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Preface

The scattering of acoustic and electromagnetic waves by periodic surfaces plays a role in many areas of applied physics and engineering. Optical diffraction gratings date from the nineteenth century and are still widely used by spectroscopists. More recently, diffraction gratings have been used as coupling devices for optical waveguides. Trains of surface waves on the oceans are natural diffraction gratings which influence the scattering of electromagnetic waves and underwater sound. Similarly, the surface of a crystal acts as a diffraction grating for the scattering of atomic beams. This list of natural and artificial diffraction gratings could easily be extended.

The purpose of this monograph is to develop from first principles a theory of the scattering of acoustic and electromagnetic waves by periodic surfaces. In physical terms, the scattering of both time-harmonic and transient fields is analyzed. The corresponding mathematical model leads to the study of boundary value problems for the Helmholtz and d'Alembert wave equations in plane domains bounded by periodic curves. In the formalism adopted here these problems are intimately related to the spectral analysis of the Laplace operator, acting in a Hilbert space of functions defined in the domain adjacent to the grating.

The intended audience for this monograph includes both those applied physicists and engineers who are concerned with diffraction gratings and those mathematicians who are interested in spectral analysis and scattering theory for partial differential operators. An attempt to address simultaneously two such disparate groups must raise the question: is there a common domain of discourse? The honest answer to this question is no! Current mathematical literature on spectral analysis and scattering theory is based squarely on functional analysis, particularly the theory of linear transformations in Hilbert spaces. This theory has been readily accessible ever since the publication of M. H. Stone's AMS Colloquium volume in 1932. Nevertheless, the theory has not become a part of the curricula of applied physics and engineering and it is seldom seen in applied science literature on wave propagation and scattering. Instead, that literature is characterized by, on the one hand, the use of heuristic non-rigorous arguments and, on the other, by formal manipulations that typically involve divergent series and integrals, generalized functions of unspecified types and the like.

The differences in style and method outlined above pose a dilemma. Can an exposition of our subject be written that is accessible and useful to both applied scientists and mathematicians? An attempt is made to do this below by dividing the work into two parts. Part 1, called Physical Theory, presents the basic physical concepts and results, formulated in the simplest and most concise form consistent with their nature. Moreover, Part 1 can be interpreted in two different ways. First, it can be interpreted in the heuristic way favored by applied physicists and engineers. When read in this way it presents a complete statement of the physical content of the theory. Second, for readers conversant with Hilbert space theory Part 1 can be interpreted as a concise statement of the principal concepts and results of a rigorous mathematical theory.

When read in the second way Part 1 serves as an introduction to and overview of the complete theory which is presented in Part 2, Mathematical Theory. This part develops the relevant concepts and results from functional analysis and the theory of partial differential equations and applies them to give complete proofs of the results formulated in Part 1. At the same time many secondary concepts and results are formulated and proved that lead to a deeper understanding of the nature and limitations of the theory.

Acknowledgments

Preliminary studies for this work began in 1974, while I was a visiting professor at the University of Stuttgart, and continued there during my tenure as an Alexander von Humboldt Foundation Senior Scientist in 1976-77. The work was completed during my sabbatical year in 1980 when I was a visiting professor at the University of Bonn with the support of the Sonderforschungsbereich 72. Throughout this period my research was supported by the U. S. Office of Naval Research. I should like to express here my appreciation for the support of the Universities of Bonn, Stuttgart and Utah, the Alexander von Humboldt Foundation and the Office of Naval Research which made the work possible. My special thanks are expressed to Professor Rolf Leis, University of Bonn, and Professor Peter Werner, University of Stuttgart, for arranging my visits to their universities.

I should also like to thank here Professor Jean Claude Guillot of the University of Paris for helpful discussions in 1977-78 of a preliminary version of this work. Finally, and most important of all, I want to express my thanks to Dr. Hans Dieter Alber of the University of Bonn for his outstanding paper of 1979 on steady-state scattering by periodic surfaces. It was the concepts introduced in this paper that led to the final, very general, theory developed here. Dr. Alber's contributions have influenced nearly every part of this work.

