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HOMOGENIZATION OF THREE-DIMENSIONAL FINITE PHOTONIC CRYSTALS

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1. INTRODUCTION

In the last decade, some advances have been made in a deeper understanding of the optical properties of photonic crytals. Such remarkable structures prohibit the propagation of light, or allow it only in certain directions at certain frequencies, or localize light in specified areas. This sort of material which affords us complete control over light propagation results when a small block of dielectric material is repeated in space. These structures, whose optical properties depend on the geometry of the crystal lattice, have been called Photonic Crystals [10–17]. PC are periodic devices which induces the so-called photonic band gaps just as electronic band gaps exist in semiconductors: light propagation is forbidden for certain frequencies in certain directions. This effect is well known and forms the basis of many devices, including Bragg mirror, dielectric Fabry-Perot filters, and distributed feedback lasers. All of these contain low-loss dielectrics that are periodic in one dimension, and therefore they are called one-dimensional photonic crystals. However, while such mirrors are tremendously useful, their reflecting properties highly depend upon the frequency of the incident wave in regard with its incidence. Actually, for some frequency range, one wishes to reflect light of any polarization at any angle (complete photonic band gap). This could be achieved with certain structures with periodicity in the three dimensions. Such a three dimensional photonic crystal has been engineered by Yablonovitch in 1987 [9]. The recent thrust in this area is partly fueled by advances in theoretical techniques, based on Fourier expansions in the vector electromagnetic Maxwell equations [7, 8], which allow non prohibiting computational calculus. This plane wave expansion method is by far the most popular theoretical tool employed for studying the photonic band gaps problem. In this paper, we adopt another point of view, based on asymptotic analysis techniques which have been used for a long time as applied to many problems of mechanic or electrostatic types [1]. Following the works of G. Bouchitté, R. Petit and D. Felbacq [2, 4, 6], we adapt these classical methods to electromagnetism for "three-dimensional finite periodic" structures.

At an atomic scale, matter behaves as if it were highly heterogeneous, but daily experiment shows it is rather homogeneous. Indeed, microscopic inhomogeneities can be smooth at a macroscopic scale (fluid aspect of fine sand...). At first sight, one can say that there are two kinds of inhomogeneities: the first ones of a periodic type (such as photonic crystals) and the others of a random type (such as amorphous glass).

In this paper we will deal with photonic structures, but it seems likely to adapt results to the stochastic case: roughly speaking, the period is changed in the mean distance between the scatterers. The incoming wave "averages" the microscopic asperities (microscopic in regard with its wavelength) whenever they are randomly or periodically arranged, provided that one makes the assumption that the obstacle is densely filled up. Indeed the incident wave "sees" the average of the asperities.

Hence, we consider a structure of constant permeability μ_0 (permeability in vacuum) lit by a monochromatic wave, whose wavelength λ is great in comparison with typical heterogeneity sizes. Consequently **the**

wavelength is great compared to the period η **of the medium**. Under such hypotheses, our goal is to replace the photonic crystal by an equivalent homogeneous structure, that is with analogous electromagnetic properties.

Thanks to our formalism, **we can treat three-dimensional structures of arbitrary shape** Ω_f **with a piecewise continuous complex valued permittivity. Such hypotheses cover the physical domains of application**. In this paper, we will pay special attention to the case where the permittivity is a piecewise constant function. Such a function describes inclusions in the scattering object we are studying. These inclusions are usually called scatterers. It is worth noting that a scatterer can possibly touch the sides of basic cells; for instance, **this allows us to study compact cubic structures such as face-centered cubic and simple cubic ones (Fig. 1) or the well-known "Yablonovite" [9–11]**. Moreover, when the number of scatterers is great, and when they are very small with regard to the wavelength, one can expect the structure to become homogeneous: that is to say that the scattering object behaves as if it were made of only one homogeneous material with a permittivity usually called effective permittivity by physicists.

From a theoretical point of view, one can only hope to obtain relevant results when the number of scatterers is infinite. Therefore, there are two ways of tackling this problem: the old one used by most of people, consists in assuming that the size of the scatterers is fixed, while the obstacle filled up by these scatterers is increasing until it covers the overall space $\mathbb{R}^3$, and the wavelength goes to infinity. It is a useful method in solid state physics, since it enables physicists to use the powerful tools of Bloch Wave Decomposition. The main drawback of this method, when applied to electromagnetism, is that the diffraction problem does not make sense anymore at the limit. In fact, **the incident field is then confined in the complementary of the overall space, and it is of null pulsatance!** On the contrary, if one considers that the obstacle and the wavelength remain fixed, while the size of scatterers goes to zero and their number to infinity, the boundary of the obstacle has still an influence at the limit, and one can still speak of incident wave. This process is much more complicated to perform than the first one, but the results it provides are closer to physical reality.

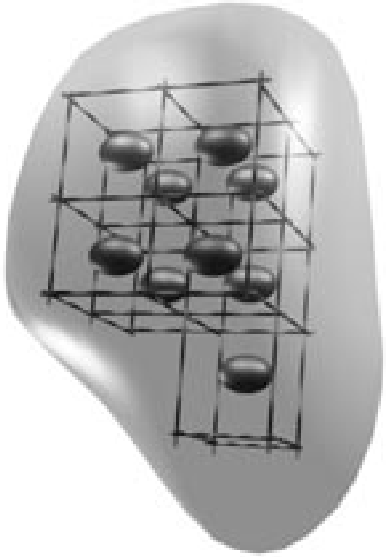

Figure 1. Homogenization of a photonic crystal made of ellipsoidal scatterers. The grid of dotted lines defines a virtual “scaffolding” Ω_η of the whole obstacle Ω_f. For the sake of simplicity, we give an example with η near from 1, i.e., with rather big scatterers and in a small number (here 9). The reader has to imagine the same body (Ω_f) filled with a great number of scatterers (on the order of 1000) of small size (η near from 0).

Homogenization techniques used in this paper, namely homogenization of diffraction, allow us to study structures of practical interest, for large wavelengths compared to the size of the scatterers of the obstacle. We achieve proofs by using a multiple scale method and, to be more precise, find what is generally called the effective permittivity of the homogeneous object. This one depends upon a local problem arising in the crystal lattice unlike the one of solid state physics which takes place in the first Brillouin zone. Contrary to the effective permittivity given by the method of Bloch waves decomposition, our permittivity also depends upon a global problem which takes into account the boundary conditions. This work is actually an extension of the ones performed in the 2D scalar cases (TE and TM) by D. Felbacq and G. Bouchitté [6], who were among the pioneers in the homogenization of diffraction.

2. SET UP OF THE PROBLEM

From now on, assuming a time dependence in $e^{-i\omega t}$, we will deal with time harmonic Maxwell equations.

For this study, we have to consider objects of opposite natures: the first ones are purely geometrical and the others merely physical.

The first approach is a geometrical description of the obstacle, which lies in a fixed domain Ω_f not necessarily simply connex. Furthermore, although our study only deals with the bounded case, it remains relevant for Ω_f infinite in one (Fig. 2) or two directions (Fig. 3). In such cases, one just has to adapt the study with "ad hoc" outgoing wave conditions (as for gratings, the reader may refer to [22]).

The second approach (a physical one) describes the optical characteristics of the material lightened by the electromagnetic wave.

Let us begin by the geometrical description of the objects involved in our study.

Let (O, x_1, x_2, x_3) be a Cartesian coordinates system of axes of origin O, $\mathbf{i} = (\mathbf{i_1}, \mathbf{i_2}, \mathbf{i_3})$ a multi-integer of $\mathbb{Z}^3$ and η a small positive real. Let $Y =]0;1[^3$ be a basic cell, and $\tau_i\,Y$ be the translation of Y by the vector $\mathbf{i}$:

$$\tau_i(Y) =]i_1, i_1+1[\times]i_2, i_2+1[\times]i_3, i_3+1[= Y + \mathbf{i}$$

Let us design by $\eta\,(\tau_i Y)$ the homothety on $\tau_i Y$ of ratio η: thus we form a box of size η and from center $\eta\mathbf{i}$ (Fig. 4).

Under such considerations, one can now define a "scaffolding" Ω_η of Ω_f in the following manner: Ω_η is defined as the greatest (in set acceptation) union of boxes of size η which is entirely enclosed in Ω_f and whose fineness is controlled by η. More precisely, the finer the scaffolding (the smaller the η), the better the imitation (Fig. 5). Obviously, as we wish to "build up" Ω_f, the number N_η of cells depends upon η, since it corresponds the following equivalence:

$$N_\eta = \frac{meas(\Omega_\eta)}{\eta^3} \simeq \frac{meas(\Omega_f)}{\eta^3}$$

where $meas(\Omega_\eta)$ and $meas(\Omega_f)$ respectively denotes the measure (volume) of Ω_η and Ω_f.

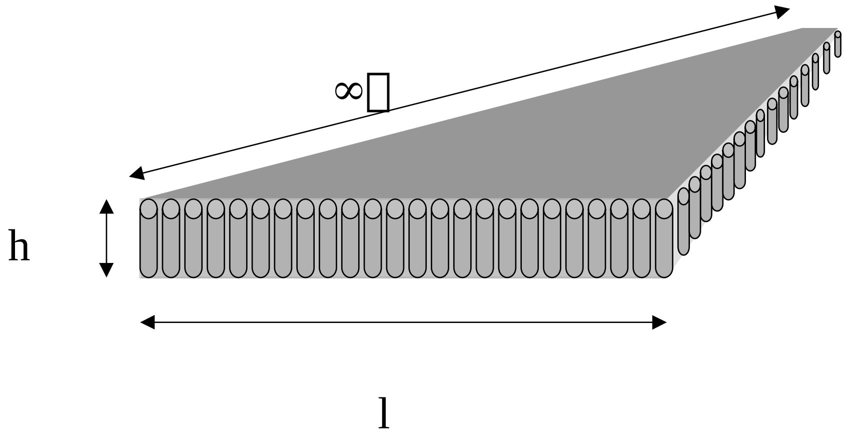

Figure 2. Band of finite parallel rods seen as a three-dimensional photonic crystal infinite in one direction.

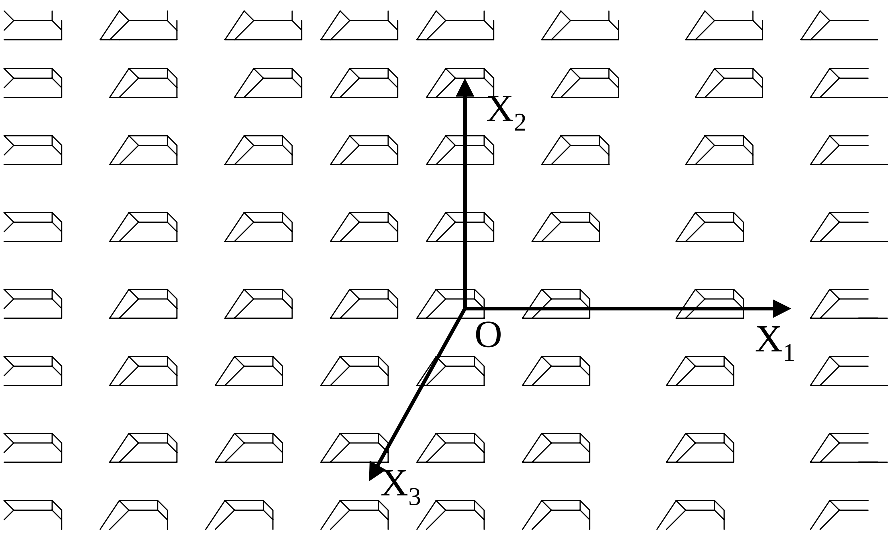

Figure 3. Bi-grating seen as a three-dimensional photonic crystal bounded in the x_3 axis.

