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A VARIATIONAL METHOD FOR ELECTROMAGNETIC DIFFRACTION IN BIPERIODIC STRUCTURES (*)

by D. C. DOBSON [1]

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Abstract — *Consider a time-harmonic electromagnetic plane wave incident on a biperiodic structure in* $\mathbb{R}^3$ *The periodic structure separates two regions with constant dielectric coefficients The dielectric coefficient inside the structure is assumed to be a general bounded measurable function The magnetic permeability is constant throughout* $\mathbb{R}^3$.

We describe a simple variational method for finding weak « quasiperiodic » solutions to Maxwell's equations in such a structure Our formulation is simple and computationally attractive because it only involves three field components The problem is formulated by constructing a variational form over a bounded region, with « transparent » boundary conditions The boundary conditions come from the Dirichlet-Neumann maps for the problem, which can be calculated explicitly We show that the variational problem admits unique solutions for all sufficiently small frequencies, and more generally for all but a discrete set of frequencies We also show that the weak solutions satisfy a conservation of energy condition Finally, we briefly discuss an implementation of a three-dimensional numerical finite element scheme which solves the discretized variational problem, and present the results of a simple numerical experiment

1. INTRODUCTION.

We consider a time-harmonic electromagnetic plane wave incident on a general biperiodic structure in $\mathbb{R}^3$. By biperiodic (or doubly periodic), we mean that the structure is periodic in each of two orthogonal directions. Such structures are sometimes called *crossed diffraction gratings* in the optics and physics literature. The periodic structure separates two regions with constant dielectric coefficients. Inside the periodic structure, the dielectric coefficient is allowed to be a general bounded measurable function. The magnetic permeability is assumed to be constant throughout the whole space.

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This problem is motivated by applications in micro-optics, where micron-scale optical diffraction structures are constructed with tools from the semiconductor industry. See the book [12] for a description of this and other mathematical problems which arise in these applications. For an introduction to the problem of electromagnetic diffraction through periodic structures (diffraction gratings), along with some numerical methods, see the interesting collection of articles edited by R. Petit [16]. Related problems have been recently studied by Nédélec and Starling [15], Bellout and Friedman [3], and Ducomet and Quang [11]. Numerical methods for the nonperiodic time-harmonic diffraction problem have also been studied ; see Bendali [2] and the references therein.

In [10], the existence and uniqueness of solutions to Maxwell's equations in biperiodic structures, consisting of two homogeneous materials separated by a piecewise C^2 interface, was established by means of an integral equation approach. The work generalized the earlier work of Chen and Friedman [8] and the approach was later implemented numerically [9]. Bruno and Reitich [5], [6], [7] have developed an elegant and extremely efficient method for solving diffraction problems in periodic structures, based on continuing the fields as analytic functions of the height of the interface.

The method presented here has the advantage that it is applicable to extremely general diffraction structures. In particular, the structure is allowed to be defined by a general bounded measurable dielectric coefficient. Thus there are no restrictions on the height, topology, or number of materials present in the interface.

A similar variational approach was recently taken by Abboud and Nédélec [1] to study Maxwell's equations in a bounded (nonperiodic) inhomogeneous medium. Our approach differs from [1] in that our variational formulation involves only the magnetic field vector. The approach of [1] allows for non-constant magnetic permeability, and is thus more general than our approach ; however for the optical applications which motivate the present work, the magnetic permeability is constant. For this case, our approach is somewhat simpler. Abboud and Nédélec mention in [1] that their work will be generalized to periodic structures in a forthcoming paper.

The outline of this paper is as follows. In Section 2, we describe the periodic Maxwell equations. We then derive in Section 3 a variational form involving only the magnetic field vector in a bounded region. To complete the variational formulation of the problem requires a description of the boundary values of the magnetic field. This is obtained in Section 4 by explicitly calculating the Dirichlet-to-Neumann map for the problem, allowing us to formulate « transparent » boundary conditions. In Section 5 we then show that the variational problem has a unique solution for all sufficiently small frequencies, and more generally for all but a discrete set of frequencies. In Section 6 we show that the weak solutions satisfy a conservation of energy condition. Finally, we briefly describe a numerical finite element method based on a discretization of the variational problem and present some illustrative numerical results.

2. THE PERIODIC MAXWELL EQUATIONS

Let L_1, L_2 be positive constants. Define the lattice

$$\Lambda = L_1 Z \times L_2 Z \times \{0\} \subset \mathbb{R}^3 , \quad Z = \{0, \pm 1, \pm 2, \ldots\} .$$

Let b be another positive constant. Define the following domains :

$$\begin{aligned} D_0 &= \{x \in \mathbb{R}^3 : -b < x_3 < b\} , \\ D_1 &= \{x \in \mathbb{R}^3 : x_3 > b\} , \\ D_2 &= \{x \in \mathbb{R}^3 : x_3 < -b\} , \end{aligned}$$

where points $x \in \mathbb{R}^3$ are denoted $x = (x_1, x_2, x_3)$. See Figure 1.

Let E, H denote complex vector fields on $\mathbb{R}^3$. The fields E, H will be called the *electric* and *magnetic* fields, respectively. We wish to solve the time-harmonic (time dependence $e^{-i\omega t}$) Maxwell equations

$$\nabla \times E - i\omega\mu H = 0 , \tag{1}$$
$$\nabla \times H + i\omega\varepsilon E = 0 , \tag{2}$$

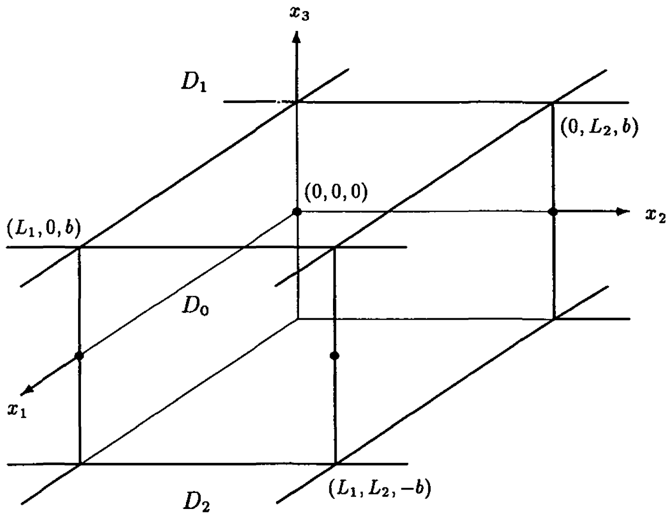

Figure 1. — Location of the three domains D_0, D_1 and D_2 relative to one periodic cell. The first few lattice points $n \in \Lambda$ are indicated by dots.

