}{\partial x_1}\left(\frac{1}{k_1^2(x)} s(x_2) \frac{\partial}{\partial x_1}\right) + \frac{\partial}{\partial x_2}\left(\frac{1}{k_1^2(x)} \frac{1}{s(x_2)} \frac{\partial}{\partial x_2}\right) + s(x_2),$$
$$\mathcal{L}_2 = \frac{\partial}{\partial x_1}\left(s(x_2) \frac{\partial}{\partial x_1}\right) + \frac{\partial}{\partial x_2}\left(\frac{1}{s(x_2)} \frac{\partial}{\partial x_2}\right) + k_2^2(x) s(x_2).$$

Let $D = \{(x_1, x_2) : 0 < x_1 < L, b_2 - \delta_2 < x_2 < b_1 + \delta_1\}$. The PML model can be formulated as follows:

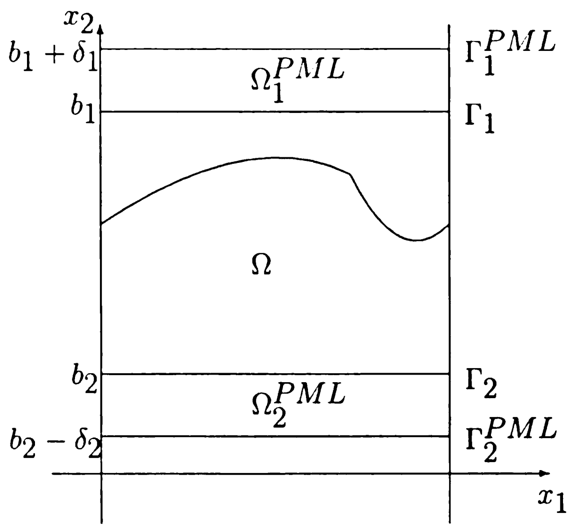


Figure 2.2. Geometry of the PML problem

$$\begin{cases} \mathcal{L}_1 \hat{H} = -g_1 \\ \mathcal{L}_2 \hat{E} = -g_2 \end{cases} \quad \text{in } D,$$

where

$$g_1 = \begin{cases} \mathcal{L}_1 u_I & \text{in } \Omega_1^{PML}, \\ 0 & \text{elsewhere}, \end{cases}$$

$$g_2 = \begin{cases} 0 & \text{in } \Omega_1^{PML} \bigcup \Omega_2^{PML}, \\ -\sum \rho_{jl} \partial x_j \hat{H} \partial x_l \hat{H} & \text{elsewhere} \end{cases}$$

with boundary conditions:

$$\hat{H}(0, x_2) = e^{-i\alpha_1 L} \hat{H}(L, x_2) \qquad \text{for } b_2 - \delta_2 < x_2 < b_1 + \delta_1,$$

$$\hat{E}(0, x_2) = e^{-i\alpha_2 L} \hat{E}(L, x_2) \qquad \text{for } b_2 - \delta_2 < x_2 < b_1 + \delta_1,$$

$$\hat{H} = u_I \qquad \text{on } \Gamma_1^{PML},$$
$$\hat{H} = 0 \qquad \text{on } \Gamma_2^{PML},$$
$$\hat{E} = 0 \qquad \text{on } \Gamma_1^{PML},$$
$$\hat{E} = 0 \qquad \text{on } \Gamma_2^{PML}.$$

Let G be any open set in D, introduce the subspace of $H^1(G)$:

$$X_j(G) = \{w \in H^1(G) : w_\alpha = we^{-\alpha_j x_1} \text{ is periodic in } x_1 \text{ with period } L\}$$

and the sesquilinear form $\mathcal{A}_{jG}$: $X_j(G) \times X_j(G) \mapsto C$ as follows:

$$\mathcal{A}_{1G}(\phi, \psi) = \int_G (\frac{1}{k_1^2(x)} s(x_2) \frac{\partial \phi}{\partial x_1} \frac{\partial \bar{\psi}}{\partial x_1} + \frac{1}{k_1^2(x)} \frac{1}{s(x_2)} \frac{\partial \phi}{\partial x_2} \frac{\partial \bar{\psi}}{\partial x_2} - s(x_2) \phi \bar{\psi}) dx,$$
$$\mathcal{A}_{2G}(\phi, \psi) = \int_G \left(s(x_2) \frac{\partial \phi}{\partial x_1} \frac{\partial \bar{\psi}}{\partial x_1} + \frac{1}{s(x_2)} \frac{\partial \phi}{\partial x_2} \frac{\partial \bar{\psi}}{\partial x_2} - k_2^2(x) s(x_2) \phi \bar{\psi}\right) dx.$$

Define $X_j^\circ(D) = \{w \in X_j(D),\ w = 0 \text{ on } \Gamma_1^{PML} \bigcup \Gamma_2^{PML}\}$. Then the weak formulation of the PML model reads as follows: Find $\hat{H} \in X_1(D)$ and $\hat{E} \in X_2^\circ(D)$, such that $\hat{H} = u_I$ on Γ_1^{PML}, $\hat{H} = 0$ on Γ_2^{PML}, and

$$\mathcal{A}_{1D}(\hat{H}, \psi) = \int_D g_1 \bar{\psi} dx \quad \forall \psi \in X_1^\circ(D), \tag{2.4.1}$$
$$\mathcal{A}_{2D}(\hat{E}, \psi) = \int_D g_2 \bar{\psi} dx \quad \forall \psi \in X_2^\circ(D). \tag{2.4.2}$$

Let $\triangle_{1j}^n = |k_{1j}^2 - (\alpha^{(n)} + \alpha_1)^2|^{\frac{1}{2}}$ and $U_{1j} = \{n : k_{1j}^2 > (\alpha^{(n)} + \alpha_1)^2\}$, $j = 1, 2$. And let

$$\triangle_{1j}^- = \min\{\triangle_{1j}^n : n \in U_{1j}\}, \quad \triangle_{1j}^+ = \min\{\triangle_{1j}^n : n \notin U_{1j}\}.$$

Introduce the following notations:

$$\sigma_1 = \int_{b_1}^{b_1 + \delta_1} s(\tau) d\tau, \quad \sigma_2 = \int_{b_2 - \delta_2}^{b_2} s(\tau) d\tau.$$

$$M_{11} = \max\left(\frac{2\Delta_{11}^-}{e^{2\sigma_1^I\Delta_{11}^-}-1}, \frac{2\Delta_{11}^+}{e^{2\sigma_1^R\Delta_{11}^+}-1}\right),$$

$$M_{12} = \begin{cases} \max\left(\frac{2\Delta_{12}^-}{e^{2\sigma_2^I\Delta_{12}^-}-1}, \frac{2\Delta_{12}^+}{e^{2\sigma_2^R\Delta_{12}^+}-1}\right) & \text{if } \Im\epsilon_2(\omega_1) = 0, \\ \frac{2|k_{12}|}{e^{2\sigma_2^R|\Im k_{12}|}-1} & \text{if } \Im\epsilon_2(\omega_1) > 0, \end{cases}$$

where σ_j^R and σ_j^I are the real and imaginary parts of σ_j, respectively. Define

$$\hat{C} = \sqrt{1+(b_1-b_2)^{-1}}.$$

It is proved in [22] that the problem (2.4.1) has a unique solution $\hat{H}$, if $(M_{11} + M_{12})\hat{C}^2 \leq \gamma_1$, and the following estimate holds:

$$\begin{aligned} |||H-\hat{H}|||_{1\Omega} &:= \sup_{0 \neq \psi \in H^1(\Omega)} \frac{|\mathcal{B}_1(H-\hat{H},\psi)|}{\|\psi\|_{H^1(\Omega)}} \\ &\leq \left(\frac{M_{11}\hat{C}}{k_{11}^2}\right)\|\hat{H}-u_I\|_{L^2(\Gamma_1)} + \left(\frac{M_{12}\hat{C}}{k_{12}^2}\right)\|\hat{H}\|_{L^2(\Gamma_2)}. \end{aligned}$$

Next we prove the existence and uniqueness of (2.4.2) and derive an error estimate between $\hat{E}$ and E. We first find an equivalent form of (2.4.2) in domain Ω. Similar to the previous argument, we write $\hat{E}$ in the expansion $\hat{E} = \sum_{n\in\mathbb{Z}} \hat{v}^{(n)}(x_2)e^{i(\alpha^{(n)}+\alpha_2)x_1}$ and deduce that

$$\hat{E} = \sum_{n\in\mathbb{Z}} \left(\hat{V}_1^{(n)} e^{i\beta_{21}^n \int_{b_1}^{x_2} s(\tau)d\tau} + \hat{\hat{V}}_1^{(n)} e^{-i\beta_{21}^n \int_{b_1}^{x_2} s(\tau)d\tau}\right) e^{i(\alpha^{(n)}+\alpha_2)x_1} \quad \text{in } \Omega_1^{PML},$$

$$\hat{E} = \sum_{n\in\mathbb{Z}} \left(\hat{V}_2^{(n)} e^{i\beta_{22}^n \int_{x_2}^{b_2} s(\tau)d\tau} + \hat{\hat{V}}_2^{(n)} e^{-i\beta_{22}^n \int_{x_2}^{b_2} s(\tau)d\tau}\right) e^{i(\alpha^{(n)}+\alpha_2)x_1} \quad \text{in } \Omega_2^{PML}.$$

Then the constants $\hat{V}_1^{(n)}$, $\hat{\hat{V}}_1^{(n)}$, $\hat{V}_2^{(n)}$ and $\hat{\hat{V}}_2^{(n)}$ can be uniquely determined by the boundary conditions $\hat{E} = 0$ on Γ_1^{PML} and Γ_2^{PML}:

$$
\begin{aligned}
&\hat{V}_1^{(n)} + \hat{\hat{V}}_1^{(n)} = \hat{v}^{(n)}(b_1), \\
&\hat{V}_1^{(n)} e^{i\beta_{21}^n \int_{b_1}^{x_2} s(\tau)d\tau} + \hat{\hat{V}}_1^{(n)} e^{-i\beta_{21}^n \int_{b_1}^{x_2} s(\tau)d\tau} = 0, \\
&\hat{V}_2^{(n)} + \hat{\hat{V}}_2^{(n)} = \hat{v}^{(n)}(b_2), \\
&\hat{V}_2^{(n)} e^{i\beta_{22}^n \int_{x_2}^{b_2} s(\tau)d\tau} + \hat{\hat{V}}_2^{(n)} e^{-i\beta_{22}^n \int_{x_2}^{b_2} s(\tau)d\tau} = 0.
\end{aligned}
$$

Thus we have:

$$
\begin{aligned}
\hat{E} &= \sum_{n \in \mathbb{Z}} \frac{\zeta_{21}^n(x_2)}{\zeta_{21}^n(b_1)} \hat{v}^{(n)}(b_1) e^{i(\alpha^{(n)} + \alpha_2)x_1} \quad \text{in } \Omega_1^{PML}, \\
\hat{E} &= \sum_{n \in \mathbb{Z}} \frac{\zeta_{22}^n(x_2)}{\zeta_{22}^n(b_1)} \hat{v}^{(n)}(b_2) e^{i(\alpha^{(n)} + \alpha_2)x_1} \quad \text{in } \Omega_2^{PML},
\end{aligned}
$$

where

$$
\begin{aligned}
\zeta_{21}^n(x_2) &= e^{-i\beta_{21}^n \int_{x_2}^{b_1 + \delta_1} s(\tau)d\tau} - e^{i\beta_{21}^n \int_{x_2}^{b_1 + \delta_1} s(\tau)d\tau}, \\
\zeta_{22}^n(x_2) &= e^{-i\beta_{22}^n \int_{b_2 - \delta_2}^{x_2} s(\tau)d\tau} - e^{i\beta_{22}^n \int_{b_2 - \delta_2}^{x_2} s(\tau)d\tau}.
\end{aligned}
$$

For any quasiperiodic function $f = \sum f^{(n)} e^{i(\alpha^{(n)} + \alpha_2)x_1}$, define

$$
(T_{2j}^{PML} f)(x_1) = \sum_{n \in \mathbb{Z}} i\beta_{2j}^n \coth(-i\beta_{2j}^n \sigma_j) f^{(n)} e^{i(\alpha^{(n)} + \alpha_2)x_1}, \quad j = 1, 2.
$$

Then

$$
\begin{aligned}
\frac{\partial \hat{E}}{\partial \nu} - T_{21}^{PML} \hat{E} = 0 \quad \text{on } \Gamma_1, \\
\frac{\partial \hat{E}}{\partial \nu} - T_{22}^{PML} \hat{E} = 0 \quad \text{on } \Gamma_2.
\end{aligned}
$$

Introduce the sesquilinear form $\mathcal{B}_2^{PML}$: $X_2(\Omega) \times X_2(\Omega) \mapsto C$ as follows:

$$\mathcal{B}_2^{PML}(\phi, \psi) = \int_\Omega (\nabla\phi\nabla\bar{\psi} - k_2^2(x)\phi\bar{\psi})dx - \sum_{j=1}^{2} \int_{\Gamma_j} (T_{2j}^{PML}\phi)\bar{\psi}dx_1.$$

We get the following variational problem: Find $\vartheta \in X_2(\Omega)$, such that:

$$\mathcal{B}_2^{PML}(\vartheta, \psi) = - \sum_{j,l=1,2} \rho_{jl} \int_\Omega \frac{\partial \hat{H}}{\partial x_j}\frac{\partial \hat{H}}{\partial x_l}\bar{\psi}dx. \tag{2.4.3}$$

The following lemma establishes the relation of this variational problem to the PML model problem (2.4.2). The proof is straight-forward from the above constructions.