Calvin H. Wilcox
Bonn
July, 1982

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Introduction

The first theoretical studies of scattering by diffraction gratings are due to Lord Rayleigh. His "Theory of Sound" Volume 2, 2nd Edition, published in 1896 [18]*, contains an analysis of the scattering of a monochromatic plane wave normally incident on a grating with a sinusoidal profile. In a subsequent paper [19] he extended the analysis to oblique incidence. Rayleigh assumed in his work that in the half-space above the grating the reflected wave is a superposition of the specularly reflected plane wave, a finite number of secondary plane waves propagating in the directions of the higher order grating spectra of optics, and an infinite sequence of evanescent waves whose amplitudes decrease exponentially with distance from the grating. The validity of Rayleigh's assumption for general grating profiles was realized in the early 1930's [10], following Bloch's work [4] on the analogous problem of de Broglie waves in crystals. Waves of this type will be called Rayleigh-Bloch waves (R-B waves for brevity) in this work.

The goal of Rayleigh's work and the literature based on it was to calculate the relative amplitudes and phases of the diffracted plane wave components of the R-B waves. Several methods for doing this have been developed. L. A. Weinstein [27] and J. A. DeSanto [5,6] gave exact solutions to the problem of the scattering of monochromatic plane waves by a comb grating; i.e., an array of periodically spaced infinitesimally thin parallel plates of finite depth mounted perpendicularly on a plane. For gratings with sinusoidal profiles, infinite systems of linear equations for the complex reflection coefficients were given by J. L. Uretsky [26] and J. A. DeSanto [7]. More recently, DeSanto [8] has extended his results to essentially arbitrary profiles. Finally, an excellent review up to 1980 of

*Numbers in square brackets denote references from the list at the end of the monograph.

both theoretical and numerical methods for determining the reflection coefficients is contained in the book Electromagnetic Theory of Gratings, edited by R. Petit [17].

The literature on diffraction gratings and their applications is very large. References to work done before 1967 may be found in the monograph by Stroke in the Handbuch der Physik [25]. A survey of the literature up to 1980 is contained in [17].

The works referenced above provide a satisfactory understanding of the scattering of the steady beams used in classical spectroscopy. However, modern applications of gratings in such areas as optical waveguides and underwater sound require an understanding of how transient electromagnetic and acoustic fields, such as pulsed laser beams and sonar signals, are scattered by diffraction gratings. The existing grating theories are inadequate for the analysis of these problems.

The purpose of this monograph is to develop a theory of the scattering of transient electromagnetic and acoustic fields by diffraction gratings. The theory is based on an eigenfunction expansion for gratings in which the eigenfunctions are R-B waves. The analysis parallels the author's work on the scattering of transient sound waves by bounded obstacles [30,31,33]. The eigenfunction expansions are generalizations of T. Ikebe's theory of distorted plane wave expansions [12], first developed for quantum mechanical potential scattering and subsequently extended to a variety of scattering problems [2,15,21,22,23,32]. The theory is based on the study of a linear operator A, called here the grating propagator, which is a selfadjoint realization of the negative of the Laplace operator acting in the Hilbert space of square integrable acoustic fields. A fundamental result of this analysis is a representation of the spectral family of A by means of R-B waves. The R-B wave expansions follow as a corollary.

The theory of scattering by gratings developed below is restricted, for brevity, to the case of two-dimensional wave propagation. Specifically, the waves are assumed to be solutions of the wave equation in a two-dimensional grating domain and to satisfy the Dirichlet or Neumann boundary condition on the grating profile. These problems provide models for the scattering of sound waves by acoustically soft or rigid gratings and of TE or TM electromagnetic waves by perfectly conducting gratings. It will be seen that the methods employed are also applicable to the scattering of scalar waves by three-dimensional (and n-dimensional) gratings and to systems such as Maxwell's equations and the equations of elasticity.