in $\mathbb{R}^3$ when the magnetic permeability μ is a real constant throughout $\mathbb{R}^3$ and the dielectric coefficient ε is periodic with respect to Λ

$$\varepsilon(x+n) = \varepsilon(x), \quad \text{for all} \quad n \in \Lambda, \quad x \in \mathbb{R}^3,$$

and satisfies

$$\varepsilon(x) = \begin{cases} \varepsilon_1 & \text{in a neighborhood containing } D_1, \\ \varepsilon_2 & \text{in a neighborhood containing } D_2, \end{cases}$$

where ε_1 and ε_2 are constants with Re (ε_1), Re $(\varepsilon_2) > 0$, Im $(\varepsilon_1) = 0$, Im $(\varepsilon_2) \geqslant 0$ Inside D_0, ε is assumed to be a bounded measurable function with Re $(\varepsilon) \geqslant a > 0$, Im $(\varepsilon) \geqslant 0$ The case Im $(\varepsilon) > 0$ accounts for materials which absorb energy , see e g [4]

We will assume that a plane wave

$$(E^*, H^*) = (s, p)\, e^{iq \cdot x}$$

is incident on D_0 from D_1 Here $p \in \mathbb{R}^3$ is the magnetic polarization vector and $q = (q_1, q_2, q_3) \in \mathbb{R}^3$ is the incidence vector The electric polarization s is given by $s = \dfrac{1}{\omega\,\varepsilon_1}(p \times q)$ The vectors p and q must satisfy the dispersion relation

$$q \cdot q = \omega^2 \varepsilon_1 \mu,$$

and the orthogonality condition

$$p \cdot q = 0$$

in order for (E^*, H^*) to satisfy (1), (2) in D_1 We also assume that (E^*, H^*) is an *incoming* wave, so $q_3 < 0$

Let $\alpha = (q_1, q_2, 0)$, and define the vector fields E_α, H_α by

$$E_\alpha(x) = e^{-i\alpha \cdot x} E(x), \quad H_\alpha(x) = e^{-i\alpha \cdot x} H(x)$$

We are interested in *quasiperiodic* solutions to (1), (2), that is, solutions such that the fields E_α, H_α are periodic with respect to Λ The Maxwell equations (1), (2) in $\mathbb{R}^3$ then become

$$\nabla_\alpha \times E_\alpha - i\,\omega\,\mu H_\alpha = 0, \tag{3}$$

$$\nabla_\alpha \times H_\alpha + i\,\omega\,\varepsilon E_\alpha = 0, \tag{4}$$

where $\nabla_\alpha = \nabla + i\,\alpha$

Since all the functions we deal with henceforth are Λ-periodic, to avoid continually referring to the periodic boundary conditions we instead view the problem as being posed over the quotient space $\mathbb{R}^3/\Lambda$. We thus define the new periodic domains

$$\begin{aligned}\Omega_0 &= D_0/\Lambda ,\\ \Omega_1 &= D_1/\Lambda ,\\ \Omega_2 &= D_2/\Lambda ,\end{aligned}$$

along with the boundaries

$$\Gamma_1 = \partial\Omega_1 , \quad \Gamma_2 = \partial\Omega_2 .$$

Note that $\bar{\Omega}_0$ is now a compact set.

For the remainder of the paper we will be studying the system (3), (4) over the quotient space $\mathbb{R}^3/\Lambda$. We shall henceforth drop the subscripts α from the fields E_α and H_α. To get solutions to the original Maxwell equations (1), (2), our solutions E and H to (3), (4) must be multiplied by $e^{i\alpha \cdot x}$.

3. VARIATIONAL FORM

Taking the ∇_α curl of $1/(\varepsilon\mu)$ times equation (4), it follows from (3), (4) that

$$\nabla_\alpha \times \left(\frac{1}{\varepsilon\mu} \nabla_\alpha \times H \right) - \omega^2 H = 0 , \tag{5}$$

$$\nabla_\alpha \times H + i\omega\varepsilon E = 0 . \tag{6}$$

Our goal is to solve (5) for H ; if a solution exists, the field E is then formally determined by (6). It is easy to check that if H and E are differentiable then (5), (6) is *equivalent* to (3), (4). More generally, (5), (6) is equivalent to (3), (4) in a weak sense.

Remark : We have chosen to study the system (5), (6) rather than the « dual » system

$$\begin{aligned}\nabla_\alpha \times (\nabla_\alpha \times E) - \omega^2 \varepsilon\mu E &= 0 ,\\ i\omega\mu H - \nabla_\alpha \times E &= 0 ,\end{aligned}$$

because, as can be shown from the weak form of (3), (4), the normal components of the E field across surfaces of discontinuity in ε are discontinuous (see e.g. [4]). By contrast, the H field is continuous across jumps in ε. Thus, given that we wish to model discontinuous ε, the H field is somewhat more amenable to approximation in simple finite element spaces. Of course, the situation would be reversed if we were considering the problem with constant ε and variable μ.

It is easy to check that the operator ∇_α satisfies the usual curl and divergence identities $\nabla_\alpha \times (\nabla_\alpha u) = \nabla_\alpha \cdot (\nabla_\alpha \times F) = 0$. Taking the ∇_α divergence of (5) then reveals that $\nabla_\alpha \cdot H = 0$. Therefore if H satisfies (5), it must also satisfy

$$\nabla_\alpha \times (\gamma \nabla_\alpha \times H) - \nabla_\alpha (\gamma \nabla_\alpha \cdot H) - \omega^2 H = 0 , \tag{7}$$

where $\gamma = 1/(\varepsilon \mu)$. Conversely, if H satisfies (7) along with the constraint $\nabla_\alpha \cdot H = 0$, then H satisfies (5).

In Section 5, we will show that (7), along with an appropriate « outgoing wave » condition, admits a unique solution H for all but a discrete set of frequencies ω. Assuming that (3), (4) also admits a solution $(\tilde{E}, \tilde{H})$ satisfying the outgoing wave condition, the two solutions H, $\tilde{H}$ must coincide since $\tilde{H}$ also solves (7). Thus under the a priori assumption of existence of solutions to the original periodic Maxwell equations (3), (4), it suffices to solve (7) ; the E field is then determined by (6). We note that the existence of solutions to the system (3), (4) is proved in [10] for structures consisting of two homogeneous materials separated by a piecewise C^2 boundary.

