Optimal Design of Periodic Diffractive Structures

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Abstract

The problem of designing a periodic interface between two different materials, which gives rise to a specified far-field diffraction pattern for a given incoming plane wave, is considered. The time harmonic waves are assumed to be TM (transverse magnetic) polarized. The diffraction problem is modeled by a generalized Helmholtz equation with transparent boundary conditions. In this paper, the design problem is relaxed to include highly oscillatory profiles. Existence of an optimal design is established. The principal method is based on homogenization theory for the model equation.

Key words. optimal design, diffractive optics, periodic structure, generalized Helmholtz equations, homogenization.

AMS subject classifications. Primary: 78A45, 49J20. Secondary: 35R30, 35J05

1 Introduction

We consider the problem of designing a periodic interface between two different materials which gives rise to a specified far-field diffraction pattern for a given incoming plane wave. Throughout, the medium is assumed to be nonmagnetic and invariant in the y direction. We study the diffraction problem in TM (traverse magnetic) polarization, *i.e.*, the magnetic field is transversal to the (x, z)-plane. The case when the electric field is transversal to the (x, z)-plane is called TE (transverse electric) polarization. These two polarizations are of primary importance since any other polarization may be decomposed into a simple combination of them. The differential equations derived from time harmonic Maxwell's equations are quite different for the TE and TM cases: In the TE case, $(\Delta + k^2)u = 0$, where the electric field $\mathbf{E} = (0, u(x, z), 0)$; In the TM case, $\nabla \cdot (\frac{1}{k^2}\nabla u) + u = 0$, where the magnetic field $\mathbf{H} = (0, u(x, z), 0)$. In both cases, k is the index of refraction of the medium. Our goal in this paper is to formulate and study aspects of the optimal shape design problem.

Because of many important applications in micro-optics, the optimal design of periodic or grating structures has recently received considerable attention. See Achdou [1], Achdou and Pironneau [2], Dobson [18] [19], and Elschner and Schmidt [13] for mathematical and computational results in the TE case. Basically, the design problem can be posed as a nonlinear least-squares problem over a set of variables that describe the class of admissible interfaces. In this work, an admissible interface is represented by the characteristic function of the set occupied by one of the dielectric materials. The interface can be very general without any smoothness assumption. In fact, it is only required to be a graph. The following difficulties arise immediately since the scattering pattern depends on the interface in a very implicit fashion:

- the set of admissible characteristic functions is not closed for the natural topology,
- the cost functional is not weakly sequentially lower semi-continuous.

As a consequence, existence of a minimizer is not guaranteed. The remedy is to consider a relaxed problem that extends the problem setting in order to take into account highly oscillatory interfaces, in such a way that well-posedness is ensured. In [1] [2] [18] [19], the design problem in the TE case was solved by using a "relaxation" technique similar to that of Kohn and Strang [21], as well as a weak convergence argument. See Cox and Dobson [12] for a recent related work on maximizing band gaps in photonic crystals in TE polarization.

This work focuses on the optimal design problem in TM polarization. The model, method, and results are quite different from the TE case. In fact, the solution in the TE case is more regular than in the TM case for $k \in L^\infty$. Also, in the TM case, the nonsmooth coefficients appear in the principal part as opposed to the lower terms for TE polarization. The analysis on the effect of the highly oscillatory coefficients in the principal part is amenable by homogenization theory. The homogenization limit is anisotropic. This is fundamentally different from the TE case in which a weak convergence analysis suffices and the resulting weak limit of the coefficients remains isotropic. We believe that the idea and method here may be extended to study the optimal design of biperiodic structures, where the model is in a 3-D vector form. An interesting future direction is to develop computational schemes for solving the design problems. Progress has been made for the TE case in [1] [2] [18] [19] [13]. However, no computational result is available in the TM case.

Homogenization theory has become the standard tool for obtaining an expression of the relaxed functional. The general approach has been applied to diffusion systems [26] [23], to the 2-D and 3-D elasticity systems [3] [20] [15], and to the biharmonic equation [22, 8]. Note that in these applications, the original sets of designs are those of all characteristic functions. In the present case, however, additional constraints induced by the choice of admissible interfaces must also be taken into account. In this regard, our work is related to that of Brizzi [10, 11] and Nevard and Keller [27] on homogenization of rough boundaries.

The diffraction theory in periodic structures has many applications in micro-optics, the reader is referred to the books [14] for a description of mathematical problems which arise in these applications. A good introduction to the problem of electromagnetic diffraction through periodic structures, along with some numerical methods, can be found in the collection of papers in [28]. Results on a related inverse diffraction problem in the TM case may be found in [7] and [5]. See also [6] for a survey of recent developments in the mathematical modeling of diffractive optics.