Lemma 2.4.1. *Any solution $\hat{E}$ of* (2.4.2) *is a solution of* (2.4.3). *Conversely, any solution ϑ of* (2.4.3) *can be uniquely extended to the whole domain D to be a solution of* (2.4.2).

Let $\triangle_{2j}^n = |k_{2j}^2 - (\alpha^{(n)} + \alpha_2)^2|^{\frac{1}{2}}$ and $U_{2j} = \{n : k_{2j}^2 > (\alpha^{(n)} + \alpha_2)^2\}$, $j = 1, 2$, then $\beta_{2j}^n = \triangle_{2j}^n$ for $n \in U_{2j}$ and $\beta_{2j}^n = i\triangle_{2j}^n$ for $n \notin U_{2j}$. Let

$$\triangle_{2j}^- = \min\{\triangle_{2j}^n, n \in U_{2j}\}, \quad \triangle_{2j}^+ = \min\{\triangle_{2j}^n, n \notin U_{2j}\}.$$

From Lemma 2.2 and Section 5 of [22], we have the following lemma which plays an important role in the subsequent analysis.

Lemma 2.4.2. *For any ϕ, $\psi \in X_2(\Omega)$, the following estimate holds:*

$$|\int_{\Gamma_j} (T_{2j}\phi - T_{2j}^{PML}\phi)\bar{\psi}dx_1| \le M_{2j}\|\phi\|_{L^2(\Gamma_j)}\|\psi\|_{L^2(\Gamma_j)}, \tag{2.4.4}$$

where

$$M_{21} = \max(\frac{2\triangle_{21}^-}{e^{2\sigma_1^I\triangle_{21}^-} - 1}, \frac{2\triangle_{21}^+}{e^{2\sigma_1^R\triangle_{21}^+} - 1}),$$

$$M_{22} = \begin{cases} \max(\frac{2\triangle_{22}^-}{e^{2\sigma_2^I\triangle_{22}^-} - 1}, \frac{2\triangle_{22}^+}{e^{2\sigma_2^R\triangle_{22}^+} - 1}) & \text{if } \Im\epsilon_2(\omega_2) = 0, \\ \frac{2|k_{22}|}{e^{2\sigma_2^R|\Im k_{22}|} - 1} & \text{if } \Im\epsilon_2(\omega_2) > 0. \end{cases}$$

Lemma 2.4.3. *For any $\psi \in X_2(\Omega)$,*

$$\|\psi\|_{L^2(\Gamma_j)} \le \|\psi\|_{H^{\frac{1}{2}}(\Gamma_j)} \le \hat{C}\|\psi\|_{H^1(\Omega)} \tag{2.4.5}$$

with $\hat{C} = \sqrt{1 + (b_1 - b_2)^{-1}}$, *if*

$$\psi(x_1, b_j) = \sum \psi_{\alpha_2}^{(n)}(b_j)e^{i(\alpha^{(n)} + \alpha_2)x_1} \quad \textit{on } \Gamma_j,$$
$$\|\psi\|_{H^{\frac{1}{2}}(\Gamma_j)} = (L \sum_{n \in \mathbb{Z}} (1 + |\alpha^{(n)} + \alpha_2|^2)^{\frac{1}{2}}|\psi_{\alpha_2}^{(n)}|^2)^{\frac{1}{2}}.$$

Theorem 2.4.1. *Let $\gamma_2 > 0$ be the constant in the inf-sup condition, and $(M_{21} + M_{22})\hat{C}^2 < \gamma_2$. Then the problem (2.4.3) attains a unique solution $\hat{E}$. Moreover, the following estimate holds:*

$$\begin{aligned} |||E - \hat{E}|||_{2\Omega} := \sup_{0 \ne \psi \in H^1(\Omega)} \frac{|\mathcal{B}_2(E - \hat{E}, \psi)|}{\|\psi\|_{H^1(\Omega)}} \\ \le \hat{C}M_{21}\|\hat{E}\|_{L^2(\Gamma_1)} + \hat{C}M_{22}\|\hat{E}\|_{L^2(\Gamma_2)} \\ + \tilde{C}\|\hat{H} - H\|_{H^1(\Omega)}[\|\hat{H}\|_{H^{1+\delta}(\Omega)} + \|H\|_{H^{1+\delta}(\Omega)}\|] \end{aligned} \tag{2.4.6}$$

for some constant $\tilde{C}$ which depends on the data of the original grating problem and some constant $\delta \in (0, \frac{1}{2})$.

Proof. It follows from Lemma 2.4.2 and Lemma 2.4.3 that

$$\begin{aligned} |\mathcal{B}_2^{PML}(\phi, \psi)| &\ge |\mathcal{B}_2(\phi, \psi)| - \sum_{j=1}^{2} \int_{\Gamma_j} (T_{2j}\phi - T_{2j}^{PML}\phi)\bar{\psi}dx_1 \\ &\ge |\mathcal{B}_2(\phi, \psi)| - (M_{21} + M_{22})\hat{C}^2\|\phi\|_{H^1(\Omega)}\|\psi\|_{H^1(\Omega)}. \end{aligned}$$

From the assumption $(M_{21} + M_{22})\hat{C}^2 \le \gamma_2$, it is obvious that the bilinear form $\mathcal{B}_2^{PML}$ satisfies the inf-sup condition, and hence the problem (2.4.3) has a unique solution. It remains to prove the estimate (2.4.6).

Clearly,

$$\begin{aligned}
\mathcal{B}_2(E-\hat{E},\psi) &= \mathcal{B}_2^{PML}(\hat{E},\psi) - \mathcal{B}_2(\hat{E},\psi) + \mathcal{B}_2(E,\psi) - \mathcal{B}_2^{PML}(\hat{E},\psi) \\
&= \int_{\Gamma_1}(T_{21} - T_{21}^{PML})\hat{E}\bar{\psi}dx_1 + \int_{\Gamma_2}(T_{22} - T_{22}^{PML})\hat{E}\bar{\psi}dx_1 \\
&\quad + \sum_{j,l=1,2} \rho_{jl}\int_\Omega (\frac{\partial \hat{H}}{\partial x_j}\frac{\partial \hat{H}}{\partial x_l} - \frac{\partial H}{\partial x_j}\frac{\partial H}{\partial x_l})\bar{\psi}dx,
\end{aligned}$$

By Hölder's inequality,

$$\begin{aligned}
&|\sum_{j,l=1,2} \rho_{jl}\int_\Omega (\frac{\partial \hat{H}}{\partial x_j}\frac{\partial \hat{H}}{\partial x_l} - \frac{\partial H}{\partial x_j}\frac{\partial H}{\partial x_l})\bar{\psi}dx| \\
&= |\sum_{j,l=1,2} \rho_{jl}\int_\Omega (\frac{\partial \hat{H}}{\partial x_j}\frac{\partial(\hat{H}-H)}{\partial x_l} + \frac{\partial(\hat{H}-H)}{\partial x_j}\frac{\partial H}{\partial x_l})\bar{\psi}dx| \\
&\leq \sum_{j,l=1,2} |\rho_{jl}|[|\int_\Omega \frac{\partial \hat{H}}{\partial x_j}\frac{\partial(\hat{H}-H)}{\partial x_l}\bar{\psi}dx| + |\int_\Omega \frac{\partial(\hat{H}-H)}{\partial x_j}\frac{\partial H}{\partial x_l}\bar{\psi}dx|] \\
&\leq \sum_{j,l=1,2} |\rho_{jl}|[\|\hat{H}-H\|_{H^1(\Omega)}(\int_\Omega (\frac{\partial \hat{H}}{\partial x_j})^2\bar{\psi}^2dx)^{\frac{1}{2}} \\
&\quad + \|\hat{H}-H\|_{H^1(\Omega)}(\int_\Omega (\frac{\partial H}{\partial x_l})^2\bar{\psi}^2dx)^{\frac{1}{2}}] \\
&\leq \sum_{j,l=1,2} |\rho_{jl}|\|\hat{H}-H\|_{H^1(\Omega)}\{[\int_\Omega (\frac{\partial \hat{H}}{\partial x_j})^{2p}dx]^{\frac{1}{2p}}(\int_\Omega \bar{\psi}^{2q}dx)^{\frac{1}{2q}} \\
&\quad + [\int_\Omega (\frac{\partial H}{\partial x_l})^{2p}dx]^{\frac{1}{2p}}(\int_\Omega \bar{\psi}^{2q}dx)^{\frac{1}{2q}}\} \\
&\qquad \text{for some } 1 < p,q < \infty, \text{ such that } \frac{1}{p} + \frac{1}{q} = 1, \\
&\leq \tilde{C_2}\sum_{j,l=1,2} |\rho_{jl}|\|\hat{H}-H\|_{H^1(\Omega)}[\|H\|_{W^{1,2p}(\Omega)} \\
&\quad + \|\hat{H}\|_{W^{1,2p}(\Omega)}]\|\psi\|_{L^{2q}(\Omega)},
\end{aligned}$$

for some constant $\tilde{C_2}$. By [12], [28], $H, \hat{H} \in H^{1+\delta}(\Omega)$ for some $\delta \in (0, \frac{1}{2})$. Take $p = \frac{1}{1-\delta}$, $q = \frac{1}{\delta}$, and using Sobolev imbedding theorem, we have:

$$| \sum_{j,l=1,2} \rho_{jl} \int_\Omega (\frac{\partial \hat{H}}{\partial x_j}\frac{\partial \hat{H}}{\partial x_l} - \frac{\partial H}{\partial x_j}\frac{\partial H}{\partial x_l})\bar{\psi} dx|$$

$$\leq \tilde{C}\|\hat{H} - H\|_{H^1(\Omega)} [\|\hat{H}\|_{H^{1+\delta}(\Omega)} + \|H\|_{H^{1+\delta}(\Omega)}\|] \|\psi\|_{H^1(\Omega)},$$

where $\tilde{C}$ depends on the data of the original grating problem. □

2.5 Discrete Problem

In this section we introduce the finite element approximation of the PML problems. Let M_h be a regular triangulation of the domain D. Recall that any triangle $T \in M_h$ is considered closed. We assume that any element T must be completely included in $\overline{\Omega_1^{PML}}$, $\overline{\Omega_2^{PML}}$ or $\bar{\Omega}$. We also require that if $(0, z)$ is a node on the left boundary, then (L, z) is also a node on the right boundary, and vice versa. Let $V_{jh}(D) \in X_j(D)$ be the conforming linear finite element spaces and $V_{jh}^\circ(D) = V_{jh}(D) \bigcap X_j^\circ(D)$. Denote by I_h: $C(\bar{D}) \mapsto V_{1h}(D)$ the standard finite element interpolation operator.

The finite element approximation to the PML problem reads as follows: Find $\hat{H}_h \in V_{1h}(D)$ and $\hat{E}_h \in V_{2h}(D)$, such that $\hat{H}_h = I_h u_I$ on Γ_1^{PML}, $\hat{H}_h = 0$ on Γ_2^{PML}, $\hat{E}_h = 0$ on Γ_1^{PML}, $\hat{E}_h = 0$ on Γ_2^{PML}, and

$$\mathcal{A}_{1D}(\hat{H}_h, \psi_h) = \int_D g_1 \bar{\psi}_h dx, \forall \psi_h \in V_{1h}^\circ(D), \quad (2.5.1)$$

$$\mathcal{A}_{2D}(\hat{E}_h, \psi_h) = \int_D g_{2h} \bar{\psi}_h dx, \forall \psi_h \in V_{2h}^\circ(D), \quad (2.5.2)$$

where

$$g_{2h} = \begin{cases} 0 & \text{in } \Omega_1^{PML} \bigcup \Omega_2^{PML}, \\ -\sum_{j,l=1,2} \rho_{jl} \partial_{x_j} \hat{H}_h \partial_{x_l} \hat{H}_h & \text{elsewhere.} \end{cases}$$

Assume the problem (2.5.1) and (2.5.2) has a unique solution $(\hat{H}_h, \hat{E}_h) \in V_{1h}(D) \times V_{2h}(D)$. Let

$$A_1(x) = \begin{pmatrix} A_{111} & 0 \\ 0 & A_{122} \end{pmatrix} = \begin{pmatrix} \dfrac{s(x_2)}{k_1^2(x)} & 0 \\ 0 & \dfrac{1}{k_1^2(x)s(x_2)} \end{pmatrix}$$

$$A_2(x) = \begin{pmatrix} A_{211} & 0 \\ 0 & A_{222} \end{pmatrix} = \begin{pmatrix} s(x_2) & 0 \\ 0 & \dfrac{1}{s(x_2)} \end{pmatrix}$$

$$B_1(x) = s(x_2),$$

$$B_2(x) = k_2^2(x)s(x_2).$$

Then

$$\mathcal{L}_1 = \nabla \cdot (A_1(x)\nabla) + B_1(x),$$

$$\mathcal{L}_2 = \nabla \cdot (A_2(x)\nabla) + B_2(x),$$

$$\mathcal{A}_{1D}(\phi, \psi) = \int_D (A_1(x)\nabla\phi\nabla\bar{\psi} - B_1(x)\phi\bar{\psi})dx,$$

$$\mathcal{A}_{2D}(\phi, \psi) = \int_D (A_2(x)\nabla\phi\nabla\bar{\psi} - B_2(x)\phi\bar{\psi})dx.$$