The reason for subtracting the term $\nabla_\alpha(\gamma \nabla_\alpha \cdot H)$ from equation (5) is to gain a coercive part in the sesquilinear form associated with the weak formulation ; this will be made clear in Section 5. We now pose the weak formulation of (7). Let F be a smooth vector field on Ω_0. From (7) we must have that

$$\int_{\Omega_0} \{\nabla_\alpha \times (\gamma \nabla_\alpha \times H)\} \cdot \bar{F} - \int_{\Omega_0} \{\nabla_\alpha (\gamma \nabla_\alpha \cdot H)\} \cdot \bar{F} - \omega^2 \int_{\Omega_0} H \cdot \bar{F} = 0 . \tag{8}$$

In equation (8), and for the remainder of the paper, bars ($\bar{F}$, etc.) denote complex-conjugation. Applying Green's formulas and some vector identities reveals that (8) is equivalent to

$$\int_{\Omega_0} (\gamma \nabla_\alpha \times H) \cdot (\overline{\nabla_\alpha \times F}) + \int_{\Omega_0} (\gamma \nabla_\alpha \cdot H)(\overline{\nabla_\alpha \cdot F}) - \omega^2 \int_{\Omega_0} H \cdot \bar{F} + \int_{\partial \Omega_0} \eta \times \{\gamma (\nabla_\alpha \times H)\} \cdot \bar{F} - \int_{\partial \Omega_0} (\gamma \nabla_\alpha \cdot H)(\bar{F} \cdot \eta) = 0 , \tag{9}$$

where η is the unit outward normal on $\partial \Omega_0 = \Gamma_1 \cup \Gamma_2$.

We wish to find a field $H \in W^1(\Omega_0)^3$ on Ω_0 such that (9) holds for all

$F \in W^1(\Omega_0)^3$. (Note : throughout the paper, given a domain D, we denote the usual L^2 Sobolev spaces $H^s(D)$ of complex-valued distributions on D by $W^s(D)$, thus avoiding the notational conflict with the field H.) To couple the variational problem (9) to the whole space $\mathbb{R}^3/\Lambda$, we must find a suitable description of the derivatives of H on $\delta \Omega_0$. That is the topic of the next section.

4. TRANSPARENT BOUNDARY CONDITIONS

For each index $n = (n_1, n_2, 0) \in \Lambda$, let

$$\alpha_n = \left(\frac{2 \pi n_1}{L_1^2}, \frac{2 \pi n_2}{L_2^2}, 0 \right).$$

Since H is Λ-periodic, we expand in a Fourier series

$$H(x) = \sum_{n \in \Lambda} H^n(x_3)\, e^{-i\alpha_n . x}, \tag{10}$$

where

$$H^n(x_3) = \frac{1}{|Q|} \int_Q H(x_1, x_2, x_3)\, e^{i\alpha_n . x}\, dx_1\, dx_2 ,$$

and $Q = [0, L_1] \times [0, L_2]$. For $n \in \Lambda$, and $j = 1, 2$, define the coefficients β_j^n by

$$\beta_j^n = e^{i\theta/2} \left| \omega^2 \varepsilon_j \mu - |\alpha_n - \alpha|^2 \right|^{1/2},$$

where

$$\theta = \arg\left(\omega^2 \varepsilon_j \mu - |\alpha_n - \alpha|^2\right), \quad 0 \leq \theta < 2\pi .$$

Notice that β_j^n is real for at most finitely many n ; for the remaining $n \in \Lambda$, β_j^n has positive imaginary part. We shall assume that $\beta_j^n \neq 0$ for all $n \in \Lambda$, $j = 1, 2$. This assumption excludes at most a discrete set of parameters ω, μ from consideration.

Since ε is constant in Ω_j, $j = 1, 2$, inside these regions equation (7) reduces to the periodic vector Helmholtz equation

$$(\Delta_\alpha + \omega^2 \varepsilon_j \mu) H = 0 \quad \text{in} \quad \Omega_j ,$$

where $\Delta_\alpha = \Delta + 2i\alpha . \nabla - |\alpha|^2$. It then follows from knowledge of the fundamental solution to the periodic Helmholtz equation (see [10]) that inside Ω_1 and Ω_2, all fields H satisfying (7) can be represented as a sum of plane waves

$$H\big|_{\Omega_j} = \sum_{n \in \Lambda} A_j^n \, e^{-i\beta_j^n x_3 - i\alpha_n \cdot x}, \quad j = 1, 2 \tag{11}$$

where the $A_j^n \in \mathbb{C}^3$ are constants. In fact, the dielectric coefficient ε is constant in neighborhoods of the boundaries Γ_j, so the representation (11) is valid in a neighborhood of Ω_j.

Notice that only the finite number of plane waves in the sum (11) which correspond to real coefficients β_j^n *propagate* outward. The remaining terms decay (or grow) exponentially as $|x_3| \to \infty$. The exponentially decaying terms are often called *evanescent*. We will insist that H is composed of bounded, outgoing plane waves in Ω_1 and Ω_2, plus the incoming incident wave $H_\alpha^* = p\, e^{-i\beta_1 x_3}$ in Ω_1. Thus we *implicitly* enforce an outgoing wave condition. Recalling that $\Gamma_1 = \{x_3 = b\}$, $\Gamma_2 = \{x_3 = -b\}$, we obtain from matching terms in (10) and (11),

$$H^n(x_3) = \begin{cases} H^n(b)\, e^{i\beta_1^n(x_3 - b)}, & n \neq 0, \quad \text{in} \quad \Omega_1, \\ H^0(b)\, e^{i\beta_1(x_3 - b)} + p\, e^{-i\beta_1 x_3} - p\, e^{i\beta_1(x_3 - 2b)}, & n = 0, \quad \text{in} \quad \Omega_1, \\ H^n(-b)\, e^{-i\beta_2^n(x_3 + b)}, & \quad \text{in} \quad \Omega_2. \end{cases} \tag{12}$$

Thus, the fields H in the domains Ω_j have the representation

$$H\big|_{\Omega_1} = \sum_{n \in \Lambda} H^n(b)\, e^{i\beta_1^n(x_3 - b) - i\alpha_n \cdot x} + p(e^{-i\beta_1 x_3} - e^{i\beta_1(x_3 - 2b)}) \tag{13}$$

$$H\big|_{\Omega_2} = \sum_{n \in \Lambda} H^n(-b)\, e^{-i\beta_2^n(x_3 + b) - i\alpha_n \cdot x}. \tag{14}$$

From (12) we calculate the normal derivatives on the boundaries Γ_j,

$$\left.\frac{\partial H^n}{\partial e_3}\right|_{\Gamma_j} = \begin{cases} i\beta_1^n H^n(b), & n \neq 0, \quad j = 1, \\ i\beta_1 H^0(b) - 2\, i\beta_1 p\, e^{-i\beta_1 b}, & n = 0, \quad j = 1, \\ -\, i\beta_2^n H^n(-b), & \quad j = 2, \end{cases} \tag{15}$$

where e_3 is the unit vector in the direction of the x_3-axis. It then follows formally from (10) and (15) that

$$\left.\frac{\partial H}{\partial e_3}\right|_{\Gamma_1} = \sum_{n \in \Lambda} i\beta_1^n H^n(b)\, e^{-i\alpha_n \cdot x} - 2\, i\beta_1 p\, e^{-i\beta_1 b}, \tag{16}$$

$$\left.\frac{\partial H}{\partial e_3}\right|_{\Gamma_2} = -\sum_{n \in \Lambda} i\beta_2^n H^n(-b)\, e^{-i\alpha_n \cdot x}. \tag{17}$$

For functions $f \in W^{1/2}(\Gamma_j)$, define the operators T_j^α, $j = 1, 2$ by

$$T_1^\alpha f = \left(\sum_{n \in \Lambda} i\beta_1^n f_n e^{-i\alpha_n . x}\right) e_3 , \tag{18}$$

$$T_2^\alpha f = -\left(\sum_{n \in \Lambda} i\beta_2^n f_n e^{-i\alpha_n . x}\right) e_3 , \tag{19}$$

where the Fourier coefficients f_n are given by

$$f_n = \frac{1}{|Q|} \int_Q f(x)\, e^{i\alpha_n . x}\, dx_1\, dx_2 ,$$

and equality in (18), (19) is interpreted in the sense of distributions.