We now outline the rest of this paper. Section 2 is devoted to a formulation of the scattering problem. Using the radiation condition and periodicity, the problem can be reduced to a bounded domain with transparent boundary conditions. In Section 3, we introduce two specific optimal design problems in TM polarization. We derive the relaxed optimization problem in Section 4 by homogenization theory. Finally, in Section 5, we obtain a characterization of the admissible generalized dielectric coefficients and establish the existence of optimal generalized designs.

2 The model problem

We first specify the problem geometry. Let S be a simple curve imbedded in the strip

$$\Omega_0 = \{(x,z) \in \mathbf{R}^2 : -b_0 < z < b_0\},$$

where b_0 is some positive constant. We assume that S defines a periodic grating in the x-direction with period 2π. For a constant $b > b_0$, let $D_1 = \{(x,z) \in \mathbf{R}^2 : z > b\}$, $D_2 = \{(x,z) \in \mathbf{R}^2 : z < -b\}$, and $\Omega = \{(x,z) \in \mathbf{R}^2 : -b < z < b\}$. Define the boundaries $\Gamma_1 = \{z = b\}$, $\Gamma_2 = \{z = -b\}$. Assume also that the curve S divides Ω into two connected components D_1^+ (which meets D_1) and D_2^+ (which meets D_2).

The whole space is filled with two materials with periodic dielectric coefficients ϵ_i of period 2π,

$$\epsilon(x) = \begin{cases} \epsilon_1 & \text{in } D_1^+ \cup \bar{D}_1 , \\ \epsilon_2 & \text{in } D_2^+ \cup \bar{D}_2 , \end{cases}$$

where ϵ_1 and ϵ_2 are constants, ϵ_1 is real and positive, and $Re\ \epsilon_2 > 0$, $Im\ \epsilon_2 \geq 0$. The case $Im\ \epsilon_2 > 0$ corresponds to a substrate which absorbs energy. For convenience, we also define the "index of refraction" $k = \sqrt{\epsilon\mu}$, where ϵ is dielectric constant and μ is the magnetic permeability constant. Note that in the literature, it is the term ωk (ω is angular frequency) that is called index of refraction. Suppose also that the media are nonmagnetic, *i.e.*, the magnetic permeability constant μ is a fixed constant (e.g. $\mu = 1$) everywhere.

We want to solve the generalized Helmholtz equation derived from Maxwell's system of equations

$$\nabla \cdot (\frac{1}{k^2}\nabla u) + \omega^2 u = 0 , \quad \text{in } \mathbf{R}^2, \tag{1}$$

when an incoming plane wave

$$u_I = e^{i\alpha x - i\beta_1 z}$$

is incident on S from D_1,

$$\alpha = \omega k_1 \sin\theta, \quad \beta_1 = \omega k_1 \cos\theta,$$

and $-\frac{\pi}{2} < \theta < \frac{\pi}{2}$ is the angle of incidence.

We seek a quasiperiodic solution, i.e., a function u such that $u_\alpha(x,z) := u(x,z)e^{-i\alpha x}$ is 2π-periodic. It is easily seen that u_α satisfies

$$\nabla_\alpha \cdot (\frac{1}{k^2}\nabla_\alpha u_\alpha) + \omega^2 u_\alpha = 0 , \quad \text{in } \mathbf{R}^2, \tag{2}$$

where the operator ∇_α is defined by

$$\nabla_\alpha = \nabla + i(\alpha, 0).$$

Due to the 2π periodicity of the problem with respect to the x-variable, we can identify Ω with the cylinder $\Omega/(2\pi Z \times \{0\})$, and similarly identify the boundaries Γ_j with $\Gamma_j/2\pi Z$. All functions defined on Ω and Γ_j will be regarded as being 2π-periodic in the x-variable.

To determine the general form of u_α far away from the interface, we expand u_α in a Fourier series:

$$u_\alpha(x,z) = \sum_{n \in Z} u_\alpha^{(n)}(z) e^{inx},$$

where

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

Define for $j = 1, 2$ the coefficients

$$\beta_j^{(n)}(\alpha) = e^{i\gamma_j^n/2}|\omega^2 k_j^2 - (n+\alpha)^2|^{1/2}, \quad n \in Z,$$

where

$$\gamma_j^n = arg(\omega^2 k_j^2 - (n+\alpha)^2), \;\; 0 \le \gamma_j^n < 2\pi.$$