For any $T \in M_h$, denote by h_T its diameter. Let B_h denote the set of all sides that do not lie on Γ_j, $j = 1, 2$. For any $e \in B_h$, h_e stands for its length. For any $T \in M_h$, introduce the residuals:

$$R_{1T} := \mathcal{L}_1 \hat{H}_h|_T + g_1|_T \tag{2.5.3}$$

$$R_{2T} := \mathcal{L}_2 \hat{E}_h|_T + g_{2h}|_T \tag{2.5.4}$$

For any interior side $e \in B_h$ which is the common side of T_1 and $T_2 \in M_h$, define the jump residuals across e as:

$$J_{1e} = (A_1 \nabla \hat{H}_h|_{T_1} - A_1 \nabla \hat{H}_h|_{T_2}) \cdot \nu_e, \tag{2.5.5}$$

$$J_{2e} = (A_2 \nabla \hat{E}_h|_{T_1} - A_2 \nabla \hat{E}_h|_{T_2}) \cdot \nu_e, \tag{2.5.6}$$

where ν_e is the unit normal vector to e pointing from T_2 to T_1. If e is the side on the left boundary and e' is the corresponding side on the right boundary which is also a side of some element of T', we define the jump residuals as:

$$J_{1e} = A_{111}[\frac{\partial}{\partial x_1}(\hat{H}_h|_T) - e^{-i\alpha_1 L}\frac{\partial}{\partial x_1}(\hat{H}_h|_{T'})], \tag{2.5.7}$$

$$J_{1e'} = A_{111}[e^{i\alpha_1 L}\frac{\partial}{\partial x_1}(\hat{H}_h|_T) - \frac{\partial}{\partial x_1}(\hat{H}_h|_{T'})], \tag{2.5.8}$$

$$J_{2e} = A_{211}[\frac{\partial}{\partial x_1}(\hat{E}_h|_T) - e^{-i\alpha_2 L}\frac{\partial}{\partial x_1}(\hat{E}_h|_{T'})], \tag{2.5.9}$$

$$J_{2e'} = A_{211}[e^{i\alpha_2 L}\frac{\partial}{\partial x_1}(\hat{E}_h|_T) - \frac{\partial}{\partial x_1}(\hat{E}_h|_{T'})]. \tag{2.5.10}$$

For any $T \in M_h$, denote by η_{jT} the local error estimator, which is defined as follows:

$$\eta_{jT} = \max_{x \in \tilde{T}} \rho_j(x_2)[h_T\|R_{jT}\|_{L^2(T)} + (\frac{1}{2}\sum_{e \in T} h_e\|J_{je}\|^2_{L^2(e)})^{\frac{1}{2}}], \quad j = 1, 2,$$

where $\tilde{T}$ is the union of all elements having nonempty intersection with T and

$$\rho_j(x_2) = \begin{cases} |s(x_2)|e^{-R_{jk}(x_2)} & x \in \overline{\Omega_k^{PML}}, k = 1, 2, \\ 1 & x \in \Omega, \end{cases} \qquad j = 1, 2$$

with $R_{jk}(x_2)$ defined as:

$$R_{j1}(x_2) = \min(\triangle_{j1}^{-}\int_{b_1}^{x_2} s_2(\tau)d\tau, \triangle_{j1}^{+}\int_{b_1}^{x_2} s_1(\tau)d\tau),$$

$$R_{j2}(x_2) = \begin{cases} \min(\triangle_{j2}^{-}\int_{x_2}^{b_2} s_2(\tau)d\tau, \triangle_{j2}^{+}\int_{x_2}^{b_2} s_1(\tau)d\tau)) & \text{if } \Im\epsilon_2(\omega_j) = 0, \\ |\Im k_{j2}|\int_{x_2}^{b_2} s_1(\tau)d\tau & \text{if } \Im\epsilon_2(\omega_j) > 0. \end{cases}$$

Define also

$$M_{13} = \max(\frac{2\triangle_{11}^{-}e^{-\triangle_{11}^{-}\sigma_1^I}}{1 - e^{-2\triangle_{11}^{-}\sigma_1^I}}, \frac{2\triangle_{11}^{+}e^{-\triangle_{11}^{+}\sigma_1^R}}{1 - e^{-2\triangle_{11}^{+}\sigma_1^R}}),$$

$$C_{j1} = \hat{C}\max(\frac{2k_{j1}\delta_1^{\frac{1}{2}}}{1-e^{-2\Delta_{j1}^{-}\sigma_1^I}}, \frac{2(1+2\delta_1(\Delta_{j1}^{+}+k_{j1}))^{\frac{1}{2}}}{1-e^{-2\Delta_{j1}^{+}\sigma_1^R}}),$$

$$C_{j2} = \begin{cases} \hat{C}\max(\frac{2k_{j2}\delta_2^{\frac{1}{2}}}{1-e^{-2\Delta_{j2}^{-}\sigma_2^I}}, \frac{2(1+2\delta_2(\Delta_{j2}^{+}+k_{j2}))^{\frac{1}{2}}}{1-e^{-2\Delta_{j2}^{+}\sigma_2^R}}) & \text{if } \Im\epsilon_2(\omega_j) = 0, \\ \hat{C}\frac{2[\max(1,|k_{j2}|)(1+2\delta_2(|\Im k_{j2}|+|k_{j2}|))]^{\frac{1}{2}}}{1-e^{-2\sigma_2^R|\Im k_{j2}|}} & \text{if } \Im\epsilon_2(\omega_j) > 0 \end{cases}$$

for $j = 1, 2$. The following is the a posterior estimate of the magnetic field at frequency ω which is proved in [22]:

Theorem 2.5.1. *There exists a constant $C > 0$, depending only on the minimum angle of the mesh M_h, such that the following a posterior error estimate is valid:*

$$|||H - \hat{H}_h|||_{1\Omega} \leq (\frac{\hat{C}M_{11}}{k_{11}^2})\|\hat{H}_h - u_I\|_{L^2(\Gamma_1)} + (\frac{\hat{C}M_{12}}{k_{12}^2})\|\hat{H}_h\|_{L^2(\Gamma_2)} \tag{2.5.11}$$

$$+ (\frac{\hat{C}M_{13}}{k_{11}^2})\|I_h u_I - u_I\|_{L^2(\Gamma_1^{PML})} \tag{2.5.12}$$

$$+ C(1 + C_{11} + C_{12})(\sum_{T\in M_h} \eta_{1T}^2)^{\frac{1}{2}}.$$

We next establish the corresponding estimate for the electric field at frequency $2\omega_1$, which is the main error estimate of this paper.

Theorem 2.5.2. *The following estimate holds:*

$$|||E - \hat{E}_h|||_{2\Omega} \leq (\hat{C}M_{21})\|\hat{E}_h\|_{L^2(\Gamma_1)} + (\hat{C}M_{22})\|\hat{E}_h\|_{L^2(\Gamma_2)} \tag{2.5.13}$$

$$+ C(1 + C_{11} + C_{12})(\sum_{T\in M_h} \eta_{2T}^2)^{\frac{1}{2}}$$

$$+ (\frac{\tilde{C}\hat{C}M_{11}}{k_{11}^2})(\|H\|_{H^{1+\delta}(\Omega)} + \|\hat{H}_h\|_{H^{1+\delta}(\Omega)})\|\hat{H}_h - u_I\|_{L^2(\Gamma_1)}$$

$$+ (\frac{\tilde{C}\hat{C}M_{12}}{k_{12}^2})(\|H\|_{H^{1+\delta}(\Omega)} + \|\hat{H}_h\|_{H^{1+\delta}(\Omega)})\|\hat{H}_h\|_{L^2(\Gamma_2)}$$

$$+ (\frac{\tilde{C}\hat{C}M_{13}}{k_{11}^2})(\|H\|_{H^1+\delta(\Omega)} + \|\hat{H}_h\|_{H^1+\delta(\Omega)})\|I_h u_I - u_I\|_{L^2(\Gamma_1^{PML})}$$

$$+ \tilde{C}C(1 + C_{21} + C_{22})(\|H\|_{H^1+\delta(\Omega)} + \|\hat{H}_h\|_{H^1+\delta(\Omega)})(\sum_{T \in M_h} \eta_{1T}^2)^{\frac{1}{2}}.$$

In order to prove this result, we first establish some lemmas. For any $\psi \in X_2(\Omega)$, we extend it to be in $X_2(D)$ denoted by $\tilde{\psi}$ as follows:

$$\tilde{\psi}(x_1, x_2) = \sum_{n \in \mathbb{Z}} \frac{\bar{\zeta}_{2j}^{(n)}(x_2)}{\bar{\zeta}_{2j}(b_i)} \psi_{\alpha_2}^{(n)}(b_j) e^{i(\alpha^{(n)} + \alpha_2)x_1} \quad \text{in } \Omega_j^{PML}, \quad j = 1, 2.$$

Lemma 2.5.1. *([22]) Let ν_j be unit outer normal to Ω_j^{PML}. Then for any ϕ, $\psi \in X_2(\Omega)$, the following identity holds:*

$$\int_{\Gamma_j} T_{2j}^{PML} \phi \bar{\psi} dx_1 = - \int_{\Gamma_j} \phi \frac{\partial \bar{\tilde{\psi}}}{\partial \nu_j} dx_1. \tag{2.5.14}$$

In what follows, for the sake of simplicity, whenever no confusion of the notation is incurred, we shall not distinguish $\tilde{\psi}$ from ψ in Ω_j^{PML}.

Lemma 2.5.2. *(error representation formula) For any $\psi \in X_2(\Omega)$, let ψ be extended to the whole domain D as above, and $\psi_h \in V_{2h}^{\circ}(D)$,*

$$\begin{aligned}
\mathcal{B}_2(E - \hat{E}_h, \psi) = & \int_D g_{2h} \overline{(\psi - \psi_h)} dx - \mathcal{A}_{2D}(\hat{E}_h, \psi - \psi_h) \\
& + \int_{\Gamma_1} (T_{21} - T_{21}^{PML}) \hat{E}_h \bar{\psi} dx_1 \\
& + \int_{\Gamma_2} (T_{22} - T_{22}^{PML}) \hat{E}_h \bar{\psi} dx_1 \\
& + \sum_{j,l=1,2} \rho_{jl} \int_\Omega (\frac{\partial \hat{H}_h}{\partial x_j} \frac{\partial \hat{H}_h}{\partial x_l} - \frac{\partial H}{\partial x_j} \frac{\partial H}{\partial x_l}) \bar{\psi} dx.
\end{aligned} \tag{2.5.15}$$

Proof. From the definition,

$$\mathcal{B}_2(E - \hat{E}_h, \psi) = \mathcal{B}_2(E - \hat{E}, \psi) + \mathcal{B}_2(\hat{E} - \hat{E}_h, \psi)$$

$$= \int_{\Gamma_1} (T_{21} - T_{21}^{PML}) \hat{E} \bar{\psi} dx_1 + \int_{\Gamma_2} (T_{22} - T_{22}^{PML}) \hat{E} \bar{\psi} dx_1$$

$$+ \sum_{j,l=1,2} \rho_{jl} \int_{\Omega} (\frac{\partial \hat{H}}{\partial x_j} \frac{\partial \hat{H}}{\partial x_l} - \frac{\partial H}{\partial x_j} \frac{\partial H}{\partial x_l}) \bar{\psi} dx$$

$$+ \mathcal{B}_2^{PML}(\hat{E} - \hat{E}_h, \psi) - \sum_{j=1}^{2} \int_{\Gamma_j} (T_{2j} - T_{2j}^{PML})(\hat{E} - \hat{E}_h) \bar{\psi} dx_1$$

$$= \int_{\Gamma_1} (T_{21} - T_{21}^{PML}) \hat{E}_h \bar{\psi} dx_1 + \int_{\Gamma_2} (T_{22} - T_{22}^{PML}) \hat{E}_h \bar{\psi} dx_1$$

$$+ \sum_{j,l=1,2} \rho_{jl} \int_{\Omega} (\frac{\partial \hat{H}}{\partial x_j} \frac{\partial \hat{H}}{\partial x_l} - \frac{\partial H}{\partial x_j} \frac{\partial H}{\partial x_l}) \bar{\psi} dx + \mathcal{B}_2^{PML}(\hat{E} - \hat{E}_h, \psi).$$

Also

$$\mathcal{B}_2^{PML}(\hat{E} - \hat{E}_h, \psi) = \mathcal{A}_{2\Omega}(\hat{E} - \hat{E}_h, \psi) - \sum_{j=1}^{2} \int_{\Gamma_j} T_{2j}^{PML}(\hat{E} - \hat{E}_h) \bar{\psi} dx_1$$

$$= \mathcal{A}_{2\Omega}(\hat{E} - \hat{E}_h, \psi) + \sum_{j=1}^{2} \int_{\Gamma_j} (\hat{E} - \hat{E}_h) \frac{\partial \bar{\psi}}{\partial \nu_j} dx_1$$

and from $\mathcal{L}_2 \bar{\psi} = 0$ and Green formula

$$\mathcal{A}_{2\Omega_j^{PML}}(\hat{E} - \hat{E}_h, \psi) = \int_{\Gamma_j} (\hat{E} - \hat{E}_h) \frac{\partial \bar{\psi}}{\partial \nu_j} dx_1.$$

Hence

$$\mathcal{B}_2^{PML}(\hat{E} - \hat{E}_h, \psi) = \mathcal{A}_{2D}(\hat{E} - \hat{E}_h, \psi)$$

$$= \int_D g_{2h} (\overline{\psi - \psi_h}) dx - \mathcal{A}_{2D}(\hat{E}_h, \psi - \psi_h) + \int_D (g_2 - g_{2h}) \bar{\psi} dx,$$

which completes the proof. $\square$

Lemma 2.5.3. *([22]) For any $\psi \in X_2(\Omega)$, let ψ be extended to D as before. Then the following estimate holds:*

$$\|s^{-1} e^{R_{2j}} \nabla \psi\|_{L^2(\Omega_j^{PML})} \leq C_{2j} \|\psi\|_{H^1(\Omega)}, \quad j = 1, 2. \tag{2.5.16}$$

We are now ready to prove Theorem 2.5.2.

