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WITH PERIODIC STRUCTURE**

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DIFFRACTIVE OPTICS IN NONLINEAR MEDIA WITH PERIODIC STRUCTURE

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Abstract

The diffraction of time-harmonic waves in a nonlinear medium with periodic structure is studied in this paper. In particular, second harmonic generation—an important phenomenon in nonlinear optics—is modeled. The model, derived from a general nonlinear system of Maxwell's equations, is shown to have a unique solution for all but a discrete number of frequencies. The problem is solved numerically by combining a method of finite elements and a fixed-point iteration scheme. Numerical experiments for some simple grating structures are presented and discussed.

Key words. nonlinear optics, nonlinear system of Helmholtz equations, harmonic generation, surface-enhanced nonlinear effects, periodic structure.

AMS(MOS) subject classifications. 35Q60, 78A45, 78A60.

1 Introduction

Since its birth in the early sixties, rapid and continuous progress has been made in the field of nonlinear optics. One of the many important applications of nonlinear optical phenomena is a method for obtaining coherent radiation at a wavelength shorter than that of available lasers, through the technology of second harmonic generation (SHG). The present work is devoted to the mathematical modeling of nonlinear optical wave mixing, or harmonic generation, a fundamental aspect of nonlinear optics. In particular, we are interested in second harmonic generation in diffraction gratings, or periodic structures, which have been shown [14], [15] to enhance certain nonlinear optical effects.

Thus, we study the diffraction of electromagnetic waves in nonlinear media. We wish to accurately predict the field intensity distribution of reflected and transmitted waves when an intense beam (pump beam) is incident on the surface of a nonlinear material with periodic structure. By assuming that the medium and grating surface are constant in one direction, the three-dimensional scattering problem can be formulated in two dimensions. Aside from the two-dimensional restriction, the geometry of the surface can be very general. We propose a model derived from a general nonlinear system of Maxwell's equations. Our overall

approach falls into the category of variational methods. We establish results on existence and uniqueness for this model problem. The problem is solved numerically by a combination of a method of finite elements and a fixed-point iteration scheme.

To the best of our knowledge, this paper provides the first analysis and computations for a fully nonlinear model of second harmonic generation in periodic structures. Existing models have so far relied on the undepleted pump approximation (UPA), which is essentially a simple linearization technique. The justification of the UPA is based on the assumption that the depletion of energy from the pump waves can be neglected. Using this approximation, the original nonlinear model may be reduced to a coupled system of linear equations. Then the corresponding well established linear theory of gratings, see for example [13], becomes applicable. Using this approximation, a French group has obtained several interesting results, see [14] and [15], and references cited there. Another common approximation in nonlinear optics is the so-called slowly varying approximation (SVA). The SVA is useful in the case where the field varies slowly in some spatial direction, relative to the wavelength of the underlying radiation. Its basic assumption is that along the slowly-varying direction (or directions), the second-order derivative is negligible compared to the product of the first-order derivative and the corresponding wave number. The advantage of the SVA is that the original second-order equation can then be approximated by a first-order equation. Unfortunately, both of these models have weaknesses. It is indicated by the theory of nonlinear optics, e.g. Shen [16], that the UPA is invalid when the output energy becomes significant compared to the pump beam. In other words, the approximation fails when high conversion efficiency is desired. The SVA is valid if the energy transfer among waves is significant only after the wave travels over a distance much longer than its wavelength. But the approximation will break down when the medium is sufficiently thin, as is the case in many applications like nonlinear coatings or nonlinear optical films.

Our model is derived from the fully nonlinear system of equations. In addition to its generality, our analysis and numerical experiments show that this model overcomes the difficulties mentioned above.

When the model is linear with periodic structure in one direction, results on existence and uniqueness were obtained by Chen and Friedman [6] assuming the dielectric coefficient ϵ is a piecewise constant function. They showed that for all but a discrete number of c 's, there exists a unique solution to the Maxwell equation by an integral equation approach, while standard jump conditions allowed them to reduce the system to a coupled pair of Fredholm equations. Similar results were obtained for Maxwell's equations in bi-periodic structures in [8].

Very little is known concerning the questions of existence and uniqueness for the nonlinear Maxwell equations that govern SHG. Recently, in [2], the authors studied second harmonic generation in nonlinear optical films by using a similar but simpler model. The problem geometry was much simpler with a flat surface and normal beam incidence, *i.e.* no grating structure was present. Under these assumptions, we showed that the problem can be treated as one-dimensional. Consequently, rigorous mathematical and computational results were obtained, with no additional constraints imposed on the solutions. In contrast, in the present work, we have to restrict to "quasiperiodic" solutions.

The variational formulation used here is motivated by the work of Achdou and Pironneau [1] (see also [7]). However, in their cases, only linear models were involved. The situation here is much more complex since we must solve a coupled nonlinear system of Helmholtz equations in periodic structures. The primary advantage of the variational formulation (as opposed, say to an integral equation formulation) is that we can easily consider very complicated structures; the material parameters only have to be bounded measurable functions.

The outline of this paper is as follows. The governing nonlinear system of Maxwell equations are introduced in Section 2. We then reduce the system to a nonlinear system of Helmholtz equations. In Section 3, the periodic structure allows us to reformulate the problem inside a “box”, with boundary conditions derived from knowledge of the fundamental solutions in linear media. We then proceed in Section 4 to formulate an equivalent variational problem over the box. The existence and uniqueness of solutions to this variational problem are established. Finally, some numerical experiments are presented and discussed in Section 5.