Assume that $\omega^2 k_j^2 \neq (n+\alpha)^2$ for all $n \in Z$, $j = 1, 2$. This condition excludes "resonance" cases and ensures that a fundamental solution for (2) exists inside D_1 and D_2. In particular, for real k_2, we have the following equivalent form of (2)

$$\beta_j^{(n)}(\alpha) = \begin{cases} \sqrt{\omega^2 k_j^2 - (n+\alpha)^2}, & \omega^2 k_j^2 > (n+\alpha)^2 \,, \\ i\sqrt{(n+\alpha)^2 - \omega^2 k_j^2}, & \omega^2 k_j^2 < (n+\alpha)^2 \,. \end{cases}$$

It follows that u_α can be expressed, inside D_1 and D_2, as a sum of plane waves in the following way :

$$u_\alpha|_{D_j} = \sum_{n\in Z} a_j^{(n)} e^{\pm i\beta_j^{(n)}(\alpha)z + inx}, \quad j = 1, 2 \,, \tag{3}$$

where the constants $a_j^{(n)}$ are complex scalars.

We next impose a radiation condition on the scattering problem. Since $\beta_j^{(n)}$ is real for at most finitely many n, there are only a finite number of propagating plane waves in the sum (3), the remaining waves are exponentially damped (so-called evanescent waves) or radiate (unbounded) as $|z| \to \infty$. We impose that u_α should contain only bounded outgoing plane waves in D_1 and D_2, plus the incident incoming wave u_I in D_1.

For functions $f \in H^{\frac{1}{2}}(\Gamma_j)$ (regarded as a complex-valued functions on the circle, with Sobolev regularity $H^{1/2}$), we consider the Dirichlet to Neumann operator T_j^α, defined by

$$(T_j^\alpha f)(x) = \sum_{n\in Z} i\beta_j^{(n)}(\alpha) f^{(n)} e^{inx}, \tag{4}$$

where $f^{(n)} = \frac{1}{2\pi}\int_0^{2\pi} f(x)e^{-inx}$, and where the equality is taken in the sense of distributions. It is easily seen [4] that the operator $T_j^\alpha : H^{\frac{1}{2}}(\Gamma_j) \to H^{-\frac{1}{2}}(\Gamma_j)$ is continuous.

Introducing the operators T_j^α allows to reformulate the scattering problem in the bounded domain Ω, in the following way : find $u_\alpha \in H^1(\Omega)$ such that

$$\nabla_\alpha \cdot (\frac{1}{k^2}\nabla_\alpha u_\alpha) + \omega^2 u_\alpha = 0 \;\; \text{in } \Omega \,, \tag{5}$$

$$(T_1^\alpha - \frac{\partial}{\partial\nu})u_\alpha = 2i\beta_1 e^{-i\beta_1 b} \;\; \text{on } \Gamma_1 \,, \tag{6}$$

$$(T_2^\alpha - \frac{\partial}{\partial\nu})u_\alpha = 0 \;\; \text{on } \Gamma_2 \,. \tag{7}$$

Theorem 2.1 *There exists a constant $\omega_0 > 0$ independent of the shape of the interface S, such that for $0 < \omega \le \omega_0$, the model problem admits a unique solution $u_\alpha \in H^1(\Omega)$. Furthermore, $||u_\alpha||_{H^1(\Omega)}$ is bounded independently of the interface S.*

We refer to [4] for a proof of the result.

Remark 2.1. For a more general function $k \in L^\infty(\Omega)$, the model problem admits a unique solution for all but possibly a discrete set of frequencies. The low frequency assumption corresponding to small period of the structure is reasonable for micro-optics applications. The assumption may be dropped in the case ϵ_2 has a positive imaginary part, *i.e.*, the substrate is absorbing.

Theorem 2.1 can be generalized. In particular, an analogous result holds in the case when the dielectric media are separated by another dielectric medium, instead of an interface : Assume that $A(x,z)$ is a positive definite, matrix-valued function in $L^\infty(\Omega)$, such that

$$\begin{cases} A(x,z) &= a_1 & \text{for } z \geq b_0 \ , \\ A(x,z) &= a_2 & \text{for } z \leq -b_0 \\ 0 < A_1 \leq A(x,z) \leq A_2 < \infty & & \text{otherwise} \ , \end{cases}$$

the last inequality being understood in the sense of quadratic forms. Then we have

Theorem 2.2 *Let $0 \leq \theta_0 < \pi/2$ be some maximum incidence angle. There exists a constant $\omega_0 > 0$ depending on the constants a_1, a_2, A_1, A_2 only, such that for incidence angles $|\theta| \leq \theta_0$ and for frequencies $0 < \omega \leq \omega_0$, the problem*

$$\nabla_\alpha \cdot (A \nabla_\alpha u_\alpha) + \omega^2 u_\alpha \ = \ 0 \quad in\ \Omega \ , \tag{8}$$

with boundary conditions (6, 7), admits a unique solution $u_\alpha \in H^1(\Omega)$. Furthermore, $||u_\alpha||_{H^1(\Omega)}$ is bounded by a constant that only depends on $a_1, a_2, A_1, A_2, b, \theta_0$ and ω_0.