Proof. Proof of Theorem 2.5.2 From the definition,

$$\begin{aligned}\mathcal{B}_2(E-\hat{E}_h,\psi) &= \int_D g_{2h}(\overline{\psi-\psi_h})dx - \mathcal{A}_{2D}(\hat{E}_h,\psi-\psi_h)\\ &+ \int_{\Gamma_1}(T_{21}-T_{21}^{PML})\hat{E}_h\bar{\psi}dx_1\\ &+ \int_{\Gamma_2}(T_{22}-T_{22}^{PML})\hat{E}_h\bar{\psi}dx_1\\ &+ \sum_{j,l=1,2}\rho_{jl}\int_\Omega\left(\frac{\partial\hat{H}_h}{\partial x_j}\frac{\partial\hat{H}_h}{\partial x_l}-\frac{\partial H}{\partial x_j}\frac{\partial H}{\partial x_l}\right)\bar{\psi}dx\\ &= III+IV+V+VI+VII.\end{aligned}$$

By integration by parts and using (2.5.3)-(2.5.10),

$$III+IV = \sum_{T\in M_h}\left(\int_T R_{2T}(\overline{\psi-\psi_h})dx + \sum_{e\subset\partial T}\frac{1}{2}\int_e J_{2e}(\overline{\psi-\psi_h})dx\right).$$

Using the interpolation estimate in [51] and Lemma 2.5.3, we get

$$\begin{aligned}|III+IV| &\le C\sum_{T\in M_h}\eta_{2T}\|\rho_2^{-1}\nabla\psi\|_{L^2(\tilde{T})}\\ &\le C(1+C_{21}+C_{22})\left(\sum_{T\in M_h}\eta_{2T}^2\right)^{\frac{1}{2}}\|\psi\|_{H^1(\Omega)}\end{aligned}$$

It follows from Lemma 2.4.2 and Lemma 2.4.3 that

$$|V+VI| \le (\hat{C}M_{21}\|\hat{E}_h\|_{L^2(\Gamma_1)} + \hat{C}M_{22}\|\hat{E}_h\|_{L^2(\Gamma_2)})\|\psi\|_{H^1(\Omega)}.$$

By an argument similar to that used in the proof of Theorem 2.4.1, we conclude that

$$\begin{aligned}|VII| &= \left|\sum_{j,l=1,2}\rho_{jl}\int_\Omega\left(\frac{\partial\hat{H}_h}{\partial x_j}\frac{\partial\hat{H}_h}{\partial x_l}-\frac{\partial H}{\partial x_j}\frac{\partial H}{\partial x_l}\right)\bar{\psi}dx\right|\\ &\le \tilde{C}(\|H\|_{H^{1+\delta}(\Omega)} + \|\hat{H}_h\|_{H^{1+\delta}(\Omega)})\||\hat{H}_h-H|\|_{1\Omega}\|\psi\|_{H^1(\Omega)},\end{aligned}$$

where $\tilde{C}$ depends on the data of the original grating problem by Theorem 2.4.1. The proof is now complete. □

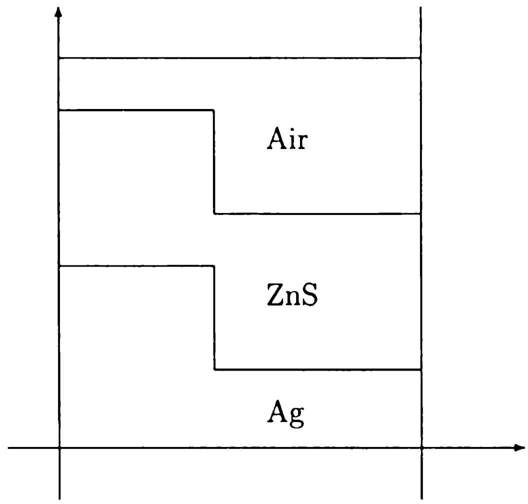


Figure 2.3. ZnS overcoated binary silver gratings

2.6 Numerical Examples

Our first example is from [12]. See also [22] for the implementation of the algorithm. This example is concerned with the grating enhancement of the SHG effects for ZnS overcoated binary silver gratings, see Figure 2.3. The enhancement of the field at 2ω is computed and shown in Figure 2.4 with respect to the associated flat structure. Here, the period of the grating is $L = 0.4\ \mu m$, the incident angle is 28.92°, and the wavelength $\lambda = 1.06\ \mu m$. The results were obtained for a thickness $t = 0.33\ \mu m$ of the coating layer, the fill factor 0.43 with respect to the groove depth d.

Another example comes from [43]. The structure is a subwavelength square grating of the period $L = 0.65\lambda$, the fill factor $F = 0.09$, and the depth varying from $d = 0.01\lambda$ to $d = 1.01\lambda$. The refractive index of the material is taken to be $n_1 = 3.346$ at the fundamental frequency and $n_2 = 3.539$ at the second harmonic frequency, corresponding to the material properties of GaAs at $\lambda_1 = 1.907\mu m$ and $\lambda_2 = 0.954\mu m$, respectively. The nonlinear coefficient is taken to be $240\mu m/V$. The incident angle is 30°. Figure 2.5 shows the enhancement of the grating structure with respect to the bulk material.

Figure 2.4. Groove depth and enhancement

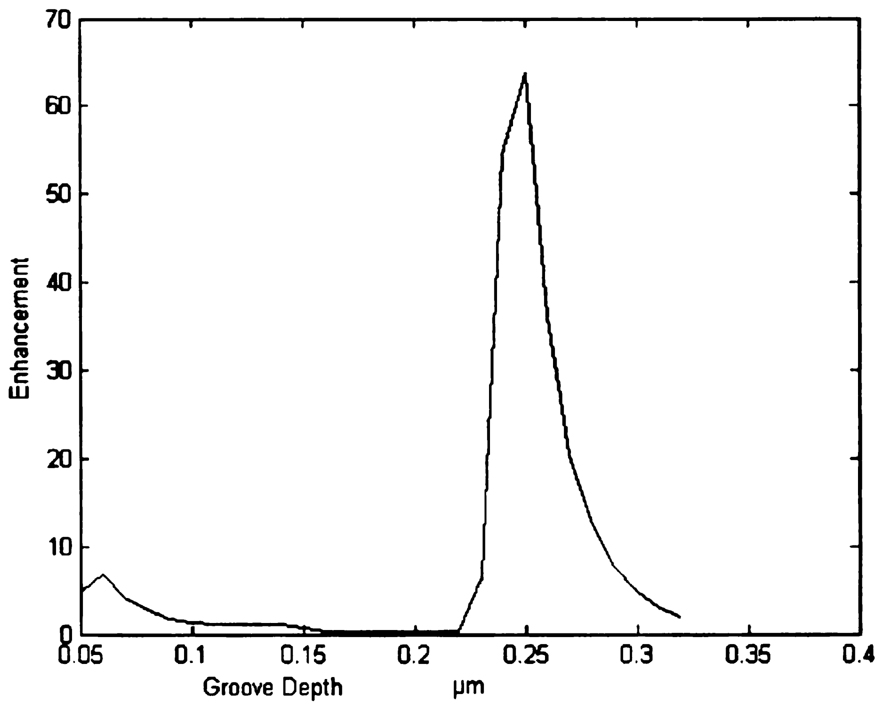
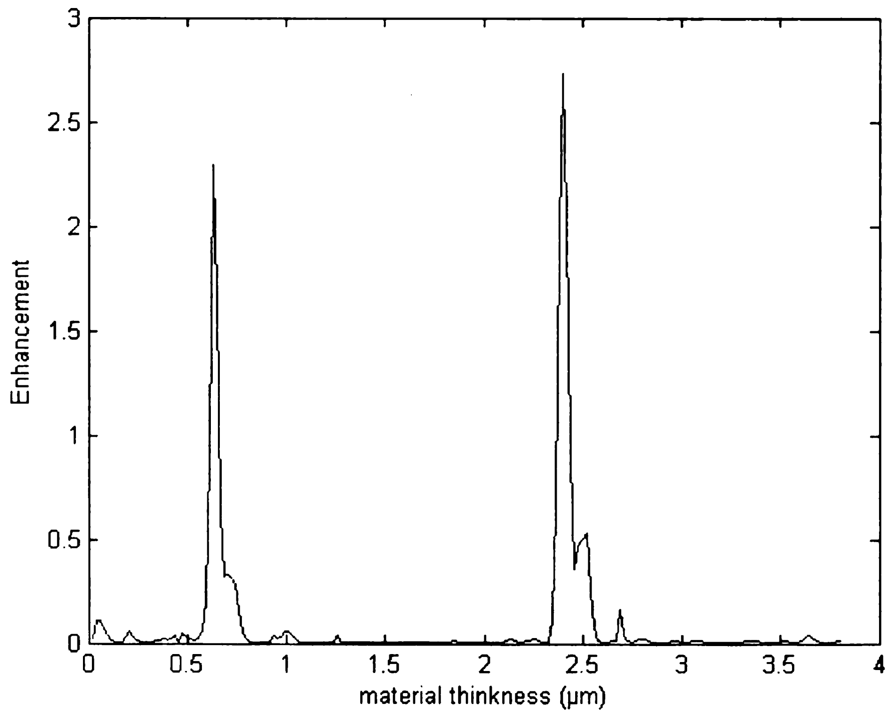


Figure 2.5. Second harmonic enhancement



CHAPTER 3

Inverse Medium Scattering in Breast Cancer Detection

3.1 Introduction

Breast cancer is a big threat to women's health. Early detection is the best way for protection. Mammography is the most effective technology presently available for breast cancer screening. According to the report from the U.S. Institute of Medicine (IOM), limitations of mammography include missing up to 15% of breast cancers, difficulty in imaging women with dense breasts, and inconclusive results. The limitations of X-ray mammography provide clear motivation for the development of a complementary breast-imaging tool to assist in detection and diagnosis. Studies show that the dielectric properties of normal breast tissues are significantly different from those of malignant breast tissues in the microwave frequency range. Other tissues in the breast, like the glandular tissue and blood vessels, also have dielectric properties different from the surrounding fatty tissue, but the difference is not nearly as significant as for the cancerous tissue. Typical dielectric properties of various tissues in the breast are listed in Table 3.1. Readers are also referred

Table 3.1. Typical dielectric properties of various tissues in the breast [27]

Media	ϵ_S	σ_S	ϵ_r(6GHz)	σ(6GHz)
skin	37.00	1.10	34.72	3.89
tumor	54.00	0.70	50.74	4.82
fatty tissue	10.00	0.15	9.80	0.40
average tissue	16.29	0.23	15.66	1.03
fibroglandular tissue	21.57	0.31	21.5	1.7

to [19] and [41] for the measurement of dielectric properties at specific radiowave and microwave frequency bands. It is apparent that there is a wide range of dielectric properties between the tumor tissue and other normal tissues in the human breast. Under microwave illumination, tissues with different dielectric properties will generate different responses. Significant dielectric contrast will lead to a high imaging contrast.

Microwave imaging for breast cancer detection has gained intense attention. Ultra-wideband (UWB) confocal microwave imaging (CMI) approach provides qualitative high resolution images of backscattered energy distributions of the interior of the breast. See [30] for a review of different approaches on CMI. See, for example, [53], [31], [44], for analysis and numerical examples on different approaches. The nonlinear inverse scattering approach is able to provide quantitative images of dielectric properties of objects with high contrasts. An iterative algorithm needs to be used. In each iteration, an equation describing electric field distribution in heterogeneous media is solved. Then the dielectric properties are adjusted by minimizing the errors between measured and calculated electric fields. An iterative reconstruction algorithm based on the Levenberg-Marquardt method is presented in [32]. In [24], the authors use Newton-type reconstruction combined with Marquardt and Tikhonov regularizations to update an initial dielectric property distribution iteratively in order to minimize the squared difference between computed and measured data. Recently the group at Rensselaer has designed and built electrical impedance tomography process that applies currents through electrodes attached to the surface of the body and measures the resulting voltages. This system uses the electrical measurements to reconstruct and display approximate pictures of the electric conductivity and permittivity inside the body. The mammography geometry is modeled as a rectangular box with electrode arrays on the top and bottom planes. The reconstruction algorithm is based on linearizing the conductivity about a constant value. In the case that the target conductivity is extremely high compared to that of the background solution, there is a large discrepancy between the true and the reconstructed conductivity values. A review of EIT techniques for breast cancer detection can be found in [56]. See also [23] for numerical implementation. By considering the tumor tissue as small inhomogeneity in the surrounding normal tissues, an algorithm using small volume asymptotics has been used to reconstruct conductivity distributions. In [4] and [5], the authors give theoretical derivation of the asymptotic formula. In [3] some numerical examples are given. Since the approach is perturbative, the significant contrast makes the reconstruction more challenging.

In this paper, we formulate the problem as an inverse scattering problem, which is to determine the dielectric property of the tissues from the measurements of electromagnetic field on the breast surface, given the incident field. Our approach follows the general idea of [20] and employ the recursive linearization algorithm from [16] and [15].