A good background on the linear theory of diffractive optics in grating structures may be found in Petit [13]. A brief description of the present problem, along with a discussion of some other mathematical problems arising from industrial applications of diffractive optics can be found in Friedman [9], Chapter 5. For the underlying physics of nonlinear optics, we refer the reader to the classic books of Bloembergen [4] and Shen [16]. Many other recent mathematical developments in nonlinear optics may be found in Newell and Moloney [12] and references cited therein. Finally, we mention that a preliminary description of the results presented here was given in the proceedings [3].

2 Nonlinear wave mixing

Throughout, the media are assumed to be nonmagnetic with constant magnetic permeability. The magnetic permeability constant is assumed to be equal to one everywhere for convenience. We also assume that no external charge or current is present in the field, and that the electric and magnetic fields are time harmonic, *i.e.*,

$$\mathbf{E} = \mathbf{E}(\mathbf{r})e^{-i\omega t}, \quad \mathbf{H} = \mathbf{H}(\mathbf{r})e^{-i\omega t}$$

where $\mathbf{r} = (x_1, x_2, x_3) \in \mathbb{R}^3$.

The Maxwell equations then take the form:

$$\begin{aligned} \nabla \times \mathbf{E} &= -\frac{i\omega}{c}\mathbf{H}, & \nabla \cdot \mathbf{H} &= 0, \\ \nabla \times \mathbf{H} &= \frac{i\omega}{c}\mathbf{D}, & \nabla \cdot \mathbf{D} &= 0, \end{aligned}$$

along with the constitutive equation:

$$\mathbf{D} = \mathbf{E} + 4\pi\mathbf{P}$$

where

- $\mathbf{E}$ = electric field,
- $\mathbf{H}$ = magnetic field,
- $\mathbf{D}$ = electric displacement,
- $\mathbf{P}$ = electric moment per unit volume,
- c = speed of the light,
- ω = angular frequency.

The vector $\mathbf{P}$ describes fully the response of the medium to the electromagnetic field and characterizes the nonlinear nature of the medium. The medium is said to be linear if $\mathbf{P} = \chi^{(1)}(\omega) \cdot \mathbf{E}$ where $\chi^{(1)}$ is the linear susceptibility tensor of the medium. The (linear) dielectric constant is defined by $\epsilon(\omega) = 1 + 4\pi\chi^{(1)}(\omega)$. In principle, essentially all optical media are nonlinear, i.e., $\mathbf{P}$ is a nonlinear function of $\mathbf{E}$. However, for most media, nonlinear optical effects are so weak that they may reasonably be ignored. The observation of nonlinear phenomena in the optical region normally can only be made by using high intensity beams, say by application of a high intensity laser.

It is usually assumed that $\mathbf{P}$ has the following power series expansion

$$\mathbf{P} = \chi^{(1)}(\omega) \cdot \mathbf{E}(\mathbf{r}, \omega) + \chi^{(2)}(\omega)(\omega = \omega_i + \omega_j) : \mathbf{E}(\mathbf{r}, \omega_i)\mathbf{E}(\mathbf{r}, \omega_j) + \cdots,$$

where $\chi^{(n)}$ are the nonlinear susceptibility tensors of the medium, which measure the non-linearity of the medium. Of particular importance is $\chi^{(2)}$, the second order nonlinear susceptibility tensor of third rank. Note that new frequency components are present in the above expression, which is the most striking difference between nonlinear and linear optics.

The simplest case of optical wave interactions in nonlinear media deals with second harmonic generation, or two wave mixing, a special case of the second-order nonlinear optical effects. In this case all $\chi^{(n)}$ with $n \geq 3$ are taken to be zero. Suppose that a pumping wave with frequency $\omega_1 = \omega$ is incident on a nonlinear medium. Let us consider the two wave fields $\mathbf{E}(\mathbf{r}, \omega_1)$ and $\mathbf{E}(\mathbf{r}, \omega_2 = \omega_1 + \omega_1)$. To simplify our notation, we denote $\mathbf{E}(\omega_i) = \mathbf{E}(\mathbf{r}, \omega_i)$. The Maxwell equations yield the following coupled system:

$$\left[\nabla \times (\nabla \times) - \frac{\omega_1^2 \epsilon_1}{c^2} \right] \mathbf{E}(\omega_1) = \frac{4\pi\omega_1^2}{c^2} \chi^{(2)}(\omega_1 = -\omega_1 + \omega_2) : \mathbf{E}^*(\omega_1)\mathbf{E}(\omega_2), \quad (2.1)$$

$$\left[\nabla \times (\nabla \times) - \frac{\omega_2^2 \epsilon_2}{c^2} \right] \mathbf{E}(\omega_2) = \frac{4\pi\omega_2^2}{c^2} \chi^{(2)}(\omega_2 = \omega_1 + \omega_1) : \mathbf{E}(\omega_1)\mathbf{E}(\omega_1), \quad (2.2)$$

where the superscript $*$ denotes the complex conjugate. As the system exhibits, through the nonlinear coupling, energy can be transferred back and forth between fields at frequencies $\omega_1 = \omega$ and $\omega_2 = 2\omega$.

Remark. The usual jump conditions of the fields are valid, see *e.g.* [4]. In fact, the tangential components of $\mathbf{E}$ and $\mathbf{H}$ must be continuous at the boundary between two homogeneous media, and the normal components of $\mathbf{D}$ and $\mathbf{H}$ must also be continuous at the boundary for all frequencies.