For simplicity, from now on, we shall remove the subscript and superscript and denote u_α, T_j^α by u, T_j, respectively.

3 The optimal design problem

We present optimal design problems in TM polarization. For simplicity, we shall restrict to the case in which the frequency ω is sufficiently small. It then follows from Theorem 2.1 that there is a unique quasi-periodic solution u_α to the model problem and $||u_\alpha||_{H^1(\Omega)}$ is bounded independent of the interface S.

Here, we consider two examples of the design problems. The rest of the paper will be devoted to a study of existence for the optimal design in a general framework which includes these two examples.

Set $a_j = \varepsilon_j^{-1}$. We can associate with each interface S a function $a_S \in L^\infty(\Omega)$ by

$$a_S(x,z) = \begin{cases} a_1 & \text{in } D_1^+ \ , \\ a_2 & \text{in } D_2^+ \ . \end{cases}$$

Example 1. We first consider the optimal design of antireflective structures. To demonstrate the idea, we further assume that the frequency ω is so small that $Im\ \beta_1^{(n)} > 0$ for all $n \neq 0$. Thus, there is only one propagating (outgoing) plane wave reflected from the structure, for a given incoming plane wave.

In this situation, it is easy to compute the reflection coefficient

$$r_0(u_\alpha) = \frac{e^{-i\beta_1 b}}{2\pi} \int_{\Gamma_1} u_\alpha - e^{-2i\beta_1 b} \ .$$

Clearly, the total reflected energy $|r_0(u_\alpha)|^2$ depends on the interface S in an implicit way.

We are now ready to present the optimal design of an antireflective structure: determine a curve S (or equivalently a distribution of material coefficients a_S) which minimizes the functional

$$Min\ J(a_S) = \int_{\alpha_1}^{\alpha_2} |r_0(u_{\alpha_k})|^2 d\alpha \tag{9}$$

over a given range of incidence angles $\theta \in [\theta_1, \theta_2]$. Here $\alpha_k = \omega k_1 sin\theta_k$ for $k = 1, 2$.

Example 2. This example is concerned with designing periodic structures with specified scattered far-field patterns (low frequency). The outward propagating modes correspond to indices n for which $\beta_j^{(n)}$ are real-valued.

Denote

$$\Lambda_j = \{n \in Z\ :\ Im(\beta_j^{(n)}) = 0\},\ \ j = 1, 2\ .$$

The coefficients of each propagating reflected mode are

$$\begin{aligned} r_n &= u_n(b)e^{-i\beta_1^{(n)}b} \ \text{ for } n \in \Lambda_1\ ,\ \ n \neq 0\ , \\ r_0 &= u_0(b)e^{-i\beta_1 b} - e^{-2i\beta_1 b} \ \text{ for } n = 0\ . \end{aligned}$$

The energy of each propagating mode is $\beta_1^{(n)}|r_n|^2/\beta_1$.

Similarly, the coefficients of each propagating transmitted mode are

$$t_m = u_m(-b)e^{-i\beta_2^{(m)}b} \ \text{ for } m \in \Lambda_2\ .$$

The energy for each transmitted mode is $\beta_2^{(n)}|t_n|^2/\beta_2$.

Define the vectors

$$r = (r_n)_{n\in\Lambda_1}\ ,\ \ t = (t_m)_{m\in\Lambda_2}\ ,$$

which clearly are functions of the interface S.

We can now state another optimal design problem. For some specified reflection and transmission vectors r^0 and t^0, determine the curve S, (or equivalently a distribution of material coefficients a_S), such that $r(S)$, $t(S)$ are close to r^0, t^0 in the least-squares sense, respectively:

$$Min\ J(a_S) = ||r(S) - r^0||^2 + ||t(S) - t^0||^2\ . \tag{10}$$

From now on, we will denote by $J(A)$ or $J(u(A))$ the above functionals associated with a material distribution $A(x, z)$ in the region Ω_0.

4 Homogenization for the design problem

This section is devoted to a formulation of the relaxed problem in the terminology of [21]. The idea is to replace the original problem with that of minimizing an extended functional over a set of generalized interfaces. The set should be closed in the weak * topology. The extended functional is required to be weakly lower semi-continuous. Also, when evaluated at an admissible original interface, it should coincide with the original functional. The form of the relaxed functional can then be determined by studying the limiting behavior of sequences of solutions $u_n = u(\chi_n)$ with respect to a sequence of admissible interfaces.

