

Calculation of electromagnetic scattering via boundary variations and analytic continuation

Oscar P. Bruno*

Fernando Reitich†

Abstract

In this paper we review and extend a numerical method we introduced recently for the solution of problems of electromagnetic scattering. Based on variations of the boundaries of the scatterers and analytic continuation, our approach yields algorithms which are applicable to a wide variety of scattering configurations. We discuss some recent applications of this method to scattering by diffraction gratings and by large two-dimensional bounded bodies. In addition, we present results of new applications to three-dimensional gratings containing corners and edges, and we further our theory to the case of three-dimensional bounded obstacles. In many cases of practical interest our algorithms give numerical results which are several orders of magnitude more accurate than those given by classical methods.

*School of Mathematics, Georgia Institute of Technology, Atlanta, Georgia 30332-0160

†Department of Mathematics and Center for Research in Scientific Computation, North Carolina State University, Raleigh, NC 27695-8205

1 Introduction

The problem of calculating the electromagnetic scattering produced by obstacles is one of utmost importance in science and engineering. Much of what we “see” —be it through visible light or x-rays, radio or microwaves— reaches us through a complicated combination of phenomena among which scattering is, in most cases, an essential element. In accordance with the substantial significance of scattering, a great deal of effort has been devoted in the last century to treating a variety of instances of this challenging mathematical problem. Among the many resulting contributions we mention exact solutions for simple geometries, high and low frequency approximations (Kirchoff and Rayleigh solutions) and rigorous numerical methods.

Consideration of exact solutions associated with simple scatterers, such as a semi-space or a spherical particle, has lead to fundamental understanding in optics and electromagnetism. Many problems encountered in practice, on the other hand, are associated with geometries for which exact solutions cannot be found and simple approximations cannot be used, and which must therefore be dealt with by means of numerical solution of Maxwell’s equations. This is the case, for example, for scattering configurations in the resonance region —where the wavelength of radiation is comparable with the size of the obstacle. The collection of scattering solvers which have been devised to treat these problems includes methods based on the solution of integral equations [16, 25, 33, 23, 20, 11] and methods based on finite elements or finite differences approximations [3, 14, 18, 26]. In this paper we review and extend a method we introduced recently. Based on variations of the boundaries of the scatterers and analytic continuation, our new perturbative approach leads to algorithms which are applicable to a wide variety of scattering configurations. In many cases of practical interest these algorithms yield numerical results which are several orders of magnitude more accurate than those given by classical methods —see §5.

For several decades perturbation methods have been considered inadequate for the treatment of problems of wave scattering, and only few of the many discussions, mainly in the area scattering by corrugated surfaces, have been based on perturbative techniques. Low order perturbative approaches include the first order calculation of Rayleigh [29] and, much more recently, that of Wait [35]. For higher order methods, the literature seems to reduce to the work of Meecham [24]. Low order methods are only appropriate for very small departures from an exactly solvable geometry, and, in particular, they cannot be applied to scatterers in the resonance region [21, 31]. The approach of Meecham, on the other hand, produces the scattering from a corrugated surface as a Neumann series whose n -th term is given by an n -fold convolution of the Green’s function. This method, which has not been implemented numerically, was thought to be mathematically incorrect [32], and dismissed.

Uretsky [32, p. 411] objected to Meecham’s approach and conjectured that the electromagnetic field for a corrugated surface does not continue analytically to the fields for a flat interface. As a specific example of this conjecture this author proposed an infinite sinusoidal corrugation of a plane. Uretsky’s conjecture was based on a certain integral ex-

pression related to the fields which appears to become meaningless as the groove depth takes on complex values. He thus suggested that series expansions in powers of the parameters controlling the shape of the scatterers could not be used in the solution of the corresponding scattering problems.

We have shown, however, that the field *does* vary analytically with respect to boundary variations [6]. Further, we have produced *explicit* recursive formulae which allow for calculation of the scattered waves *to arbitrary order* in the variation parameter. It is these observations which, together with appropriate algorithms for analytic continuation, have permitted us to introduce rigorous and accurate scattering solvers based on boundary perturbations.

In this paper we review our theory and discuss the performance of our algorithms in a number of two- and three-dimensional configurations. In particular, we present results of new applications to two-dimensional bounded obstacles and to three-dimensional gratings containing edges and corners. All of our numerical results are accompanied by reliable error estimates. Finally we present, in the Appendix, an extension of our theory to the three-dimensional bounded-body case.