LEMMA 4.1 : *The operators* $T_j^\alpha : W^{1/2}(\Gamma_j) \to W^{-1/2}(\Gamma_j)$ *are continuous.*

Proof: T_j^α is an order one pseudodifferential operator (in fact, a convolution operator). See e.g. [17]. □

We see from (16), (17) that the operators T_j^α are « Dirichlet to Neumann maps » for the field H.

Now define the vector-valued operators $R_j^\alpha : W^{1/2}(\Gamma_j) \to W^{-1/2}(\Gamma_j)^3$ by

$$R_1^\alpha f = (\partial_1^\alpha f)\, e_1 + (\partial_2^\alpha f)\, e_2 + (T_1^\alpha f)\, e_3,$$

$$R_2^\alpha f = (\partial_1^\alpha f)\, e_1 + (\partial_2^\alpha f)\, e_2 + (T_2^\alpha f)\, e_3,$$

where $\partial_j^\alpha = \partial_j + i\alpha_j$, and e_j denotes the unit vector in the x_j-direction. If $H \in W^1(\Omega_0)^3$, we see that

$$(\nabla_\alpha \times H)\big|_{\Gamma_1} = R_1^\alpha \times (H\big|_{\Gamma_1}) - 2\, i\beta_1(-p_2, p_1, 0)\, e^{-i\beta_1 b} ,$$

$$(\nabla_\alpha . H)\big|_{\Gamma_1} = R_1^\alpha . (H\big|_{\Gamma_1}) - 2\, i\beta_1 p_3\, e^{-i\beta_1 b} ,$$

$$(\nabla_\alpha \times H)\big|_{\Gamma_2} = R_2^\alpha \times (H\big|_{\Gamma_2}) ,$$

$$(\nabla_\alpha . H)\big|_{\Gamma_2} = R_2^\alpha . (H\big|_{\Gamma_2}) ,$$

where again, equality is in the sense of distributions. The operators R_j^α thus map the components of the field H restricted to Γ_j to their derivatives on Γ_j.

Substituting the expressions above into the variational form (9) then yields the equation

$$\int_{\Omega_0} (\gamma \nabla_\alpha \times H) . (\overline{\nabla_\alpha \times F}) + \int_{\Omega_0} (\gamma \nabla_\alpha . H) (\overline{\nabla_\alpha . F}) - \omega^2 \int_{\Omega_0} H . \bar{F}$$

$$+ \int_{\Gamma_1} e_3 \times \{\gamma (R_1^\alpha \times H)\} . \bar{F} - \int_{\Gamma_2} e_3 \times \{\gamma (R_2^\alpha \times H)\} . \bar{F}$$

$$- \int_{\Gamma_1} (\gamma R_1^\alpha . H) (\bar{F} . e_3) + \int_{\Gamma_2} (\gamma R_2^\alpha . H) (\bar{F} . e_3)$$

$$= - \int_{\Gamma_1} 2 i \beta_1 e^{-i\beta_1 b} \gamma (p . \bar{F}) , \tag{20}$$

where the integrals over Γ_j represent the dual pairing of $W^{-1/2}(\Gamma_j)$ with $W^{1/2}(\Gamma_j)$ and it is understood that the operators R_j^α act on the traces of H.

From (20), we define the sesquilinear form $B(H, F)$ on $W^1(\Omega_0)^3 \times W^1(\Omega_0)^3$ by

$$B(H, F) = \int_{\Omega_0} (\gamma \nabla_\alpha \times H) . (\overline{\nabla_\alpha \times F}) +$$

$$+ \int_{\Omega_0} (\gamma \nabla_\alpha . H) (\overline{\nabla_\alpha . F}) - \omega^2 \int_{\Omega_0} H . \bar{F}$$

$$+ \int_{\Gamma_1} e_3 \times \{\gamma (R_1^\alpha \times H)\} . \bar{F} - \int_{\Gamma_2} e_3 \times \{\gamma (R_2^\alpha \times H)\} . \bar{F}$$

$$- \int_{\Gamma_1} (\gamma R_1^\alpha . H) (\bar{F} . e_3) + \int_{\Gamma_2} (\gamma R_2^\alpha . H) (\bar{F} . e_3) ,$$

along with the functional $G \in [W^1(\Omega_0)^3]'$, defined by

$$G(F) = - \int_{\Gamma_1} 2 i \beta_1 e^{-i\beta_1 b} \gamma (p . \bar{F}) .$$

We then pose the variational problem : find $H \in W^1(\Omega_0)^3$ such that

$$B(H, F) = G(F) , \quad \text{for all} \quad F \in W^1(\Omega_0)^3 . \tag{21}$$

5. EXISTENCE AND UNIQUENESS OF WEAK SOLUTIONS

In this section we establish the existence and uniqueness of solutions to the variational problem (21). We show in Theorem 5.1 that a unique solution exists for all frequencies $0 < \omega < \omega_0$ where ω_0 is some positive number depending on the parameters L_1, L_2, ε, μ, and q. Then in Theorem 5.2 we show that a unique solution exists for all positive parameters ω except those in some discrete set.

THEOREM 5.1 : *There exists a frequency* $\omega_0 > 0$ *such that the variational problem* (21) *admits a unique solution* $H \in W^1(\Omega_0)^3$ *for all frequencies* $0 < \omega \leqslant \omega_0$.

Proof : For the remainder of the proof, c will denote a « generic » real constant whose value may change from line to line.

