

NEAR-FIELD IMAGING OF IMPEDANCE GRATING SURFACES

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A DISSERTATION

Submitted to
Michigan State University
in partial fulfillment of the requirements
for the degree of

Applied Mathematics – Doctor of Philosophy

2014

ABSTRACT

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This dissertation investigates the inverse rough surface scattering problem in near-field optical imaging, the purpose of which is to reconstruct a scattering surface with a resolution beyond the diffraction limit. The surface is assumed to be a small and smooth deformation of a plane surface. Based on a transformed field expansion, the boundary value problem with complex scattering surface is converted into a successive sequence of a two-point boundary value problems in the frequency domain, whereby an analytic solution for the direct scattering problem is derived from the method of integrated solution. By neglecting the high order terms in the power series expansion, the nonlinear inverse problem is linearized and an explicit inversion formula is obtained. A spectral cut-off regularization is adopted to suppress the exponential growth of the noise in the evanescent wave components, which carry high spatial frequency of the scattering surface and contribute to the super resolution in the near-field regime. The method works for sound soft, sound hard, and impedance surfaces, and requires only a single illumination at a fixed frequency and is realized efficiently by the fast Fourier transform. Numerical results show that the method is simple, stable, and effective to reconstruct scattering surfaces with sub-wavelength resolution.

To Dad and Mom

ACKNOWLEDGMENTS

First and foremost, I want to thank my parents, for loving me and taking care of me from the start of my life, for always supporting me on my dream path, and for being a wonderful family. If I look back through twenty-seven years of my life, my parents have always been there, giving me the best of everything and inspiring me. Without their love and encouragement, I would have never pursued a PhD in mathematics, let alone finished it. Without their guidance and patience, my academic path would have never have gone so far and smooth.

My greatest academic thanks goes to Professor Gang Bao, who has my thesis advisor for four years, for his guidance and support, for his kindness and patience during my graduate study at Michigan State University. I would like to thank him for giving me this interesting thesis topic and encouraging me all the time. In these four years, from the qualifying exam to dissertation defense, from thesis topic to job suggestions, from research field to trivial paperworks, he has spent so much time and effort on me that I would have never reached this point without him. In addition, his generous support of research assistantship gave me the boost to go further on my academic path without distraction.

The man with the second greatest impact on my research is Professor Peijun Li. His guidance and tutelage energized my research and set me on a path to achievement. I also learned the subtleties of research from working with him. I would like to express my gratitude to my comprehensive exam and defense committee professors, Gang Bao, Yingda Cheng, Di Liu, Jianliang Qian, Moxun Tang, Baisheng Yan, Zhengfang Zhou, for devoting time and concern to me. I also thank the Department of Mathematics for giving me so much valuable teaching experience and so many professors with whom to interact.

I also want to thank Justin Droba, for taking care of me and loving me, for teaching me physics and coding, for always being there for me and being a sweet husband, and for everything he has done for me.

I also want to thank Dennis Droba and Diane Droba, for being a sweet father-in-law and mother-in-law, for taking care of me, and for so many times of picking me up from Detroit airport and driving me the hour and a half back to Lansing and cooking for me.

My journey through graduate school would not have been nearly as enjoyable without the good company that continuously surrounded me, sharing in the good moments and providing advice and emotional support. I would especially like to acknowledge my friends, Xianfeng Hu, Jun Lai, Yuliang Wang, Zixuan Wang, Qi Tang, Eric Wolf, Hongli Gao, all of whom were always there when I needed them.

Finally, I acknowledge the alumni students and postdocs of Prof. Bao's group not already mentioned: Guanghui Hu, Xianliang Hu, Xiang Xu, Junshan Lin, Zhengfu Xu, Xinghui Zhong. I hope our paths will cross again one day.

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Introduction

The aim of this dissertation is to present an effective mathematical model and accurate computational algorithm for the grating surface problem that arises in near-field imaging with general impedance boundary condition. The impedance boundary condition has become an important concept in the modeling of wave propagation. It can be used for obstacles that are partially or totally penetrable for time-harmonic scattering problems in electromagnetism. The famous sound hard and sound soft boundary conditions are special cases of the general impedance boundary condition.

A grating surface is a periodic structure with a non-local perturbation such that the new surface lies within a small distance of the original plane. The perturbation is assumed to be smooth and very small. The input information is measured at a constant distance from above the grating surface orders in magnitude smaller than the wavelength of the incident radiation. This is the defining feature of near-field optics, which focuses on features of light or waves occurring in regions smaller than the wavelength. The hallmark of near-field optics is that it breaks the diffraction limit and is able to obtain images at subwavelength resolution. It also examines evanescent wave modes, which are crucial in near-field optical microscopes. Near-field optics also has broad application in biology, chemistry, and materials science.

This dissertation limits discussion to time-harmonic waves field incident normally incident

upon on a grating surface from above. A homogeneous medium fills the space above the grating surface. The method we will present also works for general incidence, but the computation is so much more complicated that it obscures the elegance of the method. Consequently, we limit presentation here to normal incidence only. The grating surface problem is just one kind of scattering surface problem. Scattering is a physical process in which some forms of radiation, such as light, sound, or moving particles, are redirected from their original trajectories by localized non-uniformities in the medium through which they are passing. For example, the color of the sky is formed by dispersive scattering of sunlight by particles and molecules in the atmosphere, with stronger scattering at short (blue) wavelengths leading to the sky's distinctive hue. The scattering surface problem is so important that it has been applied broadly across modern science and technology. For instance, detection of the interior of the earth is possible by measuring the travel time of waves produced by seismographs. The technique is invaluable to oil companies, who need to determine the best location to drill. Beyond applications in the energy industry, medical imaging uses X-rays, ultrasound waves, and other electromagnetic waves to help diagnose suspected tumors and other malignant growths. Scattering problems also model animal echolocation, or the bio sonar of bats, dolphins, and toothed whales. This idea can also be used to help blind humans find their way around.

Paired with every inverse problems is a forward problem. For scattering, the forward scattering problem is to determine how radiation or particles behave with preknowledge of the scatterer. That is, the goal to find the total field given complete information about the grating surface and incident wave. Conversely, inverse scattering seeks to determine the characteristics of an object, such as shape or internal structure, solely from data concerning the scattering of incoming radiation, waves, or particles. Mathematically, the inverse scattering problem is to reconstruct the function that defines the scattering surface given the total field and incident wave.

The scattering surface is called an unbounded or infinite rough surface when the perturbation is non-local and not confined to a compact region. The problem has been studied and discussed by a large number of researchers, including Voronovich[40], Chew and Warnick[41], also Chandler-Wilde and Monk[18], DeSanto and Martin[24], Li, Wu and Zheng[32], Milder[36], DeSanto and Wombell[42], Chandler-Wilde and Zhang[19], Bao and Lin[14]. Bao and Lin[14] considered an inverse scattering problem with a local perturbation on a perfect electric conductor (PEC) is considered. Since the perturbation is local, the Sommerfeld radiation condition can be imposed in their model. However, a subsequent work by Bao and Li[10] examined inverse scattering upon a PEC perturbed nonlocally. In this scenario, the usual Sommerfeld radiation condition is inapplicable. So instead, the transparent boundary condition is imposed. Two related papers examine matters arising in nonlocal PEC scatters: Bao and Li[9] analyzed the convergence and error estimate; and Li and Shen [30] proved well-posedness and uniqueness of the weak solution of the corresponding forward problem using a variational approach. Furthermore, the near-field imaging of infinite rough surface scattering problem in dielectric media was tackled by Bao and Li[11]. Other related works in near-field optics include Carney and Schotland in [17] and [16], Courjon[22], Bainier and Courjon[23].

A cavity wall is a local perturbation of a planar surface in which the perturbation lies below the unperturbed portion of the plane (cf. [26]). Many beautiful results in different offshoots of the cavity problems have been established. Among them are Li[28], Bao, Gao and Li[29], Li and Wood[31], Li, Wu and Zheng[33], Bao, Gao, Lin and Zhang[8], Ammari, Bao, and Wood[2].

If the scattering surface is periodic structure, it is called a grating surface. Bao, Cowsar, and Masters[5] and Bao, Dobson and Cox[6], Petit[39], Bao and Friedman[7] have established excellent studies on mathematical analysis and numerical approaches for diffraction gratings. Kirsch[27], Bao[3] and Ammari[1] published uniqueness theorems for grating problems. Chen

and Wu[20] and Bao, Chen and Wu[4] crafted computational strategies based on the finite element method (FEM). Bao, Li and Lv [12] and Bao, Li and Wu[13] published an elegant work about inverse diffraction grating problem. The inverse grating surface problem with PEC boundary condition has recently been studied in work of Cheng, Li and Wang[21]. This thesis focuses on grating problem with general impedance boundary condition, which is a more accurate approximation to the exact electromagnetic properties of the material.

Excepting the introduction, this dissertation is comprised of four chapters. The first introduces mathematics and physics background, and the second establishes the mathematical model and develops a solver for the forward problem. Chapter 4 derives an inversion formula for reconstruction of the grating surface function. The final chapter presents numerical experiments that highlight the accuracy and efficiency of Chapter 3's method.

As will be shown in Section 2.4, the mathematical model of the scattering problem is a two-dimensional Helmholtz equation with two different types of boundary conditions:

1. A transparent boundary condition on the inverse problem's measurement surface
2. A universally applicable impedance boundary condition on the grating surface

The placement of these boundary conditions is depicted visually below in Figure 1.1.

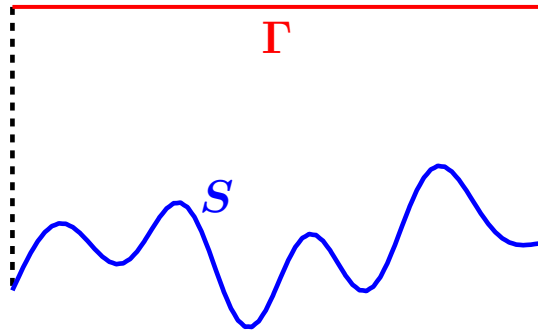


Figure 1.1 Placement of Boundary Conditions. On the measurement surface Γ , shown in red, a transparent boundary condition is placed; on the grating surface S (in blue), an impedance condition.

The necessity of the transparent boundary condition arises from the invalidity of the usual Sommerfeld radiation condition because of the nonlocal perturbation under consideration. To deal with the boundary value problem on a curved domain, a transformed field expansion is applied and the domain is transformed into a rectangular region. A formal power series expansion converts a boundary value problem concerning a complex scattering surface into a much simpler progression of two-point boundary value problems. Works by Nicholls and Reitich [38, 37], Malcolm and Nicholls[35], Bruno and Reitich[15] are the primary references for the transformed field expansion and boundary perturbation method. The boundary perturbation method and boundary integral operators are applied to an inverse problem with periodic scattering surface in Malcolm and Nicholls[34]. An explicit solution of the forward problem is obtained by the integration solution method. The uniqueness and wellposedness of the solution of this problem is proven.

Chapter 4 of this thesis derives an inversion formula for the grating surface. Discarding the high order terms in the power series creates a linearization of the nonlinear inverse problem. By calculating just the first two terms in the forward problem, an elegant yet accurate expression for grating surface is achieved. The exponential growth in the inversion formula is cured by a spectral cut-off regularization that reflects the ill-posedness of the inverse problem.

Chapter 5 of this thesis presents numerical experiments that demonstrate the accurate stability and efficiency of this method for reconstructing the grating surface with subwavelength resolution. When the deformation parameter is fixed, higher accuracy can be achieved by taking measurements closer to the surface. This reinforces the purpose of near-field imaging: measurements taken too far away lead to amplification of the exponential in the reconstruction formula and loss of valuable information contained in evanescent wave mode.

Background Knowledge

2.1 Maxwell's Theory

Maxwell's equations are precise mathematical expressions of the laws of nature. There are many different ways using different notations to display the same mathematical formulation, just like using different language to express a same idea. Here we express Maxwell equation in the following mathematical form:

$$\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J}, \quad (2.1)$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}, \quad (2.2)$$

$$\nabla \cdot \mathbf{D} = \rho, \quad (2.3)$$

$$\nabla \cdot \mathbf{B} = 0, \quad (2.4)$$

where $\mathbf{E}, \mathbf{B}, \mathbf{H}, \mathbf{D}, \mathbf{J}$ and ρ are all functions of space $\mathbf{x}$ and t .

Equation (2.1) is Ampere's law or the generalized Ampere circuit law. Equation (2.2) is Faraday's law or Faraday's magnetic induction law. Equation (2.3) is Coulomb's law or Gauss' law for electric fields. Equation (2.4) is Gauss' law or Gauss' law for magnetic fields. We refer to $\mathbf{E}$ as electric fields, $\mathbf{D}$ as electric displacement, and $\mathbf{H}$ and $\mathbf{B}$ as magnetic fields.

Symbol	Meaning	Units
$\mathbf{H}(\mathbf{x}, t)$	Magnetic field	amperes/m
$\mathbf{E}(\mathbf{x}, t)$	Electric field	volts/m
$\mathbf{B}(\mathbf{x}, t)$	Magnetic flux density	webers/m ²
$\mathbf{D}(\mathbf{x}, t)$	Electric displacement	coulombs/m ²
$\rho(\mathbf{x}, t)$	Electric charge density	coulombs/m ³
$\mathbf{J}(\mathbf{x}, t)$	Electric current density	amperes/m ²

Table 2.1 Quantities of Maxwell’s Equations. This table lists the physical quantities appearing in (2.1)–(2.4) with their meanings and their units.

Ampere’s original formulation of (2.1) lacked the electric displacement contribution $\frac{\partial \mathbf{D}}{\partial t}$, a term added by Maxwell in his pioneering 1861 work “On Physical Lines of Force.” While leading to correct results within magnetostatics, Ampere’s law without Maxwell’s correction fails when time-varying charges are present in several ways:

1. Capacitors, which result in open circuits for direct current sources, can only be employed in alternating circuit systems. When the original Ampere’s Law is applied to such a system, the result is a discontinuous current profile. Maxwell’s correction restores the proper behavior.
2. Taking the divergence of both sides of (2.1), using that $\nabla \cdot (\nabla \times \mathbf{A}) = 0$, and calling upon (2.3) results in the continuity equation

$$\nabla \cdot \mathbf{J}(\mathbf{x}, t) = -\frac{\partial}{\partial t} \rho(\mathbf{x}, t) \quad (2.5)$$

which states that if current flows out of a region (i.e., $\nabla \cdot \mathbf{J} > 0$), then the charge density in that region must correspondingly decrease. This amounts to a conservation of charge. In Ampere’s original formulation,

$$\nabla \cdot \mathbf{J}(\mathbf{x}, t) \equiv 0$$

which implies that the outward flux in space of current always vanishes. Obviously, this is correct only if charge does not vary in time—e.g., in direct current systems.

3. Faraday’s Law (2.2) states that a time-varying magnetic field induces a time-varying electric field. With the displacement term in (2.1), the corrected Ampere’s Law, in conjunction with a constitutive relation between $\mathbf{D}$ and $\mathbf{E}$, reciprocates this phenomenon: time-varying electric fields induce time-varying magnetic fields. This relationship between the time-varying electric and magnetic fields constitutes the foundation of electromagnetic wave theory and led Maxwell to prediction of electromagnetic waves.