The applications to non-smooth three-dimensional gratings given here required the introduction of a class of numerical devices which will also be needed in our forthcoming applications to three-dimensional bounded-obstacle problems, see §3.3. These methods and the derivation of recursive formulae given in the Appendix have cleared the way for the application of our perturbative approach to bounded three-dimensional scatterers. We expect the performance of our algorithms in these problems will be of a quality comparable to the one they exhibit in the various configurations considered in this paper.

2 Preliminaries

2.1 Maxwell equations

Consider a scattering configuration in which space is divided in two regions Ω^+ and Ω^- containing two different materials, such as air and a metal, of respective dielectric constants ϵ^+ and ϵ^- . The permeability of both materials is assumed to equal μ_0 , the permeability of vacuum. In the cases we consider, the region Ω^+ is of infinite extent; the scatterer Ω^- , on the other hand, may be bounded or unbounded.

We wish to determine the pattern of diffraction that occurs when an electromagnetic plane wave

$$\begin{aligned}\vec{E}^i &= \vec{A}e^{i(\alpha x_1 + \beta x_2 - \gamma x_3 - i\omega t)} \\ \vec{H}^i &= \vec{B}e^{i(\alpha x_1 + \beta x_2 - \gamma x_3 - i\omega t)}\end{aligned}$$

impinges upon Ω^- . Here, denoting by $\vec{k} = (\alpha, \beta, -\gamma)$ the wavevector, we have

$$\vec{A} \cdot \vec{k} = 0 \quad \text{and} \quad \vec{B} = \frac{1}{\omega\mu_0} \vec{k} \times \vec{A}. \quad (1)$$

Dropping the factor $e^{-i\omega t}$, the time harmonic Maxwell equations for the total fields read

$$\begin{aligned} \nabla \times \vec{E} &= i\omega\mu_0 \vec{H} \quad , \quad \nabla \cdot \vec{E} = 0 \quad , \\ \nabla \times \vec{H} &= -i\omega\epsilon \vec{E} \quad , \quad \nabla \cdot \vec{H} = 0 \quad . \end{aligned} \quad (2)$$

In particular the electromagnetic field

$$v = (\vec{E}, \vec{H}) \quad (3)$$

satisfies the Helmholtz equations

$$\Delta v + (k^\pm)^2 v = 0 \quad \text{in } \Omega^\pm, \quad (4)$$

where $k^\pm = \omega\sqrt{\mu_0\epsilon^\pm}$. The total electric and magnetic fields are given by

$$\begin{aligned} \vec{E} &= \vec{E}^{out} = \vec{E}^i + \vec{E}^+ \quad , \quad \vec{H} = \vec{H}^i + \vec{H}^+ \quad \text{in } \Omega^+ \quad \text{and} \\ \vec{E} &= \vec{E}^{in} = \vec{E}^- \quad , \quad \vec{H} = \vec{H}^- \quad \text{in } \Omega^-, \end{aligned}$$

where (\vec{E}^+, \vec{H}^+) and (\vec{E}^-, \vec{H}^-) are the reflected and refracted fields, respectively. At the interface

$$\Gamma = \partial\Omega^+ = \partial\Omega^-$$

the field satisfies the transmission conditions

$$n \times (\vec{E}^{out} - \vec{E}^{in}) = 0 \quad , \quad n \times (\vec{H}^{out} - \vec{H}^{in}) = 0 \quad \text{on } \Gamma, \quad (5)$$

where n is normal to Γ . In case the region Ω^- is filled by a perfect conductor the refracted fields vanish and the boundary conditions reduce to

$$n \times \vec{E}^{out} = n \times (\vec{E}^i + \vec{E}^+) = 0 \quad \text{on } \Gamma \quad . \quad (6)$$

Finally the field satisfies conditions of radiation at infinity, expressing the outgoing character of the scattered waves, which can be stated either in terms of the eigenfunctions expansions of §2.2, or, alternatively, in terms of the decay of the field at infinity; see e.g. [4, 17, 27].