We next want to reduce the nonlinear coupled system (2.1) and (2.2) further. Throughout the paper, we assume that all the fields are invariant in the z direction. We shall also assume that the electric fields at ω_1 and ω_2 are TE polarized, *i.e.*, they are directed along the z axis $\mathbf{E}(\mathbf{r}, \omega_1) = E(\mathbf{r}, \omega_1)\mathbf{\hat{z}}$ and $\mathbf{E}(\mathbf{r}, \omega_2) = E(\mathbf{r}, \omega_2)\mathbf{\hat{z}}$. Define

$$\begin{aligned} u &= E(\mathbf{r}, \omega_1) , \\ v &= E(\mathbf{r}, \omega_2) , \\ \chi_1 &= -\frac{4\pi\omega_1^2}{c^2}\chi_{3,3,3}^{(2)}(\omega_1 = -\omega_1 + \omega_2) , \\ \chi_2 &= -\frac{4\pi\omega_2^2}{c^2}\chi_{3,3,3}^{(2)}(\omega_2 = \omega_1 + \omega_1) . \end{aligned}$$

The system (2.1, 2.2) then reads

$$\left[\Delta + \frac{\omega_1^2 \epsilon(\omega_1)}{c^2} \right] u = \chi_1 u^* v , \quad (2.3)$$

$$\left[\Delta + \frac{\omega_2^2 \epsilon(\omega_2)}{c^2} \right] v = \chi_2 u^2 , \quad (2.4)$$

where Δ is the usual Laplacian operator. The topic of the next section is to make a more precise formulation of the scattering problem by deriving appropriate boundary conditions for the above system.

3 Problem formulation

Let us first specify the problem geometry. As shown in Figure 1, S_1 and S_2 are two simple curves imbedded in the strip

$$\Omega = \{(x, y) \in \mathbb{R}^2 : -l < y < l\} ,$$

where l is some positive constant. The medium in the region Ω between S_1 and S_2 is assumed to be nonlinear. Above the surface S_1 and below the surface S_2 , the media are assumed to be linear. The entire structure is taken to be periodic in the x -direction. More precisely, we assume that S_1 and S_2 are periodic of period 2π with respect to the integers $Z = \{0, \pm 1, \pm 2, \dots\}$ in the sense that $(S_i \cap \{(x, y)\}) + (2\pi n, 0) = S_i \cap \{(x + 2\pi n, y)\}$ for all $n \in Z$, $(x, y) \in \mathbb{R}^2$, and $i = 1, 2$.

Let $\Omega_1 = \{x \in \mathbb{R}^2 : y > l\}$, $\Omega_2 = \{x \in \mathbb{R}^2 : y < -l\}$. Define the boundaries $\Gamma_1 = \{y = l\}$, $\Gamma_2 = \{y = -l\}$. The curves S_1 and S_2 divide Ω into three connected components. Denote the component which meets Γ_1 by Ω_1^+ ; the component which meets Γ_2 by Ω_2^+ ; and let $\Omega_0 = \Omega - \Omega_1^+ - \Omega_2^+$.

Suppose that the whole space is filled with material in such a way that k_1 and k_2 satisfy

$$k_j(x) = \begin{cases} k_{j1} & \text{in } \Omega_1^+ \cup \bar{\Omega}_1 , \\ k_{j0} & \text{in } \Omega , \\ k_{j2} & \text{in } \Omega_2^+ \cup \bar{\Omega}_2 , \end{cases}$$

Figure 1: Problem geometry.

for $j = 1, 2$, where k_{j0} , k_{j1} , and k_{j2} are constants, k_{j1} are real and positive, and $\text{Re } k_{j2} > 0$, $\text{Im } k_{j2} \geq 0$. The case $\text{Im } k_{j2} > 0$ accounts for materials which absorb energy (see e.g. [5]). Suppose also that $\chi_1, \chi_2 \in L^\infty(\mathbb{R}^2)$ are supported in Ω_0 .

From the discussion in the preceding section, we wish to solve

$$\left[\Delta + \omega_1^2 k_1^2 \right] u = \chi_1 u^* v, \quad (3.1)$$

$$\left[\Delta + \omega_2^2 k_2^2 \right] v = \chi_2 u^2, \quad (3.2)$$

when an incoming plane wave

$$u_I = u_* e^{i\alpha_1 x - i\beta_{11} y}$$

is incident on S_1 from Ω_1^+ where u_* is a real constant. Here once again $\omega_1 = \omega$ and $\omega_2 = 2\omega$ are the frequencies, for $j = 1, 2$,

$$\alpha_j = \omega_j k_{j1} \sin \theta, \quad \beta_{11} = \omega k_{11} \cos \theta,$$

and $-\frac{\pi}{2} < \theta < \frac{\pi}{2}$ is the angle of incidence. Observe that the light speed has been absorbed by the frequency components by changing the length scale of the problem properly. Also note that $w_1 k_1$ and $w_2 k_2$ are the linear “indexes of refraction” often used in the literature. The benefit of pulling out the frequency components will be made clear in the following discussion.

We are interested in “quasiperiodic” solutions (u, v) , that is, solutions (u, v) such that

$$u_\alpha = u e^{-i\alpha_1 x} \quad \text{and} \quad v_\alpha = v e^{-i\alpha_2 x}$$

are 2π -periodic in the x direction.