In linear materials lacking magnetic dipole moments, $\mathbf{D}$ and $\mathbf{E}$ are related by a dielectric permittivity ε , and the magnetic fields $\mathbf{B}$ and $\mathbf{H}$ are related by a magnetic permeability μ :

$$\mathbf{D} = \varepsilon \mathbf{E} \tag{2.6}$$

$$\mathbf{B} = \mu \mathbf{H} \tag{2.7}$$

We call (2.6) and (2.7) the constitutive relations. In free space (a vacuum), $\mu = \mu_0$ and $\varepsilon = \varepsilon_0$. The numerical values of these fundamental constants are given below in Table 2.2.

Quantity	Value	Units
ε_0	8.85×10^{-12}	farad/meter
μ_0	$4\pi \times 10^{-7}$	henry/meter

Table 2.2 Fundamental Electromagnetic Constants.

Inside a material medium, the permittivity ε is determined by the electrical properties of the medium and the permeability μ is decided by the magnetic properties of the medium. In particular, for nonmagnetic materials, $\mu = \mu_0$, but there is no physical material for which $\varepsilon = \varepsilon_0$. Both ε and μ are more properly rank-2 tensors (3x3 matrices) with components that

zero out according to the material's crystal symmetry. For example, in uniaxial crystals,

$$\boldsymbol{\varepsilon}(\mathbf{x}) = \begin{pmatrix} \varepsilon_{xx}(\mathbf{x}) & 0 & 0 \\ 0 & \varepsilon_{yy}(\mathbf{x}) & 0 \\ 0 & 0 & \varepsilon_{zz}(\mathbf{x}) \end{pmatrix}$$

Only in homogeneous and isotropic materials will ε remain a scalar constant and in such materials the electric field $\mathbf{E}$ is parallel to $\mathbf{D}$ and the magnetic fields $\mathbf{B}$ and $\mathbf{H}$ are parallel[†]. In just isotropic materials, $\boldsymbol{\varepsilon}$ will be a constant tensor. Furthermore, because all materials display dispersion, $\boldsymbol{\varepsilon}$ also depends on frequency ω .

In this thesis, however, discussion will be limited to homogeneous and isotropic materials so that $\boldsymbol{\varepsilon} \equiv \varepsilon$. Because all incident waves are assumed to be monochromatic, we may ignore the effects of dispersion and set ε to its value appropriate for the input frequency.

2.2 Notations

A vector $\mathbf{A}$ has a magnitude and a direction, which can be represented graphically by a straight-line element of length proportional to the magnitude of $\mathbf{A}$ and with an arrow pointing the direction of $\mathbf{A}$. In a Cartesian coordinate system, which is also the rectangular coordinate system, $\mathbf{A}$ can be written in terms of the three Cartesian components A_x, A_y, A_z :

$$\mathbf{A} = \hat{x}A_x + \hat{y}A_y + \hat{z}A_z \tag{2.8}$$

where A_x, A_y, A_z are the projections of $\mathbf{A}$ onto the x, y, z axes. Denote the unit vector in the direction of x, y, z axes as $\hat{x}, \hat{y}, \hat{z}$. The del operator ∇ is a vector differential operator,

[†]More strictly, $\mathbf{H}$ is the magnetic field and $\mathbf{B}$ is the magnetic flux density. In nonmagnetic materials, however, the two are proportional so the distinction is not important to us. We refer to both as “magnetic field” as is common in the literature.

written as

$$\nabla = \hat{x} \frac{\partial}{\partial x} + \hat{y} \frac{\partial}{\partial y} + \hat{z} \frac{\partial}{\partial z} \quad (2.9)$$

When operating on a scalar function $\phi(x, y, z)$, the result is a vector

$$\nabla \phi = \hat{x} \frac{\partial \phi}{\partial x} + \hat{y} \frac{\partial \phi}{\partial y} + \hat{z} \frac{\partial \phi}{\partial z} \quad (2.10)$$

Since $\hat{x} \cdot \hat{x} = 1$, $\hat{y} \cdot \hat{y} = 1$, $\hat{z} \cdot \hat{z} = 1$, we have

$$\nabla^2 = \nabla \cdot \nabla = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \quad (2.11)$$

The curl of a vector field $\mathbf{H}$ is a vector defined as

$$\begin{aligned} \nabla \times \mathbf{H} &= \left(\hat{x} \frac{\partial}{\partial x} + \hat{y} \frac{\partial}{\partial y} + \hat{z} \frac{\partial}{\partial z} \right) \times \mathbf{H} = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ H_x & H_y & H_z \end{vmatrix} \\ &= \hat{x} \left(\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} \right) + \hat{y} \left(\frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} \right) + \hat{z} \left(\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} \right) \end{aligned}$$

The divergence of a vector function is a scalar, defined as

$$\begin{aligned} \nabla \cdot \mathbf{D} &= \left(\hat{x} \frac{\partial}{\partial x} + \hat{y} \frac{\partial}{\partial y} + \hat{z} \frac{\partial}{\partial z} \right) \cdot (\hat{x} D_x + \hat{y} D_y + \hat{z} D_z) \\ &= \frac{\partial D_x}{\partial x} + \frac{\partial D_y}{\partial y} + \frac{\partial D_z}{\partial z} \end{aligned}$$

2.3 Wave Propagation

In the physics of wave propagation, a plane wave (also spelled planewave) is a constant-frequency wave whose wavefronts (surfaces of constant phase) are infinite parallel planes of

constant peak-to-peak amplitude normal to the phase velocity vector.

The wavenumber (also wave number) is the spatial frequency of a wave, either in cycles per unit distance or radians per unit distance. It can be envisioned as the number of waves that exist over a specified distance—analogous to frequency being the number of cycles or radians per unit time. In terms of angular frequency, the wavenumber κ is given by

$$\kappa = \frac{2\pi}{\lambda} = \frac{\omega}{v} \quad (2.12)$$

where λ is the wavelength, ω is angular frequency of the wave.

Theorem 2.1 (Dispersion Relation). *The wavenumber κ is given by*

$$\kappa^2 = \mu_0 \varepsilon_0 \omega^2 = \omega^2 / c^2$$

where $\mu_0 \varepsilon_0 = \frac{1}{c^2}$ and $c = 3 \times 10^8$ m/sec is the speed of light in free space.

The dispersion relation provides an important connection between the spatial frequency κ and the temporal frequency ω .

Definition 2.1. *Fields for which the time variation is sinusoidal or periodic are called time-harmonic fields. Time-harmonic waves function can be written in a form of $\mathbf{A}(\mathbf{x}, t) = \mathbf{A}(\mathbf{x})e^{i\omega t}$, where ω is the wave frequency.*

Plane wave is one kind of time-harmonic fields and is called a “monochromatic” wave because it consists of a single frequency (color) of radiation. An incident wave may also be “polychromatic,” or composed of a finite number of monochromatic waves. More generally, any field $u(\mathbf{x})$ may be decomposed into an infinite combination of monochromatic waves by means of the Fourier transform:

$$\hat{u}(\xi) = \int_{\mathbb{R}} u(t) e^{-2\pi i \xi t} dt$$

By evaluating the above expression at a particular frequency $\omega = 2\pi\xi$, we can extract the component of u at that frequency.

Theorem 2.2 (Gauss's Law). *The area integral of the electric field over any closed surface is equal to the net charge enclosed in the surface divided by the permittivity of space.*

$$\oint_S \mathbf{E} d\mathbf{x} = \frac{Q_{\text{enclosed}}}{\varepsilon_0}$$

In other words, the total of the electric flux out of a closed surface is equal to the charge enclosed divided by the permittivity. It can be written in the differential form

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\varepsilon_0}$$

The electric flux through an area is defined as the electric field multiplied by the area of the surface projected in a plane perpendicular to the field. Gauss's Law is a general law applying to any closed surface. It is an important tool since it permits the assessment of the amount of enclosed charge by mapping the field on a surface outside the charge distribution. For geometries of sufficient symmetry, it simplifies the calculation of the electric field.

Remark 2.1. First taking the divergence and then integrating both sides of the constitutive relation (2.6) over a surface region S , we have in free space ($\varepsilon = \varepsilon_0$)

$$\begin{aligned} \oint_S \nabla \cdot \mathbf{D} d\mathbf{x} &= \varepsilon_0 \oint_S \nabla \cdot \mathbf{E} d\mathbf{x} \\ \oint_{\partial S} \mathbf{D} \cdot \mathbf{n} d\mathbf{x} &= Q_{\text{enclosed}} \end{aligned}$$

with the equality on the right side coming from the Divergence Theorem; the left side, from Gauss' Law. Therefore, Gauss' Law gives meaning to the electric displacement: $\mathbf{D}$ accounts for the effects of charge contained within materials. ■

2.4 The Vector Helmholtz Equation

We are interested in Maxwell equations in regions devoid of source—that is in regions where $\mathbf{J} = 0$ and $\rho = 0$. This doesn't mean there is no source anywhere in all space, instead, source exist outside the regions of interest in order to produce fields in these regions. Employing the constitutive relations (2.6) and (2.7) and this source-free assumption in (2.1)–(2.4), the Maxwell Equations become

$$\nabla \times \mathbf{H} = \varepsilon_0 \frac{\partial}{\partial t} \mathbf{E} \quad (2.13)$$

$$\nabla \times \mathbf{E} = -\mu_0 \frac{\partial}{\partial t} \mathbf{H} \quad (2.14)$$

$$\nabla \cdot \mathbf{E} = 0 \quad (2.15)$$

$$\nabla \cdot \mathbf{H} = 0 \quad (2.16)$$

In terms of scalar partial differential equations, Ampere's Law (2.13) takes the form

$$\frac{\partial}{\partial y} H_z - \frac{\partial}{\partial z} H_y = \varepsilon_0 \frac{\partial}{\partial t} E_x \quad (2.17)$$

$$\frac{\partial}{\partial z} H_x - \frac{\partial}{\partial x} H_z = \varepsilon_0 \frac{\partial}{\partial t} E_y \quad (2.18)$$

$$\frac{\partial}{\partial x} H_y - \frac{\partial}{\partial y} H_x = \varepsilon_0 \frac{\partial}{\partial t} E_z \quad (2.19)$$

Faraday's Law (2.14) becomes

$$\frac{\partial}{\partial y} E_z - \frac{\partial}{\partial z} E_y = -\mu_0 \frac{\partial}{\partial t} H_x \quad (2.20)$$

$$\frac{\partial}{\partial z} E_x - \frac{\partial}{\partial x} E_z = -\mu_0 \frac{\partial}{\partial t} H_y \quad (2.21)$$

$$\frac{\partial}{\partial x} E_y - \frac{\partial}{\partial y} E_x = -\mu_0 \frac{\partial}{\partial t} H_z \quad (2.22)$$

Finally, the two the Gauss' Laws for electric, (2.15), and magnetic, (2.16), fields are

$$\frac{\partial}{\partial x}E_x + \frac{\partial}{\partial y}E_y + \frac{\partial}{\partial z}E_z = 0 \quad (2.23)$$

$$\frac{\partial}{\partial x}H_x + \frac{\partial}{\partial y}H_y + \frac{\partial}{\partial z}H_z = 0 \quad (2.24)$$

Taking the derivative with respect to time of (2.17) and plugging in (2.21) (2.22), we get

$$\mu_0\varepsilon_0\frac{\partial^2}{\partial t^2}E_x = -\frac{\partial}{\partial y}\left(\frac{\partial}{\partial x}E_y - \frac{\partial}{\partial y}E_x\right) + \frac{\partial}{\partial z}\left(\frac{\partial}{\partial z}E_x - \frac{\partial}{\partial x}E_z\right) \quad (2.25)$$

$$= \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)E_x \quad (2.26)$$

Finally, we plug in (2.23). Similarly, we can derive the following equations:

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} - \mu_0\varepsilon_0\frac{\partial^2}{\partial t^2}\right)E_x = 0 \quad (2.27)$$

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} - \mu_0\varepsilon_0\frac{\partial^2}{\partial t^2}\right)E_y = 0 \quad (2.28)$$

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} - \mu_0\varepsilon_0\frac{\partial^2}{\partial t^2}\right)E_z = 0 \quad (2.29)$$

which can be collected into the vector expression

$$\nabla^2\mathbf{E} - \mu_0\varepsilon_0\frac{\partial^2}{\partial t^2}\mathbf{E} = 0 \quad (2.30)$$

This is the vector Helmholtz wave equation. If the wave is time-harmonic, then by means of the Fourier transform, $\frac{\partial^2}{\partial t^2}\mathbf{E}(\mathbf{x},t) = (i\omega)^2\mathbf{E}(\omega,t)$, the Helmholtz equation can be written in frequency space[†]

$$\nabla^2\mathbf{E} + \mu_0\varepsilon_0\omega^2\mathbf{E} = 0 \quad (2.31)$$

[†]We implicitly always work in frequency space (after transforming in time only), so we do not make any notational distinctions between the field and its transformed version aside from the change of symbol from t to ω .

Use the dispersion relation, $\kappa^2 = \omega^2 \mu_0 \varepsilon_0$, we have

$$(\nabla^2 + \kappa^2)\mathbf{E} = 0 \quad (2.32)$$

There is also another way to derive Helmholtz equation from Maxwell equation in free space.

For all time-harmonic wave in free space,

$$\begin{aligned} \nabla \times \mathbf{E} &= -\frac{\partial \mathbf{B}}{\partial t} = -i\omega \mathbf{B} \\ \nabla \times \mathbf{H} &= \frac{\partial \mathbf{D}}{\partial t} = i\omega \mathbf{D} = i\omega \varepsilon \mathbf{E} \end{aligned}$$

which implies

$$-\frac{1}{i\omega} \nabla \times \mathbf{E} = \mathbf{B}$$

We multiply by $\frac{1}{\mu}$ on both sides,

$$-\frac{1}{i\omega\mu} \nabla \times \mathbf{E} = \frac{1}{\mu} \mathbf{B}$$

and then take the curl. Using (2.4) and noting that $\frac{\mathbf{B}}{\mu} = \mathbf{H}$, we have

$$\begin{aligned} -\frac{1}{i\omega\mu} \nabla \times (\nabla \times \mathbf{E}) &= \nabla \times \mathbf{H} = i\omega \varepsilon \mathbf{E} \\ \Rightarrow \nabla \times (\nabla \times \mathbf{E}) - \omega^2 \varepsilon \mu \mathbf{E} &= 0 \end{aligned}$$

Using the vector identity

$$\nabla \times \nabla \times \mathbf{A} = \nabla(\nabla \cdot \mathbf{A}) - \nabla^2 \mathbf{A}$$

and calling upon the Gauss Law $\nabla \cdot \mathbf{E} = 0$ for charge-free spaces, we have

$$\nabla^2 \mathbf{E} + \omega^2 \varepsilon \mu \mathbf{E} = 0 \quad (2.33)$$

Due to the dispersion relation $\kappa^2 = \omega^2 \mu_0 \varepsilon_0$, the equation becomes

$$\nabla^2 \mathbf{E} + \kappa^2 \mathbf{E} = 0 \quad (2.34)$$

This is precisely what we had before.