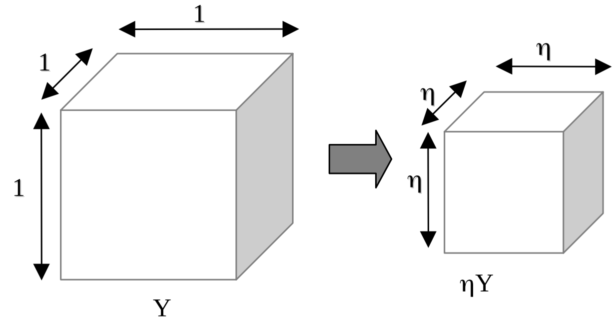

Figure 4. The elementary cell of the photonic crystal is the homothety on a unit cell of ratio η .

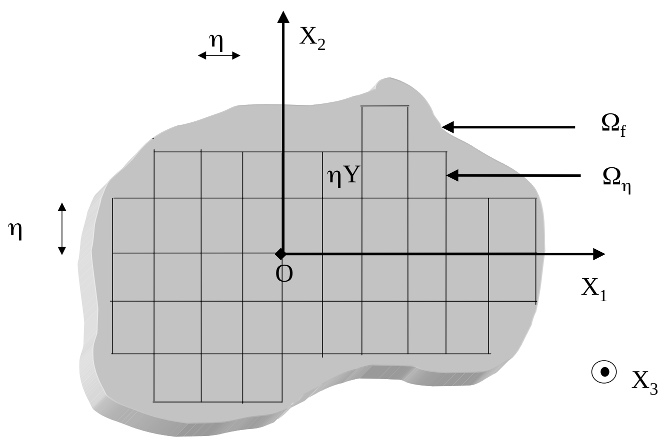

Figure 5. The process of homogenization consists in a periodic arrangement of rescaled unit cells, forming a succession of "scaffoldings" Ω_η entirely enclosed in the diffracting object Ω_f .

We can now start the description of the physical problem we are interested in.

Let us define what we will call up to the end a Scattering-Box (SB): we note B an obstacle merely defined by its relative permittivity $\varepsilon_r^B(\mathbf{x})$:

$$\forall \mathbf{x} \in \mathbb{R}^3,\ \varepsilon_r^B(\mathbf{x}) = 1 - \chi_Y + \chi_Y\, \tilde{\varepsilon}_r(\mathbf{x})\ ,$$

with χ_Y the characteristic function of Y (i.e., $\chi_Y = 1$ when $x \in Y$ and $\chi_Y = 0$ elsewhere) and where $\tilde{\varepsilon}_r(\mathbf{x})$ is a given piecewise continuous complex valued function, which denotes the relative permittivity in the overall physical space. By analogy with the geometrical study developed above, we define $\tau_i B$, $\eta\ (\tau_i B)$ and B_η . Thus, as η goes to 0, we build up a sequence of three-dimensional bounded structures B_η made of a periodic arrangement of an increasing number N_η of identical SB of decreasing size, whose global shape Ω_η tends to Ω_f .

For each obstacle B_η , we can define a total field $F_\eta = (E^d_\eta, H^d_\eta)$, corresponding to the field generated by the N_η SB when they are illuminated by a given incident monochromatic wave of wavelength λ . As explained above, our purpose is to make clear the behavior of F_η when η goes to zero. In other words, we try to understand the electromagnetic behavior of our set of SB when their size tends to zero and their number to infinity. It is obvious that for all $\mathbf{x}$ in Ω_η, $\varepsilon_r^{B_\eta}(\mathbf{x}) = \varepsilon_r^B(\frac{\mathbf{x}}{\eta})$, where ε_r^B is a Y-periodic complex valued function in Ω_f such that $0 \le arg(\omega\varepsilon) < \pi$ et Re $(i\omega\varepsilon) \le 0$. **Hence, unlike most of the articles dealing with solid state physics, we do not assume periodicity of ε_r^B in the overall space $\mathbb{R}^3$.**

Moreover, let us note the relative permittivity at every point $\mathbf{x} \in \mathbb{R}^3$ by $\varepsilon_\eta(\mathbf{x}) = \tilde{\varepsilon}(\mathbf{x}, \frac{\mathbf{x}}{\eta})$, with

$$\tilde{\varepsilon}(\mathbf{x}, \mathbf{y}) = \begin{cases} 1 & , \text{ if } \mathbf{x} \in \Omega_\eta^c \\ \varepsilon_r^{B_\eta}(\mathbf{y}) & , \text{ if } \mathbf{x} \in \Omega_\eta \end{cases}$$

where Ω_η^c denotes the complementary of the obstacle in the overall space $\mathbb{R}^3$ i.e., $\mathbb{R}^3 \setminus \bar{\Omega}_\eta$.

This is the crucial point of our discussion: unlike ε_r^B , this function can be seen as a Y-periodic function of the y variable (which continuously depends on its variable x). Therefore, we can introduce $(\mathbf{E}^d_\eta, \mathbf{H}^d_\eta)$ the diffracted field (which only makes sense outside the structure) deduced from the incident field $(\mathbf{E}^i, \mathbf{H}^i)$ lightening the structure by $(\mathbf{E}^d_\eta, \mathbf{H}^d_\eta) = (\mathbf{E}_\eta, \mathbf{H}_\eta) - (\mathbf{E}^i, \mathbf{H}^i)$. It is worth noting that we can rigorously define the diffracted field, as the structure does not cover the overall space, which emphasizes the importance of its boundary. Thus by defining the complex wave number k_0 as $k_0 = \omega(\varepsilon_0\mu_0)^{\frac{1}{2}}$, we obtain the following problem of electromagnetic scattering:

$$\mathcal{P}_\eta = \begin{cases} (1)\ \mathrm{curl}\,\mathbf{E}_\eta + i\omega\mu_0\mathbf{H}_\eta = 0 \\ (2)\ \mathrm{curl}\,\mathbf{H}_\eta - i\omega\varepsilon_0\varepsilon_\eta\mathbf{E}_\eta = 0 \\ (SM1)\ \mathbf{H}^d_\eta = O\left(\dfrac{1}{|\,\mathbf{x}\,|}\right),\ \mathbf{E}^d_\eta = O\left(\dfrac{1}{|\,\mathbf{x}\,|}\right) \\ (SM2)\ k_0\mathbf{E}^d_\eta + \omega\mu\left(\dfrac{\mathbf{x}}{|\,\mathbf{x}\,|}\wedge\mathbf{H}^d_\eta\right) = o\left(\dfrac{1}{|\,\mathbf{x}\,|}\right) \end{cases}$$

where $(SM1)$, $(SM2)$ denote the outgoing wave conditions of Silver-Müller type, which play a fundamental role by insuring existence and uniqueness of the solution of $\mathcal{P}_\eta$ (see for example Cessenat [25]).

Of course, equations (1) and (2) of the above system make sense when assuming that $\mathbf{E}_\eta$ and $\mathbf{H}_\eta$ and all their derivatives are taken in the sense of distributions in the overall space $\mathbb{R}^3$. As concerning the radiation conditions, they are relevant in $C^\infty(\mathbb{R}^3\setminus\bar{\Omega}_\eta)$. That is to say that $\mathbf{E}_\eta$ and $\mathbf{H}_\eta$ are continuous and all their derivatives outside the obstacle (it is a consequence of the Helmholtz equation arising outside the obstacle, which induces analicity of the diffracted electromagnetic field). From now on, we will always assume these hypotheses.

If we take the curl of the former equations we then have two similar problems:

$$(\mathcal{P}^E_\eta)\begin{cases} (1^E)\ \mathrm{curl}\,\mathrm{curl}\,\mathbf{E}_\eta - k_0^2\varepsilon_\eta\mathbf{E}_\eta = 0 \\ (SM1^E)\ \mathbf{E}^d_\eta = O\left(\dfrac{1}{|\,\mathbf{x}\,|}\right) \\ (SM2^E)\ \dfrac{\mathbf{x}}{|\,\mathbf{x}\,|}\wedge\mathrm{curl}\,\mathbf{E}^d_\eta + ik\mathbf{E}^d_\eta = o\left(\dfrac{1}{|\,\mathbf{x}\,|}\right) \end{cases}$$

$$(\mathcal{P}^H_\eta)\begin{cases} (1^H)\ \mathrm{curl}\,\left(\varepsilon_\eta^{-1}\mathrm{curl}\,\mathbf{H}_\eta\right) - k_0^2\mathbf{H}_\eta = 0 \\ (SM1^H)\ \mathbf{H}^d_\eta = O\left(\dfrac{1}{|\,\mathbf{x}\,|}\right) \\ (SM2^H)\ \dfrac{\mathbf{x}}{|\,\mathbf{x}\,|}\wedge\mathrm{curl}\,\mathbf{H}^d_\eta + ik\mathbf{H}^d_\eta = o\left(\dfrac{1}{|\,\mathbf{x}\,|}\right) \end{cases}$$

At this point, let us note that it appears much more difficult to perform the study of the problem $\mathcal{P}^E_\eta$ than the one of the problem $\mathcal{P}^H_\eta$: the divergence of $\mathbf{H}_\eta$ is null, contrary to $\mathrm{div}\,\mathbf{E}_\eta = O(\frac{1}{\eta})$. Indeed, $\mathrm{div}\,(\varepsilon_\eta\mathbf{E}_\eta) = \varepsilon_\eta\mathrm{div}\mathbf{E}_\eta + \nabla\varepsilon_\eta\cdot\mathbf{E}_\eta$ which implies that $\mathrm{div}\,\mathbf{E}_\eta = -\frac{\nabla_y\varepsilon(x,y)_{|y=\frac{1}{\eta}}}{\eta\varepsilon_\eta}$, by using the third Maxwell equation. The behavior of the gradient of $\mathbf{E}_\eta$ being related to the ones of the divergence and the curl of $\mathbf{E}_\eta$, it implies strong oscillations for the gradient of the electric field $\mathbf{E}_\eta$.

Hence, in the rest of the study we will exclusively deal with $\mathcal{P}_\eta^H$. Taking into account that $\mathbf{E}_\eta = \frac{i}{\omega\varepsilon_0\varepsilon_\eta}\mathrm{curl}\,\mathbf{H}_\eta$ (from equation (2)), we will come back to the couple $(\mathbf{E}_\eta, \mathbf{H}_\eta)$, solution of the initial problem $\mathcal{P}_\eta$ by taking the curl of $\mathbf{H}_\eta$, solution of the problem $\mathcal{P}_\eta^H$.