A simple calculation shows that if (u, v) satisfies the system (3.1) and (3.2), then (u_α, v_α) satisfies

$$\left[\Delta_{\alpha_1} + \omega_1^2 k_1^2 \right] u_\alpha = \chi_1 u^* v = \chi_{1\alpha} v_\alpha u_\alpha^*, \quad (3.3)$$

$$\left[\Delta_{\alpha_2} + \omega_2^2 k_2^2 \right] v_\alpha = \chi_2 u^2 = \chi_{2\alpha} u_\alpha^2, \quad (3.4)$$

where for $j = 1, 2$ the operators Δ_{α_j} are defined by

$$\Delta_{\alpha_j} = \Delta + 2i\alpha_j \partial_x - |\alpha_j|^2$$

and

$$\chi_{1\alpha} = \chi_1 e^{i(\alpha_2 - 2\alpha_1)x}, \quad \chi_{2\alpha} = \chi_2 e^{i(2\alpha_1 - \alpha_2)x}.$$

Expand u_α and v_α in a Fourier series:

$$u_\alpha(x, y) = \sum_{n \in \mathbb{Z}} u_\alpha^n(y) e^{inx}, \quad (3.5)$$

$$v_\alpha(x, y) = \sum_{n \in \mathbb{Z}} v_\alpha^n(y) e^{inx}, \quad (3.6)$$

where

$$u_\alpha^n(y) = \frac{1}{2\pi} \int_0^{2\pi} u_\alpha(x, y) e^{-inx} dx,$$

$$v_\alpha^n(y) = \frac{1}{2\pi} \int_0^{2\pi} v_\alpha(x, y) e^{-inx} dx.$$

Define for $j = 1, 2$, the coefficients

$$\beta_{1j}^n(\alpha) = e^{i\gamma_{1j}/2} \left| \omega_1^2 k_{1j}^2 - (n + \alpha_1)^2 \right|^{1/2}, \quad n \in \mathbb{Z}, \quad (3.7)$$

$$\beta_{2j}^n(\alpha) = e^{i\gamma_{2j}/2} \left| \omega_2^2 k_{2j}^2 - (n + \alpha_2)^2 \right|^{1/2}, \quad n \in \mathbb{Z}, \quad (3.8)$$

where

$$\gamma_{1j} = \arg(\omega_1^2 k_{1j}^2 - (n + \alpha_1)^2), \quad 0 \leq \gamma_{1j} < 2\pi$$

$$\gamma_{2j} = \arg(\omega_2^2 k_{2j}^2 - (n + \alpha_2)^2), \quad 0 \leq \gamma_{2j} < 2\pi.$$

We assume that $\omega_1^2 k_{1j}^2 \neq (n + \alpha_1)^2$ and $\omega_2^2 k_{2j}^2 \neq (n + \alpha_2)^2$ for all $n \in \mathbb{Z}$, $j = 1, 2$, this assumption excludes the “resonant” cases where waves can propagate along the x -axis. The assumption also ensures that a fundamental solution for (3.3) and (3.4) exists inside Ω_1 and Ω_2 . It then follows from knowledge of the fundamental solution (see eg. [6], or [8]) that inside Ω_1 and Ω_2 , u_α and v_α can be expressed as a sum of plane waves: for $j = 1, 2$

$$u_\alpha|_{\Omega_j} = \sum_{n \in \mathbb{Z}} a_j^n e^{\pm i\beta_{1j}^n(\alpha)y + inx}, \quad (3.9)$$

$$v_\alpha|_{\Omega_j} = \sum_{n \in \mathbb{Z}} b_j^n e^{\pm i\beta_{2j}^n(\alpha)y + inx}, \quad (3.10)$$

where a_j^n and b_j^n are complex scalars. Since β_{sj}^n is real for at most finitely many n , there are only a finite number of *propagating* plane waves in the sum (3.9) and (3.10); the remaining waves are exponentially damped (or unbounded) as $|y| \rightarrow \infty$. We are only interested in the case that (u_α, v_α) is composed of bounded *outgoing* plane waves in Ω_1 and Ω_2 , plus the incident incoming wave u_I in Ω_1 . From (3.5), (3.6), (3.9), and (3.10), we have

$$u_\alpha^n(y) = \begin{cases} u_\alpha^n(l)e^{i\beta_{11}^n(\alpha)(y-l)}, & n \neq 0, \text{ in } \Omega_1, \\ u_\alpha^0(l)e^{i\beta_{11}(y-l)} + u_*e^{-i\beta_{11}y} - u_*e^{i\beta_{11}(y-2l)}, & n = 0, \text{ in } \Omega_1, \\ u_\alpha^n(-l)e^{-i\beta_{12}^n(\alpha)(y+l)}, & \text{in } \Omega_2. \end{cases} \quad (3.11)$$

and

$$v_\alpha^n(y) = \begin{cases} v_\alpha^n(l)e^{i\beta_{21}^n(\alpha)(y-l)}, & \text{in } \Omega_1, \\ v_\alpha^n(-l)e^{-i\beta_{22}^n(\alpha)(y+l)}, & \text{in } \Omega_2. \end{cases} \quad (3.12)$$

Let ν be the unit outward normal vector defined by

$$\nu = \begin{cases} \vec{y} & \text{on } \Gamma_1, \\ -\vec{y} & \text{on } \Gamma_2, \end{cases}$$

where $\vec{y}$ is the unit vector of the y -axis.

One can then calculate the derivative of $u_\alpha^n(y)$ and $v_\alpha^n(y)$ with respect to ν :

$$\left. \frac{\partial u_\alpha^n}{\partial \nu} \right|_{\Gamma_j} = \begin{cases} i\beta_{11}^n u_\alpha^n(l), & n \neq 0, \text{ on } \Gamma_1, \\ i\beta_{11} u_\alpha^0(l) - 2iu_*\beta_{11}e^{-i\beta_{11}l}, & n = 0, \text{ on } \Gamma_1, \\ i\beta_{12}^n u_\alpha^n(-l), & \text{on } \Gamma_2, \end{cases} \quad (3.13)$$

and

$$\left. \frac{\partial v_\alpha^n}{\partial \nu} \right|_{\Gamma_j} = \begin{cases} i\beta_{21}^n(\alpha)v_\alpha^n(l), & \text{on } \Gamma_1, \\ i\beta_{22}^n(\alpha)v_\alpha^n(-l), & \text{on } \Gamma_2. \end{cases} \quad (3.14)$$