2.5 Fundamental Polarizations

Diffractive optics is an emerging technology with many applications. Some of the important applications include the design and fabrication of optical elements such as corrective lenses, anti-reflective interfaces, beam splitters, and sensors. A particularly important application is replacing conventional lenses by diffractive gratings which are designed and fabricated by interference fringes on holographic plates.

The basic electromagnetic theory of gratings has been studied extensively since Rayleighs time in the early 20th century. Recent advance has been greatly accelerated due to several new approaches and numerical methods including differential methods, integral methods, analytical continuation, variational method, and others.

Diffractive optical elements, as opposed to the traditional optical lenses, have many advantages. They are light, small, and inexpensive. Often diffractive structures exhibit certain periodicity. There are two classes of grating structures: linear gratings (one-dimensional gratings) and crossed gratings (biperiodic or two-dimensional gratings).

The scalar approach is valid only as long as the wavelength of the incident light is small compared with characteristic transverse dimension of the structure. However, in many ap-

plications the structure dimensions are of the order of the wavelength of the incident light. In that case, the vectorial electromagnetic character of light becomes of interest. We are then speaking of the vector theory. In the vector model, polarization properties specified by the electric and magnetic fields in accordance with Maxwells equations must be studied.

Suppose that a grating is illuminated by a plane wave which lies in the (x, y) plane. The electromagnetic fields are assumed to be independent of z . We consider the following two fundamental cases of polarizations: transverse electric (TE) polarization and transverse magnetic (TM) polarization.

In TE polarization, the electric field is parallel to the grooves or is pointed to the z direction, i.e.,

$$\mathbf{E} = \begin{pmatrix} 0 \\ 0 \\ u(x, y) \end{pmatrix} \quad (2.35)$$

It follows from the Maxwell equation for the electric field

$$\nabla \times (\nabla \times \mathbf{E}) - \kappa^2 \mathbf{E} = 0$$

that we may derive the two-dimensional scalar Helmholtz equation

$$\Delta u + \kappa^2 u = 0.$$

In TM polarization, the magnetic field is parallel to the grooves or is pointed to the z direction, i.e.,

$$\mathbf{H} = \begin{pmatrix} 0 \\ 0 \\ u(x, y) \end{pmatrix}$$

It follows from the Maxwell equation for the magnetic field

$$\nabla \times (\kappa^{-2} \nabla \times \mathbf{H}) - \mathbf{H} = 0$$

that we may derive

$$\nabla \cdot (\kappa^{-2} \nabla u) + u = 0.$$

Because κ is independent of $\mathbf{x}$, this is the same equation as for TE polarization.

2.6 Impedance Boundary Condition

The impedance boundary condition is one which relates the tangential components of the electric and magnetic fields via an impedance factor, which is a function of the properties of the surface and maybe the incident field upon it. The approximate boundary conditions can be used to simulate the material properties of a surface, and is very useful in simplifying the analytical and numerical solution of scattering problems. A simple kind of approximate boundary condition is impedance boundary condition, which is given by

$$\underbrace{\mathbf{n} \times (\nabla \times \mathbf{E})}_{\text{normal comp. of } \nabla \times \mathbf{E} \propto \mathbf{H}} - i\eta \underbrace{\mathbf{n} \times (\mathbf{n} \times \mathbf{E})}_{\text{tangential comp. of } \mathbf{E}} = 0,$$

where $\mathbf{n}$ is the unit outward normal on the surface and where η is a function of the material properties called impedance parameter.

The unit outward normal is $\mathbf{n} = (n_1, n_2, 0)$ where $n_1^2 + n_2^2 = 1$. Using the form of $\mathbf{E}$ in the TE polarization (2.35), a simple calculation yields

$$\mathbf{n} \times (\nabla \times \mathbf{E}) = \begin{pmatrix} 0 \\ 0 \\ -n_1 \frac{\partial u}{\partial x} - n_2 \frac{\partial u}{\partial y} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ -\partial_{\mathbf{n}} u \end{pmatrix}$$

where

$$\partial_{\mathbf{n}}u = \mathbf{n} \cdot \nabla u$$

Next,

$$\mathbf{n} \times (\mathbf{n} \times \mathbf{E}) = \begin{pmatrix} n_1 \\ n_2 \\ 0 \end{pmatrix} \times \begin{pmatrix} n_2 u \\ -n_1 u \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ -u \end{pmatrix}$$

Combining above identities, we obtain the impedance boundary condition for the TE polarization

$$\partial_{\mathbf{n}}u - i\eta u = 0.$$

2.7 Analysis

Denote $\alpha = (\alpha_1, \alpha_2, \dots, \alpha_N)^T \in \mathbb{Z}_+^N$, where $\mathbb{Z}_+$ is the set of non-negative integers, we set $|\alpha|_1 = \sum_{i=1}^N |\alpha_i|$ and for $u \in C^{|\alpha|_1}(\Omega)$, define

$$\frac{\partial^\alpha u}{\partial \mathbf{x}^\alpha} = \frac{\partial^{|\alpha|_1} u}{\partial x_1^{\alpha_1} \dots \partial x_N^{\alpha_N}}$$

Definition 2.2. An open, connected set $\Omega \subset \mathbb{R}^N, N = 1, 2, 3$ will be referred to as a domain.

The fundamental Sobolev spaces are denoted $W^{s,p}(\Omega)$, where $s \in \mathbb{Z}^+, 1 \leq p < \infty$ and Ω is a domain in $\mathbb{R}^N$. These spaces are defined by

$$W^{s,p}(\Omega) = \{u \in L^p(\Omega) \mid \partial^\alpha u \in L^p(\Omega) \text{ for all } |\alpha|_1 \leq s\}$$

Each of these spaces is equipped with the norm

$$\|u\|_{W^{s,p}(\Omega)} = \left(\sum_{|\alpha|_1 \leq s} \int_{\Omega} |\partial^\alpha u(x)|^p dV(x) \right)^{\frac{1}{p}} \quad (2.36)$$

An important case occurs when $p = 2$. Denote the Sobolev Spaces

$$H^s(\Omega) = \{u : D^\alpha u \in L^2(\Omega) \text{ for all } |\alpha| \leq s\}$$

and the periodic functional space

$$H_p^1(\Omega) = \{u \in H^1(\Omega) : u(0, y) = u(2\pi, y)\},$$

$H_p^1(\Omega)$ is a subspace of $H^1(\Omega)$. To define spaces on the boundary, we first need Parseval's Theorem:

Theorem 2.3 (Parseval). *Let $f, g \in L^2[0, 2\pi]$ with $f(0) = f(2\pi)$ and $g(0) = g(2\pi)$ (i.e., f and g are 2π -periodic) with Fourier series*

$$\begin{aligned} f(x) &= \sum_{n \in \mathbb{Z}} f^{(n)} e^{inx} \\ g(x) &= \sum_{n \in \mathbb{Z}} g^{(n)} e^{inx} \end{aligned}$$

Then we have

$$\int_0^{2\pi} f(x) \overline{g(x)} dx = \sum_{n \in \mathbb{Z}} f^{(n)} \overline{g^{(n)}}$$

This theorem allows us to define the trace functional space for periodic functions u defined on boundary Γ with Fourier coefficient $u^{(n)}$:

$$H^s(\Gamma) = \{u \in L^2(\Gamma) : \sum_{n \in \mathbb{Z}} (1 + n^2)^s |u^{(n)}|^2 < \infty\},$$

which is a Banach space equipped with the norm

$$\|u\|_{s, \Gamma} = \left[2\pi \sum_{n \in \mathbb{Z}} (1 + n^2)^s |u^{(n)}|^2 \right]^{1/2}$$

The dual space associated with $H^s(\Gamma)$ is the space $H^{-s}(\Gamma)$ with respect to the scalar product

in $L^2(\Gamma)$ defined by

$$\langle u, v \rangle_\Gamma = \int_\Gamma u \bar{v} dx = 2\pi \sum_{n \in \mathbb{Z}} u^{(n)} \bar{v}^{(n)}$$

The equivalence of Fourier series coefficients and the standard L^2 inner product is also established by Parseval's Theorem.

Theorem 2.4 (Trace Theorem). *Assume Ω is bounded Lipschitz domain and $\frac{1}{p} < s \leq 1$, the mapping $\gamma_T(u) = u|_{\partial\Omega}$ defined on $C^\infty(\bar{\Omega})$ has a unique continuous extension as a linear operator from $W^{s,p}(\Omega)$ onto $W^{s-1/p,p}(\partial\Omega)$. Moreover,*

$$W_0^{1,p}(\Omega) = \{u \in W^{1,p}(\Omega) \mid \gamma_T(u) = 0\}.$$

Theorem 2.5 (Lax-Milgram). *Let $\mathcal{H}$ be a Hilbert space equipped with inner product $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ and norm $\|\cdot\|_{\mathcal{H}}$. Assume that $B : \mathcal{H} \times \mathcal{H} \rightarrow \mathbb{R}$ is a bilinear mapping, for which there exist constants $\alpha, \beta > 0$ such that*

$$|B[u, v]| \leq \alpha \|u\|_{\mathcal{H}} \|v\|_{\mathcal{H}} \quad (2.37)$$

for all $u, v \in \mathcal{H}$ and

$$\beta \|u\|_{\mathcal{H}}^2 \leq B[u, u] \quad (2.38)$$

for all $u \in \mathcal{H}$. Let $f : \mathcal{H} \rightarrow \mathbb{R}$ be a bounded linear functional on $\mathcal{H}$. Then there exists a unique element $u \in \mathcal{H}$ such that

$$B[u, v] = f(v)$$

for all $v \in \mathcal{H}$.

Remark 2.2. Condition (2.37) says that the bilinear form is bounded. Condition (2.38) says that it is coercive. ■

Forward Problem

3.1 Model problem

In this chapter, we shall introduce a mathematical model, define some notations for the grating problem by a surface, and present a boundary value problem for the surface grating model. Let us first describe the problem geometry, depicted visually below in Figure 3.1.

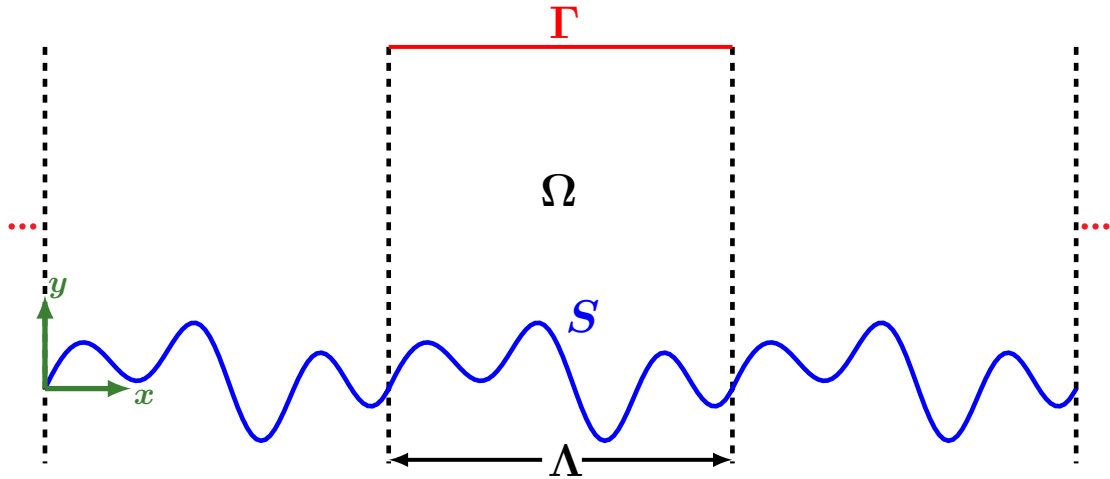


Figure 3.1 Problem Geometry. The grating surface S (in red) is assumed to be periodic with period Λ . The region Ω is the void between the scattering surface and upper boundary Γ . In the inverse problem of the next chapter, Γ will be the measurement surface.

The grating surface S is assumed to be invariant in the z direction and periodic in the x

direction with period Λ . We assume that the grating surface can be represented by the curve

$$S = \{(x, y) \in \mathbb{R}^2 : y = f(x), 0 < x < \Lambda\},$$

where f is a periodic function with period Λ . Furthermore, we assume the grating surface is small and smooth deformation of a plane surface, therefore f takes the form

$$f(x) = \varepsilon g(x), \quad g \in C^2(\mathbb{R}),$$

where ε is sufficiently small and is called the *surface deformation parameter*. This deformation is not restricted to the case of a local perturbation of a plane surface. Rather, it is considered to be a general perturbation of a planar surface, with nonlocal perturbation permitted.

Let $h > \max_{0 < x < \Lambda} f(x)$. In the next chapter, this will become the measurement distance, but this term has no meaning for the forward problem. Define the upper surface

$$\Gamma = \{(x, y) \in \mathbb{R}^2 : y = h, 0 < x < \Lambda\},$$

For now, it should just be considered a plane close to but not touching grating; eventually, a transparent boundary condition will be placed here imposed. The last region to be described is the space bounded below by the grating surface S and bounded above by the line Γ

$$\Omega = \{(x, y) \in \mathbb{R}^2 : f(x) < y < h, 0 < x < \Lambda\}.$$

The domain Ω is where the Helmholtz equation that characterizes propagation of the scattered field will be formulated.

Let Ω be filled with a homogeneous medium with a constant wavenumber $\kappa > 0$. An incoming plane wave $u^{\text{inc}} = e^{i(\alpha x - \beta y)}$ is incident upon S from the top, where $\theta \in (-\pi/2, \pi/2)$ is the

incident angle and

$$\alpha = \kappa \sin \theta \qquad \beta = \kappa \cos \theta$$

For simplicity, this thesis shall only consider normal incidence since our method requires only a single incident wave. Hence, $\alpha = 0, \beta = \kappa$ and the incident wave is reduced to

$$u^{\text{inc}} = e^{-i\kappa y}.$$

It is easily verified that the incident wave satisfies the Helmholtz equation in the whole space

$$(\Delta + \kappa^2)u^{\text{inc}} = 0 \quad \text{in } \mathbb{R}^2 \tag{3.1}$$

As derived in Section 2.5, the diffraction of a time-harmonic electromagnetic wave in the TE polarization can be modeled by the two-dimensional Helmholtz equation:

$$(\Delta + \kappa^2)u = 0 \quad \text{in } \Omega, \tag{3.2}$$

where u is the total field consisting the incident field u^{inc} and the diffracted field u^{d} , i.e.,

$$u = u^{\text{inc}} + u^{\text{d}}. \tag{3.3}$$

Adding (3.1) and (3.2) and making use of the relation (3.3), it can be seen that the diffracted field satisfies the same Helmholtz equation as u^{inc} and u :

$$(\Delta + \kappa^2)u^{\text{d}} = 0 \quad \text{in } \Omega, \tag{3.4}$$

For a grating with the impedance boundary condition, the total field u satisfies

$$(\partial_{\mathbf{n}} - i\eta)u = 0 \quad \text{on } S, \quad (3.5)$$

where $\mathbf{n} = (n_1, n_2)$ is the unit normal vector on S , given explicitly as

$$n_1 = \frac{f'(x)}{\sqrt{1 + [f'(x)]^2}}, \quad n_2 = -\frac{1}{\sqrt{1 + [f'(x)]^2}}, \quad (3.6)$$

$\eta \in \mathbb{C}$ is the impedance coefficient and is assumed to be known. To ensure existence of a unique solution for the direct problem, we assume that $\text{Re } \eta > 0$ and $\text{Im } \eta \geq 0$. When $\eta = 0$, the impedance condition becomes the sound hard condition. The impedance boundary condition will reduce to sound soft condition—perhaps better known as a perfect electric conductor (PEC)—when $\eta = \infty$. We are going to deal with the general impedance boundary condition and present a general solution for any η . Our result will be applicable to specific cases, like sound soft boundary condition and sound hard boundary condition.