In two dimensional cases, the electromagnetic intensity satisfies the Helmholtz equation:

$$\Delta u + k^2(x)(1 + q(k_0, x))u = 0, \tag{3.1.1}$$

where u is the total field; $k(x) = k_0\sqrt{\epsilon(k_0, x)}$ is the wavenumber; k_0 is the wavenumber in vacuum; $q(k_0, x)$ is the scatterer which has a compact support and

$\epsilon(k_0, x) = 1 + q(k_0, x)$ is the dielectric permittivity in dispersive medium, which is assumed to satisfy the Debye model [35]

$$\begin{aligned}\epsilon(k_0, x) &= \epsilon_r(k_0, x) - i\frac{\sigma(k_0, x)}{k_0\sqrt{\frac{\epsilon_0}{\mu_0}}} \\ &= \epsilon_\infty(x) + \frac{\epsilon_s(x) - \epsilon_\infty(x)}{1 + ik_0\sqrt{\frac{\epsilon_0}{\mu_0}}} - i\frac{\sigma_s(x)}{k_0\sqrt{\frac{\epsilon_0}{\mu_0}}},\end{aligned} \tag{3.1.2}$$

in microwave range frequencies, where ϵ_r is the relative permittivity; σ is the conductivity; $\epsilon_s = \lim_{k_0 \to 0} \epsilon$; $\epsilon_\infty = \lim_{k_0 \to \infty} \epsilon$; $\sigma_s = \lim_{k_0 \to 0} \sigma$; ϵ_0 is the permittivity in vacuum. In the following, we assume that the material is nonmagnetic, i.e., $\mu_0 = 1$.

The scatterer is illuminated by a one-parameter family of plane waves

$$u^i = e^{i\vec{k_0} \cdot \vec{x}}. \tag{3.1.3}$$

Evidently, such incident waves satisfy the homogeneous equation

$$\Delta u^i + k_0^2 u^i = 0.$$

The total electric field u consists of the incident field u^i and the scattered field u^s:

$$u = u^i + u^s.$$

It follows from the equations (3.1.1) and (3.1.3) that the scattered field satisfies

$$\Delta u^s + k^2(x)(1+q)u^s = (-k^2(x)(1+q) + k_0^2)u^i. \tag{3.1.4}$$

In free space, the scattered field is required to satisfy the following Sommerfeld radiation condition

$$\lim_{r \to \infty} \sqrt{r}\left(\frac{\partial u^s}{\partial r} - ik_0 u^s\right) = 0, \quad r = |x|,$$

uniformly along all directions $\frac{x}{|x|}$. In practice, it is convenient to reduce the problem to a bounded domain. For the sake of simplicity, we employ the first order absorbing boundary condition [36] on the surface of the breast:

$$\frac{\partial u^s}{\partial n} - ik_0 u^s = 0. \tag{3.1.5}$$

Given the incident field u^i, the direct problem is to determine the scattered field u^s for the known scatterer $q(k_0, x)$. Using the Lax-Milgram lemma and the Fredholm alternative, the direct problem is shown in [16] to have a unique solution for all $k_0 > 0$. An energy estimate for the scattered field is given in this paper, which provides a criterion for the weak scattering. Furthermore, properties on the continuity and the Fréchet differentiability of the nonlinear scattering map are examined. For the regularity analysis of the scattering map in an open domain, the reader is referred to [9], [39] and [26]. The inverse medium scattering problem is to determine the scatterer $q(k_0, x)$ from the measurements on the surface of the breast, $u^s|_{\Gamma_b}$, given the incident field u^i. Two major difficulties for solving the inverse problem by optimization methods are the ill-posedness and the presence of many local minima. In this paper we developed a continuation method based on the approach introduced in [16]. The algorithm requires multi-frequency scattering data. Using an initial guess from the Born approximation, each update is obtained via recursive linearization on the wavenumber k_0 by solving one forward problem and one adjoint problem of the Helmholtz equations.

In addition to the ill-posedness and nonlinearity of the inverse scattering problem, one major difficulty lies in the multiple scales of the problem. The tumor is comparably small in the computational domain, which makes the computation challenging. The strategy is to map the boundary data to the artificial boundary of a fairly small domain that encloses the tumor. The idea of mapping follows from [55]. The problem may be then reduced to a smaller domain which can be solved by finite element method. Suitable boundary conditions and jump conditions must then be added on the boundary of the smaller domain and the surface of the breast. Nyström

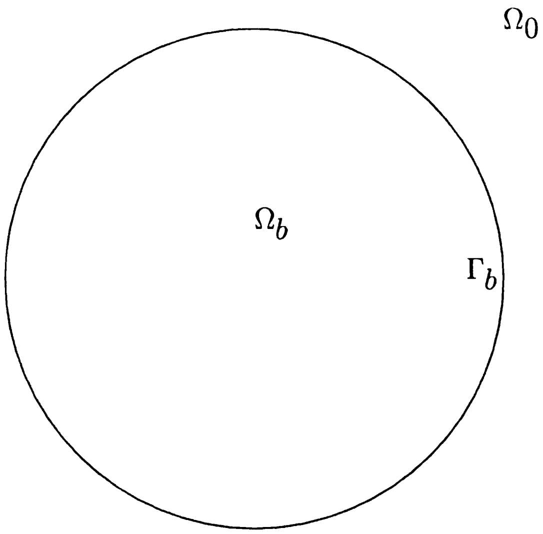


Figure 3.1. Geometry of the inverse scattering problem

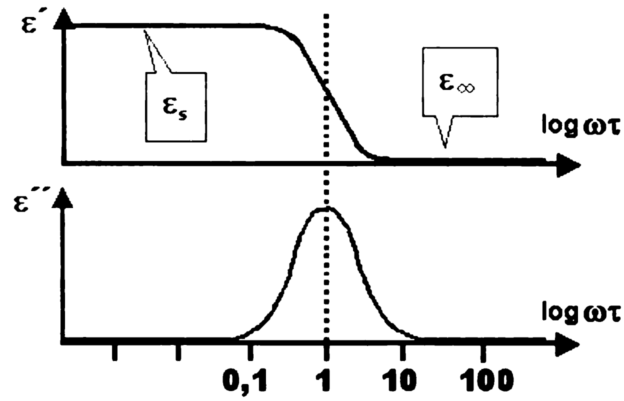
method is used on the integral equation in the annulus region between the surface and the smaller domain. Another difficulty is due to the dispersive nature of the human body. We employed the simplified Debye model:

$$\epsilon(k_0, x) = \epsilon_S(x) - i\frac{\sigma_S(x)}{k_0\sqrt{\epsilon_0}},$$

which is the approximation when the frequency is below the range of the Debye model. The Debye model (3.1.2) is suitable for dielectrics exhibiting resonance effects at the frequency $10^{11} \sim 10^{12}$Hz. The frequency used in our experiments range from $10^9 \sim 10^{10}$Hz. With this model, the reconstruction of q can be done separately for the real and imaginary part.

The plan of this paper is as follows. The analysis of the variational problem for direct scattering is presented in Section 3.2. The Fréchet differentiability of the scattering map is also given. In Section 3.3, an initial guess of the reconstruction from the Born approximation is derived in the case of weak scattering. Section 3.4 is devoted to numerical study of a regularized iterative linearization algorithm. Numerical examples are presented in Section 3.5.

Figure 3.2. Dielectric properties at frequencies described by Debye model [42]



3.2 Analysis of the Scattering Map

In this section, the direct scattering problem is studied to provide some criterion for the weak scattering, which plays an important role in the inversion method. The Fréchet differentiability of the scattering map for the problem (3.1.4), (3.1.5) is examined.

To state our boundary value problem, we introduce the bilinear form a : $H^1(\Omega_b) \times H^1(\Omega_b) \to \mathbb{C}$

$$a(\phi, \psi) = (\nabla\phi, \nabla\psi) - k^2((1+q)\phi, \psi) - ik_0\langle\phi, \psi\rangle,$$

and the linear functional on $H^1(\Omega_b)$

$$b(\psi) = ((k^2(1+q) - k_0^2)u^i, \psi).$$

Here, we have used the standard inner products

$$(\phi, \psi) = \int_{\Omega_b} \phi \cdot \overline{\psi} dx \quad \text{and} \quad \langle\phi, \psi\rangle = \int_{\Gamma_b} \phi \cdot \overline{\psi} ds,$$

where the overline denotes the complex conjugate.

Then, we have the weak form of the boundary value problem (3.1.4) and (3.1.5): find $u^s \in H^1(\Omega_b)$ such that

$$a(u^s, \xi) = b(\xi), \quad \forall \xi \in H^1(\Omega_b). \tag{3.2.1}$$

Throughout the paper, the constant C stands for a positive generic constant whose value may change step by step, but should always be clear from the contexts.

For a given scatterer q and an incident field u^i, we define the map $S(q, u^i)$ by $u^s = S(q, u^i)$, where u^s is the solution of the problem (3.1.4) and (3.1.5) or the variational problem (3.2.1). It is easily seen that the map $S(q, u^i)$ is linear with respect to u^i but is nonlinear with respect to q. Hence, we may denote $S(q, u^i)$ by $S(q)u^i$.

Concerning the map $S(q)$, a continuity result for the map $S(q)$ is presented in Lemma 3.2.3.

Lemma 3.2.1. *Given the scatterer $q \in L^\infty(\Omega_b)$, the direct scattering problem* (3.1.4) *and* (3.1.5) *has at most one solution.*

Please see [16] for the proof.

Lemma 3.2.2. *If the wavenumber k_0 is sufficiently small, the variational problem* (3.2.1) *admits a unique weak solution in $H^1(\Omega_b)$ and $S(q)$ is a bounded linear map from $L^2(\Omega_b)$ to $H^1(\Omega_b)$. Furthermore, there is a constant C dependent of Ω_b, such that*

$$\|S(q)u^i\|_{H^1(\Omega_b)} \le C\left(\frac{|k^2 - k_0^2|}{k_0} + \frac{|k|^2}{k_0}\left(1 + \frac{1}{k_0}\right)\|q\|_{L^\infty(\Omega_b)}\right)\|u^i\|_{L^2(\Omega_b)}. \tag{3.2.2}$$

Proof. Decompose the bilinear form a into $a = a_1 + k^2 a_2$, where

$$a_1(u^s, \xi) = (\nabla u^s, \nabla \xi) - ik_0\langle u^s, \xi\rangle,$$

$$a_2(u^s, \xi) = -((1+q)u^s, \xi).$$

We conclude that a_1 is coercive from

$$\begin{aligned}|a_1(u^s,u^s)| &\geq C(\|\nabla u^s\|^2_{L^2(\Omega_b)} + k_0\|u^s\|^2_{H^{1/2}(\Gamma_b)})\\ &\geq Ck_0(\|\nabla u^s\|^2_{L^2(\Omega_b)} + \|u^s\|^2_{H^{1/2}(\Gamma_b)})\\ &\geq Ck_0\|u^s\|^2_{H^1(\Omega_b)},\end{aligned}$$

where the last inequality may be obtained by applying standard elliptic estimates [34]. Next, we prove the compactness of a_2. Define an operator $\mathcal{A} : L^2(\Omega_b) \to H^1(\Omega_b)$ by

$$a_1(\mathcal{A}u^s,\xi) = a_2(u^s,\xi), \quad \forall\xi \in H^1(\Omega_b),$$

which gives

$$(\nabla\mathcal{A}u^s,\nabla\xi) - ik_0\langle\mathcal{A}u^s,\xi\rangle = -((1+q)u^s,\xi), \quad \forall\xi \in H^1(\Omega_b).$$

Using the Lax–Milgram Lemma, it follows that

$$\|\mathcal{A}u^s\|_{H^1(\Omega_b)} \leq \frac{C}{k_0}\|u^s\|_{L^2(\Omega_b)}, \tag{3.2.3}$$

where the constant C is independent of k_0. Thus $\mathcal{A}$ is bounded from $L^2(\Omega_b)$ to $H^1(\Omega_b)$ and $H^1(\Omega_b)$ is compactly imbedded into $L^2(\Omega_b)$. Hence $\mathcal{A} : L^2(\Omega_b) \to L^2(\Omega_b)$ is a compact operator.

Define a function $\phi \in L^2(\Omega_b)$ by requiring $\phi \in H^1(\Omega_b)$ and satisfying

$$a_1(\phi,\xi) = b(\xi), \quad \forall\xi \in H^1(\Omega_b).$$

It follows from the Lax–Milgram Lemma again that

$$\|\phi\|_{H^1(\Omega_b)} \leq C(\frac{|k^2-k_0^2|}{k_0} + \frac{|k|^2}{k_0}(1+\frac{1}{k_0})\|q\|_{L^\infty(\Omega_b)})\|u^i\|_{L^2(\Omega_b)}. \tag{3.2.4}$$

Using the operator $\mathcal{A}$, we can see that the problem (3.2.1) is equivalent to find $u^s \in L^2(\Omega_b)$ such that

$$(\mathcal{I} + k^2\mathcal{A})u^s = \phi. \tag{3.2.5}$$

When the wavenumber k_0 is small enough, the operator $\mathcal{I} + k^2\mathcal{A}$ has a uniformly bounded inverse. We then have the estimate

$$\|u^s\|_{L^2(\Omega_b)} \leq C\|\phi\|_{L^2(\Omega_b)}, \tag{3.2.6}$$

where the constant C is independent of k_0. Rearranging (3.2.5), we have $u^s = \phi - k^2\mathcal{A}u^s$, so $u^s \in H^1(\Omega_b)$ and, by the estimate (3.2.3) for the operator $\mathcal{A}$, we have

$$\|u^s\|_{H^1(\Omega_b)} \leq \|\phi\|_{H^1(\Omega_b)} + C\frac{|k|^2}{k_0}\|u^s\|_{L^2(\Omega_b)}.$$

The proof is complete by combining the estimates (3.2.6) and (3.2.4) and observing that $u^s = S(q)u^i$. □

For a general wavenumber $k_0 > 0$, from the equation (3.2.5), the existence follows from the Fredholm alternative and the uniqueness result. However, the constant C in the estimate (3.2.2) depends on the wavenumber.

Remark 3.2.1. It follows from the explicit form of the incident field (3.1.3) and the estimate (3.2.2) that

$$\|u^s\|_{H^1(\Omega_b)} \leq |\Omega|^{1/2}(C_1 + C_2\|q\|_{L^\infty(\Omega_b)}),$$

where Ω is the compact support of the scatterer q and the constant C_1, C_2 depends on k_0, Ω_b.