Even with the restriction to the two-dimensional case, the analytical work needed to derive and fully establish eigenfunction expansions for diffraction gratings is necessarily intricate and lengthy. This is clear from an examination of the simpler case of scattering by bounded obstacles presented in the author's monograph [30]. Therefore, to make the work more accessible to potential users, the monograph has been divided into two parts. As explained in the Preface, Part 1 can be interpreted both as a complete statement, without proofs, of the physical concepts and results of the theory and also as a summary and introduction to the complete mathematical theory developed in Part 2.

A preliminary version of the R-B wave expansion theorem of this monograph was announced by J. C. Guillot and the author in 1978 [34]. That work was based on an integral equation for the R-B waves. In this monograph an alternative method based on analytic continuation is used. A key step is the introduction of the reduced grating propagator A_p which depends on the wave momentum. The Hilbert space theory of such operators was initiated by H. D. Alber [3]. Alber's powerful method of analytic continuation of the resolvent of A_p is used in Part 2 to construct the R-B wave eigenfunctions.

Part 1
Physical Theory

This monograph develops a theory of the scattering of two-dimensional acoustic and electromagnetic fields by diffraction gratings. This Part 1 presents the principal physical concepts and results in their simplest forms and without proofs. Moreover, to avoid distracting technicalities the precise conditions for the validity of the results are not always given. Part 1 also contains no references to the literature. All of these omissions are remedied in Part 2 which contains the final mathematical formulation of the theory, together with complete proofs and indications of related literature.

§1. The Physical Problems

The propagation of two-dimensional acoustic and electromagnetic fields is studied below in unbounded planar regions whose boundaries (= the diffraction gratings) lie between two parallel lines and are periodic. In each case the medium filling the region is assumed to be homogeneous and lossless. In the acoustic case the grating is assumed to be either rigid or acoustically soft. In the electromagnetic case it is assumed to be perfectly conducting. In both cases the sources of the field are assumed to be localized in space and time. The principal goal of the theory is to calculate the "final" or large-time form of the resulting transient field.

§2. The Mathematical Formulation

Rectangular coordinates $X = (x,y) \in R^2$ will be used to describe the region adjacent to the diffraction grating. The notation

$$R_a^2 = \{X : y > a\} \tag{2.1}$$

will be used. Then with a suitable choice of coordinate axes the region

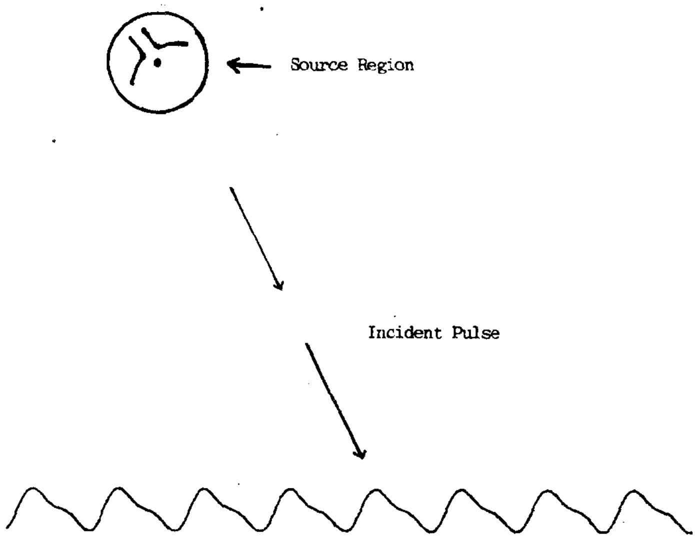

Figure 1. Grating with Source Region and Incident Pulse

above the grating will be characterized by a grating domain $G \subset R^2$ with the properties

(2.2) $$R_h^2 \subset G \subset R_0^2 ,$$

(2.3) $$G + (2\pi,0) = G$$

where $h > 0$ is a suitable constant. The choice of the constant 2π in (2.3) is simply a convenient normalization.