It is known that for any given periodic function $u(x)$ with period Λ , it has a Fourier series expansion

$$u(x) = \sum_{n \in \mathbb{Z}} u_n e^{in(\frac{2\pi}{\Lambda})x},$$

where the Fourier coefficients are given by

$$u_n = \frac{1}{\Lambda} \int_0^\Lambda u(x) e^{-in(\frac{2\pi}{\Lambda})x} dx.$$

Motivated by uniqueness, we shall seek the periodic solution of u , which implies u^d is also periodic with same period. Therefore, we may write the Fourier series of u^d in x :

$$u^d(x, y) = \sum_{n \in \mathbb{Z}} u_n^d(y) e^{in(2\pi/\Lambda)x}, \quad (3.7)$$

When (3.7) is plugged into (3.4), an ordinary differential equation of u^d is derived,

$$\frac{d^2 u_n^d}{dy^2} + \left[\kappa^2 - \left(\frac{2\pi n}{\Lambda} \right)^2 \right] u_n^d(y) = 0$$

The diffracted wave is required to be a bounded outgoing wave in Ω . Mandating this, the solution for each n can be readily obtained as

$$u_n^d(y) = A_n e^{i\beta_n y} \quad (3.8)$$

Upon substitution into the Fourier series (3.7), we see that u^d is a (infinite) combination of plane waves:

$$u^d(x, y) = \sum_{n \in \mathbb{Z}} A_n e^{i\alpha_n x + i\beta_n y}, \quad (3.9)$$

valid for $y > \max_{0 < x < \Lambda} f(x)$. A_n is a complex number and the factors in the exponent are given explicitly by

$$\alpha_n = \frac{2\pi n}{\Lambda} \quad \beta_n = \begin{cases} (\kappa^2 - \alpha_n^2)^{1/2} & \text{for } \kappa > |\alpha_n|, \\ i(\alpha_n^2 - \kappa^2)^{1/2} & \text{for } \kappa < |\alpha_n|. \end{cases}$$

Now we will introduce a transparent boundary condition on Γ . Taking the partial derivative of u^d with respect to y and then evaluating at $y = h$ yields

$$\partial_y u^d(x, h) = i\beta_n \sum_{n \in \mathbb{Z}} A_n e^{i\alpha_n x + i\beta_n h} \quad (3.10)$$

Now given any u on Γ , define a boundary operator T which maps the Dirichlet data $u(x, h)$ to the Neumann data $\partial_y u(x, h)$:

$$(Tu)(x) = \sum_{n \in \mathbb{Z}} i\beta_n u^{(n)} e^{i\alpha_n x}.$$

For u^d on Γ , we have

$$(Tu^d)(x) = \sum_{n \in \mathbb{Z}} i\beta_n A_n e^{i\alpha_n x + i\beta_n y} \quad (3.11)$$

The transparent boundary condition on Γ is

$$\partial_y u^d = Tu^d \quad (3.12)$$

which is

$$\partial_y(u - u^{inc}) = T(u - u^{inc}) \quad (3.13)$$

Equivalently, a transparent boundary condition for the total field which bridges Dirichlet data and Neumann data is derived:

$$(\partial_y - T)u = \psi \quad \text{on } \Gamma, \quad (3.14)$$

where $\psi = \partial_y u^{inc} - Tu^{inc} = -2i\kappa e^{-i\kappa h}$.

To summarize, the surface scattering model can be reduced to the following boundary value problem for the total field:

$$\begin{cases} (\Delta + \kappa^2)u = 0 & \text{in } \Omega, \\ (\partial_{\mathbf{n}} - i\eta)u = 0 & \text{on } S, \\ (\partial_y - T)u = \psi & \text{on } \Gamma, \end{cases} \quad (3.15)$$

This thesis considers two problems: the direct diffractive grating problem and the inverse diffractive grating problem. The direct problem is to determine the total field u , with knowledge of the incident field and the grating function f . The aim of this dissertation is to study the inverse diffractive grating problem, which is to reconstruct the grating surface function f from the measurement of the total field u on Γ when given the incident field u^{inc} . In particular, we are interested in the inverse problem in near-field regime, in which the measurement distance h is much smaller than the wavelength $\lambda = 2\pi/\kappa$ of the incident wave,

in the presence of noise.

We point out that $u|_{\Gamma}$ should belong to $H^{1/2}$. The trace theorem guarantees that if the variational problem has a weak solution in H^1 , then the boundary information will belong to $H^{1/2}$. Since $u|_{\Gamma} \in H^{1/2} \subset L^2(\Gamma)$, the Fourier series of u will converge in the sense of L^2 .

The forward problem has a C^∞ solution by elliptic regularity, since the boundary here Lipschitz continuous (but not smooth because of the corners).

Before proceeding further, we prove a result about the boundary operator T , below.

Lemma 3.1. *The linear boundary operator $T: H^{1/2}(\Gamma) \rightarrow H^{-1/2}(\Gamma)$ is continuous.*

Proof. For any $u, v \in H^{1/2}(\Gamma)$, we have

$$\langle Tu, v \rangle_{\Gamma} = i2\pi \sum_{n \in \mathbb{Z}} \beta_n (1+n^2)^{-1/2} (1+n^2)^{1/4} u^{(n)} (1+n^2)^{1/4} \overline{v^{(n)}} \quad (3.16)$$

Define

$$G(n) \triangleq \frac{|\beta_n|}{(1+n^2)^{1/2}} = \left| \frac{\kappa^2 - n^2}{1+n^2} \right|^{\frac{1}{2}}$$

Claim. $G(n)$ is bounded on $\mathbb{Z}$.

Proof. Extend G to all of $\mathbb{R}$ by

$$G(x) = \left| \frac{\kappa^2 - x^2}{1+x^2} \right|^{\frac{1}{2}}$$

and compute

$$G'(x) = \begin{cases} -\frac{x}{1+x^2} \left(\sqrt{\frac{1+x^2}{\kappa^2-x^2}} + \sqrt{\frac{\kappa^2-x^2}{1+x^2}} \right) & \text{if } |x| < |\kappa| \\ \frac{x}{1+x^2} \left(\sqrt{\frac{1+x^2}{x^2-\kappa^2}} + \sqrt{\frac{x^2-\kappa^2}{1+x^2}} \right) & \text{if } |x| \geq |\kappa| \end{cases}$$

Now observe that for a fixed κ , G' has the following properties:

1. $G'(x) < 0$ for $x < -\kappa$

2. $G'(x) > 0$ for $-\kappa < x < 0$

3. $G'(x) < 0$ for $0 < x < \kappa$

4. $G'(x) > 0$ for $x > \kappa$

Accordingly, $G(x)$ is increasing on $[-\kappa, 0] \cup [\kappa, \infty]$ and decreasing on $(-\infty, -\kappa) \cup (0, \kappa)$.

Consequently,

$$\begin{aligned} G(x) &\leq \max\{G(0), G(\infty), G(-\infty)\} \\ &= \max\{\kappa, 1\} \end{aligned}$$

Let $C \triangleq \max\{\kappa, 1\} + 1$ so that for all $n \in \mathbb{Z}$, $|G(n)| \leq C$. This proves the claim. ■

Now, applying the result of the previous claim to (3.16), we have

$$|\langle Tu, v \rangle_\Gamma| \leq C \left| 2\pi \sum_{n \in \mathbb{Z}} (1+n^2)^{1/4} u^{(n)} (1+n^2)^{1/4} \bar{v}^{(n)} \right|$$

Then, by the Cauchy-Schwarz inequality, the above becomes

$$\begin{aligned} |\langle Tu, v \rangle_\Gamma| &\leq 2\pi C \sqrt{\sum_{n \in \mathbb{Z}} (1+n^2)^{1/2} |u^{(n)}|^2} \sqrt{\sum_{n \in \mathbb{Z}} (1+n^2)^{1/2} |v^{(n)}|^2} \\ &\leq 2\pi C \|u\|_{1/2, \Gamma} \|v\|_{1/2, \Gamma} \end{aligned}$$

This shows that the $L^2(\Gamma)$ duality pairing of Tu with $H^{1/2}(\Gamma)$ functions forms a bounded linear functional on $H^{1/2}(\Gamma)$. Therefore, we conclude that $Tu \in (H^{1/2}(\Gamma))^* = H^{-1/2}(\Gamma)$.

Further, we have the bound

$$\begin{aligned} \|Tu\|_{-1/2, \Gamma} &\leq \sup_{v \in H^{1/2}(\Gamma)} \frac{|\langle Tu, v \rangle_\Gamma|}{\|v\|_{1/2, \Gamma}} \\ &\leq C \|u\|_{1/2, \Gamma} \end{aligned}$$

which establishes that T is continuous from $H^{1/2}(\Gamma)$ to $H^{-1/2}(\Gamma)$. ■

Lemma 3.2. *The estimates*

$$\operatorname{Re}\langle Tu, u \rangle_\Gamma \leq 0 \quad \text{and} \quad \operatorname{Im}\langle Tu, u \rangle_\Gamma \geq 0$$

hold for any $u \in H^{1/2}(\Gamma)$.

Proof. By the definition of the transparent boundary operator T , we have for any $u \in H^{1/2}(\Gamma)$ that

$$\langle Tu, u \rangle_\Gamma = i2\pi \sum_{n \in \mathbb{Z}} \beta_n |u^{(n)}|^2.$$

Taking the real part gives

$$\operatorname{Re}\langle Tu, u \rangle_\Gamma = -2\pi \sum_{|\alpha_n| > \kappa} (|\alpha_n| - \kappa^2)^{1/2} |u^{(n)}|^2 \leq 0$$

and taking the imaginary part gives

$$\operatorname{Im}\langle Tu, u \rangle_\Gamma = 2\pi \sum_{|\alpha_n| < \kappa} (\kappa^2 - |\alpha_n|^2)^{1/2} |u^{(n)}|^2 \geq 0,$$

which yields the proof. ■

We are going to focus on the variational formulation for the direct diffractive grating problem.

Define the periodic functional space

$$H_p^1(\Omega) = \{u \in H^1(\Omega) : u(0, y) = u(2\pi, y)\} \quad (3.17)$$

which is a subspace of $H^1(\Omega)$.

Now we multiply the Helmholtz equation by the complex conjugate of a test function $v \in H_p^1(\Omega)$:

$$\Delta u \bar{v} + \kappa^2 u \bar{v} = 0$$

Then we integrate over Ω and integrate by parts, obtaining

$$\int_{\Omega} \nabla u \cdot \nabla \bar{v} d\mathbf{x} - \int_{\partial\Omega} \frac{\partial u}{\partial n} \bar{v} dS = \kappa^2 \int_{\Omega} u \bar{v} d\mathbf{x}$$

Applying the boundary conditions on Γ and S , we get

$$\int_{\Omega} \nabla u \cdot \nabla \bar{v} d\mathbf{x} - \int_S \frac{\partial u}{\partial n} \bar{v} dS - \int_{\Gamma} \frac{\partial u}{\partial n} \bar{v} dS = \kappa^2 \int_{\Omega} u \bar{v} d\mathbf{x}$$

which implies

$$\int_{\Omega} \nabla u \cdot \nabla \bar{v} d\mathbf{x} - i\eta \int_S u \bar{v} dS - \langle Tu, v \rangle_{\Gamma} - \langle \rho, v \rangle_{\Gamma} = \kappa^2 \int_{\Omega} u \bar{v} d\mathbf{x}$$

Therefore we derive the variational formulation for the forward problem: find $u \in H_{S,p}^1(\Omega)$, such that

$$a_{\Omega}(u, v) = \langle \rho, v \rangle_{\Gamma} \text{ for all } v \in H_p^1(\Omega) \quad (3.18)$$

where

$$a_{\Omega}(u, v) = \int_{\Omega} \nabla u \cdot \nabla \bar{v} d\mathbf{x} - i\eta \int_S u \bar{v} dS - \langle Tu, v \rangle_{\Gamma} - \kappa^2 \int_{\Omega} u \bar{v} d\mathbf{x} \quad (3.19)$$

Lemma 3.3. *The direct scattering problem has at most one solution.*

Proof. Because the problem is linear, if u_1 and u_2 are both solutions for this direct scattering problem, then so is $u_1 - u_2$. It therefore suffices to show that $u = 0$ in Ω if $\psi = 0$ (no source term). It follows from Green's theorem that we have

$$\begin{aligned} 0 &= \int_{\Omega} (u \Delta \bar{u} - \bar{u} \Delta u) = \int_{\partial\Omega} (u \partial_{\mathbf{n}} \bar{u} - \bar{u} \partial_{\mathbf{n}} u) \\ &= \int_S (u \partial_{\mathbf{n}} \bar{u} - \bar{u} \partial_{\mathbf{n}} u) + \int_{\Gamma} (u \partial_{\mathbf{n}} \bar{u} - \bar{u} \partial_{\mathbf{n}} u) \\ &= -2i\text{Re}(\eta) \int_S |u|^2 - 2i\text{Im}\langle Tu, u \rangle_{\Gamma}, \end{aligned}$$

which yields that $u = 0$ on S since $\text{Re}(\eta) > 0$ and $\text{Im}\langle Tu, u \rangle_{\Gamma} \geq 0$. The impedance boundary

condition on S gives that $\partial_{\mathbf{n}}u = 0$ on S , which implies that $u \equiv 0$ in Ω . ■

Theorem 3.1. *The direct scattering problem has a unique weak solution in $H_{\mathbf{p}}^1(\Omega)$.*

Proof. Decompose the bilinear form into $a_{\Omega} = a_1 - \kappa^2 a_2$, where

$$a_1(u, v) = \int_{\Omega} \nabla u \cdot \nabla \bar{v} - i\eta \int_S u \bar{v} - \langle Tu, v \rangle_{\Gamma}$$

and

$$a_2(u, v) = \int_{\Omega} u \bar{v}.$$

Simple calculations yield

$$\operatorname{Re} a_1(u, u) = \int_{\Omega} |\nabla u|^2 + \operatorname{Im}(\eta) \int_S |u|^2 - \operatorname{Re} \langle Tu, u \rangle_{\Gamma} \geq \int_{\Omega} |\nabla u|^2$$

and

$$\operatorname{Im} a_1(u, u) = -\operatorname{Im}(\eta) \int_S |u|^2 - \operatorname{Im} \langle Tu, u \rangle_{\Gamma} \leq -\operatorname{Im}(\eta) \int_S |u|^2.$$

We conclude that a_1 is coercive from

$$\begin{aligned} |a_1(u, u)| &\geq C(|\operatorname{Re} a_1(u, u)| + |\operatorname{Im} a_1(u, u)|) \\ &\geq C \left(\int_{\Omega} |\nabla u|^2 + \int_S |u|^2 \right) = C \|u\|_{1, \Omega}^2, \end{aligned}$$

where the last inequality may be obtained from the Poincare inequality.