Lemma 3.2.3. *Assume that* $q_1, q_2 \in L^\infty(\Omega_b)$. *Then*

$$\|S(q_1)u^i - S(q_2)u^i\|_{H^1(\Omega_b)} \leq C\|q_1 - q_2\|_{L^\infty(\Omega_b)}\|u^i\|_{L^2(\Omega_b)}, \tag{3.2.7}$$

where the constant C *depends on* k_0, Ω_b, *and* $\|q_2\|_{L^\infty(\Omega_b)}$.

Proof. Let $u_1^s = S(q_1)u^i$ and $u_2^s = S(q_2)u^i$. It follows that for $j = 1, 2$

$$\Delta u_j^s + k^2(1 + q_j)u_j^s = (-k^2(1 + q_j) + k_0^2)u^i.$$

By setting $w = u_1^s - u_2^s$, we have

$$\Delta w + k^2(1+q_1)w = -k^2(q_1 - q_2)(u^i + u_2^s).$$

The function w also satisfies the boundary condition (3.1.5).

We repeat the procedure in the proof of Lemma 3.2.2 to obtain

$$\|w\|_{H^1(\Omega_b)} \le C\|q_1 - q_2\|_{L^\infty(\Omega_b)}\|u^i + u_2^s\|_{L^2(\Omega_b)}.$$

Using Lemma 3.2.2 again for u_2^s yields

$$\|u_2^s\|_{H^1(\Omega_b)} \le C\|q_2\|_{L^\infty(\Omega_b)}\|u^i\|_{L^2(\Omega_b)},$$

which gives

$$\|S(q_1)u_0^i - S(q_2)u^i\|_{H^1(D)} \le C\|q_1 - q_2\|_{L^\infty(D)}\|u^i\|_{L^2(\Omega_b)},$$

where the constant C depends on Ω_b, k_0, and $\|q_2\|_{L^\infty(\Omega_b)}$. □

Let γ be the restriction (trace) operator to the boundary Γ_b. By the trace theorem, γ is a bounded linear operator from $H^1(\Omega_b)$ onto $H^{1/2}(\Gamma_b)$. We can now define the scattering map $M(q) = \gamma S(q)$.

Next, consider the Fréchet differentiability of the scattering map. Recall the map $S(q)$ is nonlinear with respect to q. Formally, by using the first order perturbation theory, we obtain the linearized scattering problem of (3.1.4), (3.1.5) with respect to a reference scatterer q,

$$\Delta v + k^2(1+q)v = -k^2\delta q(u^i + u^s), \tag{3.2.8}$$

$$\frac{\partial v}{\partial n} - ik_0 v = 0, \tag{3.2.9}$$

where $u^s = S(q)u^i$.

Define the formal linearzation $T(q)$ of the map $S(q)$ by $v = T(q)(\delta q, u^i)$, where v is the solution of the problem (3.2.8), (3.2.9). The following is a boundedness result for the map $T(q)$. A proof may be given by following step by step the proofs of Lemma 3.2.2. Hence we omit it here.

Lemma 3.2.4. *Assume that $q, \delta q \in L^\infty(\Omega_b)$ and u^i is the incident field. Then $v = T(q)(\delta q, u^i) \in H^1(\Omega_b)$ with the estimate*

$$\|T(q)(\delta q, u^i)\|_{H^1(\Omega_b)} \le C\|\delta q\|_{L^\infty(\Omega_b)}\|u^i\|_{L^2(\Omega_b)}, \tag{3.2.10}$$

where the constant C depends on k_0, Ω_b, and $\|q\|_{L^\infty(\Omega_b)}$.

The next lemma is concerned with the continuity property of the map.

Lemma 3.2.5. *For any $q_1, q_2 \in L^\infty(\Omega_b)$ and an incident field u^i, the following estimate holds*

$$\begin{aligned}\|T(q_1)(\delta q, u^i) - T(q_2)(\delta q, u^i)\|_{H^1(\Omega_b)} \le C\|q_1 - q_2\|_{L^\infty(\Omega_b)}\cdot \\ \cdot\|\delta q\|_{L^\infty(\Omega_b)}\|u^i\|_{L^2(\Omega_b)},\end{aligned} \tag{3.2.11}$$

where the constant C depends on k_0, Ω_b, and $\|q_2\|_{L^\infty(\Omega_b)}$.

Proof. Let $v_j = T(q_j)(\delta q, u^i)$, for $j = 1, 2$. It is easy to see that

$$\begin{aligned}\Delta(v_1 - v_2) + k^2(1 + q_1)(v_1 - v_2) = \\ - k^2\delta q(u_1^s - u_2^s) - k^2(q_1 - q_2)v_2,\end{aligned}$$

where $u_j^s = S(q_j)u^i$.

Similar to the proof of Lemma 3.2.2, we get

$$\begin{aligned}\|v_1 - v_2\|_{H^1(\Omega_b)} \le C(\|\delta q\|_{L^\infty(\Omega_b)}\|u_1^s - u_2^s\|_{H^1(\Omega_b)} \\ + \|q_1 - q_2\|_{L^\infty(\Omega_b)}\|v_2\|_{H^1(\Omega_b)}).\end{aligned}$$

From Lemma 3.2.2, we obtain

$$\|v_1 - v_2\|_{H^1(\Omega_b)} \le C\|q_1 - q_2\|_{L^\infty(\Omega_b)}\|\delta q\|_{L^\infty(\Omega_b)}\|u^i\|_{L^2(\Omega_b)},$$

which completes the proof. □

The following result concerns the differentiability property of $S(q)$.

Lemma 3.2.6. *Assume that $q, \delta q \in L^\infty(\Omega_b)$. Then there is a constant C dependent of k, Ω_b, and $\|q\|_{L^\infty(\Omega_b)}$, for which the following estimate holds*

$$\|S(q+\delta q)u^i - S(q)u^i - T(q)(\delta q, u^i)\|_{H^1(\Omega_b)} \le C\|\delta q\|^2_{L^\infty(\Omega_b)}\|u^i\|_{L^2(\Omega_b)}. \tag{3.2.12}$$

Proof. By setting $u_1^s = S(q)u^i, u_2^s = S(q+\delta q)u^i$, and $v = T(q)(\delta q, u^i)$, we have

$$\Delta u^s + k^2(1+q)u_1^s = (-k^2(1+q) + k_0^2)u^i,$$
$$\Delta u^s + k^2(1+q+\delta q)u_2^s = (-k^2(1+q+\delta q) + k_0^2)u^i,$$
$$\Delta v + k^2(1+q)v = -k^2\delta q u_1^s - k^2 \delta q u^i.$$

In addition, u_1^s, u_2^s, and v satisfy the boundary condition (3.1.5).

Denote $U = u_2^s - u_1^s - v$. Then

$$\Delta U + k^2(1+q)U = -k^2\delta q(u_2^s - u_1^s).$$

Similar arguments as in the proof of Lemma 3.2.2 give

$$\|U\|_{H^1(\Omega_b)} \le C\|\delta q\|_{L^\infty(\Omega_b)}\|u_2^s - u_1^s\|_{H^1(\Omega_b)}.$$

From Lemma 3.2.2, we obtain further that

$$\|U\|_{H^1(\Omega_b)} \le C\|\delta q\|^2_{L^\infty(\Omega_b)}\|u^i\|_{L^2(\Omega_b)}.$$

□

Finally, by combining the above lemmas, we arrive at

Theorem 3.2.2. *The scattering map $M(q)$ is Fréchet differentiable with respect to q and its Fréchet derivative is*

$$DM(q) = \gamma T(q). \tag{3.2.13}$$

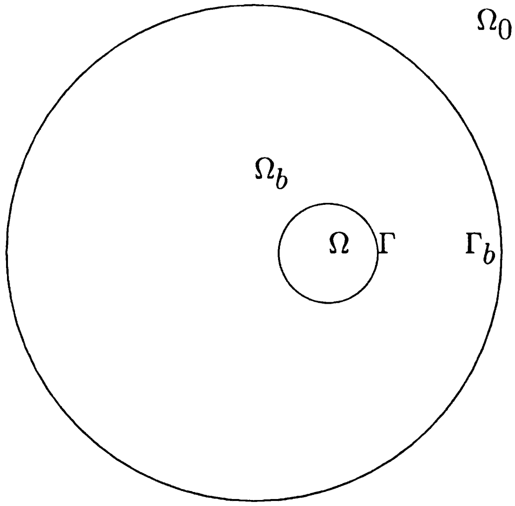


Figure 3.3. Geometry of the inverse scattering problem

3.3 Inverse Medium Scattering

In this section, a regularized recursive linearization method for solving the inverse scattering problem of the Helmholtz equation in two dimensions is proposed. The algorithm requires multi-frequency Dirichlet and Neumann scattering data, and the recursive linearization is obtained by a continuation method on the wavenumber k_0. It first solves a linear equation (Born approximation) at the lowest k_0, which gives the initial guess of $q(k_0, x)$. Updates are subsequently obtained by using a sequence of increasing wavenumbers. For each iteration, one forward and one adjoint equation are solved. Since in this specific problem, the tumor is very small compared to the breast, finite element method is time-consuming. Our strategy is to map the boundary data to the artificial boundary of a fairly small domain that encloses the tumor.

Let Ω_b be the circle that contains the breast; let $\Gamma_b = \partial\Omega_b$ be the surface of the breast; let $\Omega_0 = \mathbb{R}^2/\bar{\Omega_b}$; let Γ be the artificial boundary that contains the tumor; let Ω be the domain enclosed by Γ; let $\tilde{\Omega_b} = \Omega_b/\bar{\Omega}$. We assume

$$\epsilon = \begin{cases} \epsilon_0 & \text{in } \Omega_0, \\ \epsilon_b & \text{in } \tilde{\Omega_b}, \\ \epsilon_b(1+q) & \text{in } \Omega. \end{cases} \qquad k = \begin{cases} k_0 & \text{in } \Omega_0, \\ k_b & \text{in } \Omega_b. \end{cases}$$

The problem can be modeled as follows:

$$\Delta u + k_b^2(1+q)u = 0 \qquad \text{in } \Omega_b, \tag{3.3.1}$$

$$\Delta u^0 + k_0^2 u^0 = 0 \qquad \text{in } \Omega_0, \tag{3.3.2}$$

$$u = u^0 = u^s + u^i \qquad \text{on } \Gamma_b, \tag{3.3.3}$$

$$\frac{\partial u}{\partial n} = \epsilon_b\left(\frac{\partial u^s}{\partial n} + \frac{\partial u^i}{\partial n}\right) \qquad \text{on } \Gamma_b, \tag{3.3.4}$$

$$\frac{\partial u^s}{\partial n} - ik_0 u^s = 0 \qquad \text{on } \Gamma_b,$$

where (3.3.3) and (3.3.4) are the jump conditions on the surface of the breast.

3.3.1 Born Approximation

Define a test function $\hat{u} = e^{ik_b x \cdot \vec{d}}, \vec{d} = (\cos\theta, \sin\theta), \theta \in [0, 2\pi]$. Hence $\hat{u}$ satisfies:

$$\Delta \hat{u} + k_b^2 \hat{u} = 0 \quad \text{in } \Omega_b. \tag{3.3.5}$$

Multiplying the equation (3.3.1) by $\hat{u}$, and integrating over Ω_b on both sides, we have

$$\int_{\Omega_b} \hat{u}\Delta u dx + k_b^2 \int_{\Omega_b} (1+q)\hat{u}u dx = 0.$$

Integration by parts yields

$$\int_{\Omega_b} \Delta \hat{u} u dx + \int_{\Omega_b} k_b^2(1+q)u\hat{u} dx + \int_{\Gamma_b} \left(\hat{u}\frac{\partial u}{\partial n} - u\frac{\partial \hat{u}}{\partial n}\right) ds = 0.$$

We have by noting (3.3.5) and the jump conditions (3.3.3) and (3.3.4) that

$$\int_\Omega k_b^2 q u\hat{u} dx = \int_{\Gamma_b} \left(u^s\frac{\partial \hat{u}}{\partial n} - \epsilon_b \hat{u}\frac{\partial u^s}{\partial n}\right) ds + \int_{\Gamma_b} \left(u^i\frac{\partial \hat{u}}{\partial n} - \epsilon_b \hat{u}\frac{\partial u^i}{\partial n}\right) ds,$$

where we take into account that q has compact support in Ω. Using the special form of the incident wave and the test function, we then get

$$\int_\Omega k_b^2 q u e^{ik_b x \cdot \vec{d_1}} dx = \int_{\Gamma_b} (ik_b n \cdot \vec{d_1} e^{ik_b x \cdot \vec{d_1}} u^s - e^{ik_b x \cdot \vec{d_1}} \frac{\partial u^s}{\partial n}) ds$$
$$+ \int_{\Gamma_b} e^{ik_0 x \cdot \vec{d_2} + ik_b x \cdot \vec{d_1}} (ik_b n \cdot \vec{d_1} - \epsilon_b ik_0 n \cdot \vec{d_2}) ds. \tag{3.3.6}$$

From Lemma 3.2.2 and Remark 3.2.1, for a small wavenumber, the scattered field is weak and the inverse scattering problem becomes essentially linear. Dropping the nonlinear term of (3.3.6), we obtain the linearized integral equation

$$\int_\Omega k_b^2 q_0(x) e^{ik_0 x \cdot \vec{d_2} + ik_b x \cdot \vec{d_1}} dx = \int_{\Gamma_b} (ik_b n \cdot \vec{d} e^{ik_b x \cdot \vec{d_1}} u^s - e^{ik_b x \cdot \vec{d_1}} \frac{\partial u^s}{\partial n}) ds$$
$$+ \int_{\Gamma_b} e^{ik_0 x \cdot \vec{d_2} + ik_b x \cdot \vec{d_1}} (ik_b n \cdot \vec{d_1} - \epsilon_b ik_0 n \cdot \vec{d_2}) ds, \tag{3.3.7}$$

which is the Born approximation.