To conclude this introduction, let us recall that in this paper, we will only pass to the limit on the problem $(\mathcal{P}_\eta^H)$, for the reason explained above. Furthermore, we will say in what sense does the field $\mathbf{H}_\eta$ tend to a field $\mathbf{H}_{hom}$ generally called homogenized field, solution of the so called homogenized diffraction problem $(\mathcal{P}_{hom}^H)$, whose resolution leads with an annex problem of electrostatic type which will be explained further.

Finally, we let the conductivity tend to infinity in the homogenized problem.

3. ASYMPTOTIC ANALYSIS

The main idea of homogenization of diffraction is to select two scales in the study: a microscopic one (the size of the basic cell) and a mesoscopic one (the size of the whole obstacle of shape Ω_f). From a physical point of view, one can say that the modulus of the incident field is forced to oscillate like the permittivity in the lightened periodic structure. In fact, the smaller the size η of the SB, the faster the modulus of the field F_η oscillates. Hence, we suppose that $\mathbf{H}_\eta$, solution of the problem $\mathcal{P}_\eta^{\mathbf{H}}$ has a two-scale expansion of the form:

$$\forall \mathbf{x} \in \Omega_f, \;\; \mathbf{H}_\eta(\mathbf{x}) = \mathbf{H}_0\left(\mathbf{x}, \frac{\mathbf{x}}{\eta}\right) + \eta\mathbf{H}_1\left(\mathbf{x}, \frac{\mathbf{x}}{\eta}\right) + \eta^2\mathbf{H}_2\left(\mathbf{x}, \frac{\mathbf{x}}{\eta}\right) + \ldots$$

where $\mathbf{H}_i : \Omega_f \times Y \longmapsto \mathbb{C}^3$ is a smooth function of 6 variables, independent of η, such that $\forall \mathbf{x} \in \Omega_f,\; \mathbf{H}_i(\mathbf{x}, \cdot)$ is Y-periodic.

Our goal is to characterize the electromagnetic field when η tends to 0. If the coefficients $\mathbf{H}_i$ do not increase "too much" when η tends to 0, the limit of $\mathbf{H}_\eta$ will be $\mathbf{H}_0$, the rougher approximation of $\mathbf{H}_\eta$. Hence, we make the assumption that for all $\mathbf{x} \in \mathbb{R}^3,\; \mathbf{H}_i(\mathbf{x}, \frac{\mathbf{x}}{\eta}) = o(\frac{\mathbf{x}}{\eta^i})$, so that the expansion (also denoted by the german word "ansatz") still makes sense in neighbourhood of 0. If the above expansion is relevant, we can state the following fundamental result:

Fundamental theorem 1 *When* η *tends to zero,* $\mathbf{H}_\eta$ *solution of the problem* $(\mathcal{P}_\eta^H)$*, converges (for the norm of energy on every compact subset of* $\mathbb{R}^3$*) to the unique solution* $\mathbf{H}_{hom}$ *of the following problem* $(\mathcal{P}_{hom}^{\mathbf{H}})$ *:*

$$(\mathcal{P}_{hom}^{\mathbf{H}}) = \begin{cases} \text{curl}\,\left(\varepsilon_{hom}^{-1}(\mathbf{x})\text{curl}\,\mathbf{H}_{hom}(\mathbf{x})\right) - k_0^2\mathbf{H}_{hom}(\mathbf{x}) = 0 \\ \mathbf{H}_{hom}^d(\mathbf{x}) = O\left(\dfrac{1}{|\,\mathbf{x}\,|}\right) \\ \dfrac{\mathbf{x}}{|\,\mathbf{x}\,|} \wedge \text{curl}\,\mathbf{H}_{hom}^d(\mathbf{x}) + ik\mathbf{H}_{hom}^d(\mathbf{x}) = o\left(\dfrac{1}{|\,\mathbf{x}\,|}\right) \end{cases}$$

With

$$\begin{cases} \varepsilon_{hom}(\mathbf{x}) = \left\langle \tilde{\varepsilon}(\mathbf{x},\mathbf{y})(I - \nabla_{\mathbf{y}}\mathbf{V}_Y(\mathbf{y}))\right\rangle_Y & , \textit{ in } \Omega_f \\ \varepsilon_{hom}(\mathbf{x}) = 1 & , \textit{ in } \Omega_f^c \end{cases}$$

Where $< f >_Y$ *and* $\tilde{\varepsilon}(\mathbf{x},\mathbf{y})$ *respectively denote the average of* f *in* Y *(i.e.,* $\int_Y f(x,y)\,dy$*) and*

$$\tilde{\varepsilon}(\mathbf{x},\mathbf{y}) = \begin{cases} 1 & , \textit{ if } \mathbf{x} \in \Omega_f^c \\ \varepsilon_r^B(\mathbf{y}) & , \textit{ if } \mathbf{x} \in \Omega_f \end{cases}$$

Besides, $\mathbf{V}_Y = (V_1, V_2, V_3)$*, where* V_j*,* $j \in \{1,2,3\}$ *is the unique solution in* $H_\sharp^1(Y)/\mathbb{R}$ *(that is to say that* V_j *are defined up to an additive constant in the Hilbert space of* Y*-periodic functions* $H_\sharp^1(Y)$*) of one of the three following problems* $(\mathcal{K}_j)$ *of electrostatic type:*

$$(\mathcal{K}_j) : -\text{div}_{\mathbf{y}}\left[\varepsilon_r^B(\mathbf{y})\left(\nabla_{\mathbf{y}}(V_j(\mathbf{y}) - y_j)\right)\right] = 0\,, \quad j \in \{1,2,3\}$$

Roughly speaking, as η tends to zero, we can replace the isotropic heterogeneous diffracting obstacle of shape Ω_η, by an anisotropic homogeneous obstacle of shape Ω_f. In other terms, the effective permittivity is given by what follows.

Developed form for the matrix of effective permittivity

The relative permittivity matrix of the homogenized problem is equal to:

$$\varepsilon_{hom} = \begin{pmatrix} \langle \varepsilon(y) \rangle_Y & 0 & 0 \\ 0 & \langle \varepsilon(y) \rangle_Y & 0 \\ 0 & 0 & \langle \varepsilon(y) \rangle_Y \end{pmatrix} - \begin{pmatrix} \varphi_{11} & \varphi_{12} & \varphi_{13} \\ \varphi_{21} & \varphi_{22} & \varphi_{23} \\ \varphi_{31} & \varphi_{32} & \varphi_{33} \end{pmatrix}$$

where φ_{ij} represent corrective terms defined by:

$$\forall i, j \in \{1,2,3\},\ \varphi_{ij} = \left\langle \varepsilon \frac{\partial V_j}{\partial y_i} \right\rangle_Y = \left\langle \varepsilon \frac{\partial V_i}{\partial y_j} \right\rangle_Y = -\langle \varepsilon \bigtriangledown V_i \cdot \bigtriangledown V_j \rangle_Y$$

the brackets denoting averaging over Y, and V_j being the unique solutions in $H^1_\sharp(Y)/I\!R$ of the three partial differential equations $\mathcal{K}_j$. Hence, thanks to the symmetry of the right matrix above ($\varphi_{ij} = \varphi_{ji}$), the homogenized permittivity is given by the knowledge of six terms φ_{ij}, depending upon the resolution of three annex problems $\mathcal{K}_j$.

Proof of the corollary

As for the homogenized permittivity, $\bigtriangledown_y \mathbf{V}_Y$ denoting the Jacobian matrix $\frac{\partial V_j}{\partial y_i}$ of $\mathbf{V}_Y$, ε_{hom} clearly derives from the equation of the theorem.

Multiplying $\mathrm{div}_y (\varepsilon \bigtriangledown_y (V_i - y_i))$ by V_j, $j \in \{1,2,3\}$, and integrating by parts over the basic cell Y leads to: $\langle \varepsilon(y) (\bigtriangledown_y (V_i - y_i)) \cdot V_j \rangle_Y = 0$. Therefore, we get the equality:

$$\begin{aligned} \varphi_{ij} &= \left\langle \varepsilon \frac{\partial V_i}{\partial y_j} \right\rangle_Y \\ &= -\langle \varepsilon \bigtriangledown V_i \cdot \bigtriangledown V_j \rangle_Y \\ &= \left\langle \varepsilon \frac{\partial V_j}{\partial y_i} \right\rangle_Y , \quad i \text{ and } j \text{ playing a symmetrical role} \end{aligned}$$

Hence, we derive that $\varphi_{ij} = \varphi_{ji}$.

4. PRACTICAL APPLICATION

In most applications, one has just to consider a two valued piecewise constant permittivity in the unit cell Y and more precisely, the relative permittivity yields ε_r in what we will call, from now on, the scatterer

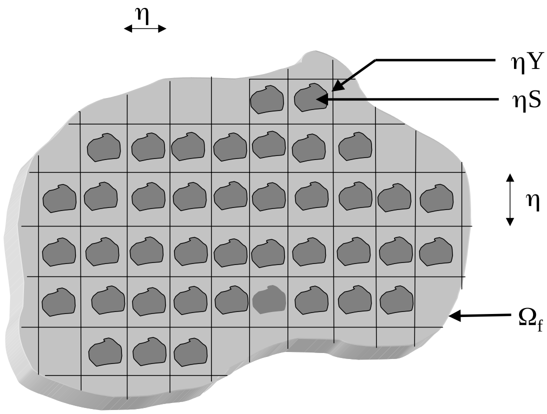

Figure 6. The elementary cell of the three-dimensional photonic crystal's lattice results of a homothety of ratio η over a unit cell.

S and 1 elsewhere. It is the case, for instance, of the structures studied by E. Yablonovitch [9]. Consequently, the problem we are dealing with is only defined by a complex number ε_{scat} and the shape of the scatterers $\Omega_S = Supp\{\varepsilon_r - 1\}$ (in other words, the scatterers lie in the volume area, support of the above function). It is worth noting that one can give many shapes to S, except the ones with very irregular boundaries: this covers most of the structures encountered in physics (cubic compact structures, Yablonovite...). Before going further, it is worth noting that the limit behavior of the complex permittivity ε_η of the set Ω_η is crucially related to the limit filling ratio of the elementary cells:

$$\theta = \lim_{\eta \to 0} \frac{meas(f(\eta)\Omega_S)}{\eta^3}$$

where $meas(f(\eta)\Omega_S)$ denotes the volume occupied by the homothety on Ω_S of ratio $f(\eta)$ i.e., $f(\eta)\Omega_S$ in Y_η (Fig. 6). Indeed, when θ equals zero the scatterers "disappear" when η tends to 0, and the effective medium is completely transparent (e.g., $f(\eta) = \eta^2$).

On the contrary, the structure becomes homogeneous (but not invisible) at the limit when $\theta \neq 0$ i.e., when $f(\eta) = \eta$ (if the reader wants to convince himself from this remark, he just has to make an expansion (ansatz) with functions $H_i(x, \frac{x}{\eta^\alpha})$, $\alpha > 1$).