Define an operator $K : L^2(\Omega) \rightarrow H^1(\Omega)$ by

$$a_1(Ku, v) = a_2(u, v) \quad \text{for all } v \in H_{\mathbf{p}}^1(\Omega).$$

Using the Lax-Milgram Theorem, we have

$$\|Ku\|_{1,\Omega} \leq C \|u\|_{0,\Omega}.$$

Thus K is bounded from $L^2(\Omega)$ to $H^1(\Omega)$. Because $H^1(\Omega)$ is compactly embedded into $L^2(\Omega)$, $K : L^2(\Omega) \rightarrow L^2(\Omega)$ is a compact operator.

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

$$a_1(\xi, v) = \langle \rho, v \rangle_\Gamma \quad \text{for all } v \in H_p^1(\Omega).$$

It follows from the Lax-Milgram theorem again that

$$\|\xi\|_{1,\Omega} \leq C \|\rho\|_{0,\Omega}.$$

Using the operator K , we can see that the direct scattering problem is equivalent to finding $u \in L^2(\Omega)$ such that

$$(I - \kappa^2 K)u = \xi.$$

It follows from the Fredholm alternative and the uniqueness result that we have

$$\|u\|_{0,\Omega} \leq C \|\xi\|_{0,\Omega},$$

which gives

$$u = \xi + \kappa^2 Ku.$$

The proof is completed by noting that K is a bounded operator from $L^2(\Omega)$ to $H^1(\Omega)$. ■

3.2 Transformed field expansion

In this section, we shall introduce the transformed field expansion to convert the domain to a rectangular region to facilitate derivation of the analytic solution for the direct problem. The expansion of solution is given as a power series of the parameter ε and is crucial in the inversion formula.

Consider the changes of variables:

$$\tilde{x} = x, \quad \tilde{y} = h \left(\frac{y - f}{h - f} \right),$$

which maps the domain Ω to the rectangle

$$D = \{(\tilde{x}, \tilde{y}) \in \mathbb{R}^2 : 0 < \tilde{y} < h, 0 < \tilde{x} < \Lambda\}.$$

Notice that the grating surface $y = f(x)$ is mapped into the plane surface $\tilde{y} = 0$ while the measurement plane $y = h$ is mapped to itself as $\tilde{y} = h$ under this change of variables. Now the grating problem can be restated in this transformed coordinate. First, we prove the following.

Theorem 3.2. *Let $w(\tilde{x}, \tilde{y}) = u(x, y)$. Then w is a periodic function with period Λ .*

Proof. For arbitrary $x \in \mathbb{R}, y \in [0, h]$, we have $w(\tilde{x} + \Lambda, \tilde{y}) = u(x + \Lambda, y)$, and $u(x + \Lambda, y) = u(x, y)$ since u is periodic, therefore $w(\tilde{x} + \Lambda, \tilde{y}) = u(x, y)$ where $u(x, y)$ is $w(\tilde{x}, \tilde{y})$ by definition. We can conclude $w(\tilde{x} + \Lambda, \tilde{y}) = w(\tilde{x}, \tilde{y})$, which implies w is periodic with Λ . ■

Now we are going to focus on the scattering problem for w . By the chain rule,

$$\begin{aligned} u_x &= \frac{\partial w}{\partial x} = \frac{\partial w}{\partial \tilde{x}} \frac{\partial \tilde{x}}{\partial x} + \frac{\partial w}{\partial \tilde{y}} \frac{\partial \tilde{y}}{\partial x} \\ &= \frac{\partial w}{\partial \tilde{x}} + \frac{\partial w}{\partial \tilde{y}} h(y - h) \frac{-f'}{(h - f)^2} \end{aligned}$$

$$= \frac{\partial w}{\partial \tilde{x}} + \frac{\partial w}{\partial \tilde{y}} h f' \frac{h-y}{(h-f)^2}$$

and

$$\begin{aligned} u_y &= \frac{\partial w}{\partial y} = \frac{\partial w}{\partial \tilde{x}} \frac{\partial \tilde{x}}{\partial y} + \frac{\partial w}{\partial \tilde{y}} \frac{\partial \tilde{y}}{\partial y} \\ &= \frac{\partial w}{\partial \tilde{y}} \frac{h}{h-f} \end{aligned}$$

So we have

$$\begin{aligned} \partial x &= \partial \tilde{x} - f' \left(\frac{h-\tilde{y}}{h-f} \right) \partial \tilde{y}, \\ \partial y &= \left(\frac{h}{h-f} \right) \partial \tilde{y}. \end{aligned}$$

Therefore,

$$\begin{aligned} u_{xx} &= \left(\frac{\partial w}{\partial \tilde{x}} + \frac{\partial w}{\partial \tilde{y}} h f' \frac{h-y}{(h-f)^2} \right)'_x \\ &= \frac{\partial^2 w}{\partial \tilde{x} \partial x} + \frac{\partial^2 w}{\partial \tilde{y} \partial x} h f' \frac{h-y}{(h-f)^2} + \frac{\partial w}{\partial \tilde{y}} \left(h f' \frac{h-y}{(h-f)^2} \right)'_x \\ &= \frac{\partial^2 w}{\partial \tilde{x}^2} + 2 \frac{\partial^2 w}{\partial \tilde{x} \partial \tilde{y}} h f' \frac{h-y}{(h-f)^2} + \frac{\partial^2 w}{\partial \tilde{y}^2} \left(h f' \frac{h-y}{(h-f)^2} \right)^2 + \frac{\partial w}{\partial y} \left(h f' \frac{h-y}{(h-f)^2} \right)'_x \end{aligned}$$

where the derivative in the last term

$$\begin{aligned} \left(h f' \frac{h-y}{(h-f)^2} \right)'_x &= \frac{h(h-y)f''(h-f)^2 + h f'(h-y)2(h-f)f'}{(h-f)^4} \\ &= (f''(h-f) + 2f'^2) \frac{h(h-y)}{(h-f)^3} \end{aligned}$$

Note that

$$\frac{h(h-y)}{(h-f)^3} = \frac{h(h-f+f-y)}{(h-f)^3} = \frac{h \frac{h-f}{h-f} - h \frac{y-f}{h-f}}{(h-f)^2} = \frac{h-\tilde{y}}{(h-f)^2}$$

So

$$\left(hf' \frac{h-y}{(h-f)^2} \right)'_x = (f''(h-f) + 2f'^2) \frac{h-\tilde{y}}{(h-f)^2}$$

We may differentiate again and obtain the needed second derivatives:

$$\begin{aligned} u_{xx} &= \frac{\partial^2 w}{\partial \tilde{x}^2} + 2 \frac{\partial^2 w}{\partial \tilde{x} \partial \tilde{y}} hf' \frac{h-y}{(h-f)^2} + \frac{\partial^2 w}{\partial \tilde{y}^2} \left(hf' \frac{h-y}{(h-f)^2} \right)^2 + \left[(f''(h-f) + 2f'^2) \frac{h-\tilde{y}}{(h-f)^2} \right] \frac{\partial w}{\partial y} \\ &= \frac{\partial^2 w}{\partial \tilde{x}^2} + 2f' \frac{h-\tilde{y}}{h-f} \frac{\partial^2 w}{\partial \tilde{x} \partial \tilde{y}} + \left(f' \frac{h-\tilde{y}}{h-f} \right)^2 \frac{\partial^2 w}{\partial \tilde{y}^2} + \left[(f''(h-f) + 2f'^2) \frac{h-\tilde{y}}{(h-f)^2} \right] \frac{\partial w}{\partial y} \end{aligned}$$

$$\begin{aligned} u_{yy} &= \frac{\partial}{\partial y} \left(\frac{\partial w}{\partial \tilde{y}} \frac{h}{h-f} \right) \\ &= \frac{h^2}{(h-f)^2} \frac{\partial^2 w}{\partial \tilde{y}^2} \end{aligned}$$

Since $u_{xx} + u_{yy} + \kappa^2 u = 0$, it can be derived that w , upon dropping the tilde, satisfies the following equation in D :

$$(c_1 \partial_{xx} + c_2 \partial_{yy} + c_3 \partial_{xy} + c_4 \partial_y + c_1 \kappa^2) w = 0, \quad (3.20)$$

where

$$\begin{aligned} c_1 &= (h-f)^2 & c_3 &= -2f'(h-y)(h-f) \\ c_2 &= [f'(h-y)]^2 + h^2 & c_4 &= -(h-y)[f''(h-f) + 2(f')^2]. \end{aligned}$$

Combing (3.5) and (3.6), the impedance boundary condition becomes

$$\begin{aligned} &f' \left(1 - \frac{f}{h} \right) \partial_x w - (1 + (f')^2) \partial_y w \\ &- i\eta (1 + (f')^2)^{1/2} \left(1 - \frac{f}{h} \right) w = 0 \quad \text{on } y = 0. \end{aligned} \quad (3.21)$$

The transparent boundary condition (3.14) reduces to

$$\partial_y w = \left(1 - \frac{f}{h}\right) (Tw + \rho) \quad \text{on } y = h. \quad (3.22)$$

By the small perturbation assumption, we consider a formal expansion of w in a power series of ε :

$$w(x, y; \varepsilon) = \sum_{k=0}^{\infty} w_k(x, y) \varepsilon^k. \quad (3.23)$$

Substituting $f = \varepsilon g$ into each of c_1 , c_2 , c_3 , and c_4 and inserting the power series expansion (3.23) into (3.20)–(3.22), we derive the recursion equation for w_k :

$$(\Delta + \kappa^2)w_k = v_k \quad \text{in } D, \quad (3.24)$$

where

$$\begin{aligned} v_k = & \frac{1}{h} \left[2g\partial_{xx} + 2g'(h-y)\partial_{xy} + g''(h-y)\partial_y + 2\kappa^2 g \right] w_{k-1} \\ & - \frac{1}{h^2} \left[g^2\partial_{xx} + (g')^2(h-y)^2\partial_{yy} + 2gg'(h-y)\partial_{xy} - (2(g')^2 - gg'')(h-y)\partial_y + \kappa^2 g^2 \right] w_{k-2}. \end{aligned}$$

The impedance boundary condition (3.21) becomes

$$(\partial_y + i\eta)w_k = \varphi_k \quad \text{on } y = 0, \quad (3.25)$$

where

$$\begin{aligned} \varphi_k = & \left[g'\partial_x - i\eta \left(\frac{g}{h} \right) \right] w_{k-1} - \left[g' \left(\frac{g}{h} \right) \partial_x + (g')^2 \partial_y \right] w_{k-2} \\ & - i\eta \sum_{l=1}^{\lfloor \frac{k}{2} \rfloor} \binom{\frac{1}{2}}{l} (g')^{2l} \times \left[w_{k-2l} - \left(\frac{g}{h} \right) w_{k-2l-1} \right]. \end{aligned}$$

Here $\lfloor l \rfloor$ is the largest integer not greater than m and the generalized binomial coefficient

$$\binom{\frac{1}{2}}{l} = \frac{\frac{1}{2}(\frac{1}{2}-1)\cdots(\frac{1}{2}-l+1)}{l!}.$$

The transparent boundary condition (3.22) reduces to

$$\partial_y w_k - Tw_k = \psi_k \quad \text{on } y = h, \quad (3.26)$$

where

$$\left. \begin{aligned} \psi_0 &= \psi, \\ \psi_1 &= -\left(\frac{g}{h}\right)(Tw_0 + \psi), \\ \psi_k &= -\left(\frac{g}{h}\right)Tw_{k-1}, \quad k \geq 2. \end{aligned} \right\} \quad (3.27)$$

It is understood that $w_k = 0$ for all $k < 0$ in the above recurrence relations. For each w_k , the equation (3.24) and the boundary conditions (3.25) and (3.26) require only the previous solutions $w_{k-1}, w_{k-2}, \dots, w_0$. Hence the transformed diffraction problem (3.24)–(3.27) can be solved recursively starting from $k = 0$.

3.3 Fourier series expansion

For fixed k , we shall derive an analytic solution of w_k for the problem (3.24)–(3.27), considering v_k, φ_k, ψ_k as known functions. Since $w_k, v_k, \varphi_k, \psi_k$ are periodic functions in x with period Λ , they have the following Fourier series expansions

$$\begin{aligned} w_k(x, y) &= \sum_{n \in \mathbb{Z}} w_k^{(n)}(y) e^{i\alpha_n x}, \\ v_k(x, y) &= \sum_{n \in \mathbb{Z}} v_k^{(n)}(y) e^{i\alpha_n x}, \\ \varphi_k(x, y) &= \sum_{n \in \mathbb{Z}} \varphi_k^{(n)}(y) e^{i\alpha_n x}, \\ \psi_k(x) &= \sum_{n \in \mathbb{Z}} \psi_k^{(n)} e^{i\alpha_n x}. \end{aligned}$$

Substituting these expansions into (3.24), (3.25), and (3.26), we obtain a two-point boundary value problem for $w_k^{(n)}$:

$$\left. \begin{aligned} \frac{d^2 w_k^{(n)}}{dy^2} + \beta_n^2 w_k^{(n)} &= v_k^{(n)}, \quad 0 < y < h, \\ \frac{dw_k^{(n)}}{dy} + i\eta w_k^{(n)} &= \varphi_k^{(n)}, \quad y = 0, \\ \frac{dw_k^{(n)}}{dy} - i\beta_n w_k^{(n)} &= \psi_k^{(n)}, \quad y = h. \end{aligned} \right\} \quad (3.28)$$

By taking the Fourier series, the two-dimensional grating problem for the Helmholtz equation reduces to a one-dimensional two-point boundary value problem in the y direction, which can be solved analytically. Using Theorem B.1 in Appendix, we obtain an explicit solution of (3.28).

Theorem 3.3. *The two-point boundary value problem (3.28) has a unique solution, which is given by*

$$w_k^{(n)}(y) = K_1^{(n)}(y)\varphi_k^{(n)} - K_2^{(n)}(y)\psi_k^{(n)} + \int_0^h K_3^{(n)}(y, z)v_k^{(n)}(z) dz \quad (3.29)$$

where

$$\begin{aligned} K_1^{(n)}(y) &= \frac{e^{i\beta_n y}}{i(\beta_n + \eta)} \\ K_2^{(n)}(y) &= \frac{e^{i\beta_n(h-y)}}{i(\beta_n + \eta)} K^{(n)}(y) \\ K_3^{(n)}(y, z) &= \begin{cases} \frac{e^{i\beta_n(y-z)}}{i(\beta_n + \eta)} K^{(n)}(z), & z < y, \\ \frac{e^{i\beta_n(z-y)}}{i(\beta_n + \eta)} K^{(n)}(y), & z > y, \end{cases} \end{aligned}$$

and

$$K^{(n)}(t) = \frac{(\beta_n + \eta)}{2\beta_n} + \frac{(\beta_n - \eta)}{2\beta_n} e^{2i\beta_n t}.$$

It follows from Theorem 3.3 that the power series (3.23) along with the solution representation (3.29) gives an analytic solution of the direct grating problem (3.20)–(3.22).