Since the scatterer $q_0(k_0, x)$ has a compact support, we use the notation

$$\hat{q_0}(\xi) = \int_\Omega q_0(x) e^{ik_0 x \cdot \vec{d_2} + ik_b x \cdot \vec{d_1}} dx,$$

where $\hat{q}_0(\xi)$ is the Fourier-Laplace transform of $q_0(x)$ with $\xi = (k_0 \vec{d_1} + k_b \vec{d_2})$, due to the presence of the evanescent waves. Choose

$$\vec{d_j} = \left(\cos\theta_j, \sin\theta_j\right), \quad j = 1, 2,$$

where θ_j are spherical angles. It is obvious that the domain $[0, 2\pi]$ of $\theta_j, j = 1, 2,$ corresponds to the ball $\{\xi \in \mathbb{R}^2 : |\xi| \leq k_0 + |k_b|\}$. Thus, the Fourier modes of $\hat{q}_0(\xi)$ may be beyond the disk with radius $2k$. Please refer to [17] for detailed analysis. The scattering data with the higher wavenumber must be used in order to recover more modes of the true scatterer.

The integral equation (3.3.7) can be written as the operator form

$$A(k_0, \theta; x) q(x) = f(k_0, \theta). \tag{3.3.8}$$

It is implemented by using the method of least squares with Tikhonov regularization [29]

$$q_0(k_0, x) = (A * A + \alpha I)^{-1} f,$$

where α is a small positive number, $A*$ is the adjoint operator of A. q_0 is used as the starting point of the following recursive linearization algorithm.

3.3.2 Recursive Linearization

As discussed in the previous section, when the wavenumber is small, the Born approximation allows a reconstruction of those Fourier modes less than or equal to $k_0 + |k_b|$ for the function $q(x)$. We now describe a procedure that recursively determines q_{k_0} at $k_0 = k_j$ for $j = 1, 2, ...$ with the increasing wavenumbers. Suppose now that the scatterer $q_{\tilde{k}}$ has been recovered at some wavenumber $\tilde{k}$, and that the wavenumber k is slightly larger than $\tilde{k}$. We wish to determine q_k, or equivalently, to determine the perturbation

$$\delta q = q_k - q_{\tilde{k}}.$$

For the reconstructed scatterer $q_{\tilde{k}}$, we solve at the wavenumber k the forward scattering problem

$$\begin{aligned}
&\Delta \tilde{u} + k_b^2(1 + q_{\tilde{k}}(k, x))\tilde{u} = 0 && \text{in } \Omega_b, \\
&\Delta \tilde{u}^0 + k_0^2 \tilde{u}^0 = 0 && \text{in } \Omega_0, \\
&\tilde{u} = \tilde{u}^0 = \tilde{u}^s + u^i && \text{on } \Gamma_b, \\
&\frac{\partial \tilde{u}}{\partial n} = \epsilon_b\left(\frac{\partial \tilde{u}^s}{\partial n} + \frac{\partial u^i}{\partial n}\right) && \text{on } \Gamma_b, \\
&\frac{\partial \tilde{u}^s}{\partial n} - ik_0\tilde{u}^s = 0 && \text{on } \Gamma_b.
\end{aligned} \tag{3.3.9}$$

For the scatterer q_k, we have

$$\Delta u + k_b^2(1 + q_k(k, x))u = 0 \qquad \text{in } \Omega_b,$$

$$\begin{aligned}
&\Delta u^0 + k_0^2 u^0 = 0 && \text{in } \Omega_0, \\
&u = u^0 = u^s + u^i && \text{on } \Gamma_b, \\
&\frac{\partial u}{\partial n} = \epsilon_b\left(\frac{\partial u^s}{\partial n} + \frac{\partial u^i}{\partial n}\right) && \text{on } \Gamma_b, \\
&\frac{\partial u^s}{\partial n} - ik_0 u^s = 0 && \text{on } \Gamma_b.
\end{aligned} \tag{3.3.10}$$

Subtracting (3.3.9) from (3.3.10) and omitting the second-order smallness in δq and in $\delta u = u - \tilde{u}$, we obtain

$$\begin{aligned}
&\Delta \delta u + k_b^2(1 + q_{\tilde{k}}(k, x))\delta u = -k_b^2 \delta q \tilde{u} && \text{in } \Omega_b, \\
&\Delta \delta u^0 + k_0^2 \delta u^0 = 0 && \text{in } \Omega_0, \\
&\delta u = \delta u^0 = \delta u^s && \text{on } \Gamma_b, \\
&\frac{\partial \delta u}{\partial n} = \epsilon_b \frac{\partial \delta u^s}{\partial n} && \text{on } \Gamma_b, \\
&\frac{\partial \delta u^s}{\partial n} - ik_0 \delta u^s = 0 && \text{on } \Gamma_b.
\end{aligned} \tag{3.3.11}$$

For the scatterer q_k and the incident wave u^i, we define the map $S(q_k, u^i)$ by

$$S(q_k, u^i) = u^0,$$

where u^0 is the total field data corresponding to the incident wave u^i. Let γ be the trace operator to the boundary Γ_b. Define the scattering map

$$M(q_k, u^i) = \gamma S(q_k, u^i).$$

For simplicity, denote $M(q_k, u^i)$ by $M(q_k)$. By the definition of the trace operator, we have

$$M(q_k) = u^0|_{\Gamma_b}.$$

Let $DM(q_k)$ be the Fréchet derivative of $M(q_k)$ and denote the residual operator by

$$R(q_{\tilde{k}}) = u^0|_{\Gamma_b} - \tilde{u}^0|_{\Gamma_b}.$$

It follows from Theorem 3.2.13 that

$$DM(q_{\tilde{k}})\delta q = R(q_{\tilde{k}}). \tag{3.3.12}$$

In order to reduce the computation cost and instability, we consider the Landweber iteration of (3.3.12), which has the form

$$\delta q = \beta DM^*(q_{\tilde{k}})R(q_{\tilde{k}}), \tag{3.3.13}$$

where β is a relaxation parameter and $DM^*(q_{\tilde{k}})$ is the adjoint operator of $DM(q_{\tilde{k}})$.

In order to compute the correction δq, we need some efficient way to compute $DM^*(q_{\tilde{k}})R(q_{\tilde{k}})$, which is given by the following theorem.

Theorem 3.3.1. *Given residual $R(q_{\tilde{k}})$, there exists a function ϕ such that the adjoint Fréchet derivative $DM^*(q_{\tilde{k}})$ satisfies*

$$[DM^*(q_{\tilde{k}})R_j(q_{\tilde{k}})](x) = \bar{\tilde{u}}(x) \cdot \bar{\phi}\frac{1}{\bar{\epsilon}_b}, \tag{3.3.14}$$

where $\tilde{u}$ is the solution of (3.3.9).

Proof. Let $\tilde{u}$ be the solution of (3.3.9). Consider the following problem

$$\begin{aligned}
&\Delta\delta u + k_b^2(1 + q_{\tilde{k}}(k,x))\delta u = -k_b^2\delta q\tilde{u} && \text{in } \Omega_b, \\
&\Delta\delta u^0 + k_0^2\delta u^0 = 0 && \text{in } \Omega_0, \\
&\delta u = \delta u^0 = \delta u^s && \text{on } \Gamma_b, \\
&\frac{\partial\delta u}{\partial n} = \epsilon_b\frac{\partial\delta u^s}{\partial n} && \text{on } \Gamma_b, \\
&\frac{\partial\delta u^s}{\partial n} - ik_0\delta u^s = 0 && \text{on } \Gamma_b.
\end{aligned} \tag{3.3.15}$$

and the adjoint problem

$$\begin{aligned}
&\Delta\psi + \bar{k}_b^2(1 + \bar{q}_{\tilde{k}}(k,x))\psi = 0 && \text{in } \Omega_b, \\
&\Delta\psi^0 + k_0^2\psi^0 = 0 && \text{in } \Omega_0, \\
&\frac{\partial\psi^0}{\partial n} + ik_0\psi^0 = (u^0 - \tilde{u}^0)\bar{k}_b^2. && \text{on } \Gamma_b.
\end{aligned} \tag{3.3.16}$$

Since the existence and uniqueness of the weak solution for the adjoint problem may be established by following the same proof of Lemma 3.2.2, we omit the proof here.

Multiplying the equation (3.3.15) with the complex conjugate of ψ and integrating over Ω_b on both sides, we obtain

$$\int_{\Omega_b} \Delta\delta u\bar{\psi}dx + \int_{\Omega_b} k_b^2(1+q_{\tilde{k}})\delta u\bar{\psi}dx = \int_{\Omega_b} -k_b^2\delta q\tilde{u}\bar{\psi}dx.$$

Integration by parts yields

$$\int_{\Gamma_b}(\bar{\psi}\frac{\partial\delta u}{\partial n} - \delta u\frac{\partial\bar{\psi}}{\partial n})ds = -k_b^2\int_{\Omega_b}\delta q\tilde{u}\bar{\psi}dx.$$

It follows from (3.3.12) and the boundary conditions of (3.3.15) and the adjoint problem that

$$\int_{\Gamma_b}(u^0-\tilde{u}^0)k_b^2\epsilon_b\delta u ds = k_b^2\int_{\Omega}\delta q\tilde{u}\bar{\psi}dx,$$

$$\int_{\Gamma_b} DM(q_{\tilde{k}})\delta q\overline{R(q_{\tilde{k}})}\epsilon_b ds = \int_{\Omega}\delta q\tilde{u}\bar{\psi}dx.$$

We know from the adjoint operator $DM^*(q_{\tilde{k}})$ that

$$\int_{\Omega_b}\delta q\epsilon_b\overline{DM(q_{\tilde{k}})R(q_{\tilde{k}})}ds = \int_{\Omega}\delta q\tilde{u}\bar{\psi}dx.$$

Since it holds for any δq and since q has compact support in Ω, we have

$$\overline{DM^*(q_{\tilde{k}})R(q_{\tilde{k}})} = \frac{1}{\epsilon_b}\tilde{u}\bar{\psi}.$$

Taking the complex conjugate of the above equation and letting $\phi = \bar{\psi}$ yields the result. □

Using this theorem, we can rewrite (3.3.13) as

$$\delta q = \frac{\beta}{\bar{\epsilon}_b}\bar{\tilde{u}}\bar{\phi}. \qquad (3.3.17)$$

So for each incident wave and each wavenumber k_0, we have to solve one forward problem (3.3.9) along with one adjoint problem (3.3.16). Since the adjoint problem has a similar variational form as the forward problem, essentially, we need to compute two forward problems at each sweep. Once δq is determined, $q_{\tilde{k}}$ is updated by $q_{\tilde{k}} + \delta q$.

3.4 Implementation

In this section, we discuss the numerical solution of the forward scattering problem and the computational issues of the recursive linearization algorithm.

The scattering data are obtained by numerical solution of the forward scattering problem. To implement the algorithm numerically, we employ Nyström's method in the annulus region $\tilde{\Omega}_b$ and add some suitable boundary conditions on Γ and Γ_b. Readers are referred to [40] for a detailed description of Nyström's method. See also [26] for the implementation of Nyström's method on integral equations generated by Helmholtz equation. Based on Kirsch and Monk's idea in [37] and [38], the exterior problem is solved by integral equation with radiation condition.

