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RECENT MATHEMATICAL STUDIES IN THE MODELING OF OPTICS AND ELECTROMAGNETICS *1)

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Dedicated to Professor Zhong-ci Shi on the occasion of his 70th birthday

Abstract

This work is concerned with mathematical modeling, analysis, and computation of optics and electromagnetics, motivated particularly by optical and microwave applications. The main technical focus is on Maxwell's equations in complex linear and nonlinear media.

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1. Micro-optics

Micro diffractive optics is a fundamental and vigorously growing technology which continues to be a source of novel optical devices. Significant recent technology developments of high precision micromachining techniques have permitted the creation of gratings (periodic structures) and other diffractive structures with tiny features. Current and potential application areas include corrective lenses, microsensors, optical storage systems, optical computing and communications components, and integrated opto-electronic semiconductor devices. Because of the small structural features, light propagation in micro-optical structures is generally governed by diffraction. In order to accurately predict the energy distributions of an incident field in a given structure, the numerical solution of full Maxwell's equations is required. Computational models also allow the exciting possibility of obtaining completely new structures through the solution of optimal design problems. General discussion and recent advances on the diffraction problem may be found in [32], [19], [16] and references therein.

1.1. Computation and Analysis of the Diffraction Problem

The diffraction problem is to predict the electromagnetic field distributions when a time-harmonic plane wave is incident on a given grating or periodic structure. Because of the small structural features, wave propagation is dominated by the system of Maxwell's equations. Here, the diffractive structure is periodic either in one direction – linear grating (2-D model) or in two orthogonal directions – biperiodic structure (3-D model). In the two-dimensional case, convergence analysis for the finite element methods in TE (transverse electric) and TM (transverse magnetic) polarization was first carried out in Bao [11] and [12]. In both cases, existence and uniqueness for the continuous and discreet model problems were established. In general, to model the diffraction of biperiodic diffractive structures, *i.e.,* a three-dimensional geometry, it is essential to study Maxwell's equations in vector form. In Bao and Dobson [18],

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a new variational formulation for the diffraction problem in biperiodic structures (3D) was introduced. Using the formulation, we established the well-posedness of the weak solutions (the magnetic fields) in H^1. In contrast, the classical approach only gives rise to the existence and uniqueness of $H(curl)$ solutions. This presents a severe difficulty in numerical analysis since the imbedding from $H(curl)$ to L^2 is not compact. It was established in [27] the well-posedness of the discretized problem. Error estimates for the variational (finite element) approximation of the model problem was obtained. These convergence estimates are quite general since little smoothness is assumed on the coefficients and the geometry.

A related project is on least-squares finite element analysis of diffraction problems. In the two-dimensional case, a least-squares finite element method was first proposed in [26] that incorporates the jump conditions at interfaces into the objective functional. Optimal error estimates were obtained. The results indicate that significantly better error estimates than standard finite element methods may be obtained for sufficiently smooth interfaces. More recently, for the two-dimensional diffraction problem, Chen and Wu [30] have developed a new approach by combining the adaptive finite element method and a perfectly matched layer (PML) boundary condition.

1.2. Chiral Gratings

Chiral gratings provide an exciting combination of the medium and structure, which gives rise to new features and applications. For instance, chiral gratings are capable of converting a linearly polarized incident field into two nearly circularly polarize diffracted modes in different directions. Mathematically, in a chiral medium, the Maxwell equations remain the same form. However, the constitutive equations are now coupled. Therefore, the model equations are necessarily of vector form and much more complicated than standard Maxwell's equations. A variational approach was developed by Ammari and Bao [1]. We established the existence and uniqueness of weak solutions by a combination of a variational approach and the Hodge decomposition of the electric field.

1.3. Scattering by a Perturbed Periodic Structure

Consider a time-harmonic electromagnetic plane wave incident on a periodic (grating) structure. An inhomogeneous (subwavelength) object is placed inside the periodic structure. The scattering problem is to study the electromagnetic field distributions. The problem arises in the study of near-field optics and has many physical and biological applications. In [2], we developed an integral representation approach to solve the model problem. It was shown particularly that the perturbation due to the object decays exponentially along the periodic direction of the structure, provided that no surface waves occur. Based on the approach, a general solution method may be introduced. More recently, the approach has been generalized to study the three dimensional Maxwell equation model [4].