This remark seems trivial at first glance, but one has to be careful with the behavior of the structure in the case where it is filled up

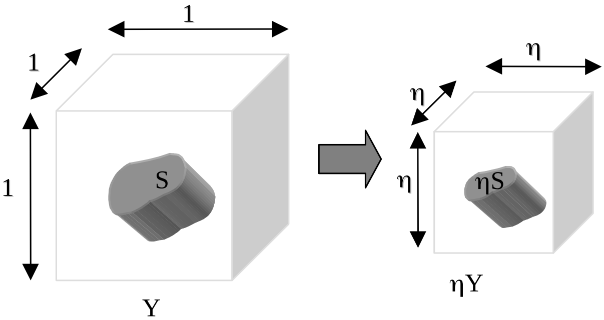

Figure 7. The imitation of the photonic crystal results when a small scatterer ηS is periodically distributed in the whole diffracting object Ω_f .

by infinite conducting scatterers. Indeed, having regard to the results obtained by D. Felbacq and G. Bouchitté, in [6], in the two-dimensional case, we can see that, even if θ equals zero, (the scatterers therefore vanish at the limit), their influence is still sensible on the effective medium.

In daily experiments, scatterers are made of one isotropic material characterized by a permittivity ε_{scat} (Fig. 7). Then, for every point $\mathbf{x} \in \mathbb{R}^3$, the permittivity is defined by:

$$\tilde{\varepsilon}_\eta(\mathbf{x}) = \varepsilon_{scat} \,, \text{ if } \mathbf{x} \in \eta\Omega_S \,, \; \tilde{\varepsilon}_\eta(\mathbf{x}) = 1 \text{ if } \mathbf{x} \notin \eta\Omega_S$$

where ε_{scat} is a bounded function, supposed to be Y-periodic with:

$$\text{Re } (\varepsilon_{scat}(y)) > 0 \,, \; \text{Im } (\varepsilon_{scat}(y)) \geq 0$$

Dielectric case

As η tends to zero, the collection of scatterers may be replaced by an anisotropic homogeneous obstacle of shape Ω_f . The relative permittivity is then given by the following lemma:

Lemma 1 *The resolution of the three annex problems $\mathcal{K}_i$ introduced in the fundamental theorem 1 amounts to look for functions V_i solutions of the following system (Fig. 8), where derivatives are taken in the usual sense:*

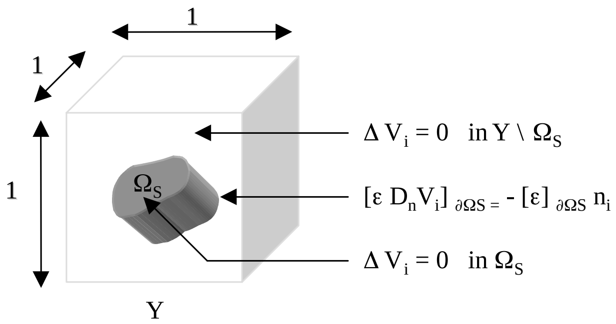

Figure 8. Description of the annex problem in the dielectric case. The scatterer can possibly touch the boundary of the elementary cell, which allows us studying dielectric structures made for example of parallel rods (Fig. 2).

$$\begin{cases} \Delta V_i & = 0 \ , \ in \ Y \setminus \partial\Omega_S \\ \left[\varepsilon \ \dfrac{\partial V_i}{\partial n} \right]_{\partial\Omega_S} & = -[\varepsilon]_{\partial\Omega_S} \ n_i \\ [V_i]_{\partial\Omega_S} & = 0 \end{cases}$$

with

$$\varepsilon = \begin{cases} \varepsilon_{scat} & , \text{in } \Omega_S \\ 1 & , \text{in } Y \setminus \bar{\Omega}_S \end{cases}$$

$[f]_{\partial\Omega_S}$ *denotes the jump of* f *across the boundary* $\partial\Omega_S$ *, and* n_i *,* $i \in \{1,2,3\}$ *, denotes the projection on the axis* e_i *of a normal of* $\partial\Omega_S$ *.*

Proof:

Let us denote by e_i , $i \in \{1,2,3\}$ the three vectors of the orthonormal base of $\mathbb{R}^3$. As already seen, the problem verified by V_i can be written:

$$\mathcal{K}_i : \ \text{div}_y \left(\varepsilon(y) \left(\nabla_y V_i + e_i \right) \right) = 0 \ , i \in \{1,2,3\}$$

This expression must be taken in the sense of distributions. Applying the formula of derivatives in the sense of distributions and keeping in mind that all functions of $H^1_\sharp(Y)/\mathbb{R}$ are continuous leads to:

$$\varepsilon \nabla V_i = \varepsilon \{ \nabla V_i \}$$

Where the derivatives in the left member must be taken in distribution sense and the ones in the right member in usual sense (brackets).

Taking the divergence of this expression we get:

$$\mathrm{div}(\varepsilon \bigtriangledown V_i + \varepsilon e_i) = \varepsilon\{\Delta V_i\} + [\varepsilon]_{\partial\Omega_S} n \cdot e_i \delta_{\partial\Omega_S} + \underbrace{[\varepsilon \bigtriangledown V_i] n}_{\left[\varepsilon \frac{\partial V_i}{\partial n}\right]} \delta_{\partial\Omega_S}$$

Equaling on the one hand the regular part and on the other hand the singular part of the above distribution we obtain the expected result.

These results call for further comments detailed in the two following remarks.

Remark about the physical sense of the annex problem

Coming back for a while to the general case, the annex problem can be rewritten as $\mathrm{div}_y(\varepsilon(y) \bigtriangledown_y V_i) = -\mathrm{div}_y(\varepsilon \bigtriangledown_y y_i)$ which can be seen as an electrostatic problem with a volumic distribution of charges $\rho_i = \mathrm{div}_y(\varepsilon \bigtriangledown_y y_i)$.

In a similar way, in the case were ε is a two valued piecewise constant function (the case encountered in most manufactured optical devices), we can write that:

$$\mathrm{div}_y(\varepsilon(y) \bigtriangledown_y V_i) = -\sigma_i \delta_{\partial\Omega_S}$$

where σ_i is a surfacic distribution of charges defined by $\sigma_i = [\varepsilon] n_i \delta_{\partial\Omega_S}$.

Solving the annex problem for a two valued piecewise constant permittivity, reduces then to look for potential induced by surfacic density of charges on the edge of the scatterer. This result is not surprising, unlike the following remark which plays a fundamental role in numerical implementations.

Remark about the numerical calculus of the permittivity

In the fundamental theorem we have seen that the relative permittivity matrix of the homogenized problem is deduced from 6 numbers φ_{ij} defined as follows:

$$\varphi_{ij} = \int_Y \varepsilon(y) \frac{\partial V_i}{\partial y_j} \, dy \; ,$$

ε being a two-valued piecewise permittivity, we then deduce that:

$$\varphi_{ij} = 1 \int_{Y - \bar{\Omega}_S} \frac{\partial V_i}{\partial y_j} \, d\mathbf{y} - \varepsilon_{scat} \int_{\Omega_S} \left\{ \frac{\partial V_i}{\partial y_j} \right\} \, d\mathbf{y}$$

It then follows that:

$$\varphi_{ij} = 1 \int_{Y-\bar{\Omega}_S} \mathrm{div}(V_i e_j)\, d\mathbf{y} - \varepsilon_{scat} \int_{\Omega_S} \mathrm{div}(V_i e_j)\, d\mathbf{y}$$
$$= \int_Y \mathrm{div}(V_i e_j)\, dy + (\varepsilon_{scat} - 1) \int_{\Omega_s} \mathrm{div}(V_i e_j)\, dy$$

Applying the Green formula, due to the antiperiodicity of the outer normal $\mathbf{n}$ to ∂Y the integral over Y vanishes, and we obtain that:

$$\varphi_{ij} = (\varepsilon_{scat} - 1) \int_{\partial\Omega_S} V_i\, n_j\, ds = [\varepsilon] \int_{\partial\Omega_S} V_i\, n_j\, ds$$

Let us remark that V_i is well defined on $\partial\Omega_S$ because it doesn't suffer a jump across the boundary of the scatterer. This last formula is very important for numerical implementations: it is not necessary to compute the gradient of V (which gives rise to numerical inaccuracy) to perform the calculus of the homogenized permittivity, which is far beyond our first thoughts on the matter. We can then hope a faster convergence as that was first expected.

The reader may be surprised of the last expression which seems to give a permittivity depending upon the choice of the potential V (V is defined up to an additive constant). In fact thanks to the nullity of $\int_{\partial\Omega_S} n_i\, ds$, the permittivity is well defined.

As concerning the numerical implementations, a method of fictitious sources is being adapted to the resolution of the annex problem on the torus $\boldsymbol{T}_Y$ [19]. Roughly speaking, $\boldsymbol{T}_Y = Y/\mathbb{R}^3$ is a unit cell whose opposite sides are stuck together. This geometrical vision enables us to take once more into account the boundedness of the whole obstacle. Indeed, when speaking of a unit cell periodically arranged in space, we come back to the paradox of Fourier expansion when applied to a diffraction problem.

Infinite conducting case

Let us first notice that in this section, we do not pretend to achieve the study of homogenization of photonic crystals with metallic inclusions. Here, we just study a case consisting in letting the conductivity tends to infinity in the homogenized problem. Therefore, we are not face to problems of cohomology type when deriving the expression of $\mathbf{E}_0$ from $\mathrm{curl}_{\mathbf{y}}\,(\mathbf{E}_0(\mathbf{x},\mathbf{y})) = 0$ (see next section).

That is to say that we cannot deal with problems involving surface currents. Works are in progress in this much more complicated case

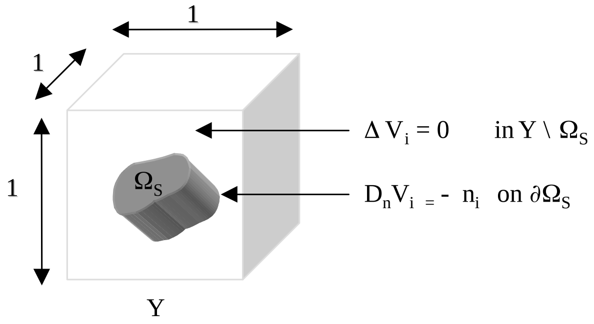

Figure 9. Description of the annex problem in the metallic case. One has to be carefull if the scatterer touch the boundary of the unit cell: when some scatterers are stuck together to form a set of parallel rodes, there are numerical inaccuracies.

by D. Felbacq and G. Bouchitté. Following the results obtained by these authors in the two dimensional case, it can be seen that the limit problem rely on the manner in which the scatterers vanish face to the volume of the basic cells.

Lemma 2 *If we assume that* $\Theta \neq 0$ *, we get the following expression for the effective permittivity (note that the average is taken on the complementary of the metallic scatterer):*

$$\varepsilon_{hom} =< (I - \bigtriangledown_y \mathbf{V}_Y >_{Y \setminus \Omega_S}$$

with

$$\left\{ \begin{array}{l} \Delta V_i = 0 \ , \ in \ Y \setminus \Omega_S \\ \dfrac{\partial V_i}{\partial n} = -n_i \ , \ on \ \partial\Omega_S \end{array} \right.$$

Denoting by Ψ_{ij} *the average* $\left\langle \frac{\partial V_i}{\partial y_j} \right\rangle_{Y \setminus \Omega_S}$*, as for the dielectric case, we prove that:*

$$\forall i, j \in \{1, 2, 3\},$$
$$\varphi_{ij} = \left\langle \frac{\partial V_j}{\partial y_i} \right\rangle_{Y \setminus \Omega_S} = \left\langle \frac{\partial V_i}{\partial y_j} \right\rangle_{Y \setminus \Omega_S} = - \left\langle \bigtriangledown V_i \cdot \bigtriangledown V_j \right\rangle_{Y \setminus \Omega_S}$$

A heuristic method to get this system (Fig. 9) is to let the conductivity tend to infinity in the annex problem of the dielectric case.