Therefore

$$\left. \frac{\partial u_\alpha}{\partial \nu} \right|_{\Gamma_1} = \sum_{n \in \mathbb{Z}} i\beta_{11}^n u_\alpha^n(l)e^{inx} - 2iu_*\beta_{11}e^{-i\beta_{11}l}, \quad (3.15)$$

$$\left. \frac{\partial u_\alpha}{\partial \nu} \right|_{\Gamma_2} = \sum_{n \in \mathbb{Z}} i\beta_{12}^n u_\alpha^n(-l)e^{inx}, \quad (3.16)$$

$$\left. \frac{\partial v_\alpha}{\partial \nu} \right|_{\Gamma_1} = \sum_{n \in \mathbb{Z}} i\beta_{21}^n v_\alpha^n(l)e^{inx}, \quad (3.17)$$

$$\left. \frac{\partial v_\alpha}{\partial \nu} \right|_{\Gamma_2} = \sum_{n \in \mathbb{Z}} i\beta_{22}^n v_\alpha^n(-l)e^{inx}. \quad (3.18)$$

Since the fields u_α and v_α are 2π -periodic in x , without loss of generality, we can move the problem from $\mathbb{R}^2$ to the quotient space (cylinder) $\mathbb{R}^2/(2\pi\mathbb{Z} \times \{0\})$. For the remainder of the paper, we shall identify Ω with the cylinder $\Omega/(2\pi\mathbb{Z} \times \{0\})$, and similarly for the boundaries $\Gamma_j \equiv \Gamma_j/2\pi\mathbb{Z}$. Thus from now on, all functions defined on Ω and Γ_j are implicitly 2π -periodic in the x variable.

For functions $f \in H^{\frac{1}{2}}(\Gamma_j)$ (the Sobolev space of complex valued functions on the circle), define the operator Λ_{sj}^α by

$$(\Lambda_{sj}^\alpha f)(x) = \sum_{n \in \mathbb{Z}} i\beta_{sj}^n(\alpha) f^n e^{inx}, \quad (3.19)$$

for $s, j = 1, 2$, where $f^n = \frac{1}{2\pi} \int_0^{2\pi} f(x) e^{-inx}$, and equality is taken in the sense of distributions.

Lemma 3.1 *For $s, j = 1, 2$, the operator $\Lambda_{sj}^\alpha : H^{\frac{1}{2}}(\Gamma_j) \rightarrow H^{-\frac{1}{2}}(\Gamma_j)$ is continuous.*

Proof. From (3.19), and the definition of $\beta_{sj}^n(\alpha)$, it is clear that Λ_{sj}^α is a standard pseudodifferential operator (in fact, a convolution operator) of order one. The conclusion follows from the Sobolev continuity properties of pseudodifferential operators as stated in Taylor [17]. $\square$

From (3.15-3.18), we see that for $j = 1, 2$,

$$\begin{aligned} \Lambda_{11}^\alpha(u_\alpha|_{\Gamma_1}) &= \frac{\partial u_\alpha}{\partial \nu}|_{\Gamma_1} + 2iu_*\beta_{11}e^{-i\beta_{11}l}, \\ \Lambda_{12}^\alpha(u_\alpha|_{\Gamma_2}) &= \frac{\partial u_\alpha}{\partial \nu}|_{\Gamma_2}, \\ \Lambda_{2j}^\alpha(v_\alpha|_{\Gamma_j}) &= \frac{\partial v_\alpha}{\partial \nu}|_{\Gamma_j}, \end{aligned}$$

that is, Λ_{sj}^α is a Dirichlet–Neumann map. We will use the abbreviated notation $\Lambda_{1j}^\alpha u_\alpha$ and $\Lambda_{2j}^\alpha v_\alpha$ to mean $\Lambda_{1j}^\alpha(u_\alpha|_{\Gamma_j})$ and $\Lambda_{2j}^\alpha(v_\alpha|_{\Gamma_j})$, respectively. We may use the operators Λ_{sj}^α to define “transparent” boundary conditions on the bounded region Ω .

Thus, we have reformulated the scattering problem as follows: find u_α and $v_\alpha \in H^1(\Omega)$ such that

$$(\Delta_\alpha + \omega_1^2 k_1^2)u_\alpha = \chi_{1\alpha} v_\alpha u_\alpha^* \text{ in } \Omega, \quad (3.20)$$

$$(\Delta_\alpha + \omega_2^2 k_2^2)v_\alpha = \chi_{2\alpha} u_\alpha^2 \text{ in } \Omega, \quad (3.21)$$

$$(\Lambda_{11}^\alpha - \frac{\partial}{\partial \nu})u_\alpha = 2iu_*\beta_{11}e^{-i\beta_{11}l} \text{ on } \Gamma_1, \quad (3.22)$$

$$(\Lambda_{12}^\alpha - \frac{\partial}{\partial \nu})u_\alpha = 0 \text{ on } \Gamma_2, \quad (3.23)$$

$$(\Lambda_{21}^\alpha - \frac{\partial}{\partial \nu})v_\alpha = 0 \text{ on } \Gamma_1, \quad (3.24)$$

$$(\Lambda_{22}^\alpha - \frac{\partial}{\partial \nu})v_\alpha = 0 \text{ on } \Gamma_2. \quad (3.25)$$