Define the space

$$W(\mathbb{R}\backslash\bar{\Omega}_b) = \{u^s \in H^1_{\rm loc}(\mathbb{R}\backslash\bar{\Omega}_b) | \quad \lim_{r\to\infty} \sqrt{r}\left(\frac{\partial u^s}{\partial r} - ik_0 u^s\right) = 0, \quad r = |x|\}.$$

Define the operators

$$\begin{aligned} G_i: &\quad H^{-\frac{1}{2}}(\Gamma) \to H^1(\Omega), \\ Gm: &\quad H^{-\frac{1}{2}}(\Gamma) \times H^{-\frac{1}{2}}(\Gamma_b) \to H^1(\tilde{\Omega}_b), \\ Ge: &\quad H^{-\frac{1}{2}}(\Gamma_b) \to W(\mathbb{R}\backslash\bar{\Omega}_b) \end{aligned}$$

by the following boundary problems. Given $\lambda_\Gamma \in H^{-\frac{1}{2}}(\Gamma)$ and $\lambda_{\Gamma_b} \in H^{-\frac{1}{2}}(\Gamma_b)$, define $G_i\lambda_\Gamma = w$ where $w \in H^1(\Omega)$ is the weak solution of

$$\begin{aligned} &\Delta w + k_b^2(1 + q_{\tilde{k}}(k, x))w = 0 && \text{in } \Omega, \\ &\frac{1}{\epsilon_b}\frac{\partial w}{\partial n} + ik_0 w = \lambda_\Gamma && \text{on } \Gamma. \end{aligned} \tag{3.4.1}$$

Define $G_m(\lambda_\Gamma, \lambda_{\Gamma_b})$ as the weak solution of

$$\begin{aligned} &\Delta w + k_b^2 w = 0 && \text{in } \tilde{\Omega}_b, \\ &\frac{1}{\epsilon_b}\frac{\partial w}{\partial n} + ik_0 w = \lambda_\Gamma && \text{on } \Gamma, \\ &\frac{1}{\epsilon_b}\frac{\partial w}{\partial n} + ik_0 w = \lambda_{\Gamma_b} && \text{on } \Gamma_b. \end{aligned} \tag{3.4.2}$$

Similarly define $G_e\lambda_{\Gamma_b} = w$ as the weak solution of

$$\begin{aligned} &\Delta w + k_0^2 w = 0 && \text{in } \mathbb{R}\backslash\Omega_b, \\ &\frac{\partial w}{\partial n} + ik_0 w = \lambda_{\Gamma_b} && \text{on } \Gamma_b, \\ &\lim_{r \to \infty} \sqrt{r}\left(\frac{\partial w}{\partial r} - ik_0 w\right) = 0, \quad r = |x|. \end{aligned} \tag{3.4.3}$$

To ensure continuity of solution of the forward problem across Γ and Γ_b, it suffices to choose $\lambda_\Gamma \in H^{-\frac{1}{2}}(\Gamma)$ and $\lambda_{\Gamma_b} \in H^{-\frac{1}{2}}(\Gamma_b)$ such that

$$G_i\lambda_\Gamma + G_i(\frac{\partial u^i}{\partial n} + ik_0 u^i) = G_m\lambda_\Gamma + G_m(\frac{\partial u^i}{\partial n} + ik_0 u^i) \qquad \text{on } \Gamma, \tag{3.4.4}$$

$$G_m\lambda_{\Gamma_b} + G_m(\frac{\partial u^i}{\partial n} + ik_0 u^i) = G_e\lambda_{\Gamma_b} + u^i \qquad \text{on } \Gamma_b. \tag{3.4.5}$$

The function λ_Γ and λ_{Γ_b} are approximated by trigonometric polynomials of order N. Represent Γ by $x(t) = (r_\Gamma \cos\theta_1, r_\Gamma \sin\theta_1), 0 \leq \theta_1 \leq 2\pi$, Γ_b by $x(t) = (r_{\Gamma_b}\cos\theta_2, r_{\Gamma_b}\sin\theta_2), 0 \leq \theta_2 \leq 2\pi$. Write $\lambda_\Gamma = \sum_{n=-N}^{N-1} b_n e^{in\theta_1}$ and $\lambda_{\Gamma_b} = \sum_{n=-N}^{N-1} a_n e^{in\theta_2}$. Thus for (3.4.4), $2N+1$ finite element problems need to be solved on the left hand side, and $2N+1$ Nyström problems need to be solved on the right hand side. Similarly for (3.4.5), $2N+1$ Nyström problems need to be solved on the left hand side, and since Γ_b is a circle, we can compute $Ge\lambda_{\Gamma_b}$ explicitly as a finite linear combination of Hankel functions:

$$Ge\lambda_{\Gamma_b} = \frac{1}{k_0} \sum_{n=-N}^{N-1} \frac{a_n e^{in\theta_2}}{(H_n^{(1)})'(k_0 r_{\Gamma_b}) + iH_n^{(1)}(k_0 r_{\Gamma_b})} H_n^{(1)}(k_0 r)$$

As for the adjoint problem, the continuity conditions are:

$$G_i\lambda_\Gamma + G_i((\overline{u-\tilde{u}})k_b^2) = Gm\lambda_\Gamma - Gm((\overline{u-\tilde{u}})k_b^2) \quad \text{on } \Gamma,$$
$$Gm\lambda_{\Gamma_b} + Gm((\overline{u-\tilde{u}})k_b^2) = Ge\lambda_{\Gamma_b} - Ge((\overline{u-\tilde{u}})k_b^2) \quad \text{on } \Gamma_b,$$

where the data on the artificial boundary Γ can be obtained from the data on Γ_b by a least square method introduced in [55].

3.5 Numerical Experiments

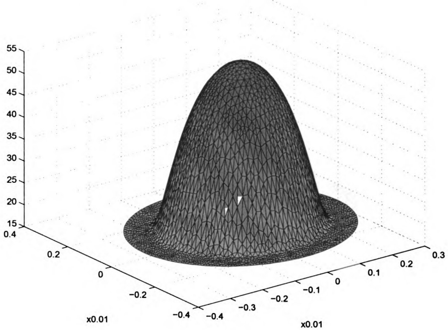
In the following, to illustrate the performance of the algorithm, two numerical examples are presented for reconstructing the scatterer of the Helmholtz equation in two dimensions. Assume the dielectric constants $\epsilon_{\text{tumor}}(k_0, x) = 54 - i\frac{2.63714}{k_0}$ and $\epsilon_{\text{normal}}(k_0, x) = 16.29 - i\frac{0.866489}{k_0}$ (see [27]).

Example 1. Define

$$q(k_0, x) = \begin{cases} (\frac{\epsilon_{\text{tumor}}}{\epsilon_{\text{normal}}} - 1)e^{\frac{|x|^2}{|x|^2 - 0.0025^2}} & |x| < 0.0025 \quad \text{in } \Omega, \\ 0 & \text{elsewhere in } \Omega. \end{cases}$$

See Figure 3.4 and 3.5 for the surface plot of the real and imaginary part of scatterer function in the domain $|x| < 0.003$. Figure 3.8 and 3.9 are the final reconstructions using the wavenumber $k_0 = 7.1$, which has relative error 6%. Figure 3.6 and 3.7 shows the result of the Born approximation.

Figure 3.4. Real part of smooth scatterer function



Example 2. [31] Assume the diameter of the breast is 10cm and a 6-mm-diameter tumor is located in the center.

$$q(k_0, x) = \begin{cases} \dfrac{\epsilon_{\text{tumor}}}{\epsilon_{\text{normal}}} - 1 & x_1^2 + x_2^2 \leq 0.003^2 \quad \text{in } \Omega, \\ 0 & \text{elsewhere in } \Omega. \end{cases}$$

See Figure 3.10 and 3.11 for the surface plot of the real and imaginary part of scatterer function in the domain $\Omega = \{x : x_1^2 + x_2^2 \leq 0.006^2\}$. Figure 3.14 and 3.15 are the final reconstructions using the wavenumber $k_0 = 6.1$, which has relative error 26.66%. Figure 3.12 and 3.13 shows the result of the Born approximation. It is easily seen that this scatterer is difficult to reconstruct because of the discontinuity.

Figure 3.5. Imaginary part of smooth scatterer function

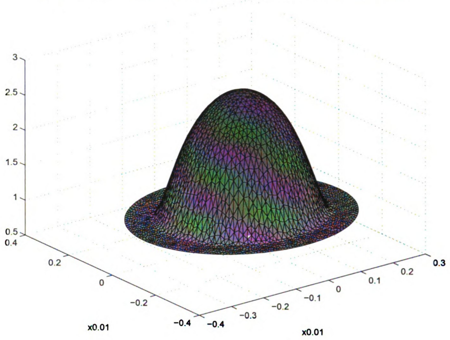


Figure 3.6. Born Approximation of the real part of smooth scatterer function

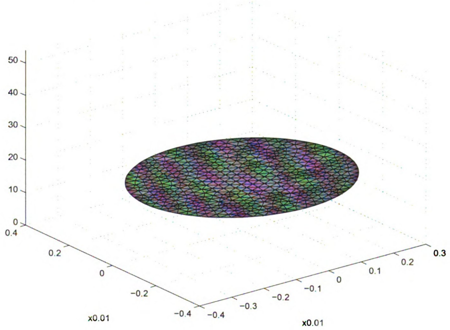


Figure 3.7. Born Approximation of the imaginary part of smooth scatterer function

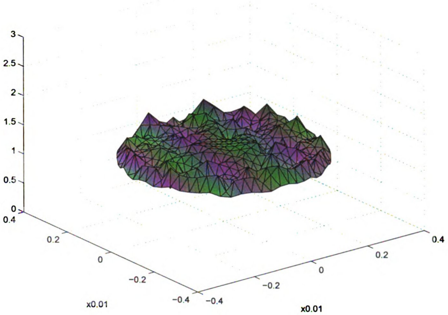


Figure 3.8. Final construction of the real part of smooth scatterer function

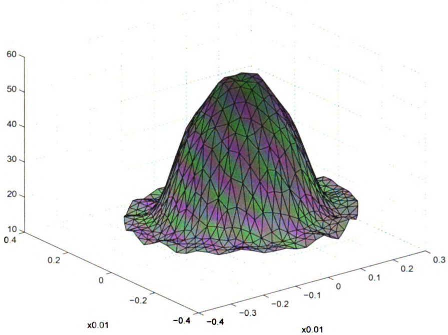


Figure 3.9. Final construction of the imaginary part of smooth scatterer function

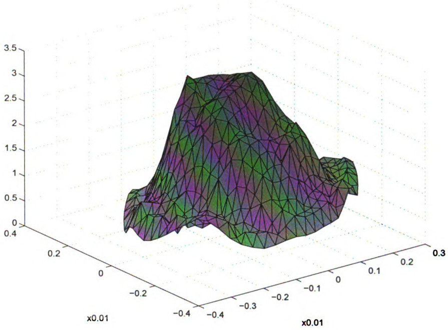


Figure 3.10. Real part of piecewise scatterer function

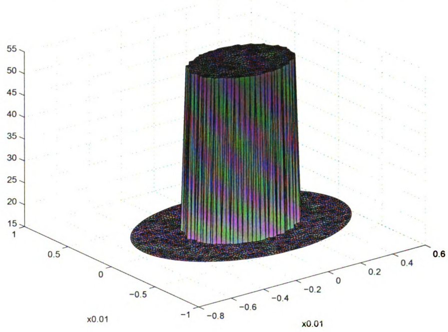


Figure 3.11. Imaginary part of piecewise scatterer function

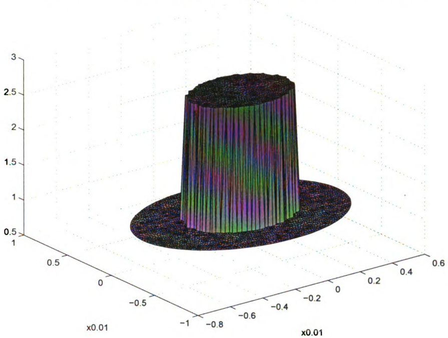


Figure 3.12. Born Approximation of the real part of piecewise scatterer function

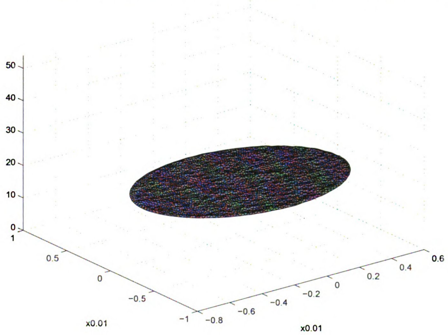


Figure 3.13. Born Approximation of the imaginary part of piecewise scatterer function

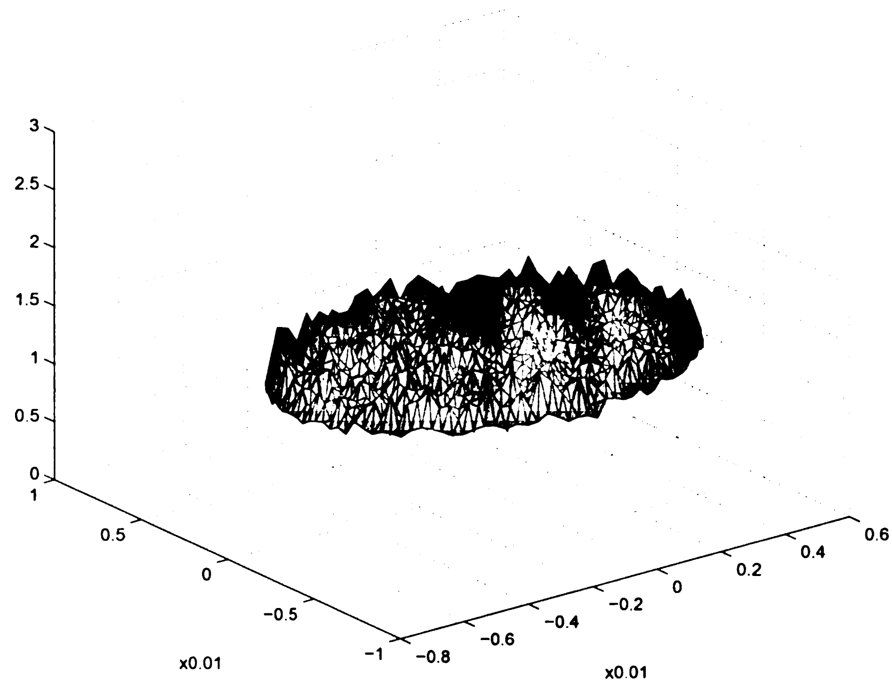


Figure 3.14. Final construction of the real part of piecewise scatterer function

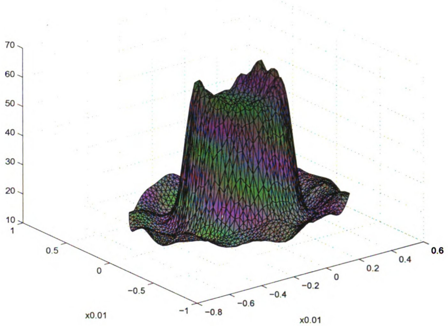
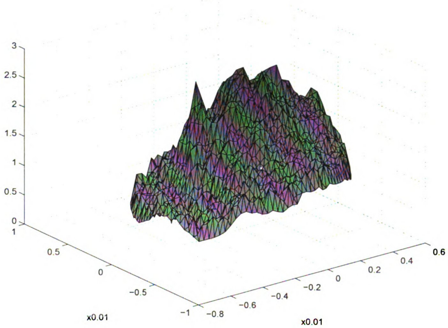


Figure 3.15. Final construction of the imaginary part of piecewise scatterer function



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