One has to be careful in the sense given to this result: the natural homogenization process would be to study the behavior of a sequence of diffraction problems $\mathcal{P}_\eta$ modelizing diffraction of obstacles with metallic inclusions. Whereas in our method, we artificially let the conductivity tend to infinity in the homogenized diffraction problem. Hence, it is very likely that letting the conductivity tend to infinity and then passing to the limit over η will lead to another problem at the limit. Nevertheless, although different, our limit problem is interesting by itself (it gives an idea on the behavior of metallic photonic crystals at large wavelengths when the basic cell and its scatterer vanish in the same way).

The case of spherical scatterers

In that case, for both dielectric and metallic scatterers, the homogenized medium is isotropic, and the tensor of the effective permittivity reduces to a scalar which appears to be $\varepsilon_{hom} = <\varepsilon(y)>_Y - \varphi_{11}$, in the dielectric case and $\varepsilon_{hom} = (1-\Theta) - \Psi_{11}$ in the metallic case, since $\varphi_{ii} = \varphi_{jj}$ (resp. $\Psi_{ii} = \Psi_{jj}$) and $\varphi_{ij} = 0$ (resp. $\Psi_{ij} = 0$) for $i \neq j,\ i,j \in \{1,2,3\}$.

5. CONCLUSION

In this paper, we present an alternative to the use of the plane-wave-expansion method as applied to the homogenization of three-dimensional finite photonic crystals. The so called multiple scale expansion allows us to consider, unlike the Fourier expansion method, taking into account the effects of the crystal's boundary on the diffracted field. Furthermore, we give explicitly the expression of the effective permittivity which characterizes an anisotropic medium and thus that may exhibit sizable birefringence. We then propose a numerical approach to give the terms of the tensor of permittivity: it consists in deriving its terms from the resolution of three annex problems of electrostatic type by using a method of fictitious sources [18] on a torus (the annex problem obtained by D. Felbacq and G. Bouchitté in the $H \parallel$ case [6] has been recently resolved by this way). It is to be noticed that our asymptotic analysis still holds when applied to the study of crystals bounded solely in one direction (bi-gratings) or two directions (rods). It is then straightforward to study the homogenization of bigratings: (the reader may refer to [21] or [22] to find adapted radiation conditions), which is a natural extension of the works led in

[3] and [5]. Work is also proceeding on the homogenization of finite photonic crystals, whose basic cell is not paralellepipedical, by the use of differential forms.

APPENDIX

A.1 The Multiple-Scale Expansion of H_η

Taking into account that $\varepsilon_\eta(\mathbf{x}) = \tilde{\varepsilon}(\mathbf{x}, \frac{\mathbf{x}}{\eta})$ in the formulation of the problem $\mathcal{P}_\eta^H$, we get the following problem: find $\mathbf{H}_\eta$ a sequence of locally square integrable functions on $\mathbb{R}^3$ solutions of

$$\mathcal{P}_\eta^H \begin{cases} \operatorname{curl} \tilde{\varepsilon}^{-1}\left(\mathbf{x}, \dfrac{\mathbf{x}}{\eta}\right) \operatorname{curl} \mathbf{H}_\eta - k_0^2 \mathbf{H}_\eta = 0 & \text{, in } \mathcal{D}'(\mathbb{R}^3) \\ \mathbf{H}_\eta^d = O\left(\dfrac{1}{|\,\mathbf{x}\,|}\right) & \text{, in } C^\infty(\mathbb{R}^3 - \bar{\Omega}_\eta) \\ \dfrac{\mathbf{x}}{|\,\mathbf{x}\,|} \wedge \operatorname{curl} \mathbf{H}_\eta^d + ik\mathbf{H}_\eta^d = o\left(\dfrac{1}{|\,\mathbf{x}\,|}\right) & \text{, in } C^\infty(\mathbb{R}^3 - \bar{\Omega}_\eta) \end{cases}$$

For η fixed, $\mathbf{H}_\eta$ is the unique solution of the above problem (the reader may refer to [25] for existence and uniqueness theorems). Let us now assume that $\mathbf{H}_\eta$ satisfies the following two-scale expansion:

$$\mathbf{H}_\eta = \mathbf{H}_0\left(\mathbf{x}, \frac{\mathbf{x}}{\eta}\right) + \eta \mathbf{H}_1\left(\mathbf{x}, \frac{\mathbf{x}}{\eta}\right) + \eta^2 \mathbf{H}_2\left(\mathbf{x}, \frac{\mathbf{x}}{\eta}\right) + \dots + \eta^N \mathbf{H}_\eta\left(\mathbf{x}, \frac{\mathbf{x}}{\eta}\right) + o(\eta^N) \qquad (1)$$

where $\mathbf{H}_i : \Omega_f \times \mathbb{R}^3 \longmapsto \mathbb{C}^3$ are smooth complex valued functions of the variables $(\mathbf{x}, \mathbf{y})$, independent of η, periodic in $\mathbf{y}$ of period 1. The introduction of the variable $\mathbf{y} = \frac{\mathbf{x}}{\eta}$ takes into account the periodic dependance on $\mathbf{x}$ of the permittivity ε_η in the "bounded periodic" structure.

Assuming that the above expansion is relevant, we can state the following lemma:

Lemma 1 *The Maxwell operator* $A_\eta = \operatorname{curl} \tilde{\varepsilon}_\eta^{-1} \operatorname{curl}$ *associated to the problem* $\mathcal{P}_\eta$ *satisfies the following operator expansion* $A_\eta = \eta^{-2} A_{\mathbf{yy}} + \eta^{-1} A_{\mathbf{xy}} + \eta^0 A_{\mathbf{xx}} + o(1)$, *where* $A_{\mu,\nu}$ *denotes the operator* $\operatorname{curl}_\mu \tilde{\varepsilon}^{-1}(\mathbf{x}, \mathbf{y})$ curl_ν, *the couple* $(\mu,\ \nu)$ *being in* $\{\mathbf{x}, \mathbf{y}\} \times \{\mathbf{x}, \mathbf{y}\}$.

Besides, the asymptotic terms of A_η *are solutions of:*

$$\mathcal{S}_0 = \begin{cases} A_{\mathbf{yy}}\mathbf{H}_0 = 0 & \text{(2a)} \\ A_{\mathbf{yy}}\mathbf{H}_1 + A_{\mathbf{xy}}\mathbf{H}_0 + A_{\mathbf{yx}}\mathbf{H}_0 = 0 & \text{(2b)} \\ A_{\mathbf{yy}}\mathbf{H}_2 + A_{\mathbf{xy}}\mathbf{H}_1 + A_{\mathbf{yx}}\mathbf{H}_1 + A_{\mathbf{xx}}\mathbf{H}_0 - k_0^2\mathbf{H}_0 = 0 & \text{(2c)} \end{cases}$$

Proof:

For convenience in the following calculations, we denote by R_η the operator of restriction onto the overplane $\{\mathbf{y} = \frac{\mathbf{x}}{\eta}\}$:

$$R_\eta : f(\mathbf{x},\mathbf{y}) \longmapsto f\left(\mathbf{x}, \frac{\mathbf{x}}{\eta}\right)$$

where $f(\mathbf{x},\mathbf{y})$ and $f(\mathbf{x},\frac{\mathbf{x}}{\eta})$ are respectively locally square integrable functions of $\Omega \times \mathbb{R}^3 \rightarrow \mathbb{C}^3$ and $\Omega \rightarrow \mathbb{C}^3$ of finite energy.

It is worth noting that R_η obeys the following rules of calculation:

properties of R_η**: the operator** R_η *is a "distributive operator", that is to say that*

$$R_\eta(f)\ R_\eta(g) = R_\eta(fg)$$

Furthermore, we can define the action of the differential operator on the restriction R_η *by:*

$$\frac{\partial}{\partial \mathbf{x}_i}\left(R_\eta f(\mathbf{x},\mathbf{y})\right) = R_\eta\left(\frac{\partial}{\partial \mathbf{x}_i} f(\mathbf{x},\mathbf{y})\right) + \frac{1}{\eta} R_\eta\left(\frac{\partial}{\partial \mathbf{y}_i} f(\mathbf{x},\mathbf{y})\right)$$

that is to say that $\left[\frac{\partial}{\partial \mathbf{x}_i}, R_\eta\right] = \frac{1}{\eta} R_\eta \frac{\partial}{\partial \mathbf{y}_i}$.

With the help of the operator R_η , (1) can be rewritten in the form:

$$\begin{aligned} \mathbf{H}_\eta(\mathbf{x}) &= R_\eta \mathbf{H}_0(\mathbf{x},\mathbf{y}) + \eta R_\eta \mathbf{H}_1(\mathbf{x},\mathbf{y}) + \ldots + \eta^N R_\eta \mathbf{H}_N(\mathbf{x},\mathbf{y}) + o(\eta^N) \\ &= R_\eta \left\{ \sum_{j=0}^{N} \eta^j\ \mathbf{H}_j(\mathbf{x},\mathbf{y}) \right\} + o(\eta^N) \qquad (3) \end{aligned}$$

Thus, the partial differential operator $\frac{\partial}{\partial \mathbf{x}_i}$ acting on $\mathbf{H}_\eta(\mathbf{x})$ satisfies the following equality:

$$\frac{\partial}{\partial \mathbf{x}_i}\mathbf{H}_\eta(\mathbf{x}) = \frac{\partial}{\partial \mathbf{x}_i} R_\eta \left\{ \sum_{j=0}^{N} \eta^j \ \mathbf{H}_j(\mathbf{x},\mathbf{y}) \right\} + o(\eta^N)$$
$$= \left(R_\eta \frac{\partial}{\partial \mathbf{x}_i} + \frac{1}{\eta} R_\eta \frac{\partial}{\partial \mathbf{y}_i} \right) \left\{ \sum_{j=0}^{N} \eta^j \ \mathbf{H}_j(\mathbf{x},\mathbf{y}) \right\} + o(\eta^{N-1})$$

We now want to deduce the action of the second order differential operator $\mathrm{curl}\,(\varepsilon_\eta^{-1}\mathrm{curl})$ involved in the problem $\mathcal{P}_\eta^H$, on the field $\mathbf{H}_\eta$. Taking into account that $[\mathrm{curl}_\mathbf{x}, \mathrm{R}_\eta] = \frac{1}{\eta} R_\eta \mathrm{curl}_\mathbf{y}$, we obtain that:

$$\mathrm{curl}_\mathbf{x}\left((R_\eta \tilde{\varepsilon}^{-1}(\mathbf{x},\mathbf{y}))(\mathrm{curl}_\mathbf{x} R_\eta \mathbf{H}_j) \right)$$
$$= \mathrm{curl}_\mathbf{x}\left((R_\eta \tilde{\varepsilon}^{-1}(\mathbf{x},\mathbf{y}))(R_\eta \mathrm{curl}_\mathbf{x} \mathbf{H}_j + \frac{1}{\eta} R_\eta \mathrm{curl}_\mathbf{y} \mathbf{H}_j) \right)$$