Remark 3.1. Theorems 3.1 and 3.3 together give an explicit analytic solution of the grating surface problem. From the definition of $K_j^{(n)}$, it is clear that when $|\alpha_n| < \kappa$, the solution component at n is a propagating wave. When $|\alpha_n| > \kappa$, the solution component becomes an evanescent wave, which decays exponentially in the y direction. ■

Remark 3.2. Notice that $\operatorname{Re} \eta \neq 0$ and $\operatorname{Im} \eta \neq 0$ while β_n is either a real number or a pure imaginary number. Hence we have $\eta \neq \beta_n$ for all $n \in \mathbb{Z}$. ■

Remark 3.3. When the impedance boundary condition is reduced to sound soft condition and $f \in C^2$, the convergence of power series for w has been proved in [9]. ■

Based on (3.29), we shall derive explicit expressions for solutions $w_0^{(n)}$ and $w_1^{(n)}$, which play an important role in the reconstruction formula.

Inverse Problem

4.1 Reconstruction formula

The previous chapter presented an analytic solution of forward problem based on a transformed field expansion and power series. We turn attention to the inverse problem. Suppose that the total field is measured on the boundary Γ with noise. Assume that the noisy data takes the form

$$u_\delta(x, h) = u(x, h) + \mathcal{O}(\delta),$$

where $u(x, h)$ is the exact data and δ is the noise level.

Since the the information is collected on $y = h$, it is natural to evaluate the power series (3.23) at $y = h$. Noting $w(x, h) = u(x, h)$ and $w_\delta(x, h) = u_\delta(x, h)$, we have

$$w_\delta(x, h) = w_0(x, h) + \varepsilon w_1(x, h) + \mathcal{O}(\varepsilon^2) + \mathcal{O}(\delta). \quad (4.1)$$

Rearranging (4.1), and dropping $\mathcal{O}(\varepsilon^2)$ and $\mathcal{O}(\delta)$ yield

$$\varepsilon w_1(x, h) = w_\delta(x, h) - w_0(x, h), \quad (4.2)$$

which is the linearization of the nonlinear inverse problem and enables us to find an explicit reconstruction formula for the linearized inverse problem.

Based on (4.2), we next shall derive the analytical solution for the leading term w_0 and then deduce an equation relating w_1 . From there, we can obtain the scattering surface function f for an explicit inversion formula.

Recalling (3.2), (3.26), and (3.27), we have

$$v_0 = 0, \quad \varphi_0 = 0, \quad \psi_0 = -2i\kappa e^{-i\kappa h},$$

whose Fourier coefficients are

$$v_0^{(n)} = 0, \quad \varphi_0^{(n)} = 0, \quad \psi_0^{(n)} = -2i\kappa e^{-i\kappa h} \delta_{0n}.$$

Here δ_{kn} is the Kronecker delta. It follows from (3.29) that

$$w_0^{(n)}(y) = -K_2^{(n)} \psi_0^{(n)} = 2i\kappa e^{-i\kappa h} K_2^{(n)}(y) \delta_{0n}, \quad (4.3)$$

which gives

$$\begin{aligned} w_0(x, y) &= \sum_{n \in \mathbb{Z}} w_0^{(n)}(y) e^{i\alpha_n x} = 2i\kappa e^{-i\kappa h} K_2^{(0)}(y) \\ &= e^{-i\kappa y} + \left(\frac{\kappa + \eta}{\kappa - \eta} \right) e^{i\kappa y}. \end{aligned} \quad (4.4)$$

Denote $u^{\text{ref}}(x, y) = \left(\frac{\kappa + \eta}{\kappa - \eta} \right) e^{i\kappa y}$. It is clear that u^{ref} represents an outgoing reflected field, that is, $w_0(x, y) = u^{\text{inc}} + u^{\text{ref}}$. It can also be verified that w_0 satisfies the impedance condition on the flat plane $y = 0$.

Remark 4.1. Physically, the leading term w_0 shows how incident field u^{inc} interacts with the impedance plane surface. It provides insight into how the incident wave is reflected by

the grating surface without any deformation (i.e., $\varepsilon = 0$), or when S is a smooth flat plane. Mathematically, it satisfies the Helmholtz equation,

$$(\Delta + \kappa^2)w_0 = 0 \quad \text{in } D,$$

with the impedance boundary condition

$$(\partial_y - i\eta)w_0 = 0 \quad \text{on } y = 0,$$

and transparent boundary condition

$$\partial_y w_0 - Tw_0 = \psi \quad \text{on } y = h,$$

where $\psi = -2i\kappa e^{-i\kappa h}$. It can be verified that the solution w_0 consists of the incident u^{inc} and the reflected field u^{ref} . ■

Now we are going to derive w_1 using (3.2) and the equations of Remark 4.1,

$$\begin{aligned} v_1(x, y) &= \frac{1}{h} \left[g''(x)(h - y)\partial_y + 2\kappa^2 g \right] w_0 \\ &= \frac{2\kappa^2}{h} \left[e^{-i\kappa y} + \left(\frac{\kappa + \eta}{\kappa - \eta} \right) e^{i\kappa y} \right] g(x) - \frac{i\kappa(h - y)}{h} \left[e^{-i\kappa y} - \left(\frac{\kappa + \eta}{\kappa - \eta} \right) e^{i\kappa y} \right] g''(x) \end{aligned}$$

and its Fourier coefficient

$$v_1^{(n)}(y) = \frac{2\kappa^2}{h} \left[e^{-i\kappa y} + \left(\frac{\kappa + \eta}{\kappa - \eta} \right) e^{i\kappa y} \right] g_n + \frac{i\kappa \alpha_n^2 (h - y)}{h} \left[e^{-i\kappa y} - \left(\frac{\kappa + \eta}{\kappa - \eta} \right) e^{i\kappa y} \right] g_n, \quad (4.5)$$

where g_n is the Fourier coefficient of g (note the difference in notation from the usual $g^{(n)}$!).

Following (3.26) and (4.4) yield

$$\varphi_1(x) = \left[g' \partial_x - i\eta \left(\frac{g}{h} \right) \right] w_0(x, 0)$$

$$= -\frac{i\eta g(x)}{h}w_0(x,0) = -\left[\frac{2i\kappa\eta}{h(\kappa-\eta)}\right]g(x)$$

which has Fourier coefficients

$$\varphi_1^{(n)} = -\left[\frac{2i\kappa\eta}{h(\kappa-\eta)}\right]g_n. \quad (4.6)$$

Similarly, we have from (3.27) and (4.4) that

$$\begin{aligned} \psi_1(x) &= -\left(\frac{g}{h}\right)(Tw_0 + \psi_0) = -\left(\frac{g}{h}\right)(Tw_0 + \psi) \\ &= -\left(\frac{g}{h}\right)\partial_y w_0(x, h) = \frac{i\kappa}{h}\left[e^{-i\kappa h} - \left(\frac{\kappa + \eta}{\kappa - \eta}\right)e^{i\kappa h}\right]g(x) \end{aligned}$$

which has Fourier coefficients

$$\psi_1^{(n)} = \frac{i\kappa}{h}\left[e^{-i\kappa h} - \left(\frac{\kappa + \eta}{\kappa - \eta}\right)e^{i\kappa h}\right]g_n. \quad (4.7)$$

Letting $k = 1$ and evaluating at $y = h$ in (3.29), we get

$$w_1^{(n)}(h) = K_1^{(n)}(h)\varphi_1^{(n)} - K_2^{(n)}(h)\psi_1^{(n)} + \int_0^h K_3^{(n)}(h, z)v_1^{(n)}(z)dz. \quad (4.8)$$

where

$$\begin{aligned} K_1^{(n)}(h) &= \frac{ie^{i\beta_n h}}{\eta - \beta_n}, \\ K_2^{(n)}(h) &= \frac{i}{\eta - \beta_n}K^{(n)}(h) \\ &= -\frac{i}{2\beta_n} + \frac{i}{2\beta_n}\frac{\eta + \beta_n}{\eta - \beta_n}e^{2i\beta_n h} \\ K_3^{(n)}(h, z) &= \frac{e^{i\beta_n(h-z)}}{i(\beta_n - \eta)}K^{(n)}(z) \\ &= \frac{e^{i\beta_n(h-z)}}{2i\beta_n} + \frac{e^{i\beta_n(h+z)}}{2i\beta_n}\frac{\beta_n + \eta}{\beta_n - \eta} \end{aligned}$$

By letting $M_1 = K_1^{(n)}(h)\varphi_1^{(n)}$, $M_2 = K_2^{(n)}(h)\psi_1^{(n)}$, $M_3 = \int_0^h K_3^{(n)}(h, z)v_1^{(n)}(z)dz$, (4.8) could

be rewritten as $w_1^{(n)}(h) = M_1 - M_2 + M_3$. We continue simplifying M_1, M_2 , and M_3 :

$$\begin{aligned} M_1 &= K_1^{(n)}(h) \varphi_1^{(n)} \\ &= \frac{2\kappa\eta e^{i\beta_n h}}{(\eta - \beta_n)(\kappa - \eta)h} g_n, \end{aligned}$$

$$\begin{aligned} M_2 &= K_2^{(n)}(h) \psi_1^{(n)} \\ &= \frac{\kappa g_n}{2\beta_n h(\kappa - \eta)(\eta - \beta_n)} \left[(\eta - \beta_n)(\kappa - \eta) e^{-i\kappa h} + (\eta + \beta_n) e^{2i\beta_n h} (\kappa + \eta) e^{i\kappa h} \right. \\ &\quad \left. - (\eta - \beta_n)(\kappa + \eta) e^{i\kappa h} - (\eta + \beta_n) e^{2i\beta_n h} (\kappa - \eta) e^{-i\kappa h} \right], \end{aligned}$$

$$\begin{aligned} M_3 &= \int_0^h K_3^{(n)}(h, z) v_1^{(n)}(z) dz \\ &= \underbrace{\frac{\kappa^2 g_n e^{i\beta_n h}}{ih\beta_n(\beta_n - \eta)(\kappa - \eta)} \underbrace{\int_0^h \mathcal{K}_n^+(z; \eta) dz}_{\mathcal{I}_+}}_{\triangleq N_1} + \underbrace{\frac{\kappa e^{i\beta_n h}}{(\beta_n - \eta)(\kappa - \eta)} \frac{\alpha_n^2}{2h\beta_n} \underbrace{\int_0^h (h - z) \mathcal{K}_n^-(z; \eta) dz}_{\mathcal{I}_-}}_{\triangleq N_2} \end{aligned}$$

where

$$\mathcal{K}_n^\pm(z; \eta) = \left[(\beta_n - \eta) e^{-i\beta_n z} + (\beta_n + \eta) e^{i\beta_n z} \right] \times \left[e^{-i\kappa z} (\kappa - \eta) \pm e^{i\kappa z} (\kappa + \eta) \right]$$

Performing the integration yields

$$\begin{aligned} \mathcal{I}_+ &= \frac{(\beta_n + \eta)(\kappa + \eta)}{(\beta_n + \kappa)} (1 - e^{i(\beta_n + \kappa)h}) + \frac{(\beta_n + \eta)(\kappa - \eta)}{(\beta_n - \kappa)} (1 - e^{i(\beta_n - \kappa)h}) \\ &\quad - \frac{(\beta_n - \eta)(\kappa - \eta)}{(\beta_n + \kappa)} (1 - e^{-i(\beta_n + \kappa)h}) - \frac{(\beta_n - \eta)(\kappa + \eta)}{(\beta_n - \kappa)} (1 - e^{-i(\beta_n - \kappa)h}) \end{aligned}$$

$$\mathcal{I}_- = 2i(\kappa^2 - \eta^2) + \frac{1}{2h\beta_n} \mathcal{A}$$

with

$$\begin{aligned}\mathcal{A} = & \frac{(\beta_n + \eta)(\kappa + \eta)(\beta_n - \kappa)}{(\beta_n + \kappa)}(1 - e^{+i(\beta_n + \kappa)h}) - \frac{(\beta_n + \eta)(\kappa - \eta)(\beta_n + \kappa)}{(\beta_n - \kappa)}(1 - e^{+i(\beta_n - \kappa)h}) \\ & - \frac{(\beta_n - \eta)(\kappa - \eta)(\beta_n - \kappa)}{(\beta_n + \kappa)}(1 - e^{-i(\beta_n + \kappa)h}) + \frac{(\beta_n - \eta)(\kappa + \eta)(\beta_n + \kappa)}{(\beta_n - \kappa)}(1 - e^{-i(\beta_n - \kappa)h})\end{aligned}$$

Combining N_1 and N_2 , we get

$$\begin{aligned}M_3 = & \frac{2i\kappa(\kappa^2 - \eta^2)e^{i\beta_n h}}{(\eta - \beta_n)(\kappa - \eta)}g_n + \frac{\kappa e^{i\beta_n h}}{2h\beta_n(\beta_n - \eta)(\kappa - \eta)} \times \\ & g_n \left[(\beta_n + \eta)(\kappa + \eta)(1 - e^{+i(\beta_n + \kappa)h}) - (\beta_n + \eta)(\kappa - \eta)(1 - e^{+i(\beta_n - \kappa)h}) \right. \\ & \left. - (\beta_n - \eta)(\kappa - \eta)(1 - e^{-i(\beta_n + \kappa)h}) + (\beta_n - \eta)(\kappa + \eta)(1 - e^{-i(\beta_n - \kappa)h}) \right]\end{aligned}$$

Subtracting M_2 from M_3 leads to

$$M_3 - M_2 = \frac{2i\kappa(\kappa^2 - \eta^2)e^{i\beta_n h}}{(\eta - \beta_n)(\kappa - \eta)}g_n + \frac{2\eta\kappa e^{i\beta_n h}}{h(\beta_n - \eta)(\kappa - \eta)}g_n$$

Finally, we calculate $M_1 - M_2 + M_3$.

$$\begin{aligned}w_1^{(n)}(h) &= M_1 - M_2 + M_3 \\ &= \frac{2\kappa\eta e^{i\beta_n h}}{h(\eta - \beta_n)(\kappa - \eta)}g_n - \frac{2i\kappa(\kappa^2 - \eta^2)e^{i\beta_n h}}{(\beta_n - \eta)(\kappa - \eta)}g_n + \frac{2\eta\kappa e^{i\beta_n h}}{h(\beta_n - \eta)(\kappa - \eta)}g_n \\ &= \frac{-2i\kappa(\kappa + \eta)e^{i\beta_n h}}{(\beta_n - \eta)}g_n\end{aligned}$$

Therefore, an elegant equation relating Fourier coefficient of w_1 and g is obtained:

$$w_1^{(n)}(h) = \frac{2i\kappa(\eta + \kappa)}{(\eta - \beta_n)}e^{i\beta_n h}g_n. \quad (4.9)$$