The formulation (3.20-3.25) admits a variational form. In particular, taking a test function $\phi \in H^1(\Omega)$, we can restate (3.20-3.25) in the equivalent weak form

$$\begin{aligned} & \int_\Omega \nabla u_\alpha \cdot \nabla \bar{\phi} - \int_\Omega (\omega^2 k_1^2 - \alpha_1^2) u_\alpha \bar{\phi} - 2i\alpha_1 \int_\Omega (\partial_x u_\alpha) \bar{\phi} - \int_{\Gamma_1} (\Lambda_{11}^\alpha u_\alpha) \bar{\phi} - \int_{\Gamma_2} (\Lambda_{12}^\alpha u_\alpha) \bar{\phi} \\ &= - \int_{\Gamma_1} 2iu_*\beta_{11}e^{-i\beta_{11}l} \bar{\phi} - \int_{\Gamma_1} \chi_{1\alpha} v_\alpha u_\alpha^* \bar{\phi} \end{aligned} \quad (3.26)$$

and

$$\begin{aligned} & \int_{\Omega} \nabla v_{\alpha} \cdot \nabla \bar{\phi} - \int_{\Omega} (\omega_2^2 k_2^2 - \alpha_2^2) v_{\alpha} \bar{\phi} - 2i\alpha_2 \int_{\Omega} (\partial_x v_{\alpha}) \bar{\phi} - \int_{\Gamma_1} (\Lambda_{21}^{\alpha} v_{\alpha}) \bar{\phi} - \int_{\Gamma_2} (\Lambda_{22}^{\alpha} v_{\alpha}) \bar{\phi} \\ &= - \int_{\Gamma_1} \chi_{2\alpha} u_{\alpha}^2 \bar{\phi}. \end{aligned} \quad (3.27)$$

4 Existence and uniqueness

Recall that χ_1 , and χ_2 supported in Ω_0 are fixed L^{∞} functions in Ω . We assume that k_1 and k_2 are fixed L^{∞} functions in Ω . For $j = 1, 2$, let $A_j : H^1(\Omega) \rightarrow H^{-1}(\Omega)$ be the linear operator defined by $B_j(u_1, u_2) = \langle A_j u_1, u_2 \rangle$, where

$$B_j(u_1, u_2) = \int_{\Omega} \nabla u_1' \cdot \nabla \bar{u}_2' - \int_{\Omega} (\omega_j^2 k_j^2 - \alpha_j^2) u_1 \bar{u}_2 - 2i\alpha_j \int_{\Omega} (\partial_x u_1) \bar{u}_2 - \int_{\Gamma_1} (\Lambda_{j1}^{\alpha} u_1) \bar{u}_2 - \int_{\Gamma_2} (\Lambda_{j2}^{\alpha} u_1) \bar{u}_2.$$

Recall that $\omega_1 = \omega$ and $\omega_2 = 2\omega$ are the frequencies.

Theorem 4.1 *For all but a discrete set of frequencies ω , there exist constants $C_j(\omega, \Omega)$ such that*

$$\|A_j^{-1}\| \leq C_j, \quad j = 1, 2.$$

Proof. Since the argument is the same for both operators A_j , $j = 1, 2$, we shall choose $j = 1$ as the representative. The same arguments can be carried over to the $j = 2$ case. Write $B_1 = B_1^1 + \omega_1^2 B_1^2$ where

$$\begin{aligned} B_1^1(u_1, u_2) &= \int_{\Omega} \nabla u_1 \cdot \nabla \bar{u}_2 + \int_{\Omega} \alpha^2 u_1 \bar{u}_2 - 2i\alpha \int_{\Omega} (\partial_x u_1) \bar{u}_2 - \int_{\Gamma_1} (\Lambda_{11}^{\alpha} u_1) \bar{u}_2 - \int_{\Gamma_2} (\Lambda_{12}^{\alpha} u_1) \bar{u}_2, \\ B_1^2(u_1, u_2) &= - \int_{\Omega} k_1^2 u_1 \bar{u}_2. \end{aligned}$$

Integrating by parts in x , we have by periodicity

$$\int_{\Omega} (\partial_x u) \bar{u} = 0.$$

Thus

$$B_1^1(u, u) = \int_{\Omega} |\nabla u|^2 + \int_{\Omega} \alpha^2 |u|^2 - \int_{\Gamma_1} (\Lambda_{11}^{\alpha} u) \bar{u} - \int_{\Gamma_2} (\Lambda_{12}^{\alpha} u) \bar{u}. \quad (4.1)$$

Next for $j = 1, 2$, let $\Pi_j^+(\alpha) = \{n \in Z : \text{Im } \beta_{1j}^n(\alpha) = 0\}$, $\Pi_j^-(\alpha) = Z - \Pi_j^+(\alpha)$. Each $\Pi_j^+(\alpha)$ is a finite set (corresponding to indices of the propagating outgoing orders), and $0 \in \Pi_1^+(\alpha)$. We find

$$- \int_{\Gamma_j} (\Lambda_{1j}^{\alpha} u) \bar{u} = - \int_{\Gamma_j} \sum_{n \in \Pi_j^+(\alpha)} i\beta_{1j}^n(\alpha) u_n e^{inx} \bar{u} - \int_{\Gamma_j} \sum_{n \in \Pi_j^-(\alpha)} i\beta_{1j}^n(\alpha) u_n e^{inx} \bar{u}. \quad (4.2)$$

Noticing that because of the assumption on the outgoing plane waves all $\beta_{1j}^n(\alpha) \in \Pi_j^-(\alpha)$ satisfy $-i\beta_{1j}^n(\alpha) \geq 0$, we see that the second term on the right-hand side of (4.2) is real and nonnegative. Furthermore, we have

$$\text{Im} \left\{ \int_{\Gamma_j} (\Lambda_{1j}^{\alpha} u) \bar{u} \right\} = 2\pi \sum_{n \in \Pi_j^+(\alpha)} \beta_{1j}^n |u_n|^2.$$