For simplicity, admissible interfaces are chosen to be graphs of L^∞ functions $h(x)$ in the x variable with values in a fixed band $[-b_0, b_0]$. Recall that b_0 is a fixed constant satisfying $0 < b_0 < b$.

We can describe an admissible interface by the characteristic function χ of its subgraph, i.e., for $h \in L^\infty(0, 2\pi)$ with $||h||_\infty \le b_0$,

$$\chi(S)(x,z) = \begin{cases} 1 & \text{if } h(x) \le z , \\ 0 & \text{if } z < h(x) . \end{cases} \tag{11}$$

Let X denote the set of those characteristic functions.

This choice is certainly not the most general one that can be handled by our method. In fact, the proofs below remain valid, provided that admissible minimizing sequences of characteristic functions satisfy

$$\partial_z \chi_n \text{ is compact in } H^{-1}(\Omega) . \tag{12}$$

We will show that the set X satisfies this property. From a manufacturing point of view, it is a natural choice since gratings of small scales are usually fabricated by micro-lithographic techniques. The constraints on the values of h are also natural from the point of view of design. After all, the boundaries $z = \pm b$ of Ω are artificial.

Let $\{\chi_n\} \subset X$ be a sequence that converges weakly * in $L^\infty(\Omega)$ to some function η. For simplicity, we set $a_{\chi_n}(x,z) = \varepsilon(x,z)^{-1} = \chi_n(x,z)a_1 + (1 - \chi_n(x,z))a_2$. We also denote by $m(x,z)$ and $c(x,z)$ the arithmetic and harmonic averages of the weak-* limit of a_n, i.e.,

$$m(x,z) = \eta(x,z)a_1 + (1 - \eta(x,z))a_2 = \text{w*lim } a_{\chi_n} , \tag{13}$$

$$c(x,z) = \left(\frac{\eta(x,z)}{a_1} + \frac{1-\eta(x,z)}{a_2}\right)^{-1} = (\text{w*lim } a_{\chi_n}^{-1})^{-1} , \tag{14}$$

and let A^* denote the tensor

$$A^*(\eta) = \begin{pmatrix} c(x,z) & 0 \\ 0 & m(x,z) \end{pmatrix} . \tag{15}$$

Let $u_n = u(\chi_n)$ denote the solution to

$$\nabla_\alpha \cdot (a_{\chi_n} \nabla_\alpha u_n) + \omega^2 u_n = 0 ,$$

with the boundary conditions (6,7). and let $u = u(\eta)$ denote the solution to

$$\nabla_\alpha \cdot (A^*(\eta) \nabla_\alpha u) + \omega^2 u = 0 ,$$

with the boundary conditions (6,7).

Theorem 4.1 *Assume that $\omega \le \omega_0$ and $|\theta| \le \theta_0$, where ω_0 and θ_0 are given by Theorem 2.2. Assume $\chi_n \rightharpoonup \eta$ weakly * in $L^\infty(\Omega)$. Then the corresponding sequence of solutions $\{u_n\}$ converges weakly in $H^1(\Omega)$ to $u = u(\eta)$. Moreover, if J is weakly continuous with respect to u, then*

$$J(u_n) \longrightarrow J(u(\eta)) .$$

Remark 4.1. In particular, for the functionals defined in Section 3, we have

$$J(a_{\chi_n}) \longrightarrow J(A^*(\eta)) . \tag{16}$$

In order to prove the theorem, we need the following two lemmas.

Lemma 4.1 *Let $\{\chi_n\} \subset X$ satisfy $\chi_n \rightharpoonup \eta$ in $L^\infty(\Omega)$ weak*. Then, $\partial_z \chi_n \longrightarrow \partial_z \eta$ strongly in $H^{-1}(\Omega)$.*

Proof : The proof relies on the following classical result of Murat [24]: Assume that $\{f_n\}$ is a sequence of positive distributions and is bounded in $W^{-1,p}(\Omega)$, for some $p > 2$. Then f_n lies in a compact set of $H^{-1}(\Omega)$.