1.4. Inverse Diffraction and Optimal Design Problems

Consider scattering of electromagnetic waves by a doubly periodic structure. Above the structure, the medium is assumed to be homogeneous with a constant dielectric coefficient. The medium is a perfect conductor below the structure. An inverse problem arises and may be described as follows [10]. For a given incident plane wave, the tangential electric field is measured away from the structure. To what extent can one determine the location of the periodic structure that separates the dielectric medium from the conductor? This inverse problem which arises naturally in the optimal design of gratings has received much attention recently. However, most of the progress has been made only in the 2-D or scalar case where the structure and material are assumed to be invariant in one direction. In this 2-D setting, Friedman and Bao obtained by using a variational method and index theory in [21] the first set of stability results for a large class of inverse diffraction problems. The result indicates that for small h, if the boundary measurements of a perturbed problem are $O(h)$ close to the scattered fields in a suitable norm, then the grating structure of the perturbed problem is $O(h)$ close to the original grating structure measured in the Hausdorff distance. More recently, Bao and Zhou [28] made some important progress in characterizing uniqueness and stability in the general biperiodic case, where the model PDE is three dimensional and in vector form. The main idea was to formulate the problem as an estimation problem of the first eigenvalue for the Laplacian and then use the fact that the eigenspaces are finite dimensional. In particular, our stability result leads to a nontrivial extension of a theorem proved in [21].

Given the incident field, the optimal design problem is to determine a periodic structure which gives rise to some specified diffraction patterns away from the structure. The problem can be posed as a nonlinear least-squares problem. Difficulties arise since the scattering pattern depends on the interface in a very implicit and nonlinear fashion and in general the set over which the function is minimized is neither convex nor closed. Recently, Bao and Bonnetier [13] studied the design problem in TM (transverse magnetic) polarization by developing a homogenization approach. The main idea is to allow the grating profiles to be highly oscillating and to use relaxed formulation [31] of the optimization problem. In the present case, the relaxed formulation involves materials, the effective dielectric properties of which need be determined. When considering optimal design problems involving diffraction gratings, it is useful to have some *a priori* characterization of the range of possible reflectances one can achieve for given material parameters. More recently, we have also examined [20] the limiting case of a rapidly oscillating dielectric grating and show that such gratings can have reflectance no greater than that of a flat interface, regardless of the shape of the grating interface.

2. Nonlinear Diffractive Optics

A remarkable application of nonlinear optics is to generate powerful coherent radiation at a frequency that is twice that of available lasers (so called *second-harmonic generation*) [34]. Nonlinear optics also has applications in laser technology, spectroscopy, optical switching, parametric amplifiers and oscillators, optical computing, and communications. Our focus is on modeling and enhancements of the most useful second order nonlinear optical effects, especially second harmonic generation (SHG). In general, nonlinear optical effects are so weak that the observation of nonlinear phenomena in the optical region can only be made by using high intensity lasers. Recently, it has been found experimentally by physicists and engineers that diffraction gratings can greatly enhance nonlinear optical effects [33] .

2.1. Well-posedness of the Model

The electromagnetic fields in a nonlinear medium are governed by the following Maxwell equations:

$$\begin{aligned} \nabla \times E &= i\omega H, \quad \nabla \cdot H = 0 \,, \\ \nabla \times H &= -i\omega (E + 4\pi P), \ \nabla \cdot E = -4\pi \nabla \cdot P, \end{aligned}$$

where the new term P is the polarization vector. In general, P is a nonlinear function of E. The simplest nonlinear optical wave interaction deals with second harmonic generation, a special case of the second-order nonlinear optical effects. When a pumping wave with frequency $\omega_1 = \omega$ is incident on a nonlinear medium, second harmonic generation leads to two wave fields $E(x, \omega_1)$ and $E(x, \omega_2 = \omega_1 + \omega_1)$. Note that new frequency components are present in the above expression, which is the most striking difference between nonlinear and linear optics. In this case,

$$\begin{aligned} P(\omega_1) &= \chi^{(1)}(\omega_1) \cdot E(x, \omega_1) + \chi^{(2)}(\omega_1)(\omega_1 = \omega_2 - \omega_1) : \overline{E}(x, \omega_1) E(x, \omega_2) \,, \\ P(\omega_2) &= \chi^{(1)}(\omega_2) \cdot E(x, \omega_2) + \chi^{(2)}(\omega_2)(\omega_2 = \omega_1 + \omega_1) : E(x, \omega_1) E(x, \omega_1) \,, \end{aligned}$$

where $\chi^{(2)}$ is the second order nonlinear susceptibility tensor which measures the nonlinearity of the medium, and $\chi^{(2)} : E\ E$ is a vector whose i-th component is $\sum_{j,k} \chi^{(2)}_{ijk} E_j E_k$.