Since $0 \in \Pi_1^+(\alpha)$, $B_1^1(u, u)$ satisfies

$$\operatorname{Re} B_1^1(u, u) \geq \|\nabla u\|_{L^2(\Omega)}^2, \quad -\operatorname{Im} B_1^1(u, u) \geq 2\pi\beta_{11}|u_0|^2,$$

and hence from the definition of β_{11} ,

$$|B_1^1(u, u)| \geq \omega c_1 \|u\|_{H^1(\Omega)}^2. \quad (4.3)$$

Thus B_1^1 is a bounded coercive sesquilinear form over $H^1(\Omega)$. The Lax-Milgram lemma then gives the existence of a bounded invertible map $A_{1,1} : H^1(\Omega_0) \rightarrow H^{-1}(\Omega_0)$ such that $\langle A_{1,1}u, v \rangle_{H^1} = B_1^1(u, v)$. From (4.3), $A_{1,1}^{-1}$ is bounded and $\|A_{1,1}^{-1}\| \leq \frac{1}{\omega_1 c_1}$. To emphasize that $A_{1,1}$ depends on the frequency ω_1 , we write $A_{1,1}(\omega_1)$. Notice that the operator $A_{1,2} : H^1(\Omega) \rightarrow H^{-1}(\Omega)$ defined by $\langle A_{1,2}u_1, u_2 \rangle = B_1^2(u_1, u_2)$ is compact.

Holding ω_0 fixed, consider the operator $A_1(\omega_0, \omega) = A_{1,1}(\omega_0) + \omega^2 A_{1,2}$. We see that $A_1(\omega_0, \omega)^{-1}$ exists by Fredholm theory for all $\omega \notin \mathcal{E}(\omega_0)$, where $\mathcal{E}(\omega_0)$ is some discrete set. It is clear that

$$\|A_{1,1}(\omega) - A_{1,1}(\omega_0)\| \rightarrow 0, \quad \text{as } \omega \rightarrow \omega_0.$$

Thus, since $\|A_1(\omega, \omega) - A_1(\omega_0, \omega)\| = \|A_{1,1}(\omega) - A_{1,1}(\omega_0)\|$ is small for $|\omega - \omega_0|$ sufficiently small, it follows from the stability of bounded invertibility (see e. g. Kato [11], Theorem IV-1.16) that $A_1(\omega, \omega)^{-1}$ exists and is bounded for $|\omega - \omega_0|$ sufficiently small, $\omega \notin \mathcal{E}(\omega_0)$. Since $\omega_0 > 0$ can be taken to be any real number, we have shown that $A_1(\omega, \omega)^{-1}$ exists for all but a discrete set of points. $\square$

Therefore, we only need to solve the following problem: find u_α and $v_\alpha \in H^1(\Omega)$ such that for $f \in H^{-1}(\Omega)$, and $\chi_{1\alpha}, \chi_{2\alpha} \in L^\infty(\Omega)$, the system

$$A_1 u_\alpha = \chi_{1\alpha} v_\alpha u_\alpha^* + f, \quad (4.4)$$

$$A_2 v_\alpha = \chi_{2\alpha} u_\alpha^2, \quad (4.5)$$

holds.

Consider the following fixed-point iteration. Set $u_{\alpha,0} = 0$ and for $k = 0, 1, \dots$, define

$$\begin{aligned} v_{\alpha,k} &= A_2^{-1}(\chi_{2\alpha} u_{\alpha,k}^2), \\ u_{\alpha,k+1} &= A_1^{-1}(\chi_{1\alpha} u_{\alpha,k}^* v_{\alpha,k} + f). \end{aligned}$$

Further

$$u_{\alpha,k+1} = F(u_{\alpha,k})$$

where

$$F(u) = A_1^{-1}\{\chi_{1\alpha} u^* A_2^{-1}(\chi_{2\alpha} u^2) + f\}.$$

It is easy to see that F maps $H^1(\Omega)$ to $H^1(\Omega)$.

Theorem 4.2 *Given $f \in H^{-1}(\Omega)$ there exists a constant $\epsilon > 0$ depending only on $\|f\|_{H^{-1}}$ and Ω , such that if $\|\chi_{1\alpha}\|_{L^\infty} \|\chi_{2\alpha}\|_{L^\infty} \leq \epsilon$ then the model problem, (4.4), (4.5), admits a unique solution $u_\alpha, v_\alpha \in H^1(\Omega)$.*

Proof. For the sake of simplicity, we shall drop all the subscripts α in the proof.

The proof of Theorem 4.2 follows from the contraction mapping principle, see for example [10]. All we need to do is verify the hypotheses in the contraction principle. Therefore we may separate the proof into two parts:

First, we prove that if the product of $\|\chi_1\|_{L^\infty}$ and $\|\chi_2\|_{L^\infty}$ sufficiently small, then there exists $R > 0$ such that $\|u\|_{H^1} \leq R$ implies $\|F(u)\|_{H^1} \leq R$.

Let $g = A_1^{-1}f$, then $g \in H^1$. Write

$$F(u) - g = A_1^{-1}\{\chi_1(u - g)^* A_2^{-1}(\chi_2 u^2)\} + A_1^{-1}\{\chi_1 g^* A_2^{-1}(\chi_2 u^2)\}.$$

Then using Schauder's lemma on the algebraic properties of Sobolev spaces, we can estimate

$$\begin{aligned} \|F(u) - g\|_{H^1} &\leq C\|\chi_1(u - g)^* A_2^{-1}(\chi_2 u^2)\|_{L^2} + C\|\chi_1 g^* A_2^{-1}(\chi_2 u^2)\|_{L^2} \\ &\leq C\|\chi_1\|_{L^\infty}(\|(u - g)^* A_2^{-1}(\chi_2 u^2)\|_{L^2} + \|g\|_{H^1}\|A_2^{-1}(\chi_2 u^2)\|_{H^1}) \\ &\leq \|\chi_1\|_{L^\infty}\|\chi_2\|_{L^\infty}(C_1\|u\|_{H^1}^2\|u - g\|_{H^1} + C_2\|u\|_{H^1}^2). \end{aligned}$$