We then use the distributivity of R_η to get:

$$\mathrm{curl}_\mathbf{x}\left((\mathrm{R}_\eta \tilde{\varepsilon}^{-1}(\mathbf{x},\mathbf{y}))(\mathrm{curl}_\mathbf{x} \mathrm{R}_\eta \mathbf{H}_\mathrm{j}) \right)$$
$$= \mathrm{curl}_\mathbf{x} \mathrm{R}_\eta (\tilde{\varepsilon}^{-1} \mathrm{curl}_\mathbf{x} \mathbf{H}_\mathrm{j}) + \frac{1}{\eta} \mathrm{curl}_\mathbf{x} \mathrm{R}_\eta (\tilde{\varepsilon}^{-1} \mathrm{curl}_\mathbf{y} \mathbf{H}_\mathrm{j})$$

We iterate the process, by taking into account once more that $\mathrm{curl}_\mathbf{x}$ and R_η do not commute:

$$\mathrm{curl}_\mathbf{x}\left((\mathrm{R}_\eta \tilde{\varepsilon}^{-1}(\mathbf{y}))(\mathrm{curl}_\mathbf{x} \mathrm{R}_\eta \mathbf{H}_\mathrm{j}) \right)$$
$$= R_\eta \left[\mathrm{curl}_\mathbf{x} (\tilde{\varepsilon}^{-1} \mathrm{curl}_\mathbf{x} \mathbf{H}_\mathrm{j}) + \frac{1}{\eta} \mathrm{curl}_\mathbf{y} (\tilde{\varepsilon}^{-1} \mathrm{curl}_\mathbf{x} \mathbf{H}_\mathrm{j} \right]$$
$$+ \frac{1}{\eta} R_\eta \left[\mathrm{curl}_\mathbf{x} (\tilde{\varepsilon}^{-1} \mathrm{curl}_\mathbf{y} \mathbf{H}_\mathrm{j}) + \frac{1}{\eta} \mathrm{curl}_\mathbf{y} (\tilde{\varepsilon}^{-1} \mathrm{curl}_\mathbf{y} \mathbf{H}_\mathrm{j}) \right]$$

We then apply this two-scale second order operator in the expansion of the magnetic field $\mathbf{H}_\eta$. Assuming that the terms of the development of the powers higher than 2 are bounded, we can write:

$$\mathrm{curl}_\mathbf{x}\left(\tilde{\varepsilon}^{-1} \mathrm{curl}_\mathbf{x} (\mathbf{H}_0 + \eta \mathbf{H}_1) \right) + \frac{1}{\eta} \mathrm{curl}_\mathbf{x} \left(\tilde{\varepsilon}^{-1} \mathrm{curl}_\mathbf{y} (\mathbf{H}_0 + \eta \mathbf{H}_1) \right)$$
$$+ \frac{1}{\eta} \left(\mathrm{curl}_\mathbf{y} \tilde{\varepsilon}^{-1} \mathrm{curl}_\mathbf{x} (\mathbf{H}_0 + \eta \mathbf{H}_1) \right)$$
$$+ \frac{1}{\eta} \mathrm{curl}_\mathbf{y} \left(\tilde{\varepsilon}^{-1} \mathrm{curl}_\mathbf{y} (\mathbf{H}_0 + \eta \mathbf{H}_1 + \eta^2 \mathbf{H}_2) \right)$$
$$- k_0^2 (\mathbf{H}_0 + \eta \mathbf{H}_1) + O(\eta) = 0$$

In a neighborhood of $\eta = 0$, we express the vanishing of the coefficients of successive powers of $\frac{1}{\eta}$. Thus, we have to consider the following system:

$$\mathcal{S}_0 = \begin{cases} \eta^{-2} : & A_{\mathbf{yy}}\mathbf{H}_0 = 0 \quad (4a) \\ \eta^{-1} : & A_{\mathbf{yy}}\mathbf{H}_1 + A_{\mathbf{xy}}\mathbf{H}_0 + A_{\mathbf{yx}}\mathbf{H}_0 = 0 \quad (4b) \\ \eta^{0} \quad : & A_{\mathbf{yy}}\mathbf{H}_2 + A_{\mathbf{xy}}\mathbf{H}_1 + A_{\mathbf{yx}}\mathbf{H}_1 + A_{\mathbf{xx}}\mathbf{H}_0 - k_0^2\mathbf{H}_0 = 0 \quad (4c) \end{cases}$$

where $A_{\mu,\nu}$ denotes the operator $\mathrm{curl}_\mu \tilde{\varepsilon}^{-1}(\mathbf{x},\mathbf{y})\mathrm{curl}_\nu$, the couple (μ, ν) being in $\{\mathbf{x},\mathbf{y}\} \times \{\mathbf{x},\mathbf{y}\}$.

Let us consider the first equality of the previous system $\mathcal{S}_0$:

$$\mathrm{curl}_\mathrm{y}\left(\tilde{\varepsilon}^{-1}(\mathbf{x},\mathbf{y})\mathrm{curl}_\mathrm{y}\mathbf{H}_0\right) = 0 \quad (5)$$

The next step in the asymptotic expansion is to show that $\mathbf{H}_0$ only depend on the macroscopic variable $\mathbf{x}$. This property follows from two lemmae.

Lemma 2 *Let* $\mathbf{H}_0$ *be a* Y *periodic function in* $\mathbf{y}$*, solution of the equation (5). Then*

$$\textit{For almost every } \mathbf{y} \textit{ in } Y, \ \ \mathrm{curl}_\mathbf{y}\mathbf{H}_0(\mathbf{x},\mathbf{y}) = 0 \quad (6)$$

Proof:

Multiplying equation (5) by the conjugate of $\mathbf{H}_0$ and integrating over Y leads to:

$$\int_Y \mathrm{curl}_\mathbf{y}\left[\tilde{\varepsilon}^{-1}(\mathbf{x},\mathbf{y})\left(\mathrm{curl}_\mathbf{y}\mathbf{H}_0(\mathbf{x},\mathbf{y})\right)\right] \cdot \mathbf{H}_0^*(\mathbf{y})\,\mathrm{d}\mathbf{y} = 0$$

By applying the Poynting Identity ($\mathrm{div}(A \wedge B) = -A \cdot \mathrm{curlB} + \mathrm{B} \cdot \mathrm{curlA}$) and summing on Y, we have:

$$\int_Y \left[\tilde{\varepsilon}^{-1}(\mathbf{x},\mathbf{y})\left(\mathrm{curl}_\mathbf{y}\mathbf{H}_0(\mathbf{x},\mathbf{y})\right)\right] \cdot \mathrm{curl}_\mathbf{y}\mathbf{H}_0^*(\mathbf{x},\mathbf{y})\,\mathrm{d}\mathbf{y} \\ - \int_Y \mathrm{div}_\mathbf{y}\left[\tilde{\varepsilon}^{-1}(\mathbf{x},\mathbf{y})\left(\mathrm{curl}_\mathbf{y}\mathbf{H}_0(\mathbf{x},\mathbf{y})\right) \wedge \mathbf{H}_0^*(\mathbf{y})\right] d\mathbf{y} = 0$$

The Green-Ostrogradsky formula then gives us:

$$\int_Y \left[\tilde{\varepsilon}^{-1}(\mathbf{x},\mathbf{y})\left(\mathrm{curl}_\mathbf{y}\mathbf{H}_0(\mathbf{x},\mathbf{y})\right)\right] \cdot \mathrm{curl}_\mathbf{y}\mathbf{H}_0^*(\mathbf{x},\mathbf{y})\,\mathrm{d}\mathbf{y} \\ - \int_{\partial Y} \left[\tilde{\varepsilon}^{-1}(\mathbf{x},\mathbf{y})\left(\mathrm{curl}_\mathbf{y}\mathbf{H}_0(\mathbf{x},\mathbf{y})\right) \wedge \mathbf{H}_0^*(\mathbf{x},\mathbf{y})\right] \cdot \mathbf{n}\,ds = 0$$

From the anti-periodicity of the unit outgoing normal $\mathbf{n}$ to ∂Y and the periodicity in the $\mathbf{y}$ variable of $\mathbf{H}_0$, we deduce that:

$$\int_Y \tilde{\varepsilon}^{-1}(\mathbf{x},\mathbf{y})\,[\mathrm{curl}_{\mathbf{y}}\mathbf{H}_0(\mathbf{x},\mathbf{y})]^2\,d\mathbf{y} = 0$$

Let us assume that the real or imaginary parts of ε^{-1} keep a constant sign. We deduce that:

$$a.e.\mathbf{y} \in Y,\ \ \mathrm{curl}_{\mathbf{y}}\mathbf{H}_0(\mathbf{x},\mathbf{y}) = 0$$

This auxiliary lemma is applied to perform the proof of the following fundamental lemma.

Lemma 3 *H_0 solution of the system $\mathcal{S}_0$ is independent of the microscopic variable y. That is to say there exists a function, namely $\mathbf{H}_{hom}$, such as:*

$$\textit{For almost every } \mathbf{y} \textit{ in } Y,\ \ \mathbf{H}_{hom}(\mathbf{x}) = \mathbf{H}_0(\mathbf{x},\mathbf{y}) \tag{7}$$

Proof:

From the lemma 2, we deduce the following equation:

$$a.e.\mathbf{y} \in Y\ \ \mathrm{curl}_{\mathbf{y}}\mathbf{H}_0(\mathbf{x},\mathbf{y}) = 0 \tag{8}$$

Furthermore, from equations (4b) and (8) we have that:

$$\mathrm{curl}_{\mathbf{y}}\left(\tilde{\varepsilon}^{-1}(\mathbf{x},\mathbf{y})\mathrm{curl}_{\mathbf{x}}\mathbf{H}_0(\mathbf{x},\mathbf{y})\right) + \mathrm{curl}_{\mathbf{y}}\left(\tilde{\varepsilon}^{-1}(\mathbf{x},\mathbf{y})\mathrm{curl}_{\mathbf{y}}\mathbf{H}_1(\mathbf{x},\mathbf{y})\right) = 0 \tag{9}$$

By applying $\mathrm{div}_{\mathbf{y}}$ to (4c) we derive that:

$$\begin{aligned}
&\mathrm{div}_{\mathbf{y}}\left(\mathrm{curl}_{\mathbf{x}}\left(\tilde{\varepsilon}^{-1}\mathrm{curl}_{\mathbf{x}}\mathbf{H}_0\right)\right) + \mathrm{div}_{\mathbf{y}}\left(\mathrm{curl}_{\mathbf{x}}\left(\tilde{\varepsilon}^{-1}\mathrm{curl}_{\mathbf{y}}\mathbf{H}_1\right)\right)\\
&+ \mathrm{div}_{\mathbf{y}}\left(\mathrm{curl}_{\mathbf{y}}\left(\tilde{\varepsilon}^{-1}\mathrm{curl}_{\mathbf{x}}\mathbf{H}_1\right)\right) + \mathrm{div}_{\mathbf{y}}\left(\mathrm{curl}_{\mathbf{y}}\left(\tilde{\varepsilon}^{-1}\mathrm{curl}_{\mathbf{y}}\mathbf{H}_2\right)\right)\\
&- k_0^2\mathrm{div}_{\mathbf{y}}\mathbf{H}_0 = 0
\end{aligned}$$