In the two dimensional case in which Ω^- is a cylinder and $\beta = 0$, the fields \vec{E} and \vec{H} are independent of x_2 and the system of equations (2),(5) (or (2),(6)) can be reduced to a pair of decoupled equations for two scalar unknowns [19]. Indeed, the functions $u_1(x_1, x_3)$

and $u_2(x_1, x_3)$ equal to the transverse components E_{x_2} (Field Transverse Electric, TE) and H_{x_2} (Field Transverse Magnetic, TM), which satisfy equation (4), determine completely the electromagnetic field through equations (2). The boundary conditions (6), (5) can be translated into appropriate boundary conditions for the unknowns u_i . In case Ω^- contains a perfect conductor, we have

$$u_1 = -e^{i\alpha x_1 - i\gamma x_3} \quad , \quad \text{and} \quad (7)$$

$$\frac{\partial u_2}{\partial n} = -\frac{\partial}{\partial n}(e^{i\alpha x_1 - i\gamma x_3}), \quad \text{on } \Gamma. \quad (8)$$

In the case where Ω^- contains a finitely conducting metal or dielectric u_1 satisfies the transmission conditions

$$u_1^+ - u_1^- = -e^{i\alpha x_1 - i\gamma x_3} \quad , \quad \text{and}$$

$$\frac{\partial u_1^+}{\partial n} - \frac{\partial u_1^-}{\partial n} = -\frac{\partial}{\partial n}(e^{i\alpha x_1 - i\gamma x_3}) \quad , \quad \text{on } \Gamma, \quad (9)$$

while u_2 satisfies

$$u_2^+ - u_2^- = -e^{i\alpha x_1 - i\gamma x_3} \quad , \quad \text{and}$$

$$\frac{\partial u_2^+}{\partial n} - \left(\frac{k^+}{k^-}\right)^2 \frac{\partial u_2^-}{\partial n} = -\frac{\partial}{\partial n}(e^{i\alpha x_1 - i\gamma x_3}) \quad \text{on } \Gamma. \quad (10)$$

2.2 Eigenfunction expansions

In addition to Taylor series, our analytic approach is based on the series expansions of the electromagnetic field which result from separation of variables. Such expansions are most frequently found in solutions associated with simple objects such as a circle, a sphere or a semispace. This is in part due to the fact that, for such simple scatterers, the functions resulting from restriction of the separated solutions to the scattering boundaries form a complete orthonormal system, and thus boundary conditions can easily be accounted for by means of Fourier analysis.

It is interesting to note, however, that expansions in series of separated variables may be useful even when their restrictions to the boundary of the scatterer do not form an orthogonal system. The first occurrence of an approach of this type can be found in the work of Rayleigh [29]. After evaluating such expansions at the scattering boundaries, this

author used appropriate approximations and found first order corrections to the scattered field for geometries which result from small perturbations from an exactly solvable one. With the advent of computers attempts were made to extend Rayleigh's approach of evaluating series expansions at the boundary of the obstacles to general scattering solvers which do not assume small departures from an exact geometry. These attempts did not succeed since, indeed, the series may not converge at the obstacle boundaries, that is, Rayleigh's hypothesis may not be satisfied. This fact was first established by Petit and Cadilhac [28] by consideration of a sinusoidal corrugation on a plane.

Our method is not unrelated to Rayleigh's hypothesis. In fact, we established [6] the convergence of the eigenfunction expansions throughout the boundary for sufficiently small but otherwise arbitrary (analytic) perturbations of the exactly solvable geometry. Whereas these "sufficiently small" perturbations for which Rayleigh's hypothesis can be used may be too small, they are certainly sufficient to allow for calculation of derivatives of arbitrary order with respect to boundary perturbations.

The series expansions obtained from separation of variables are well known. For example, a solution to the two-dimensional Helmholtz equation outside a circular cylinder is given, in polar coordinates, by an expansion of the form

$$u(\rho, \theta) = \sum_{r=-\infty}^{\infty} B_r (-i)^r H_r^{(1)}(k\rho) e^{ir\theta}. \quad (11)$$

where $H_r^{(1)}$ denotes the first Hankel function of order r . The principle of conservation of energy can be given a simple form in terms of the amplitudes B_r in this expansion. Indeed, any solution u to a scattering problem from a perfectly conducting obstacle *of any shape* admits a representation (11) and we have

$$\sum_r |B_r|^2 + \operatorname{Re} \left(\sum_r B_r \right) = 0. \quad (12)$$

Relation (12), which holds independently of whether or not the series (11) converges at the boundary of the obstacle, can be made into a useful estimator for errors in the numerical calculation of the fields, see §5.

For a solution in three dimensional space and outside a sphere we have

$$E^+(R, \theta, \phi) = \sum_{r=0}^{\infty} \sum_{s=-r}^r \vec{B}_{rs} h_r^{(1)}(kR) P_r^s(\cos(\theta)) e^{is\phi} \quad (13)$$

where (R, θ, ϕ) are spherical coordinates, P_r^s are the Legendre functions of the first kind and $h_r^{(1)}$ are the first spherical Hankel functions [17].