Choosing $R = 2\|g\|_{H^1}$, since $\|\chi_1\|_{L^\infty}\|\chi_2\|_{L^\infty}$ is sufficiently small we then have

$$\|F(u)\|_{H^1} \leq \|F(u) - g\|_{H^1} + \|g\|_{H^1} \leq R.$$

For the second part, we claim that given a radius R , we can take $\|\chi_1\|_{L^\infty}\|\chi_2\|_{L^\infty}$ small enough so that F is a contraction on

$$B_R = \{u \in H^1 : \|u\|_{H^1} \leq R\}$$

i.e.,

$$\|F(u_1) - F(u_2)\|_{H^1} \leq C_0\|u_1 - u_2\|_{H^1}$$

for all $u_1, u_2 \in B_R$ where $C_0 < 1$. This is obvious from the following estimates:

$$\begin{aligned} \|F(u_1) - F(u_2)\|_{H^1} &= \|A_1^{-1}\{\chi_1 u_1^* A_2^{-1}(\chi_2 u_1^2) - \chi_1 u_2^* A_2^{-1}(\chi_2 u_2^2)\}\|_{H^1} \\ &\leq C\|\chi_1\{u_1^* A_2^{-1}(\chi_2 u_1^2) - u_2^* A_2^{-1}(\chi_2 u_2^2)\}\|_{L^2} \\ &= C\|\chi_1\{(u_1 - u_2)^* A_2^{-1}(\chi_2 u_1^2) - u_2^* A_2^{-1}(\chi_2(u_2^2 - u_1^2))\}\|_{L^2} \\ &\leq C\|\chi_1\|_{L^\infty}\{\|u_1 - u_2\|_{H^1} \cdot \|A_2^{-1}(\chi_2 u_1^2)\|_{H^1} \\ &\quad + \|u_2\|_{H^1} \cdot \|A_2^{-1}(\chi_2(u_2^2 - u_1^2))\|_{H^1}\} \\ &\leq C\|\chi_1\|_{L^\infty}\|\chi_2\|_{L^\infty}(\|u_1\|_{H^1}^2 + \|u_2\|_{H^1}^2)\|u_1 - u_2\|_{H^1}. \end{aligned}$$

Thus one may choose the constant

$$C_0 = 2CR^2\|\chi_1\|_{L^\infty}\|\chi_2\|_{L^\infty},$$

where the constant C is identical to the one in the previous estimates. It follows that for $\|\chi_1\|_{L^\infty}\|\chi_2\|_{L^\infty}$ sufficiently small, we have $C_0 < 1$. $\square$

Figure 2: The grating profile.

5 Numerical experiments

The model problem is solved by a combination of a finite element method and fixed-point iterations. The finite element scheme follows directly from the variational form of the problem and was implemented with piecewise bilinear basis functions over a uniform rectangular grid. An Orthomin algorithm was used to solve the resulting linear equations. The fixed-point procedure was then implemented as described in the last section. We generally found that the fixed-point procedure converged rapidly, on the order of ten iterations for most examples.

As an illustration, we compare the results obtained using our scheme with those obtained from the UPA. For the simple grating profile shown in Figure 2, the electric field intensities at the pump frequency and at the doubled frequency are shown in Figure 3 and Figure 5, respectively.

The differences of the field intensities obtained using our method and those obtained by the UPA are given in Figure 4 and Figure 6. For the experiment shown here, there is a 13-15% difference (in the l_2 norm) between the fields given by the two models. We point out that the UPA is in fact just the first step of our fixed-point iteration. Other experiments we have done indicate that the UPA becomes less accurate when either the nonlinear susceptibilities, the depth of the material, or the intensity of the pump beam is increased. On the other hand, as one might hope, UPA is quite accurate in cases where little energy is transferred to the second-harmonic field.

Figure 7 exhibits how the conversion efficiency of the SH field varies as one varies the incidence angle. For this example, there is a critical angle (0.225) corresponding to a resonant point (a so-called “Rayleigh point” in optics). The figure shows that near this critical point, high nonlinear conversion efficiencies may be expected. The energies of the pump fields and doubled frequency wave fields for an incident angle close to the resonant angle are illustrated

Figure 3: Our model: energy of the pump frequency wave.

Figure 4: The energy difference between our model and the UPA at the pump frequency.

Figure 5: Our model: energy of the doubled frequency wave.

Figure 6: The energy difference between our model and the UPA at the doubled frequency.

Figure 7: The conversion efficiency of the SH fields versus incident angles.

in Figure 8 and Figure 9. For comparison, the energies of the pump fields and doubled frequency wave fields for an incident angle that is away from the resonant region are shown in Figure 9 and Figure 10. Note the much higher intensity of the pump field inside the nonlinear material in the near-resonant case. The higher pump intensity presumably leads to greater energy transfer between the fields.

We intend to further investigate the nonlinear conversion efficiency obtained for various grating parameters and shapes. The objective is to maximize the conversion efficiency subject to the grating parameters, nonlinear materials, intensity of the incident laser beam, incident angles, and frequencies. We anticipate that the best conversion efficiency may be achieved near the resonant regions. A detailed study will be reported in a forthcoming paper.

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Figure 8: The energy of the pump frequency wave when the incident angle is near the resonant point.

Figure 9: The energy of the doubled frequency wave when the incident angle is near the resonant point.

Figure 10: The energy of the pump frequency wave when the incident angle is away from the resonant point.

Figure 11: The energy of the doubled frequency wave when the incident angle is away from the resonant point.

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