Now, since $\{\chi_n\}$ is bounded in $L^\infty(\Omega)$, $\partial_z \chi_n$ is bounded in $W^{-1,p}(\Omega)$, for any $p \geq 1$. Moreover, for $\phi \in \mathcal{D}(\Omega)$, $\phi \geq 0$, we have

$$\begin{aligned} < \partial_z \chi_n, \phi > &= -\int_\Omega \chi_n \partial_z \phi_n \\ &= -\int_0^{2\pi} dx \int_{h(x)}^b \partial_z \phi_n(x,z) dz \\ &= \int_0^{2\pi} \phi(x, h(x)) dx \ \geq \ 0 \ , \end{aligned}$$

and the Lemma follows. □

Lemma 4.2 *(The div-curl Lemma of Murat and Tartar [26]) Assume that $\{f_n\}$, $\{g_n\}$ are two bounded sequences in $L^2(\Omega_0)^2$, such that*

$$f_n \rightharpoonup f \ , \ \ g_n \rightharpoonup g \ , \quad \textit{weakly in } L^2(\Omega_0)^2$$

and

$$\begin{aligned} div(f_n) &\to div(f) \ \textit{ strongly in } H^{-1}(\Omega_0) \ , \\ curl(g_n) &\to curl(g) \ \textit{ strongly in } H^{-1}(\Omega_0)^2 \ . \end{aligned}$$

Then

$$f_n g_n \rightharpoonup fg \ \textit{in } \mathcal{D}'(\Omega_0) \ .$$

Proof of Theorem 4.1. By Theorem 2.2, $\{u_n\}$ is uniformly bounded in $H^1(\Omega)$. A subsequence can be extracted with the properties that

$$\begin{cases} u_n \rightharpoonup u & \text{weakly in } H^1(\Omega) \\ \xi_n = a_n \nabla_\alpha u_n \rightharpoonup \xi^* & \text{weakly in } L^2(\Omega) \ . \end{cases}$$

We subdivide Ω into three parts :

$$\begin{aligned} \Omega_1 &= (0, 2\pi) \times (b_0, b) \ , \\ \Omega_0 &= (0, 2\pi) \times (-b_0, b_0) \ , \\ \Omega_2 &= (0, 2\pi) \times (-b, -b_0) \ . \end{aligned}$$

Since the dielectric coefficients are constant for $|z| > b_0$, it is obvious that

$$\xi^* \ = \ a_i \nabla_\alpha u \ \text{ in } \Omega_i \ , \ \text{for } \ i = 1, 2 \ .$$

Also, since the operators T_i are linear, one can verify directly that u and ξ^* satisfy

$$\begin{aligned} \nabla_\alpha \cdot \xi^* + \omega^2 u &= 0 \text{ in } \Omega , \\ \frac{\partial u}{\partial \nu} - T_1(u) &= 2i\beta_1 e^{-i\beta_1 b} \text{ on } \Gamma_1 , \\ \frac{\partial u}{\partial \nu} - T_2(u) &= 0 \text{ on } \Gamma_2 . \end{aligned}$$

To identify the relationship between ξ^* and $\nabla_\alpha u$ in the remaining part Ω_0, we choose $f_n = \xi_n$ in Lemma 4.2. Since

$$\operatorname{div}(\xi_n) = -i\,\alpha \xi_{1,n} - \omega^2\, u_n ,$$

is uniformly bounded in $L^2(\Omega_0)$, which is compactly embedded in $H^{-1}(\Omega_0)$, we have

$$\operatorname{div}(\xi_n) \longrightarrow \operatorname{div}(\xi^*) \text{ strongly in } H^{-1}(\Omega_0) .$$

On the other hand, let $g_n = (1/a_n(x,z), 0)$. By Lemma 4.1, $\operatorname{curl}(g_n) = (1/a_1 - 1/a_2)\partial_z \chi_n$ converges strongly in $H^{-1}(\Omega_0)$. It follows that

$$(\partial_x + i\,\alpha)\, u_n = 1/a_n\, \xi_{1,n} = f_n \cdot g_n \rightharpoonup f \cdot g = c^{-1}(x,z)\, \xi_1^* ,$$

hence $\xi_1^* = c(x,z)\,(\partial_x + i\,\alpha)\, u$. For the identification of ξ_2^*, let $\phi \in \mathcal{D}(\Omega)$ and consider

$$\begin{aligned} \int_\Omega \xi_{2,n}\phi &= \int_\Omega a_n \partial_z u_n\, \phi \\ &= -\int_\Omega u_n\, (\partial_z(\chi_n a_1 + (1-\chi_n)a_2)\, \phi + a_n\, \partial_z \phi) . \end{aligned}$$

As $u_n \rightharpoonup u$, weakly in $H^1(\Omega)$, Lemma 4.1 shows that

$$\begin{aligned} \int_\Omega u_n\, \partial_z(\chi_n a_1 + (1-\chi_n)a_2)\, \phi &\longrightarrow \int_\Omega u\, \partial_z(\eta a_1 + (1-\eta)a_2)\, \phi \\ &= \int_\Omega u\, \partial_z m\, \phi , \end{aligned}$$

while the strong convergence of u_n in $L^2(\Omega)$ and the weak convergence of a_n to m imply that

$$\int_\Omega u_n\, a_n\, \partial_z \phi \longrightarrow \int_\Omega u\, m\, \partial_z \phi .$$