This expression confines itself to:

$$-\mathrm{div}_{\mathbf{x}}\Big(\underbrace{\mathrm{curl}_{\mathbf{y}}\left(\tilde{\varepsilon}^{-1}\mathrm{curl}_{\mathbf{x}}\mathbf{H}_0\right) + \mathrm{curl}_{\mathbf{y}}\left(\tilde{\varepsilon}^{-1}\mathrm{curl}_{\mathbf{y}}\mathbf{H}_1\right)}_{=0 \text{ from } (9)}\Big) - k_0^2\mathrm{div}_{\mathbf{y}}\mathbf{H}_0 = 0$$

Finally, we get the following formulation:

$$k_0^2 \mathrm{div}_{\mathbf{y}} \mathbf{H}_0 = 0$$

From the positivity of k_0^2, and the relation $\mathrm{curl}_{\mathbf{y}}\mathrm{curl}_{\mathbf{y}} = -\boldsymbol{\Delta}_{\mathbf{y}} + \nabla_{\mathbf{y}}\mathrm{div}_{\mathbf{y}}$, we derive that:

$$\boldsymbol{\Delta}_{\mathbf{y}} \mathbf{H}_0(\mathbf{x}, \mathbf{y}) = 0$$

We develop $\mathbf{H}_0$ in Fourier series in the $\mathbf{y}$ variable which is Y-periodic.

$$\mathbf{H}_0(\mathbf{x}, \mathbf{y}) = \sum_{\mathbf{m} \in \mathbb{Z}^3} c_{\mathbf{m}}(\mathbf{x}) e^{-2i\pi(\mathbf{m}\cdot\mathbf{y})}$$

Taking the vectorial Laplacien of $\mathbf{H}_0$ in the $\mathbf{y}$ variable we get:

$$\sum_{\mathbf{m} \in \mathbb{Z}^3} -4\pi^2(\mid \mathbf{m} \mid^2) c_{\mathbf{m}}(\mathbf{x}) e^{-2i\pi(\mathbf{m}\cdot\mathbf{y})} = 0$$

By positivity of $\mid \mathbf{m} \mid^2$ we deduce that:

$$c_{\mathbf{m}}(\mathbf{x}) = 0 \quad , \forall \mathbf{m} \in \mathbb{Z}^3 \setminus \{0, 0, 0\}$$

This leads us to the following result:

$$a.e.\ \mathbf{y} \in Y \ , \exists\ \mathbf{H}_{hom} \ , \mathbf{H}_{hom}(\mathbf{x}) = \mathbf{H}_0(\mathbf{x}, \mathbf{y})$$

From expression (9) of the lemma 3, we get:

$$\mathrm{curl}_{\mathbf{y}} \left(\tilde{\varepsilon}^{-1}(\mathbf{x}, \mathbf{y}) \left(\mathrm{curl}_{\mathbf{y}} \mathbf{H}_1(\mathbf{x}, \mathbf{y}) + \mathrm{curl}_{\mathbf{x}} \mathbf{H}_{\mathrm{hom}}(\mathbf{x}, \mathbf{y}) \right) \right) = 0 \qquad (10)$$

For reasons of coherence in the physical units, we can state that:

$$\mathbf{E}_0(\mathbf{x}, \mathbf{y}) = \frac{i}{\omega \varepsilon_0} \tilde{\varepsilon}^{-1}(\mathbf{x}, \mathbf{y}) (\mathrm{curl}_{\mathbf{y}} \mathbf{H}_1(\mathbf{x}, \mathbf{y}) + \mathrm{curl}_{\mathbf{x}} \mathbf{H}_{hom}(\mathbf{x})) \qquad (11)$$

This is just a definition, since it has not been proved that $\mathbf{E}_\eta$ were converging towards $\mathbf{E}_0$. Consequently, the equation (10) can be written as:

$$\mathrm{curl}_{\mathbf{y}} \left(-i\omega\varepsilon_0\ \mathbf{E}_0(\mathbf{x}, \mathbf{y}) \right) = 0 \qquad (12)$$

$\tilde{\varepsilon}$ goes in the left side of the expression (11), and we take its divergence in the $\mathbf{y}$ variable:

$$\operatorname{div}_{\mathbf{y}}\left(\tilde{\varepsilon}\mathbf{E}_0(\mathbf{x},\mathbf{y})\right) = 0 \tag{13}$$

The results derived from the equations (7) and (9) are thus summed up in the following system:

$$\begin{cases} \operatorname{curl}_{\mathbf{y}}\left(\mathbf{E}_0(\mathbf{x},\mathbf{y})\right) = 0 \\ \operatorname{div}_{\mathbf{y}}\left(\tilde{\varepsilon}\mathbf{E}_0(\mathbf{x},\mathbf{y})\right) = 0 \end{cases}$$

Making the obvious remark that the average of $\mathbf{E}_0$ on Y gives us a field independant of the microscopic variable, we denote by $\mathbf{E}_{hom}$ the following quantity:

$$\mathbf{E}_{hom}(\mathbf{x}) = \langle \mathbf{E}_0 \rangle_Y = \frac{1}{meas(Y)} \int_Y \mathbf{E}_0(\mathbf{x},\mathbf{y})\, d\mathbf{y} \tag{14}$$

Where $meas(Y)$ denotes the volume area of the unit cell Y.

Hence, $\operatorname{curl}_{\mathbf{y}}\left(\mathbf{E}_0 - \mathbf{E}_{\text{hom}}\right) = 0$. In general, it merely implies that $\mathbf{E}_0 = \mathbf{E}_{hom}(\mathbf{x}) - \bigtriangledown_{\mathbf{y}} V(\mathbf{x},\mathbf{y}) + \mathbf{E}_{cohom}(\mathbf{x})$, where $\mathbf{E}_{cohom}$ belongs to the so called cohomology space whose dimension depends upon the number of cuts made in the complex plane to obtain a simply connected open set $\tilde{Y}$. As for us, $< \mathbf{E}_0 >_Y = < \mathbf{E}_{hom} >_Y$ and $< \bigtriangledown_{\mathbf{y}} V >_Y = 0$ which implies that $\mathbf{E}_{cohom} = 0$. Then, $\mathbf{E}_0 - \mathbf{E}_{hom}$ derives from a scalar potential denoted by V. That is to say that there exists a Y-periodic function $V(\mathbf{x},\mathbf{y})$ such as:

$$\mathbf{E}_0 = \mathbf{E}_{hom} - \bigtriangledown_{\mathbf{y}} V \tag{15}$$

It is worth noting that this deduction would not hold anymore if there were currents in the Scattering-Box. This would be the case for a domain Ω_f filled up by diffracting objects of infinite conductivity.

Injecting (15) in (13), leads us to:

$$\operatorname{div}_{\mathbf{y}}\left(\tilde{\varepsilon}\left(\mathbf{E}_{hom} - \bigtriangledown_{\mathbf{y}} V\right)\right) = 0 \tag{16}$$

By linearity of the divergence, we can write that:

$$\begin{aligned} -\operatorname{div}_{\mathbf{y}}\left(\tilde{\varepsilon}\left(\bigtriangledown_{\mathbf{y}} V\right)\right) &= -\operatorname{div}_{\mathbf{y}}\left(\tilde{\varepsilon}\mathbf{E}_{hom}\right) \\ &= -\operatorname{div}_{\mathbf{y}}\left(\tilde{\varepsilon}\sum_{j=1}^{3} \mathbf{E}_{hom,j} e_j\right) \\ &= -\sum_{j=1}^{3} \operatorname{div}_{\mathbf{y}}\left(\tilde{\varepsilon}(\mathbf{x},\mathbf{y}) e_j\right) \mathbf{E}_{hom,j}(\mathbf{x}) \end{aligned}$$

We are thus led to solve an annex problem of electrostatic type $\mathcal{K}_j$:

$$\mathcal{K}_j : \ -\mathrm{div}_{\mathbf{y}} \left(\tilde{\varepsilon}(\mathbf{x},\mathbf{y}) \left(\bigtriangledown_{\mathbf{y}} V_j - e_j\right)\right) = 0 \ , \ j \in \{1,2,3\} \tag{17}$$

The variational form associated to this problem having the good properties (sesquilinear, continue and coercive) in the Hilbert space $H^1_\sharp(Y)/\mathbb{R}$, Lax-Milgram lemma assures the existence and uniqueness of the solution of this problem in $H^1_\sharp(Y)/\mathbb{R}$, that is, up to an additive constant.

Let us remark that $\tilde{\varepsilon}(\mathbf{x},\mathbf{y})$ being a data of the problem $\mathcal{P}_\eta$, $\mathrm{div}_{\mathbf{y}}(\tilde{\varepsilon}(\mathbf{x},\mathbf{y})e_j)$ is a known function. Therefore, we have to solve an annex problem where the unknowns are the three components of the potential V_j. The solutions of (16) are given by the functions:

$$V(\mathbf{x},\mathbf{y}) = \sum_{j=1}^{3} V_j(\mathbf{y}) E_{hom,j}(\mathbf{x}) = \mathbf{V}_Y \cdot \mathbf{E}_{hom} \tag{18}$$

where $\mathbf{V}_Y = (V_1, V_2, V_3)$ and V_j denote respectively the vectorial potential of the basic cell and one of the scalar potentials associated with the density of charges $\mathrm{div}_{\mathbf{y}}(\varepsilon(\mathbf{y})e_j)$. Before going further, it is worth noting that the problem $\mathcal{K}_j$ is of interest by itself. Works are in progress to solve it by a method of fictitious sources [18–20], but it is not the object of the present paper.

We still have to precise the link between $\mathbf{E}_{hom}$ and $\mathbf{H}_{hom}$.

From (15) and (18) we get that:

$$\mathbf{E}_0 = (I - \bigtriangledown_{\mathbf{y}} \mathbf{V}_Y) \mathbf{E}_{hom} \tag{19}$$

where I denotes the identity matrix and $\bigtriangledown_{\mathbf{y}} \mathbf{V}_Y$ denotes the jacobian of $\mathbf{V}_Y$.