Remark 4.2. The impedance boundary condition (3.5) reduces to the perfectly conducting

boundary condition $u = 0$ on S as $\eta \rightarrow \infty$, and (4.9) becomes

$$w_1^{(n)}(h) = 2i\kappa e^{i\beta_n h} g_n,$$

which is consistent with the result in [10]. ■

We recall that $f = \varepsilon g$ so that $f_n = \varepsilon g_n$, where f_n is the Fourier coefficient of f . Plugging (4.3) and (4.9) into (4.2), we deduce that

$$f_n = \frac{i(\beta_n - \eta)}{2\kappa(\kappa + \eta)} \left[w_\delta^{(n)}(h) - w_0^{(n)}(h) \right] e^{-i\beta_n h}, \quad (4.10)$$

where $w_\delta^{(n)}(h)$ is the Fourier coefficient of the noisy data $w_\delta(x, h)$ and $w_0^{(n)}(h)$ is the Fourier coefficient of $w_0(x, h)$ given as

$$w_0^{(n)}(h) = \left[e^{-i\kappa h} + \left(\frac{\kappa + \eta}{\kappa - \eta} \right) e^{i\kappa h} \right] \delta_{0n}.$$

Remark 4.3. The inversion formula (4.10) includes cases for sound soft and sound hard boundary conditions. For sound hard boundary conditions, i.e., $\eta = 0$, the inversion formula reduces to

$$f_n = \frac{i\beta_n}{2\kappa^2} \left[w_\delta^{(n)}(h) - w_0^{(n)}(h) \right] e^{-i\beta_n h},$$

For the sound soft boundary condition, $\eta = \infty$, the inversion formula reduces to

$$f_n = -\frac{i}{2\kappa} \left[w_\delta^{(n)}(h) - w_0^{(n)}(h) \right] e^{-i\beta_n h}.$$

■

Remark 4.4. The inversion formula (4.10) accounts for both propagation wave modes and

evanescent wave modes. More explicitly, we have

$$f_n = \begin{cases} \frac{i(\sqrt{\kappa^2 - \alpha_n^2} - \eta)}{2\kappa(\kappa + \eta)} [w_\delta^{(n)}(h) - w_0^{(n)}(h)] e^{-i\sqrt{\kappa^2 - \alpha_n^2}h} & \text{for } |\alpha_n| < \kappa \\ -\frac{\sqrt{\alpha_n^2 - \kappa^2} + i\eta}{2\kappa(\kappa + \eta)} [w_\delta^{(n)}(h) - w_0^{(n)}(h)] e^{\sqrt{\alpha_n^2 - \kappa^2}h} & \text{for } |\alpha_n| > \kappa \end{cases} \quad (4.11)$$

The low frequency modes of the scattering surface function f come from propagating (bounded) waves, while the evanescent modes generate the high frequency modes. The factor on the right hand side of (4.10), $e^{-i\beta_n h}$, reflects the ill-posedness of this problem. In other word, the measurement noise will be exponentially amplified for high frequency modes $|\alpha_n| > \kappa$.

It follows from the definition of β_n and (4.10) that it is a well-posed problem to seek reconstruction of the Fourier coefficients f_n for which $|\alpha_n| < \kappa$, since small variations in the measured data will not be amplified and lead to large errors in the reconstruction. However, the resolution of the reconstruction f is limited by the given wavenumber κ . In contrast, it is severely ill-posed to reconstruct those Fourier coefficients f_n with $|\alpha_n| > \kappa$, since small variations in the data will be exponentially amplified and lead to huge errors in the reconstruction. However, these ill-behaving modes contribute to the super resolution of the reconstructed function f .

To obtain a stable and super-resolved reconstruction, we may adopt a regularization to suppress the exponential growth. One remedy is to make h as small as possible, i.e., measure the data at the distance which is as close as possible to the grating surface, or bring the scanning tip close to the scattering surface. This is exactly the idea of near-field optics. The other remedy is to adopt a commonly used regularization, such as cut-off regularization or Tikhonov regularization[25]. Following [14], we consider the spectral cut-off regularization. Define the signal-to-noise ratio (SNR) by

$$\text{SNR} = \min\{\varepsilon^{-2}, \delta^{-1}\}.$$

For fixed h , the cut-off frequency ω is chosen in such a way that

$$e^{(\omega^2 - \kappa^2)^{1/2}h} = \text{SNR},$$

which implies that the spatial frequency will be cutoff for those below the noise level and the surface deformation parameter. More explicitly, we have

$$\frac{\omega}{\kappa} = \left[1 + \left(\frac{\log \text{SNR}}{\kappa h} \right)^2 \right]^{1/2}, \quad (4.12)$$

which indicates $\omega > \kappa$ as long as $\text{SNR} > 0$ and super resolution may be achieved.

Taking into account the frequency cut-off, we may have a regularized reconstruction formulation:

$$f_n = \frac{i(\beta_n - \eta)}{2\kappa(\kappa + \eta)} \left[w_\delta^{(n)}(h) - w_0^{(n)}(h) \right] e^{-i\beta_n h} \chi_n(\alpha_n), \quad (4.13)$$

where the characteristic function

$$\chi_n(\alpha_n) = \begin{cases} 1 & \text{for } |\alpha_n| \leq \omega, \\ 0 & \text{for } |\alpha_n| > \omega. \end{cases}$$

Once f_n have been computed, the grating surface function can be approximated by

$$f(x) \approx \sum_{|\alpha_n| \leq \omega} f_n e^{i\alpha_n x}. \quad (4.14)$$

Hence, only two fast Fourier transforms are needed to reconstruct the grating surface function: one for the data to obtain $w_\delta^{(n)}(h)$ and another to obtain the approximated f .

Remark 4.5. When the impedance boundary condition reduces to sound hard boundary

condition, i.e. $\eta = 0$, the regularized inversion formula (4.13) is reduced to

$$f_n = \frac{i\beta_n}{2\kappa^2} \left[w_\delta^{(n)}(h) - w_0^{(n)}(h) \right] e^{-i\beta_n h} \chi_n(\alpha_n), \quad (4.15)$$

For the sound soft boundary condition, i.e., $\eta = \infty$, the regularized inversion formula (4.13) is reduced to

$$f_n = -\frac{i}{2\kappa} \left[w_\delta^{(n)}(h) - w_0^{(n)}(h) \right] e^{-i\beta_n h} \chi_n(\alpha_n) \quad (4.16)$$

■

This completes solution to the inverse problem.

Numerical Experiments

We have already derived an elegant reconstruction formula for the inverse problem. In this chapter, we are going to present two numerical examples to illustrate the effectiveness of our method for algorithmic implementation and dependence of resolution on parameters measurement distance h , surface deformation parameter ε , and the noise level δ .

The near-field data $u(x, h)$ is created by solving the direct grating problem using the finite element method with a perfectly matched layer. The wavenumber is taken as $\kappa = 2\pi$ which corresponds to the wavelength $\lambda = 1$. The grating period is $\Lambda = 1$, i.e., $\Lambda = \lambda$, and the impedance constant $\eta = 2\pi(1 + i)$, which is merely illustrative and stands for a complex impedance. To get the data we need on boundary Γ , we use synthetic data: first, we solve the forward problem by FEM then get the solution, then use these data as information to reconstruct the scattering function $f(x)$. We present two numerical examples. The first example only contains low Fourier modes and the second example contains high frequency modes which necessitate cut-off regularization will be applied.

In all the figures, the plots are rescaled with respect to the wavelength λ . Due to the unstructured triangular meshes, the wave field data $u(x, h)$ is not equally spaced with respect to x . We construct a curve $u(x, h)$ by using the natural cubic spline interpolation formula based on the computed discrete data $u(x, h)$. The curve $u(x, h)$ is evaluated at equally

spaced points x_j and used as our synthetic scattering data. For the stability test, some relative random noise is added to the data, i.e., the near-field measurement is updated with

$$u_\delta(x, h) = u(x, h)(1 + \delta \text{rand}),$$

where rand represents a normally distributed random number in $[-1, 1]$. In the examples, approximately 1% noise is added to the data.

5.1 Numerical Example 1: Low Frequency

The exact grating surface is given by $f(x) = \varepsilon g(x)$, where

$$g(x) = 0.5 \sin(4\pi x) + 0.5 \sin(6\pi x).$$

This is a simple example since the grating profile function g only contains a couple of low Fourier modes. We examine the dependence of reconstruction results on the parameters h and ε . Figures 5.1 and 5.2 display the reconstructed surfaces against the exact surfaces.

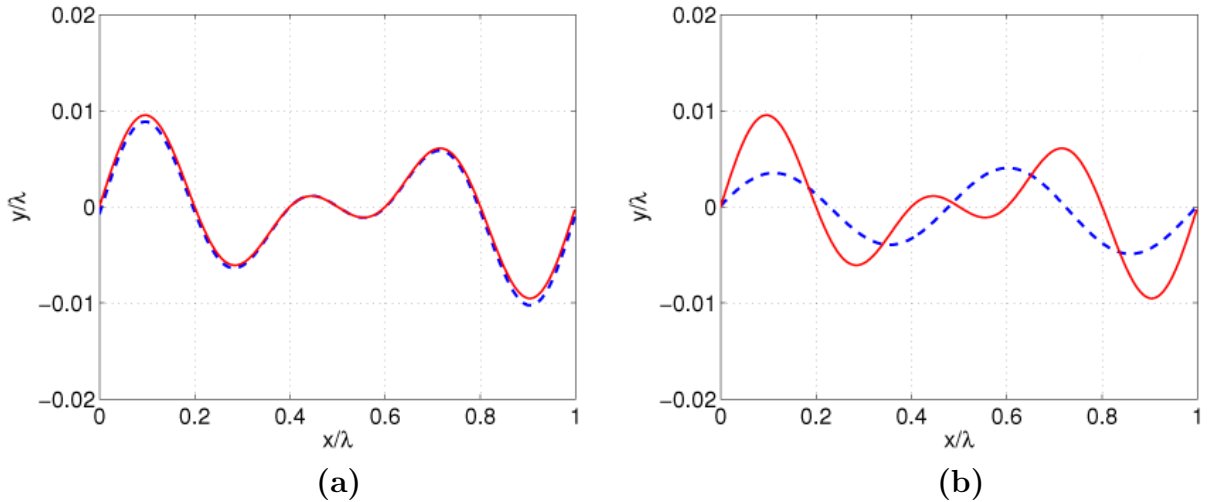


Figure 5.1 Numerical Experiment #1: $\varepsilon = 0.01$. Reconstruction of a grating with finite Fourier modes: the exact surface (solid line) is plotted against the reconstructed surface (dashed line) using different h and the same $\varepsilon = 0.01$: (a) $h = 0.1\lambda$; (b), $h = 0.2\lambda$.

Figure 5.1 above compares the reconstruction using two different measurement distances. The examples of this figure fix $\varepsilon = 0.01$. (a) and (b) plot the reconstructed surfaces by using $h = 0.1\lambda$ and $h = 0.2\lambda$, respectively. It is clear that smaller h of (a) gives a better reconstruction than what is seen in (b). In particular, the fine features of the grating surface are completely recovered and sub-wavelength resolution is achieved when using $h = 0.1\lambda$. A larger cut-off frequency ω may be used in the reconstruction when the measurement distance h is smaller, allowing for inclusion of higher-frequency modes, and hence, more detail.

The next comparison fixes $h = 0.1\lambda$ and consider reconstructions for two different ε . The result is displayed in Figure 5.2 below.

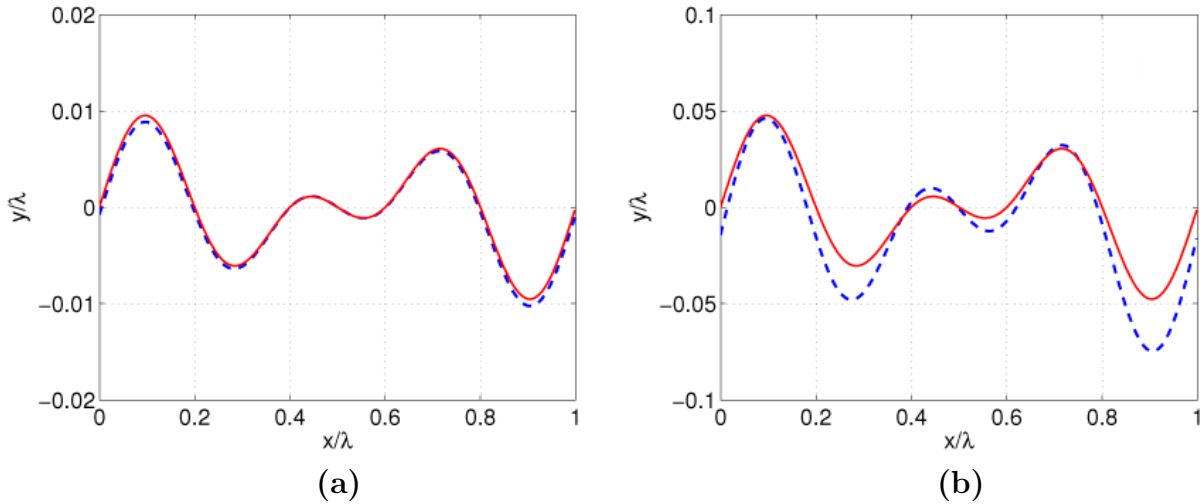


Figure 5.2 Numerical Experiment #1: $h = 0.1\lambda$. Reconstruction of a grating with finite Fourier modes: the exact surface (solid line) is plotted against the reconstructed surface (dashed line) using different ε and the same $h = 0.1\lambda$: (a) $\varepsilon = 0.01$; (b), $\varepsilon = 0.05$.

Figure 5.2 shows the reconstruction surfaces from using $\varepsilon = 0.01$ and $\varepsilon = 0.05$ in (a) and (b), respectively. Our method yields better results with the smaller ε of (a) than with larger ε of (b). Because we use a linearized model (i.e., truncate all terms of ε^2 or higher), smaller ε gives a more accurate approximation of the original nonlinear model problem.

5.2 Numerical Example 2: High Frequency

This time, the exact grating surface is given by $f(x) = \varepsilon g(x)$, where

$$g(x) = 0.5e^{\sin(4\pi x)} + 0.4e^{\sin(6\pi x)} - 1.5.$$

This is a harder example as the grating profile function g contains much higher Fourier modes. It is expected that larger cut-off frequency ω is desirable and thus even smaller h is necessary in order to capture all the surface features. As in the preceding example, we present comparisons of different ε and h values.