Let us write the variational form B in (21) as $B(H, F) = B_1(H, F) - \omega^2 B_2(H, F)$ where

$$B_1(H, F) = \int_{\Omega_0} (\gamma \nabla_\alpha \times H) \cdot (\overline{\nabla_\alpha \times F}) + \int_{\Omega_0} (\gamma \nabla_\alpha \cdot H)(\overline{\nabla_\alpha \cdot F})$$
$$+ \int_{\Gamma_1} e_3 \times \{\gamma (R_1^\alpha \times H)\} \cdot \bar{F} - \int_{\Gamma_2} e_3 \times \{\gamma (R_2^\alpha \times H)\} \cdot \bar{F}$$
$$- \int_{\Gamma_1} (\gamma R_1^\alpha \cdot H)(\bar{F} \cdot e_3) + \int_{\Gamma_2} (\gamma R_2^\alpha \cdot H)(\bar{F} \cdot e_3),$$

and

$$B_2(H, F) = \int_{\Omega_0} H \cdot \bar{F} .$$

Applying some vector identities and integrating by parts in the x_1 and x_2 directions reveals that

$$\int_{\Omega_0} \gamma \, |\nabla_\alpha \times H|^2 + \int_{\Omega_0} \gamma \, |\nabla_\alpha \cdot H|^2$$
$$= \int_{\Omega_0} \gamma \sum_{j,k} |\partial_j^\alpha H_k|^2 + 2 \operatorname{Re} \left\{ \int_{\partial\Omega_0} \gamma \eta_3 H_3 (\overline{\partial_2^\alpha H_2}) + \int_{\partial\Omega_0} \gamma \eta_3 H_3 (\overline{\partial_1^\alpha H_1}) \right\},$$

where the subscripts on H denote vector components and η_3 is the x_3-component of the unit outward normal η. With similar manipulations one can show that

$$\int_{\partial\Omega_0} \eta \times \{\gamma (\nabla_\alpha \times H)\} \cdot \bar{H} - \int_{\partial\Omega_0} (\gamma \nabla_\alpha \cdot H)(\bar{H} \cdot \eta)$$
$$= - \int_{\partial\Omega_0} \gamma \eta_3 (\partial_3 H) \cdot \bar{H} + 2 \operatorname{Re} \left\{ \int_{\partial\Omega_0} \gamma \eta_3 (\partial_1^\alpha H_3) \bar{H}_1 \right.$$
$$\left. + \int_{\partial\Omega_0} \gamma \eta_3 (\partial_2^\alpha H_3) \bar{H}_2 \right\} .$$

Thus, integrating by parts on the boundary terms and combining we obtain

$$B_1(H, H) = \int_{\Omega_0} \gamma \sum_{j,k} |\partial_j^\alpha H_k|^2 - \int_{\Gamma_1} \gamma (T_1^\alpha H) . \bar{H} - \int_{\Gamma_2} \gamma (T_2^\alpha H) . \bar{H} . \quad (22)$$

For $j = 1, 2$, let $\Lambda_j^+ = \{n \in \Lambda : \operatorname{Im} \beta_j^n = 0\}$; define $\Lambda_j^- = \Lambda - \Lambda_j^+$. The sets Λ_j^+ are finite and contain the indices of the outward propagating modes. The sets Λ_j^- contain the indices of the exponentially damped modes. Let us expand the terms involving the operators T_j^α :

$$- \int_{\Gamma_j} \gamma (T_j^\alpha H) . \bar{H} =$$

$$= - \int_{\Gamma_j} \gamma \sum_{n \in \Lambda_j^+} i\beta_j^n H^n e^{-i\alpha_n . x} . \bar{H} - \int_{\Gamma_j} \gamma \sum_{n \in \Lambda_j^-} i\beta_j^n H^n e^{-i\alpha_n . x} . \bar{H}.$$

Since $\operatorname{Im}(\varepsilon) \geq 0$, we can write $\gamma = \frac{1}{\varepsilon\mu} = \gamma' - i\gamma''$ where $\gamma' > 0$, $\gamma'' \geq 0$. Let us first consider the case where ε_2 is real. We then have from (22) that

$$\operatorname{Re} \{B_1(H, H)\} =$$

$$= \int_{\Omega_0} \gamma' \Sigma |\partial_j^\alpha H_k|^2 + \gamma_1 \sum_{n \in \Lambda_1^-} |\beta_1^n| |H^n(b)|^2 + \gamma_2 \sum_{n \in \Lambda_2^-} |\beta_2^n| |H^n(-b)|^2 ,$$

$$\operatorname{Im} \{B_1(H, H)\} =$$

$$= - \int_{\Omega_0} \gamma'' \Sigma |\partial_j^\alpha H_k|^2 - \gamma_1 \sum_{n \in \Lambda_1^+} |\beta_1^n| |H^n(b)|^2 - \gamma_2 \sum_{n \in \Lambda_2^+} |\beta_2^n| |H^n(-b)|^2 .$$

It is easy to check that for ω sufficiently small, there is a constant $c > 0$ such that

$$|\beta_j^n| \geq c\omega (1 + |n|^2)^{1/2} , \quad \text{for all} \quad n \in \Lambda , \quad j = 1, 2 .$$

Furthermore, $\int_{\Omega_0} |\partial_j^\alpha H_k|^2 \geq c \int_{\Omega_0} |\partial_j H_k|^2$ and hence

$$|B_1(H, H)| \geq c \left(\int_{\Omega_0} \Sigma |\partial_j H_k|^2 + \omega \|H\|^2_{W^{1/2}(\Gamma_1)} + \omega \|H\|^2_{W^{1/2}(\Gamma_2)} \right) . \quad (23)$$

The case where ε_2 has positive imaginary part is only a little more complicated. In this case let $q_n = -i\gamma_2 \beta_2^n$ and split q_n into real and imaginary parts $q_n = q_n' - i q_n''$. It is easy to check that $q_n'' > 0$ for all $n \in \Lambda$. Let $\tilde{\Lambda} = \{n \in \Lambda : q_n' < 0\}$. One can also check that $\tilde{\Lambda}$ is a finite set and for all $n \in \tilde{\Lambda}$, we have $|q_n''| > |q_n'|$. It follows that

$$|B_1(H, H)| \geqslant c \left(\int_{\Omega_0} \Sigma \, |\partial_j H_k|^2 + \omega \, \|H\|^2_{W^{1/2}(\Gamma_1)} \right.$$
$$\left. + \sum_{n \in \tilde{\Lambda}} (|q_n''| - |q_n'|) \, |H^n(-b)|^2 + \sum_{n \in (\Lambda - \tilde{\Lambda})} |q_n''| \, |H^n(-b)|^2 \right) .$$

We can also check that there is a constant c such that

$$q_n'' \geqslant c\omega \, (1 + |n|^2)^{1/2} , \quad \text{for all} \quad n \in \Lambda , \quad j = 1, 2 ,$$

and so the bound (23) still holds.