We conclude that

$$\int_\Omega \xi_{2,n}\phi \longrightarrow -\int_\Omega u\,(\partial_z m\, \phi + m\, \partial_z \phi) = \int_\Omega m\, \partial_z u\, \phi .$$

Since the limit is unique, it is the whole sequence u_n that converges weakly to u. This establishes the first part of Theorem 4.1. □

Remark 4.2. The weak lower semi-continuity of J with respect to u yields (16) for the functional of Example 2 of Section 3. For Example 1, the convergence (16) can be shown by a combination of the fact that $r_\alpha(u_{\alpha,\chi_n}) \longrightarrow r_\alpha(u_{\alpha,\eta})$ for a.e. $\alpha \in (\alpha_1, \alpha_2)$ and the Lebesgue Dominated Convergence Theorem. □

Remark 4.3. Theorem 4.1 extends previous results of R. Brizzi [10] [11] (see also [27]) about homogenization of a periodic transmission problem, *i.e.*, assuming that $a_n(x,z) = a(nx,z)$, the function a being 1-periodic in $x \in \mathbb{R}^N$, for any dimension $N > 0$. We believe that the method may be modified to study the biperiodic structures case (3-D), *i.e.*, the case of periodic coefficients in (x, y). In this situation, due to the local character of H-convergence, the local value of the effective matrix in the non-periodic case, is equal to an effective matrix that can be obtained by periodic homogenization [16]. The effective matrix takes a more complicated form

$$A^*(x,z) = \begin{bmatrix} B^* & 0 \\ 0 & m(x,z) \end{bmatrix} ,$$

where B^* is a 2×2 matrix, the eigenvalues of which can be described in terms of $\eta(x, y, z)$ [29].

5 The relaxed problem and existence of a generalized minimizer

Theorem 4.1 gives useful indications for the proper form of the relaxed problem. Let $J^*(\eta) = J(A^*(\eta))$, where $u(\eta)$ is the solution to (8) with $A = A^*$ and the boundary conditions (6,7). The original problem, $\min_{\chi \in X} J(a_\chi)$ is replaced with the problem of minimizing $J^*(\eta)$ over the set of densities which are weak* limits of admissible characteristic functions of X. In this section, we characterize this set of densities and show that the relaxed problem is well-posed, i.e., has a minimum.

Let X^*, be the set of L^∞ functions η, such that

$$0 \le \eta \le 1 \ , \quad \begin{cases} \eta(x,z) = 0 & \text{for } z < -b_0 \\ \eta(x,z) = 1 & \text{for } z > b_0 \end{cases} \quad \text{and } \partial_z \eta \ge 0 \ \text{ in } \mathcal{D}'(\Omega) \ .$$

X^* is obviously closed for the L^∞ weak* topology.

Lemma 5.1 *The set X^* is the L^∞ weak* closure of X.*

Proof : Obviously, $X \subset X^*$. Given $\eta \in X^*$, let H be the function defined on $(0, 1) \times \Omega$ by

$$H(\zeta, x, z) = \begin{cases} 1 & \text{if } \zeta \le \eta(x,z) \\ 0 & \text{if } \eta(x,z) < \zeta \end{cases} ,$$

and extend H as a 1-periodic function of ζ on $\mathbb{R} \times \Omega$. Define $\chi_n(x, z) = H(nx, x, z)$. For fixed n, since $\eta(x, z)$ is increasing with z, χ_n defines an interface in X. Indeed, if $\chi_n(x, z) = 0$ then for $z' < z$ we have

$$\eta(x,z') \le \eta(x,z) \le nx - [nx]$$

thus $\chi_n(x, z') = 0$ also. Conversely, if $\chi_n(x, z) = 1$ then for $z' > z$ we have

$$nx - [nx] \le \eta(x,z) \le \eta(x,z')$$

thus $\chi_n(x, z') = 1$. Let $\phi \in L^1(\Omega)$. It follows from the Fubini Theorem that for *a.e.* $z \in (-b, b)$, $\phi(., z) \in L^1(0, 2\pi)$. Lemma A.1 in the Appendix of [9] shows that for a.e. $z \in \Omega$,

$$\int_0^{2\pi} H(nx,x,z)\phi(x,z)dx \longrightarrow \int_0^{2\pi} \eta(x,z)\phi(x,z)dx \ . \tag{17}$$

Note that no extraction of subsequences is needed here, *i.e.*, (17) holds pointwise. Furthermore, the absolute value of the right hand side is uniformly bounded by $\int_0^{2\pi} |\phi(x, z)|dx$ which is a L^1 function of z. It follows from the Fubini and Lebesgue Dominated Convergence Theorems that

$$\int_\Omega \chi_n \phi \longrightarrow \int_\Omega \eta\phi \ . \qquad \square$$

In the next two lemmas, we show that J^* is weakly continuous.