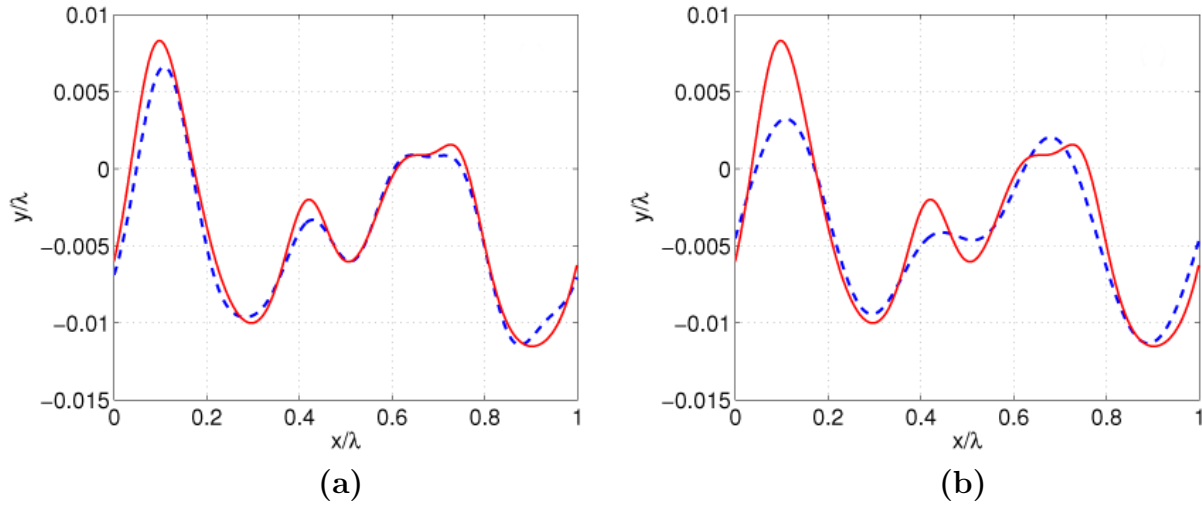


Figure 5.3 Numerical Experiment #2: $\varepsilon = 0.01$. Reconstruction of a grating with infinite Fourier modes: the exact surface (solid line) is plotted against the reconstructed surface (dashed line) using different h and the same $\varepsilon = 0.01$: (a) $h = 0.05\lambda$; (b), $h = 0.1\lambda$.

Figure 5.3 shows the reconstructed surfaces for $h = 0.05\lambda$ and $h = 0.1\lambda$, respectively, both with $\varepsilon = 0.01$. For the larger h value in (b), the reconstruction is unable to capture the fine features in the middle part of the exact grating surface. Recall that this choice of h was sufficient for the grating surface in Example 1 (the wavelength is the same in both examples). In contrast, all the detailed features are almost reconstructed in (a) when using $h = 0.05\lambda$ because larger ω is indeed allowed to be taken.

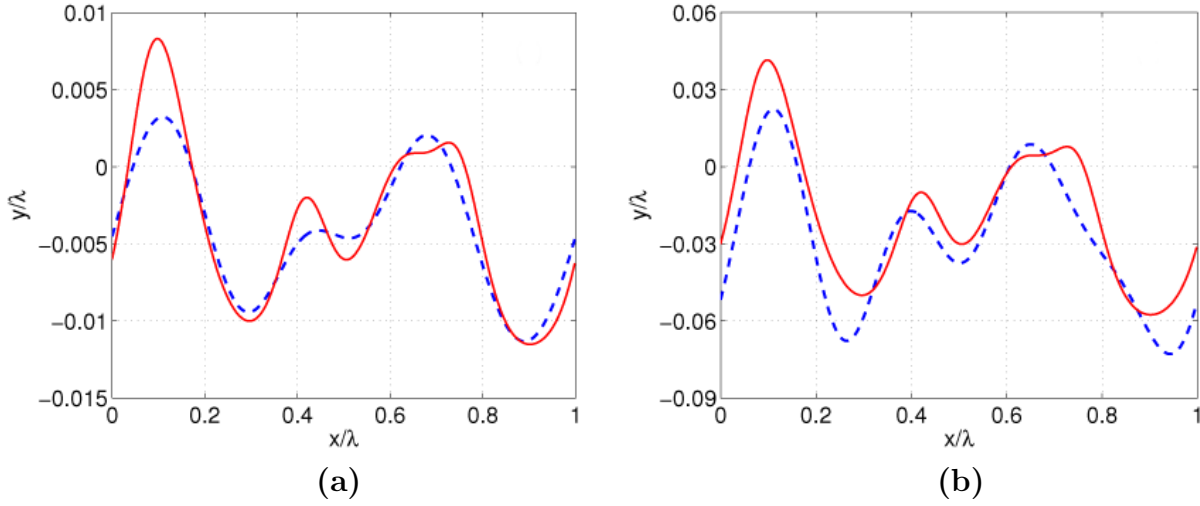


Figure 5.4 Numerical Experiment #2: $h = 0.1\lambda$. Reconstruction of a grating with infinite Fourier modes: the exact surface (solid line) is plotted against the reconstructed surface (dashed line) using different ε and the same $h = 0.1\lambda$: (a) $\varepsilon = 0.01$; (b), $\varepsilon = 0.05$.

Our final comparison, above in Figure 5.4, compares the results by using different ε . Taking the same $h = 0.1\lambda$, (b) and (c) show the reconstructed surfaces using $\varepsilon = 0.01$ and $\varepsilon = 0.05$, respectively. Again, it can be seen from the subplots of Figure 5.4 that smaller ε yields better reconstruction than larger ε due to the approximation error in the linearization procedure. Nonlinear corrections may be needed in order to improve the reconstructions.

5.3 Summary and Conclusion

We have presented a simple, stable, and effective computational method for the imaging of impedance grating surfaces and achieved sub-wavelength resolution. The grating surface model was assumed to be a small and smooth deformation of a planar surface. Using the transformed field expansion, the complex grating surface problem was converted into a forward-marching sequence of two-point boundary value problems. Thanks to the power series expansion and integration method, we were able deduce an analytic solution for the direct problem. By dropping higher order terms in power series, we linearized the nonlinear inverse problem and obtained an explicit reconstruction formula for both propagation

and evanescent wave modes. To suppress the exponential growth, an appropriate cut-off frequency was chosen from SNR analysis after proper consideration of the deformation parameter, noise level, and the measurement distance. Fast Fourier transforms contributed to implementing the reconstruction formula.

In conclusion, we have shown that the method presented works for general impedance grating surfaces. We presented two examples, one of which has finite Fourier modes and another one has infinite Fourier modes, and investigated how the parameters influence the reconstructions. The numerical results show that super resolution may be achieved by using small measurement distance, which is exactly the principle of near-field optical imaging.

APPENDIX

APPENDIX

A.1 Integration solution method

For self-containedness, the integrated solution method is briefly introduced to solve a two-point boundary value problem. We refer to Zhang [43] for the details of the integrated solutions of ordinary differential equation system and two-point boundary value problems.

Consider the two-point boundary value problem

$$\begin{cases} \mathbf{u}'(y) + M(y)\mathbf{u}(y) = \mathbf{f}(y), \\ A_0\mathbf{u}(y)|_{y=0} = \mathbf{r}_0, \\ B_1\mathbf{u}(y)|_{y=h} = \mathbf{s}_1, \end{cases} \quad (\text{A.1})$$

where $\mathbf{f}(y) \in \mathbb{C}^m$ are m -dimensional vector fields, $\mathbf{r}_0 \in \mathbb{C}^{m_1}$ and $\mathbf{s}_1 \in \mathbb{C}^{m_2}$ are given m_1 - and m_2 -dimensional vector fields, respectively, $M(y) \in \mathbb{C}^{m \times m}$ is an $m \times m$ matrix, and $A_0 \in \mathbb{C}^{m_1 \times m}$ and $B_1 \in \mathbb{C}^{m_2 \times m}$ are full rank matrices with $m_1 + m_2 = m$, i.e., $\text{rank} A_0 = m_1$ and $\text{rank} B_1 = m_2$.

Let $\Phi(y)$ be the fundamental matrix of the system

$$\begin{cases} c\Phi'(y) + M(y)\Phi(y) = \mathbf{0}, \\ \Phi(0) = I_m, \end{cases} \quad (\text{A.2})$$

where I_m is the $m \times m$ identity matrix.

Theorem A.1. *The two-point boundary value problem (A.1) has a unique solution if and only if*

$$\det \begin{bmatrix} A_0 \\ B_1\Phi(h) \end{bmatrix} \neq 0. \quad (\text{A.3})$$

Let the pair of functions $\{A(y), \mathbf{r}(y)\}$ and $\{B(y), \mathbf{s}(y)\}$ be the integrated solutions of the problems (A.1), then there exist $D_0(A, y) \in \mathbb{C}^{m_1 \times m_1}$ and $D_1(B, y) \in \mathbb{C}^{m_2 \times m_2}$ such that

$$\begin{cases} A' = AM + D_0 A, & A(0) = A_0, \\ \mathbf{r}' = A\mathbf{f} + D_0 \mathbf{r}, & \mathbf{r}(0) = \mathbf{r}_0, \end{cases} \quad (\text{A.4})$$

$$\begin{cases} B' = BM + D_1 B, & B(h) = B_1, \\ \mathbf{s}' = B\mathbf{f} + D_1 \mathbf{s}, & \mathbf{s}(h) = \mathbf{s}_1. \end{cases} \quad (\text{A.5})$$

Theorem A.2. *If the two-point boundary value problem (A.1) has a unique solution, then the matrix*

$$\begin{bmatrix} A(y) \\ B(y) \end{bmatrix} \in \mathbb{C}^{m \times m}$$

is nonsingular.

Theorem A.3. *The two-point boundary value problem (A.1) is equivalent to the linear system*

$$\begin{bmatrix} A(y) \\ B(y) \end{bmatrix} \mathbf{u}(y) = \begin{bmatrix} \mathbf{r}(y) \\ \mathbf{s}(y) \end{bmatrix}. \quad (\text{A.6})$$

A.2 A two-point boundary value problem

Consider a two-point boundary value problem

$$\begin{cases} u'' + \beta^2 u = v, & 0 < y < h, \\ u' - i\eta u = \varphi, & y = 0, \\ u' - i\beta u = \psi, & y = h, \end{cases} \quad (\text{B.1})$$

where $\beta \in \mathbb{C}, \eta \in \mathbb{C}$, and $\eta \neq \beta$.

Let $u_1 = u$ and $u_2 = u'$. The two-point boundary value problem (B.1) can be equivalently formulated into

$$\begin{cases} \mathbf{u}' + M\mathbf{u} = \mathbf{v}, \\ A_0\mathbf{u}(0) = \varphi, \\ B_1\mathbf{u}(h) = \psi, \end{cases} \quad (\text{B.2})$$

where

$$\mathbf{u} = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}, \quad \mathbf{v} = \begin{bmatrix} 0 \\ v \end{bmatrix}, \quad M = \begin{bmatrix} 0 & -1 \\ \beta^2 & 0 \end{bmatrix},$$

and

$$A_0 = [-i\eta \quad 1], \quad B_1 = [-i\beta \quad 1].$$

Theorem A.4. *The two-point boundary value problem (B.1) has a unique solution given by*

$$u(y) = K_1(y)\varphi - K_2(y)\psi + \int_0^h K_3(y, z)v(z)dz, \quad (\text{B.3})$$

where

$$K_1(y) = \frac{e^{i\beta y}}{i(\beta - \eta)}, \quad K_2(y) = \frac{e^{i\beta(h-y)}}{i(\beta - \eta)}K(y),$$

$$K_3(y, z) = \begin{cases} \frac{e^{i\beta(y-z)}}{i(\beta - \eta)}K(z), & z < y, \\ \frac{e^{i\beta(z-y)}}{i(\beta - \eta)}K(y), & z > y. \end{cases}$$

Here

$$K(t) = \frac{(\beta - \eta)}{2\beta} + \frac{(\beta + \eta)}{2\beta}e^{2i\beta t}.$$

Proof. It can be verified that there exists a non-singular matrix P such that

$$P^{-1}MP = N,$$

where

$$N = \begin{bmatrix} -i\beta & 0 \\ 0 & i\beta \end{bmatrix}, \quad P = \begin{bmatrix} 1 & 1 \\ i\beta & -i\beta \end{bmatrix}, \quad P^{-1} = \frac{1}{2i\beta} \begin{bmatrix} i\beta & 1 \\ i\beta & -1 \end{bmatrix}.$$

A simple calculation yields that the fundamental matrix of (A.2) is

$$\Phi(y) = P \begin{bmatrix} e^{i\beta y} & \\ & e^{-i\beta y} \end{bmatrix} P^{-1},$$

which gives

$$\det \begin{bmatrix} A_0 \\ B_1 \Phi(h) \end{bmatrix} = \begin{vmatrix} -i\eta & 1 \\ -i\beta e^{-i\beta h} & e^{-i\beta h} \end{vmatrix} = i(\beta - \eta)e^{-i\beta h} \neq 0.$$

It follows from Theorem A.1 that the two-point boundary value problem (B.2) and thus (B.1) has a unique solution.

Let $\{A(y), r(y)\}$ and $\{B(y), s(y)\}$ be the integrated solutions of the problems (B.2). Taking

$$D_0 = i\beta, \quad D_1 = -i\beta,$$

we obtain from (A.4) that the integrated solutions satisfy

$$\begin{cases} A' = AM + i\beta A, & A(0) = A_0, \\ r' = A\mathbf{v} + i\beta r, & r(0) = \varphi, \end{cases} \quad (\text{B.4})$$

and

$$\begin{cases} B' = BM - i\beta B, & B(h) = B_1, \\ s' = B\mathbf{v} - i\beta s, & s(h) = \psi. \end{cases} \quad (\text{B.5})$$

Upon solving the initial value problems (B.4) and (B.5), we obtain the integrated solutions for A and B :

$$A = [A_1(y) \ A_2(y)], \quad B = [B_1(y) \ B_2(y)], \quad (\text{B.6})$$

where

$$\begin{aligned} A_1(y) &= \frac{i(\beta - \eta)}{2} - \frac{i(\beta + \eta)}{2} e^{2i\beta y}, \\ A_2(y) &= \frac{(\beta - \eta)}{2\beta} + \frac{(\beta + \eta)}{2\beta} e^{2i\beta y}, \end{aligned}$$

and

$$B_1(y) = -i\beta, \quad B_2(y) = 1.$$

Once A and B are available, we may solve the initial value problems (B.4) and (B.5) and obtain the integrated solutions for r and s :

$$r(y) = e^{i\beta y} \varphi + \int_0^y e^{i\beta(y-z)} A_2(z) v(z) dz, \quad (\text{B.7})$$

$$s(y) = e^{i\beta(h-y)} \psi - \int_y^h e^{i\beta(z-y)} v(z) dz. \quad (\text{B.8})$$

It follows from Theorem A.3 that the two-point boundary value problem (B.2) is equivalent to the linear system

$$\begin{bmatrix} A_1 & A_2 \\ B_1 & B_2 \end{bmatrix} \begin{bmatrix} u \\ u' \end{bmatrix} = \begin{bmatrix} r \\ s \end{bmatrix}.$$

An application of Cramer's rule yields

$$u = \frac{rB_2 - sA_2}{A_1B_2 - B_1A_2}. \quad (\text{B.9})$$

A simple calculation yields

$$A_1B_2 - B_1A_2 = \mathbf{i}(\beta - \eta).$$

Substituting (B.6)–(B.8) into (B.9), we deduce (B.3). ■

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