Finally let us consider scatterers which are given by a biperiodic corrugation of a plane

$$\Omega^- = \{z < f(x_1, x_2)\}, \quad (14)$$

where f is a biperiodic function of periods d_1 and d_2 in the variables x_1 and x_2 , respectively. The periodicity of the structure implies that the fields must be (α, β) quasi-periodic, i.e., they must verify equations of the form

$$v(x_1 + d_1, x_2, x_3) = e^{i\alpha d_1} v(x_1, x_2, x_3) \quad \text{and} \quad v(x_1, x_2 + d_2, x_3) = e^{i\beta d_2} v(x_1, x_2, x_3).$$

In this case, separation of variables leads to expansions of the form

$$\vec{E}^\pm = \sum_{r=-\infty}^{\infty} \sum_{s=-\infty}^{\infty} \vec{B}_{r,s}^\pm e^{i\alpha_r x_1 + i\beta_s x_2 \pm i\gamma_{r,s}^\pm x_3}. \quad (15)$$

The expansion for \vec{E}^+ (resp. \vec{E}^-) converges to the field in the region $\{x_3 > \max(f(x_1, x_2))\}$ (resp. $\{x_3 < \min(f(x_1, x_2))\}$). Here we have put

$$\alpha_r = \alpha + rK_1, \quad \beta_s = \beta + sK_2, \quad \alpha_r^2 + \beta_s^2 + (\gamma_{r,s}^\pm)^2 = (k^\pm)^2 \quad (16)$$

where $\gamma_{r,s}^\pm$ is determined by $\text{Im}(\gamma_{r,s}^\pm) > 0$ or $\gamma_{r,s}^\pm \geq 0$,

$$(k^\pm)^2 = \omega^2 \epsilon^\pm \mu_0$$

and

$$K_1 = \frac{2\pi}{d_1}, \quad K_2 = \frac{2\pi}{d_2}.$$

It is clear from (16) that only a finite number of modes propagate away from the grating, since the remaining modes decay exponentially. The main quantities of interest here are the *grating efficiencies*

$$e_{r,s}^\pm = \frac{|B_{r,s}^\pm|^2 \gamma_{r,s}^\pm}{\gamma_{0,0}^+} \quad (17)$$

for the finitely many propagating modes, i.e. the modes (r, s) such that $\gamma_{r,s}^\pm$ is real.

In this case the principle of conservation of energy can be stated as follows: if we let U^\pm denote the set of indices corresponding to the non-evanescent modes in Ω^\pm , then

$$\sum_{(r,s) \in U^+} e_{r,s}^+ + \sum_{(r,s) \in U^-} e_{r,s}^- = 1, \quad (18)$$

provided the dielectric constants ϵ^+ and ϵ^- are real.

In the two dimensional case we shall consider gratings of the form

$$\Omega^- = \{x_3 < f(x_1)\}, \quad (19)$$

for which the expansion above reduces to

$$u^\pm = \sum_{r=-\infty}^{\infty} B_r^\pm e^{i\alpha_r x_1 \pm \gamma_r^\pm x_3}. \quad (20)$$

The principle of conservation of energy now reads

$$\sum_{r \in U^+} e_r^+ + \sum_{r \in U^-} e_r^- = 1, \quad (21)$$

where the efficiencies are now given by $e_r^\pm = \gamma_r^\pm |B_r^\pm|^2 / \gamma_0^\pm$.

3 Analyticity and Taylor coefficients

3.1 Overview

As we said, our algorithms are based on a theorem we established recently [6] of analyticity of the electromagnetic field with respect to boundary variations. To describe our results assume Ω_δ^- is a family of scatterers, one for each value of the real parameter δ —see e.g. Figure 1 and equations (24)–(27) below. Further, assume the boundaries Γ_δ of these obstacles admit a parametrization

$$\vec{r} = H(s_1, s_2, \delta) \quad (22)$$

where the function H is jointly analytic in the spatial parameters (s_1, s_2) and the perturbation parameter δ . Our theorems state that both the values $v = v(\vec{r}, \delta)$ of the electromagnetic field at a fixed point in space as well as the values at a point *on the varying boundary* depend analytically on the boundary variations. More precisely, if \vec{r} is a point in space away from

Γ_δ and $\vec{r}_\delta \in \Gamma_\delta$ is a point on the interface which varies analytically with δ , then $v(\vec{r}, \delta)$ is jointly analytic in (\vec{r}, δ) , and $v(\vec{r}_\delta, \delta)$ is an analytic function of δ for all real values of δ for which the surface (22) does not self intersect.