Little is known mathematically on the nonlinear problem. In [17], we studied second harmonic generation in periodic structures. The model, derived from a general nonlinear system of time harmonic Maxwell's equations, was shown to have a unique solution for all but a discrete number of frequencies. The problem was solved numerically by combining a method of finite elements and a fixed-point iteration scheme. Our numerical experiments confirmed that it is possible to use gratings to enhance nonlinear optical effects. Furthermore, we analyzed [14] another model that deals with nonlinear optical materials with more practical group symmetry properties than in [17]. The PDE is a coupled system of Maxwell's equations derived by the linearization of the nonlinear model. Using a pair of transparent boundary conditions, we reformulated the problem in a bounded domain. A technical difficulty for this model is the appearance of jumps in the leading coefficients of the PDE. By using a variational technique, we established well-posedness and regularity of the system.

Another recent project is concerned with the well-posedness of the mathematical model for second harmonic generation of nonlinear optics in biperiodic structures. The governing equation is a system of nonlinear Maxwell's equations. The well-posedness of the model has been studied by Bao, Minut, and Zhou [23]. A crucial step is to establish interior and global L^p-type estimates for the solutions of Maxwell's equations with source term in a domain filled with two different materials separated by an interface. The usual elliptic estimates cannot be applied directly, due to the singularity of the dielectric permittivity. A special curl-div decomposition is introduced for the electric field to reduce the problem to an elliptic equation in divergence form with jump coefficients. The potential analysis and the jump condition lead to the interior L^p estimates which are superior to the straightforward Nash-Moser estimates. The reduction procedure is expected to be useful for future numerical simulation. Because of the natural physical requirements, the boundary condition is nonlocal and involves a first order pseudo differential operator, the boundary estimate is established by novel maximum principles and Riesz convexity arguments.

2.2. Thin Coatings

In many applications, diffractive structures are coated with one or more thin dielectric layers to enhance diffraction efficiency and, in the case of metallic structures, to prevent the metal surface from tarnishing. Another application of great interest is the antireflective coating. Coated structures present certain difficulties. The coatings are usually very thin in contrast to the structure features (wavelength, period, height of the grating). Thus, the diffraction problem involves at least two scales. A direct numerical solution of the multiple scale problem is difficult with our current finite element method due to the scale of computation. The standard finite element method attempts to resolve the small scale features of the problem, which is very expensive in terms of CPU time and computer memory. Thin nonlinear coatings are also of great interest. The effect of thin coatings of nonlinear material on gratings structures in second harmonic generation has been studied recently by Ammari, Bao, and Hamdache [6]. Asymptotic expansions of the fields inside a thin nonlinear coating are performed. The convergence of these formal expansions is established. Our asymptotic analysis reveals the physical nature of this nonlinear problem. It also provides an effective method for overcoming the computational difficulties that arise in thin nonlinear coatings.

2.3. Optimal Design

The optimal design of nonlinear gratings arises in the study of surface enhanced nonlinear optical effects of second harmonic generation. The problem has been studied in [24] by an optimization approach. In order to apply certain gradient based optimization methods, an explicit formula for the partial derivatives of the Rayleigh coefficients with respect to the parameters of the grating profile has been derived. Using the formula, numerical results have been obtained on an optimal design problem of nonlinear binary gratings.

3. Electromagnetics

Significant progress has been made in a diverse set of research topics with industrial, medical, and millitary applications.

3.1. Electromagnetic Cavities

As a measure of the detectability of a target by radar systems, the *radar cross section* (RCS) of the target has always been an important subject of study in electromagnetics. Mathematical and computational methods to accurately predict the RCS of complex objects such as aircraft are of great interest to designers. Of particular importance is the prediction of the RCS of cavities due to its dominance to the target's overall RCS. Examples of cavities include jet engine inlet ducts, exhaust nozzles, and cavity-backed antennas.

Consider a time-harmonic electromagnetic plane wave incident on an arbitrarily shaped open cavity embedded in an infinite ground plane. The ground plane and the walls of the open cavity are perfect electric conductors, and the interior of the open cavity is filled with a nonmagnetic material which may be inhomogeneous. The half-space above the ground plane is filled by free-space characterized by its permittivity ε_0 and permeability μ_0. An important project is to study the propagation of the scattered waves from the cavity, and hence its RCS.

There are a large number of articles in the engineering literature available on computation and design of cavities. However, little is known about the analysis of the problem. In the general two-dimensional setting, we have recently established the well-posedness of the scattering problem in [8] by a variational approach, and in [7] by an integral equation method. The analysis of the three-dimensional scattering problem from a cavity has been conducted in [9] by extending the variational approach of [8] to solve the scattering problem. However, the situation here is more difficult: Because of the three dimensional geometry, we must study directly the vector form of Maxwell's equations. A Hodge decomposition is needed here due to a lack of compactness of the solution functional space. In comparison, the compactness is trivial in the two-dimensional case. We are also interested in the optimal design of cavities with desirable features.