Let $U \in W^1(\Omega_0)^3$ be a vector-valued function with harmonic components and Dirichlet data $U = H$ on $\partial\Omega_0$. Then $(H - U) \in W_0^1(\Omega_0)$ and by elliptic estimates (e.g. [13]),

$$\|U\|_{W^1(\Omega_0)} \leqslant c(\|H\|_{W^{1/2}(\Gamma_1)} + \|H\|_{W^{1/2}(\Gamma_2)}) .$$

Applying the Poincaré inequality and (23) we have

$$\begin{aligned}
\|H\|^2_{L^2(\Omega_0)^3} &\leqslant c \left(\int_{\Omega_0} |\nabla (H - U)|^2 + \|U\|^2_{L^2(\Omega_0)} \right) \\
&\leqslant c \left(\int_{\Omega_0} |\nabla H|^2 + \|U\|^2_{W^1(\Omega_0)} \right) \\
&\leqslant c \left(\int_{\Omega_0} |\nabla H|^2 + \|H\|^2_{W^{1/2}(\Gamma_1)} + \|H\|^2_{W^{1/2}(\Gamma_2)} \right) \\
&\leqslant c\omega^{-1} \, |B_1(H, H)| ,
\end{aligned}$$

with the last inequality holding for ω sufficiently small. Thus for small ω, B_1 satisfies the coercivity bound

$$|B_1(H, H)| \geqslant c_1 \, \omega \, \|H\|^2_{W^1(\Omega)} . \tag{24}$$

Let us define the operator $A_1 : W^1(\Omega)^3 \to [W^1(\Omega)^3]'$ by $\langle A_1 H, F \rangle = B_1(H, F)$. From (24), we see that A_1 is invertible with $\|A_1^{-1}\| \leqslant \dfrac{1}{c_1 \, \omega}$. Notice also that the operator $A_2 : W^1(\Omega)^3 \to [W^1(\Omega)^3]'$ defined by

$\langle A_2 H, F \rangle = B_2(H, F)$ is bounded (and in fact, compact). Defining $A = A_1 - \omega^2 A_2$ and bounding $\|A_1^{-1} A_2\| \leq \frac{c_2}{c_1 \omega}$ we then have

$$\|A^{-1}\| \leq \frac{\|A_1^{-1}\|}{1 - \omega^2 \|A_1^{-1} A_2\|} \leq \frac{1}{c_1 \omega - c_2 \omega^2}.$$

Hence for ω sufficiently small, A^{-1} exists. □

THEOREM 5.2 : *The variational problem* (21) *admits a unique solution* $H \in W^1(\Omega_0)^3$ *for all but a discrete set of parameters* $\omega > 0$.

Proof : Let $\mathcal{R} = \{\omega : \beta_j^n = \omega^2 \varepsilon_j \mu - |\alpha_n - \alpha|^2 \neq 0$ for all $n \in \Lambda, j = 1, 2\}$, so $\mathcal{R}$ is a discrete set of points. Recall that we excluded parameters such that $\omega \in \mathcal{R}$ in Section 4 when we defined the boundary operators T_j^α.

Note that the sesquilinear form B_1 depends on ω through the coefficients β_j^n defining the operators T_j^α. Nevertheless, for any *fixed* $\omega \notin \mathcal{R}$, we can bound

$$|\beta_j^n| \geq c(1 + |n|^2)^{1/2}, \quad \text{for all} \quad n \in \Lambda, \quad j = 1, 2,$$

and so with the same argument used in Theorem 5.1 we can establish a bound

$$|B_1(H, \bar{H})| \geq c \ \|H\|^2_{W^1(\Omega_0)},$$

so that the associated operator A_1 is bounded and invertible. To emphasize that A_1 depends on ω, we write $A_1(\omega)$. The compact operator A_2 does not depend on ω.

Holding $\omega_1 \notin \mathcal{R}$ fixed, now consider the operator $A(\omega_1, \omega) = A_1(\omega_1) - \omega^2 A_2$. By Fredholm theory, we see that $A(\omega_1, \omega)^{-1}$ exists for all $\omega \notin \mathcal{E}(\omega_1)$, where $\mathcal{E}(\omega_1)$ is some discrete set. We will first show that $A(\omega, \omega)^{-1}$ exists for ω near ω_1, except possibly for $\omega \in \mathcal{E}(\omega_1)$, thus proving the theorem for ω near ω_1.

It is easy to check that

$$\|A_1(\omega) - A_1(\omega_1)\| \to 0, \quad \text{as} \quad \omega \to \omega_1;$$

indeed, one need only show that the boundary maps $T_j^\alpha(\omega)$, $T_j^\alpha(\omega_1)$ converge as operators on $W^{1/2}(\Gamma)$ and this follows from the definition of the coefficients β_j^n. Thus, since $\|A(\omega, \omega) - A(\omega_1, \omega)\| = \|A_1(\omega) - A_1(\omega_1)\|$ is small for $|\omega - \omega_1|$ sufficiently small, it follows from the stability of bounded invertibility (see e.g. [14], Theorem IV-1.16) that $A(\omega, \omega)^{-1}$ exists and is bounded for all ω near ω_1 with $\omega \notin \mathcal{E}(\omega_1)$.

Since ω_1 can be taken at any point outside $\mathscr{R}$, it follows that $A(\omega, \omega)^{-1}$ exists for all but a discrete set of frequencies ω. $\square$

6. CONSERVATION OF ENERGY

In this section we show that the weak solutions of the variational problem (21) conserve energy in the sense that the energy radiated away from Ω_0 is the same as that of the incident wave, provided there is no material present which absorbs energy (i.e. provided $\operatorname{Im}(\varepsilon) \equiv 0$).

From the expansion (11) and the representation (13), we see that the coefficients of each propagating reflected plane wave are

$$r_n = H^n(b)\, e^{-i\beta_1 b} \qquad \text{for} \quad n \neq 0\,, \quad n \in \Lambda_1^+\,,$$
$$r_0 = H^0(b)\, e^{-i\beta_1 b} - p\, e^{-2i\beta_1 b} \quad \text{for} \quad n = 0\,,$$

where $\Lambda_1^+ = \{n \in \lambda : \operatorname{Im} \beta_1^n = 0\}$. The « energy » of each reflected mode can be defined [16] by $\beta_1^n\, |r_n|^2/\beta_1$. (Note : there are many different ways to define the energy of electromagnetic waves. Our definition is equivalent, up to a multiplicative constant, to the usual definition involving the Poynting vector.) Similar to the reflected modes, the coefficients of each propagating transmitted more are

$$t_m = H^m(-b)\, e^{-i\beta_2 b} \quad \text{for} \quad m \in \Lambda_2^+\,,$$

where $\Lambda_2^+ = \{m \in \Lambda : \operatorname{Im} \beta_2^m = 0\}$. Note that propagating transmitted modes only exist when $\gamma_2 = 1/(\mu\,\varepsilon_2)$ is real, for otherwise Λ_2^+ is empty. The energy of each transmitted mode is similarly defined as

$$\frac{\gamma_2\, \beta_2^m\, |t_m|^2}{\gamma_1\, \beta_1}\,, \quad m \in \Lambda_2^+\,.$$

Conservation of energy states that the total energy of the reflected and transmitted waves must equal the energy of the incident wave H^*. The energy of the incident wave is $|p|^2$, where p is the magnetic polarization vector. The conservation of energy condition can thus be written

$$\frac{1}{\beta_1}\left(\sum_{m \in \Lambda_1^+} \beta_1^n\, |r_n|^2 + \frac{\gamma_1}{\gamma_2} \sum_{m \in \Lambda_2^+} \beta_2^m\, |t_m|^2\right) = |p|^2\,. \tag{25}$$

THEOREM 6.1 : (*Conservation of energy*). *Assume that the coefficients γ, γ_1, and γ_2 are real. Then the reflection ans transmission coefficients r_n, t_m corresponding to solutions $H \in W^1(\Omega)^3$ of* (21) *satisfy* (25).