It follows from these theorems that the field can be expanded in a series in powers of δ

$$v^\pm(\vec{r}, \delta) = \sum_{n=0}^{\infty} v_n^\pm(\vec{r}) \delta^n \quad (23)$$

which converges for δ small enough. The vector field v_n^\pm satisfies Maxwell's equations (2) as well conditions of radiation at infinity. They also satisfy boundary conditions on $\Gamma_0 = \Gamma_\delta|_{\delta=0}$ which can be obtained by differentiation as we show below. Such differentiations and use of the chain rule are permissible, as it follows from the analyticity theorems mentioned above and related extension theorems [6]. The solution of the boundary value problems for the v_n 's then easily leads to a numerical algorithm for the calculation of the scattered field.

In the following section we derive recursive formulae for the calculation of the Taylor coefficients of the amplitudes $B_r = B_r(\delta)$ associated with a two dimensional bounded obstacle

$$\Omega^- = \Omega_\delta^- = \{\rho < a + \delta f(\theta)\}; \quad (24)$$

the problem of summation of such series is considered in §5 below. Corresponding formulae for Taylor coefficients associated to the various kinds of diffraction gratings

$$\Omega_\delta^- = \{x_3 < \delta f(x_1)\} \quad (25)$$

in two dimensions, or

$$\Omega_\delta^- = \{x_3 < \delta f(x_1, x_2)\} \quad (26)$$

in three dimension were given in [7, 8, 9]. The case of a three dimensional bounded obstacle

$$\Omega_\delta^- = \{\rho < a + \delta f(\theta, \phi)\} \quad (27)$$

is considered in the Appendix. In some cases the algebraic manipulations required by these derivations are minimal and the resulting formulae simple; in others the algebra and the resulting expressions are substantially involved. In the simplest case of a two dimensional grating (25) in TE polarization, for example, the recursive formula takes the form

$$d_{n,r} = -(-i\beta)^n C_{n,r} - \sum_{k=0}^{n-1} \sum_{q=\max(-kF, r-(n-k)F)}^{\min(kF, r+(n-k)F)} C_{n-k, r-q} (i\beta_q)^{n-k} d_{k,q}, \quad (28)$$

($-nF \leq r \leq nF$). Here $d_{n,r}$ are the coefficients in the power series

$$B_r(\delta) = \sum_{k=0}^{\infty} d_{k,r} \delta^k \quad (29)$$

of the amplitudes $B_r(\delta)$ in the eigenfunction expansion of the function $u_1 = E_{x_2}$, see §2.2; and $C_{n,r}$ is the r -th Fourier coefficient of the $f^n/n!$.

The difficulty in these derivations increases with the spatial dimension. Also, problems involving a perfectly conducting scatterer lead to fewer unknowns and simpler calculations than the corresponding problem for a finitely conducting one. Further, a substantially greater difficulty arises in the derivations corresponding to three dimensional obstacles — due to the character of the special functions associated to that case. In the Appendix we discuss this derivation, which is rather complex and leads to cumbersome recursive formulae. Fortunately, we found the calculation amenable to treatment by means of a symbolic manipulator. We also found it useful to take advantage of the ability symbolic manipulators have of translating their output formulae into expressions in various languages of scientific programming. With these provisos the challenge of producing a three dimensional bounded obstacle code based on our theory is reduced to the ordinary range of difficulties in small scale programming.

3.2 Recursive formulae: bounded obstacles in two dimensions

Let us derive formulae for a perfectly conducting and bounded two dimensional object (24) under TE radiation. The interface Γ_δ is given by

$$\Gamma_\delta = \{(\rho, \theta) : \rho = a + \delta f(\theta)\}. \quad (30)$$

(Here we view our obstacle as two dimensional perturbation of a circular cylinder. In some circumstances it may be advantageous to use perturbations from other particular geometries for which exact solutions are known, such as, for example, an appropriate elliptic cylinder or ellipsoid.) In the TE case considered here the transverse component $u = E_{x_2}$ of \vec{E} , ($u = u_1$ in the notation of §2), satisfies the Helmholtz equation (4) and the boundary condition

$$u = -e^{\alpha x_1 - \gamma x_3} \text{ on } \Gamma_\delta. \quad (31)$$

It is clearly sufficient to consider the case in which the direction of our incident wave is that of the negative x_1 -axis, and we thus have

$$\vec{E}^i = \hat{x}_2 e^{-ikx_1}, \quad \vec{H}^i = \hat{x}_3 \sqrt{\frac{\epsilon^+}{\mu}} e^{-ikx_1}.$$