The acoustic or electromagnetic field in G can be described by a real-valued function $u = u(t,X)$ that is a solution of the initial-boundary value problem

(2.4) $$D_t^2 u - \Delta u = 0 \text{ for all } t > 0 \text{ and } X \in G ,$$

(2.5) $$D_\nu u \equiv \vec{\nu} \cdot \nabla u = 0 \text{ (resp., } u = 0) \text{ for all } t \geq 0 \text{ and } X \in \partial G ,$$

(2.6) $$u(0,X) = f(X) \text{ and } D_t u(0,X) = g(X) \text{ for all } X \in G .$$

Here t is a time coordinate, $D_t = \partial/\partial t$, $D_x = \partial/\partial x$, $D_y = \partial/\partial y$, $\nabla u = (D_x u, D_y u)$, $\Delta u = D_x^2 u + D_y^2 u$, ∂G denotes the boundary of G and $\vec{\nu} = \vec{\nu}(X)$ is a unit normal vector to ∂G at X. In the acoustic case $u(t,X)$ is interpreted as a potential for an acoustic field with velocity $\vec{v} = -\nabla u$ and acoustic pressure

$p = D_t u$. Then the boundary condition (2.5) corresponds to an acoustically hard (resp., soft) boundary. Alternatively, if u satisfies the Neumann condition $D_\nu u = 0$ on ∂G then

$$E_x = D_y u,\ E_y = -D_x u,\ H_z = D_t u \tag{2.7}$$

describes a TM electromagnetic field in a domain G bounded by a perfect electrical conductor. Similarly, if u satisfies the Dirichlet condition $u = 0$ on ∂G then

$$H_x = -D_y u,\ H_y = D_x u,\ E_z = D_t u \tag{2.8}$$

describes a TE electromagnetic field in the same kind of domain. The functions f(X) and g(X) in (2.6) characterize the initial state of the field. They are assumed to be given or calculated from the prescribed wave sources, and to be localized:

$$\text{supp } f \cup \text{supp } g \subset \{X : x^2 + (y - y_0)^2 \le \delta_0^2\} \tag{2.9}$$

where $y_0 > h + \delta_0$.

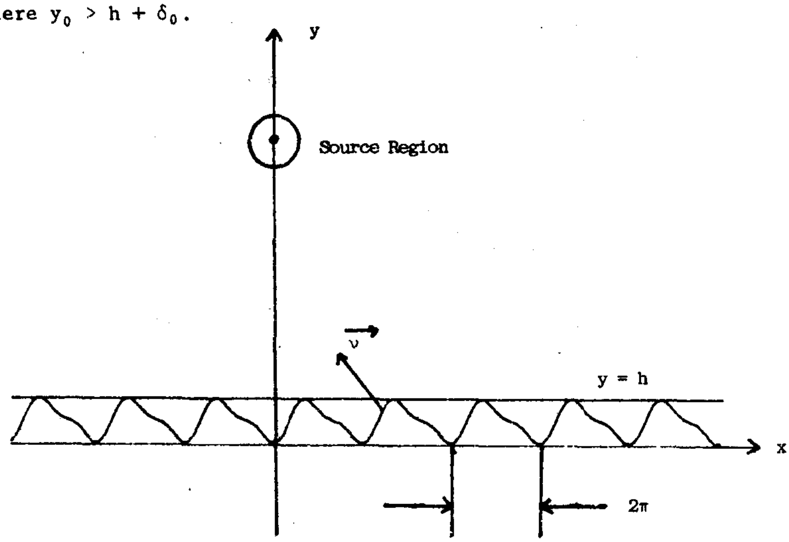

Figure 2. Grating Domain with Coordinate System

In both the acoustic and the electromagnetic interpretations the integral

$$E(u,K,t) = \int_K \{|\nabla u(t,X)|^2 + |D_t u(t,X)|^2\}\ dX \tag{2.10}$$

is interpreted as the wave energy in the set K at time t ($dX = dxdy$). Solutions of the wave equation satisfy the energy conservation law $E(u,G,t) = E(u,G,0)$ under both boundary conditions (2.5). It will be assumed that the initial state has finite energy:

$$\int_G \{|\nabla f(X)|^2 + |g(X)|^2\}\, dX < \infty \tag{2.11}$$

§3. Solution of the Initial-Boundary Value Problem

The initial-boundary value problem in its classical formulation (2.4) -(2.6) will have a solution only if ∂G and the functions f and g are sufficiently smooth. However, for arbitrary domains G the problem is known to have a unique solution with finite energy whenever the initial state f,g has this property. A formal construction of the solution may be based on the linear operator $A = -\Delta$, acting in the Hilbert space $\mathcal{H} = L_2(G)$. If the domain of A is defined to be the set of $u \in \mathcal{H}$ such that $\nabla u \in \mathcal{H}$, $\Delta u \in \mathcal{H}$ and one of the boundary conditions (2.5) holds then A is a selfadjoint non-negative operator. Moreover,

$$u(t,\cdot) = (\cos t\, A^{1/2})\, f + (A^{-1/2} \sin t\, A^{1/2})\, g \tag{3.1}$$

is the solution with finite energy whenever the initial state has finite energy. It will be convenient to write (3.1) as

$$u(t,X) = \text{Re}\, \{v(t,X)\}\ , \quad v(t,\cdot) = e^{-itA^{1/2}}\, h \tag{3.2}$$

where

$$h = f + i\, A^{-1/2}\, g\ . \tag{3.3}$$

This representation is valid if f and g are real-valued and $A^{1/2} f$, f, g and $A^{-1/2} g$ are in $\mathcal{H}$. A rigorous interpretation of relations (3.1)-(3.3) can be based on the calculus of selfadjoint operators in Hilbert spaces.

§4. The Reference Problem and Its Eigenfunctions

In the class of grating domains defined by (2.2), (2.3) there is a special case for which the scattering problem is explicitly solvable. This is the case of the degenerate grating $G = R_0^2$ ($h = 0$). The problem (2.4) -(2.6) with $G = R_0^2$ and the Neumann boundary condition will be called the reference problem. The corresponding reference propagator is the operator $A_0 = -\Delta$ in $\mathcal{H}_0 = L_2(R_0^2)$ with Neumann boundary condition. The solution of the scattering problem for non-degenerate gratings is developed below as a perturbation of the reference problem.

A_0 has a pure continuous spectrum filling the half-line $\lambda \geq 0$. This is easily verified by separation of variables which yields the family of generalized eigenfunctions

(4.1) $$\psi_0(x,y,p,q) = \frac{1}{\pi} e^{ipx} \cos q\, y = \frac{1}{2\pi} e^{i(px-qy)} + \frac{1}{2\pi} e^{i(px+qy)}$$

where $(x,y) \in R_0^2$ and also $(p,q) \in R_0^2$. Clearly

(4.2) $$A_0\, \psi_0(x,y,p,q) = -\Delta\, \psi_0(x,y,p,q) = \omega^2(p,q)\, \psi_0(x,y,p,q)$$

where

(4.3) $$\omega^2(p,q) = p^2 + q^2 \geq 0$$

and

(4.4) $$D_\nu\, \psi_0(x,y,p,q) = D_y\, \psi_0(x,y,p,q) = 0 \text{ on } \partial R_0^2 \;.$$

The decomposition of (4.1) illustrates the physical interpretation of ψ_0. If $(p,q) \in R_0^2$ then $q > 0$ and the first term represents a monochromatic plane wave incident on the plane boundary in the direction $(p,-q)$, while the second term represents the specularly reflected wave propagating in the direction (p,q).