Proof : From (21) we see that

$$\operatorname{Im} B(H, H) = -2\,\beta_1 \operatorname{Re}\left\{e^{i\beta_1 b}\int_{\Gamma_1}\gamma\,(p\,.\,\bar{H})\right\}.$$

Expanding the operators T_1^α, T_2^α we see that the imaginary part of B is given by

$$-\gamma_1 \sum_{n\in\Lambda_1^+}\beta_1^n\,|H^n(b)|^2 - \gamma_2\sum_{m\in\Lambda_2^+}\beta_2^m\,|H^m(-b)|^2 =$$

$$= -2\,\beta_1\,\gamma_1 \operatorname{Re}\left\{e^{i\beta_1 b}p\,.\,\bar{H}^0(b)\right\},$$

from which (25) follows immediately. □

Remark : Scaling the incident wave energy to $|p|^2 = 1$, the numbers $(\beta_1^n\,|r_n|^2)/\beta_1$ and $(\gamma_2\,\beta_2^m\,|t_m|^2)/(\gamma_1\,\beta_1)$ are often referred to in the optics and engineering literature as *efficiencies*. They represent the proportion of energy radiated in each propagating mode. Given a solution H to problem (21), the efficiencies can be easily calculated from the Fourier coefficients of the traces $H|_{\Gamma_j}$.

7. FINITE ELEMENT METHOD AND NUMERICAL EXPERIMENTS

In this section, we briefly describe a finite element method for solving the variational problem (21). We will not prove any convergence theorems or make error estimates here. Such estimates should be facilitated by the fact that the underlying operator A has a bounded inverse, as established in Theorems 5.1 and 5.2, although in the case of rough dielectric coefficients, the lack of regularity may preclude « optimal » global error esimates for standard schemes. Rather than delve into these issues here, we merely wish to describe a particular finite element scheme and illustrate qualitatively, with a simple numerical experiment, the kinds of results one can expect with such a scheme.

It is very convenient that the domain Ω_0 is a periodic « box ». We discretized Ω_0 with a uniform rectangular grid, say with N_k grid points in each x_k direction, and used the piecewise-trilinear finite element basis with elements $\phi\,(x - X^j)$, where $\{X^j\}$ is the set of $N_1\,.\,N_2\,.\,N_3$ grid points, and

$$\phi\,(x) = \begin{cases}\left(1 - \left|\dfrac{x_1}{h_1}\right|\right)\left(1 - \left|\dfrac{x_2}{h_2}\right|\right)\left(1 - \left|\dfrac{x_3}{h_3}\right|\right) & \text{if} \quad |x_k| \leq h_k,\ k = 1, 2, 3\,, \\ 0 & \text{otherwise}\,.\end{cases}$$

Here, h_k denotes the grid spacing in the k-th direction, i.e., $h_1 = L_1/N_1$, $h_2 = L_2/N_2$, $h_3 = 2\,b/(N_3 - 1)$. The basis elements centered at grid points which lie on the boundaries Γ_j are restricted to Ω_0.

The equations were discretized using the standard Galerkin approximation with a simple gaussian quadrature formula to compute the integrals over the cells. The boundary conditions were calculated by truncating the Fourier transform representation of the operators T_j^{α}.

The resulting linear system is large and sparse, but not necessarily Hermitian or positive definite. We chose to solve the system with an « Orthomin » iterative solver. We experimented with several generic preconditioners, for example diagonal scaling and incomplete LU decomposition, but generally observed quicker convergence without a preconditioner. An important topic for future research is the design of effective preconditioners for this problem.

Our numerical experiment is meant to solve a prototypical electromagnetic scattering problem which could be encountered in micro-optics. We are given a biperiodic structure such as the one pictured in Figure 2. This particular structure illustrates qualitatively the features of devices we wish to model.

The goal is to predict the diffracted field which results when a plane wave of a particular frequency, polarization, and incidence angle impinges on the

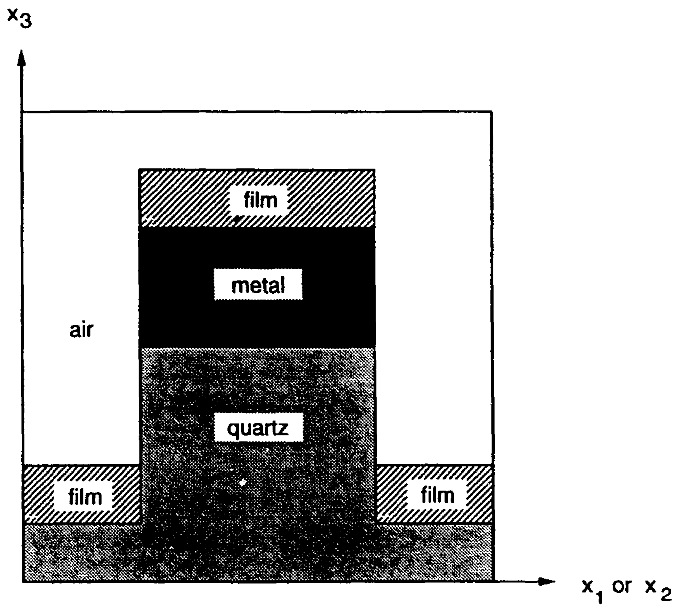

Figure 2. — Cross-section through the center of one periodic cell of the prototypical biperiodic structure. The profile is the same in both the (x_1, x_3) and (x_2, x_3) cross-sections.

structure from above. In micro-optical applications, the period of the structure is usually comparable to the wavelength of the incident radiation. We have chosen the wavelength of the incoming wave to be 0.55 μm, roughly in the center of the visible electromagnetic spectrum. We have taken the period of the structure to be 0.5 μm in both the x_1 and x_2-directions. The