3.2. Helmholtz and Maxwell's Equations with High Wavenumbers

It is well known that wave propagation problems for the Helmholtz equations involving high wavenumbers are notoriously difficult to solve numerically. The very short wave problem governed by the Helmholtz equations has recently been recognized by O. C. Zienkiewitz as one of the remaining unsolved problems for modern numerical approaches. As observed recently by I. Babuska, J. B. Keller, and many others, the existing approaches lead to some numerically non-robust behavior, known as "the pollution effect".

Along with G. W. Wei and S. Zhao, we have investigated [25] the pollution effect, and explore the feasibility of a local spectral method, the discrete singular convolution (DSC) algorithm for solving the Helmholtz equation with high wavenumbers. The algorithm is designed by using a novel regularized Shannon's sampling theorem. The Fourier analysis is employed to study the dispersive error of the DSC algorithm. Our analysis of dispersive errors indicates that the DSC algorithm yields a dispersion vanishing scheme. The dispersion analysis is further confirmed by the numerical results. For one and higher-dimensional Helmholtz equations, the DSC algorithm is shown to be an essentially pollution free scheme. Furthermore, for large scale computation, the grid density of the DSC algorithm can be close to the optimal two grid points per wavelength. The present study reveals that the DSC algorithm is accurate and efficient for solving the Helmholtz equation with high wavenumbers.

3.3. Inverse Source Problems in Brain Imaging

Understanding the human brain, the most complex organized structure known to exist, presents a great challenge to the scientific community. The project is devoted to the study of an inverse source problem that arises in determining locations of epileptic foci in the living human brain. At present, the only way to cure a patient with an epileptic focus permanently is to remove a small part of the brain surgically or by use of gamma-rays. Therefore, accurate location of the epileptic focus is of great clinical interest. The data is measured via magnetoencephalography (MEG) – a noninvasive technique for investigating neuronal activity of the living human brain.

A new computational method has been developed for solving the inverse problem in [5]. Our main idea is to conduct a low frequency asymptotic analysis of the fields for Maxwell's equations. Our method is constructive and computationally attractive. In fact, the method only requires a small number of solutions to the Maxwell equations. To the best of our knowledge, all of the existing modeling methods are based on least-squares type optimization procedures which are iterative (non-constructive) and often require solutions of the model equations many times. A crucial step of our method is to construct special test functions which relate the source locations and direction vectors to the boundary measurements of the magnetic fields. Such a construction relies on a careful study of the asymptotic behavior of Maxwell's equations. The Maxwell equations may be solved by a finite element approach developed in our previous research on the electromagnetic scattering. Our preliminary analysis and computational experiments indicate that the method is accurate and robust.

3.4. Inverse Medium Problems

Recently, we have obtained significant results in the development of solution methods for inverse scattering problems motivated by optimal design of electromagnetic cavities and optical devices. Other applications of inverse scattering problems include non-destructive testing, optical measurements, ultrasound tomography, seismic imaging, submarine detection, and medical imaging.

In Bao and Liu [22], we have introduced a general regularized homotopy continuation method is for numerical solution of nonlinear inverse problems. A major difficulty for solving these inverse problems by an optimization method is the ill-posedness due to the presence of many local minima. Classic iterative methods, such as Gauss-Newton or Levenberg-Marquardt algorithms, offer fast local convergence but might not be able to compute the global minimum. Based on a natural concept of multi-experimental data, a regularized homotopy continuation method is constructed to compute the global minimum. As the experimental index t increases continuously, the global minimizer can be computed continuously by using local optimization methods. By discretizing the continuous homotopy method, various recursive linearization algorithms may be developed. These algorithms can be applied to numerical solution of an inverse medium scattering problem which reconstructs the refractive index of an inhomogeneous medium from limited aperture measurements of the far field pattern of the scattered fields. It is assumed that the data is measured at multiple frequencies. Our results in particular provide a general framework for the work of Chen [29] on recursive linearization of inverse medium problems.

Another interesting problem is to solve the inverse scattering problems when the data are only measured along one or a few directions, the limited aperture case. The model is obviously more practical. The inverse scattering problem with limited aperture is also challenging, since without full aperture measurements, the ill-posedness and nonlinearity of the inverse problem become more severe. An efficient regularized iterative linearization method (recursive lineriza- tion with respect to the wave number) has been developed for solving the inverse problem. The convergence of the iterative method has been illustrated through numerical examples.

Results on regularity and stability of the inverse medium problem were proved by Bao, Ma, and Chen [15] in the two-dimensional case. Initial progress on the regularity and stability analysis of the inverse medium problem in electromagnetics has been made in Ammari and Bao [3] where the forward problem is governed by the Maxwell equations. A crucial step is to establish interior estimates for the non-elliptic Maxwell equations.

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