Lemma 5.2 *Assume that* $\{\eta_n\} \subset X^*$ *with* $\eta_n \rightharpoonup \eta \in X^*$, *weakly* $*$ *in* $L^\infty(\Omega)$. *Then,*

$$\partial_z \eta_n \quad \longrightarrow \quad \partial_z \eta \quad \textit{strongly in } H^{-1}(\Omega) \ . \tag{18}$$

Proof : We first show that if $\rho(z) \in L^\infty(-b,b)$ is an increasing function and if $\phi \in \mathcal{D}(-b,b)$, $\phi \geq 0$, then

$$< \partial_z \rho, \phi >_{H^{-1},H^1(-b,b)} \ \geq \ 0 \, . \tag{19}$$

Indeed, the right-hand side is equal to $-\int_{-b}^{b} \rho(z)\partial_z\phi(z)dz$. For N large enough, there exists a subdivision $-b < z_1 < \cdots < z_j < \cdots < z_N < b$ of $(-b,b)$ and a piecewise constant function

$$\rho_N(z) \quad = \quad \sum_{j=1}^{N} r_j \, \chi_{(z_j, z_j+1)}$$

with $r_j \leq r_{j+1}$, that approximates ρ in L^2. Since

$$\left| \int (\rho(z) - \rho_N(z))\partial_z\phi \right| \leq ||\rho - \rho_N||_{L^2} \, ||\partial_z\phi||_{L^2}$$

and

$$-\int \rho_N(z)\partial_z\phi = \sum_j (r_j - r_{j-1})\phi(z_j) \ \geq \ 0 \, ,$$

the inequality (19) follows.

To prove the lemma, consider now $\phi \in \mathcal{D}(\Omega)$, $\phi \geq 0$. For a.e. $x \in (0, 2\pi)$, the inequality (19) implies that

$$-\int_{-b}^{b} \eta_n(x,z)\partial_z\phi(x,z)dz \quad \geq \quad 0 \, ,$$

which yields $< \partial_z\eta_n, \phi >_{H^{-1},H^1(\Omega)} \geq 0$. Finally, the proof is complete by an application of Murat's Lemma as in the proof of Lemma 4.1. □

Lemma 5.3 *Assume that* $\{\eta_n\} \subset X^*$, *such that* $\eta_n \rightharpoonup \eta$ *weakly* in* L^∞. *Then*

$$J^*(\eta_n) \quad \longrightarrow \quad J^*(\eta) \ .$$

Proof : Since the effective matrix $A^*(\eta_n)$ is diagonal and η_n satisfies the right compactness property (from Lemma 5.2), the proof follows exactly that of Theorem 4.1. From the weak convergence of η_n to η, we get

$$\left\{ \begin{array}{lcl} m(\eta_n) & \rightharpoonup & m(\eta) \\ c^{-1}(\eta_n) & \rightharpoonup & c^{-1}(\eta) \end{array} \right. \quad \text{weak-}* \ \ L^\infty(\Omega) \, .$$

This convergence result is sufficient to verify that the effective limit of $A^*(\eta_n)$ is $A^*(\eta)$. □

Combining Theorem 4.1, Lemmas 5.1 and 5.3, we arrive at the following relaxation result.

Theorem 5.1 *Let J be the cost functional introduced in Section 3. The relaxed problem $min_{\eta \in X^*} J^*(\eta)$ has a solution. In addition*

$$inf_{\chi \in X} J(a_\chi) \quad = \quad min_{\eta \in X^*} J^*(\eta) \ .$$

Proof : Assume that $\{\eta_n\} \subset X^*$ is a minimizing sequence. Upon extracting a subsequence that converges weakly * to some $\eta \in X^*$, Lemma 5.3 yields $\liminf_{n\to\infty} J^*(\eta_n) = \liminf_{n\to\infty} J(A^*(\eta_n)) \geq J(A^*(\eta)) = J^*(\eta)$.

Consider now a minimizer $\eta \in X^*$. From Lemma 5.1, there exists a sequence of characteristic functions χ_n that define admissible interfaces, such that

$$\chi_n \rightharpoonup \eta \ .$$

It is immediate from Theorem 4.1 that $\lim_{n\to\infty} J(\chi_n) = J^*(\eta)$. □

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