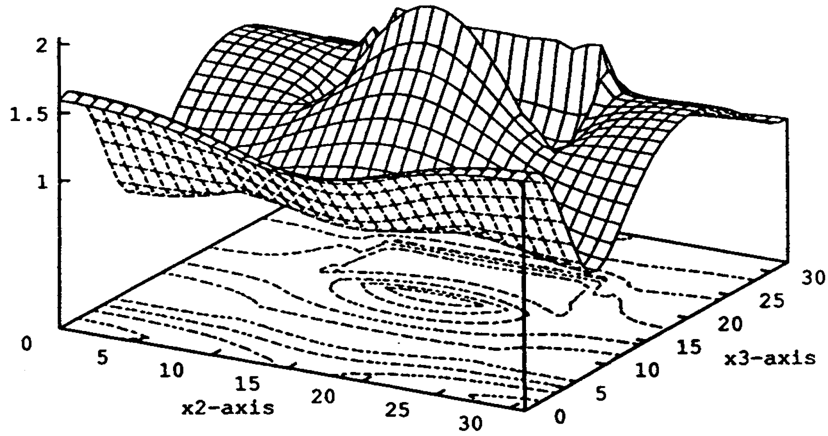

Figure 3. — Cross-section of the amplitude $|H|$, taken through the metal region in the (x_2, x_3) plane.

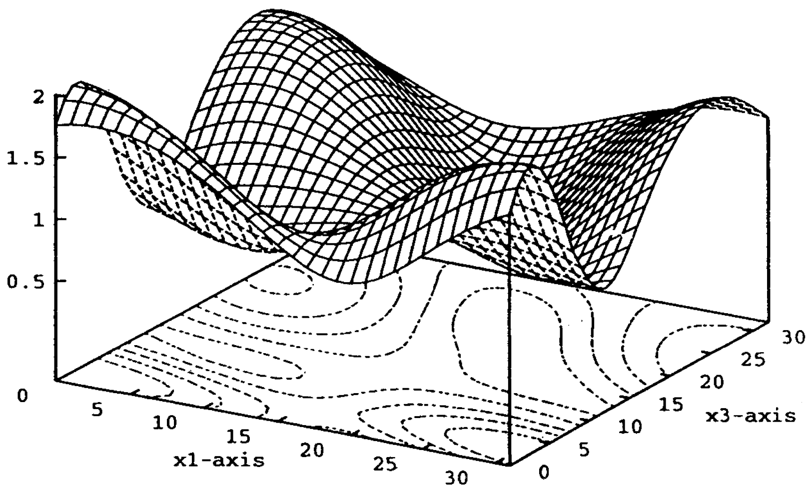

Figure 4. — Cross-section of the amplitude $|H|$, taken through the non-absorbtive region in the (x_1, x_3) plane.

height of the computational box is also 0.5 μm. We used a $32 \times 32 \times 33$ grid. The grid lines are aligned with the discontinuities in the dielectric coefficient ε, since this is where we expect discontinuities in the derivatives of H.

Figures 3 through 6 show cross-sections of the amplitude of the H field inside the computational box when an incoming plane wave,

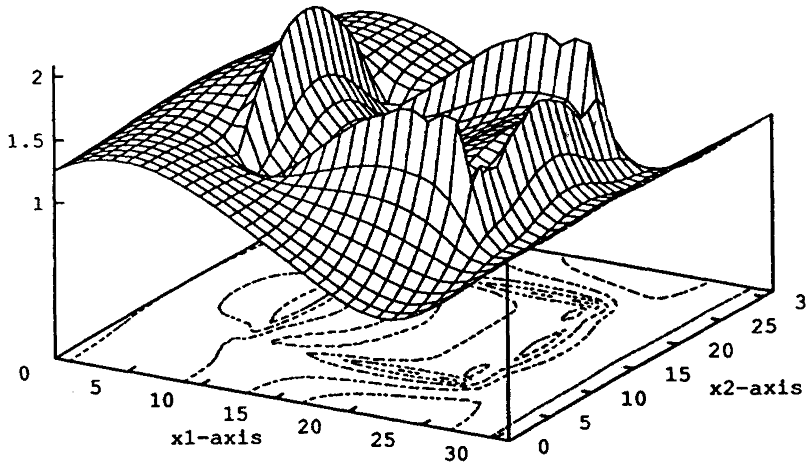

Figure 5. — **Cross-section of the amplitude $|H|$, taken through the metal region in the (x_1, x_2) plane.**

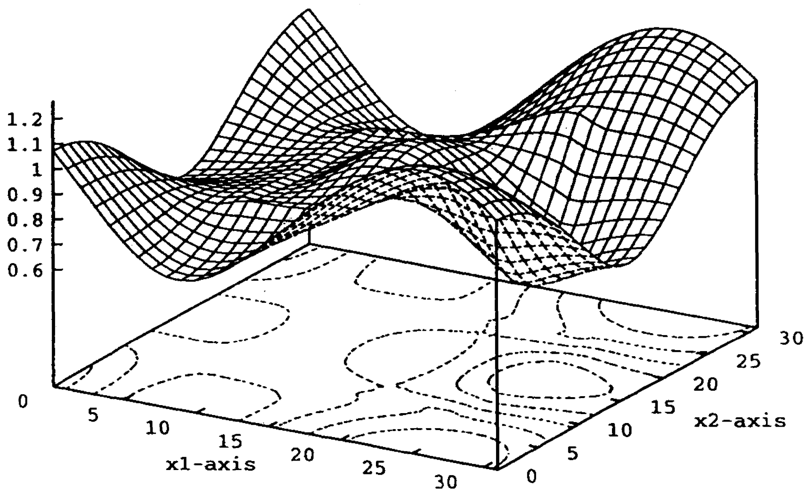

Figure 6. — **Cross-section of the amplitude $|H|$, taken below the metal region in the (x_1, x_2) plane.**

polarized such that the E field is pointing in the x_2 direction, is incident on the structure at an angle of 30° with respect to the x_3-axis. Perhaps the most striking feature of the figures is the sharp drop in field intensity inside the metallic material (which we chose to be gold), compared to the relatively smooth « waves » in the other media. Notice that the intensity is symmetric in the x_2-direction, but asymmetric in the x_1-direction ; this is because the incoming wavevector is orthogonal to the x_2-axis.

The primary advantages of this scheme are its generality and simplicity. Perhaps the biggest disadvantage at present is the large cost associated with complicated simulations. In general, as the ratio of the wavelength to the size of the structure decreases, the waves inside the box become more complicated and therefore more difficult to approximate accurately in finite element spaces. Since we must use a 3-dimensional mesh, the cost of adding more grid points in each direction is large. As it stands, the method is certainly feasible for « medium sized » problems (say $20 \times 20 \times 20$ mesh) on the current generation of workstations. Hopefully, with improvements in preconditioners and iterative methods for solving the discretized equations, the cost can be reduced significantly.

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