The functions $\{\psi_0(X,P) : P = (p,q) \in R_0^2\}$ form a complete family of generalized eigenfunctions for A_0. This means that for every $h \in \mathcal{H}_0$ one has

(4.5) $$\hat{h}_0(P) = \ell.\text{i.m.} \int_{R_0^2} \overline{\psi_0(X,P)}\, h(X)\, dX \text{ exist in } \mathcal{H}_0$$

and

(4.6) $$h(X) = \ell.\text{i.m.} \int_{R_0^2} \psi_0(X,P)\, \hat{h}_0(P)\, dP \text{ in } \mathcal{H}_0 \;.$$

The $\ell.\text{i.m.}$ notation in (4.5) means that the integral converges not pointwise but in $\mathcal{H}_0$; i.e.,

(4.7) $$\lim_{M\to\infty} \int_{R_0^2} \left| \hat{h}_0(P) - \int_0^M \int_{-M}^M \overline{\psi_0(X,P)}\, h(X)\, dX \right|^2 dP = 0 \;.$$

Equation (4.6) has the analogous interpretation. Moreover, Parseval's relation holds:

$$(4.8) \qquad \int_{R_0^2} |\hat{h}_0(P)|^2 \, dP = \int_{R_0^2} |h(X)|^2 \, dX .$$

In fact, if a linear operator Φ_0 in $\mathcal{H}_0$ is defined by

$$(4.9) \qquad \Phi_0 h = \hat{h}_0$$

then Φ_0 is unitary.

The eigenfunction expansion (4.6) is useful because it diagonalizes A_0. In particular, the solution $v_0(t,\cdot) = e^{-itA_0^{1/2}} h$ of the reference problem has the expansion

$$(4.10) \qquad v_0(t,X) = \ell.\text{i.m.} \int_{R_0^2} \psi_0(X,P)\, e^{-it\omega(P)}\, \hat{h}_0(P)\, dP$$

where $\omega(P) = |P| = \sqrt{p^2+q^2}$.

§5. Rayleigh-Bloch Diffracted Plane Waves for Gratings

In analogy with the case of the degenerate grating, the generalized eigenfunctions of the grating propagator A may be defined as the response of the grating to a monochromatic plane wave $(2\pi)^{-1} \exp\{i(px - qy)\}$. It will be shown that there are two distinct families which will be denoted by $\psi_+(X,P)$ and $\psi_-(X,P)$, respectively. It will be convenient to write them as perturbations of the eigenfunctions $\psi_0(X,P)$ for the degenerate grating:

$$(5.1) \qquad \psi_\pm(X,P) = \psi_0(X,P) + \psi_\pm^{sc}(X,P) \ , \ X \in G \ , \ P \in R_0^2 \ .$$

They are characterized by the conditions

$$(5.2) \qquad A\, \psi_\pm(X,P) = -\Delta\, \psi_\pm(X,P) = \omega^2(P)\, \psi_\pm(X,P) \ , \ X \in G \ ,$$

$$(5.3) \qquad D_\nu\, \psi_\pm = 0 \ (\text{resp.}, \ \psi_\pm = 0) \ \text{for } X \in \partial G \ ,$$

(5.4) $\psi_+^{sc}(X,P)$ is outgoing and $\psi_-^{sc}(X,P)$ is incoming for $X \to \infty$.

The last condition is based on the Fourier series representation in x of $\psi_\pm^{sc}(x,y,P)$ which is valid for $y > h$. It can be written (with $P = (p,q)$)

$$(5.5) \qquad \psi_\pm^{sc}(X,P) = \frac{1}{2\pi} \sum_{(p+\ell)^2 < p^2+q^2} c_\ell^\pm(P)\, e^{i(p_\ell x \pm q_\ell y)} + \frac{1}{2\pi} \sum_{(p+\ell)^2 \ge p^2+q^2} c_\ell^\pm(P)\, e^{ip_\ell x}\, e^{-y\{(p+\ell)^2 - p^2 - q^2\}^{1/2}}$$