That is to say that:

$$\mathbf{E}_0 = \left(I - \begin{bmatrix} \dfrac{\partial V_1}{\partial y_1} & \dfrac{\partial V_2}{\partial y_1} & \dfrac{\partial V_3}{\partial y_1} \\ \dfrac{\partial V_1}{\partial y_2} & \dfrac{\partial V_2}{\partial y_2} & \dfrac{\partial V_3}{\partial y_2} \\ \dfrac{\partial V_1}{\partial y_3} & \dfrac{\partial V_2}{\partial y_3} & \dfrac{\partial V_3}{\partial y_3} \end{bmatrix} \right) \mathbf{E}_{hom}$$

Furthermore, from (11) we know that:

$$\mathbf{E}_0 = \frac{i}{\omega \varepsilon_0} \tilde{\varepsilon}^{-1} \left(\mathrm{curl}_{\mathbf{y}} \mathbf{H}_1 + \mathrm{curl}_{\mathbf{x}} \mathbf{H}_{hom}\right)$$

We then deduce from (19) that:

$$\left(I - \nabla_{\mathbf{y}} \mathbf{V}_Y\right) \mathbf{E}_{hom} = \frac{i}{\omega \varepsilon_0} \tilde{\varepsilon}^{-1} \left(\mathrm{curl}_{\mathbf{y}} \mathbf{H}_1 + \mathrm{curl}_{\mathbf{x}} \mathbf{H}_{hom}\right)$$

Making the sum over Y of this expression leads us to:

$$\mathrm{curl}_{\mathbf{y}} \left(\langle \mathbf{H}_1 \rangle (\mathbf{x})\right) + \mathrm{curl}_{\mathbf{x}} \mathbf{H}_{hom}(\mathbf{x}) = -i\omega\varepsilon_0 \langle \tilde{\varepsilon} \left(I - \nabla_{\mathbf{y}} \mathbf{V}_Y\right) \rangle_Y \mathbf{E}_{hom} \quad (20)$$

The first term of the left member is obviously null. Then, we are led to the following system:

$$\begin{cases} \mathrm{curl}_{\mathbf{x}} \mathbf{H}_{hom}(\mathbf{x}) = -i\omega\varepsilon_0 \varepsilon_{hom} \mathbf{E}_{hom} \\ \varepsilon_{hom} = \langle \tilde{\varepsilon}(I - \nabla_{\mathbf{y}} \mathbf{V}_Y) \rangle_Y \end{cases} \quad (21)$$

It remains to give the equation verified by $\mathbf{H}_{hom}(\mathbf{x})$. Summing the equation (4c) in the system $\mathcal{S}_0$ over Y, we derive that:

$$\begin{aligned} &\int_Y \left(\mathrm{curl}_{\mathbf{y}} \left(\tilde{\varepsilon}^{-1} \left(\mathrm{curl}_{\mathbf{y}} \mathbf{H}_2\right)\right)\right) d\mathbf{y} \\ &\quad = k_0^2 \int_Y \mathbf{H}_{hom} \, d\mathbf{y} - \int_Y \left(\mathrm{curl}_{\mathbf{x}} \left(\tilde{\varepsilon}^{-1} \left(\mathrm{curl}_{\mathbf{x}} \mathbf{H}_{\mathrm{hom}}\right)\right)\right) d\mathbf{y} \\ &\qquad - \int_Y \left(\mathrm{curl}_{\mathbf{x}} \left(\tilde{\varepsilon}^{-1} \left(\mathrm{curl}_{\mathbf{y}} \mathbf{H}_1\right)\right)\right) d\mathbf{y} \\ &\qquad - \int_Y \left(\mathrm{curl}_{\mathbf{y}} \left(\tilde{\varepsilon}^{-1} \left(\mathrm{curl}_{\mathbf{x}} \mathbf{H}_1\right)\right)\right) d\mathbf{y} \end{aligned} \quad (22)$$

Due to periodicity of $\mathbf{H}_1$, $\mathbf{H}_2$ and $\tilde{\varepsilon}$, and due to the antiperiodicity of the outer normal $\mathbf{n}$ to ∂Y, by virtue of the Green formula ($\int_Y \mathrm{curlA} \, \mathrm{d}\mathbf{y} = \int_{\partial \mathrm{Y}} \mathrm{n} \wedge \mathrm{A} \, \mathrm{ds}$), we get that:

$$\int_Y \mathrm{curl}_{\mathbf{y}} \left(\tilde{\varepsilon}^{-1} \left(\mathrm{curl}_{\mathbf{x}} \mathbf{H}_1(\mathbf{x}, \mathbf{y})\right)\right) = \int_{\mathrm{Y}} \mathrm{curl}_{\mathbf{y}} \left(\tilde{\varepsilon}^{-1} \left(\mathrm{curl}_{\mathbf{y}} \mathbf{H}_2(\mathbf{x}, \mathbf{y})\right)\right) = 0$$

Therefore, the equation (22) reduces to:

$$\begin{aligned} &- k_0^2 \int_Y \mathbf{H}_{hom} \, d\mathbf{y} + \int_Y \left(\mathrm{curl}_{\mathbf{x}} \left(\tilde{\varepsilon}^{-1} \left(\mathrm{curl}_{\mathbf{x}} \mathbf{H}_{\mathrm{hom}}\right)\right)\right) d\mathbf{y} \\ &+ \int_Y \left(\mathrm{curl}_{\mathbf{x}} \left(\tilde{\varepsilon}^{-1} \left(\mathrm{curl}_{\mathbf{y}} \mathbf{H}_1\right)\right)\right) d\mathbf{y} = 0 \end{aligned}$$

Taking into account the equation (11), we get:

$$-\int_Y k_0^2 \mathbf{H}_{hom}\, d\mathbf{y} - i\omega\varepsilon_0 \int_Y \mathrm{curl}_{\mathbf{x}} \mathbf{E}_0 = 0$$

The two integrands being independent of the $\mathbf{y}$ variable, and by definition of E_{hom}, we obtain:

$$k_0^2 \mathbf{H}_{hom}(\mathbf{x}) + i\omega\varepsilon_0 \mathrm{curl}\mathbf{E}_{\mathrm{hom}} = 0$$

The homogenized equation then clearly follows from the system (21):

$$\mathrm{curl}\left(\varepsilon_{\mathrm{hom}}^{-1}\left(\mathrm{curl}\mathbf{H}_{\mathrm{hom}}(\mathbf{x})\right)\right) - \mathrm{k}_0^2 \mathbf{H}_{\mathrm{hom}}(\mathbf{x}) = 0$$

with the effective permittivity defined by:

$$\varepsilon_{hom} = < \tilde{\varepsilon}(I - \nabla_{\mathbf{y}} \mathbf{V}_Y) >_Y$$

Comments:

The multiple-scale method which relies on the boundedness of the asymptotic terms of the expansion (1), risks to be mathematically unsound, and hence to lead to untrue equations. Nevertheless, in our case, the multiple-scale method gives the good form of the homogenized equation: we get the same results using the so called two-scale convergence method relying on the following theorem:

Let $\mathbf{u}(\mathbf{x}, \mathbf{y})$ be a function $\Omega_f \times \mathbb{R}^3 \longmapsto \mathbb{C}^3$ periodic and regular in $\mathbf{y}$ with period $Y =]0;1[^3$ and square integrable on Ω_f. Then, the sequence $(\mathbf{u}_\eta)$ defined by $\mathbf{u}_\eta(\mathbf{x}) = \mathbf{u}(\mathbf{x}, \frac{\mathbf{x}}{\eta})$, which of course fails to converge everywhere, tends weakly in $L^2(\Omega_f)$ to the "average function" $< \mathbf{u} > (\mathbf{x}) = \int_Y \mathbf{u}(\mathbf{x}, \mathbf{y})\, d\mathbf{y}$ that is to say that *we can extract a subsequence of* u_η *still denoted by* u_η, such that:

$$\forall \varphi \in L^2(\Omega_f)\ ,\ \int_{\Omega_f} \mathbf{u}_\eta(\mathbf{x})\varphi(\mathbf{x})\, d\mathbf{x} \to \left(\int_{\Omega_f} \left(\int_Y \mathbf{u}(\mathbf{x}, \mathbf{y})\, d\mathbf{y}\right)\varphi(\mathbf{x})\, d\mathbf{x}\right).$$

Roughly speaking, this method is based on a variational approach of the problem and uses suitable test functions of the form:

$$\varphi_\eta(\mathbf{x}) = \varphi_0(\mathbf{x}, \frac{\mathbf{x}}{\eta}) + \eta\varphi_1(\mathbf{x}, \frac{\mathbf{x}}{\eta})\ ,$$

which can be seen as an ansatz of the first order. This is the object of an article in preparation with G. Bouchitté devoted to mathematicians.

Coming back to the multiple scale method, the first order term $\mathbf{H}_1$ provides the likely form of a corrector $\mathbf{C}_1$ chosen in such a way that $\|\mathbf{H}_\eta - (\mathbf{H}_{hom} + \eta\mathbf{C}_1)\|_{H^1(\Omega_f)} \to 0$. In other words, this expression converges to 0 for the Hilbert norm L^2 and for the L^2 norm of its gradient. Roughly speaking, the corrector $\mathbf{C}_1$ is given for correcting strong oscillations near the obstacle. It is very important in numerical computation since it gives a convergence criterion. At this time, we have not been able to prove this choice to be in agreement with the requirement $\|\mathbf{H}_\eta - (\mathbf{H}_{hom} + \eta\mathbf{H}_1)\|_{H^1(\Omega_f)} \to 0$, since $\mathbf{H}_\eta$ belongs to another Hilbert space (which is very close to H^1).

In conclusion, the multiple-scale method leads here to the right formula, which is probably the essential point for most physicists. In fact, it remains to relate the limit of the inner field in the finite obstacle (given by the multiple-expansion) to the one of the diffracted field. For the interested reader, we hence give a sketch of this proof: our aim is to enlighten the reader on a few technical points with underlying physical phenomena.

A.2 On the Convergence of the Diffracted Field

Our purpose is to study the behavior of the electromagnetic field $\mathbf{F}_\eta = (\mathbf{E}_\eta, \mathbf{H}_\eta)$ in order to answer the following question: does this function converge, in some sense which remains to be cleared up, to some function $\mathbf{F}_0$? If so, is it possible to characterize $\mathbf{F}_0$ as solution of the problem of diffraction of incident wave $\mathbf{F}^i$ by a certain structure which we are able to give "clearly"? This can be done using some powerful mathematical tools which have been successfully applied, among others, by G. Bouchitté and R. Petit in the electromagnetic theory of gratings [2, 4] and by G. Bouchitté and D. Felbacq in the case of a two-dimensional finite photonic crystal [6].

Forgetting physics for a while, let us consider the Hilbert space $H(\mathrm{curl}, \Omega_\mathrm{f}) = \{\mathrm{v} \in \mathrm{L}^2(\Omega_\mathrm{f})\ ,\ \mathrm{curl}\,\mathrm{v} \in \mathrm{L}^2(\Omega_\mathrm{f})\}$ and its Hilbert subspace $H^1(\Omega_f) = \{v \in L^2(\Omega_f)\ ,\ \bigtriangledown v \in L^2(\Omega_f)\}$. It is well-known, in functional analysis [25], that the Hilbert space $H^1(\Omega_f)$ has got a behavior close to $H^1(\mathrm{curl}, \Omega_\mathrm{f})$'s provided one gets some control on the divergence in $L^2(\Omega_f)$ norm. In fact, if we want to control the gradient of a function in $L^2(\Omega_f)$, we just have to keep controlling its curl and divergence in $L^2(\Omega_f)$. That is to say that the vectorial aspect of the diffraction by three dimensional photonic structures appears in the decomposition of the gradient on its tangential (curl) and normal (divergence) components. Our battle plan is then to get enough information on the curl and on the divergence of the field to realize a study similar to the one of the two-dimensional case [6].

It is for this reason that we will give preference to the study of the magnetic field $\mathbf{H}_\eta$, whose divergence is null in Ω_f, contrary to the one of $\mathbf{E}_\eta$.

Let us repeat once more that the mutiple-scale method which rests upon the existence of the expansion (1) risks to be mathematically unsound in homogenization process dealing with metallic inclusions. Hence, it remains to show that the heuristic calculus of the preceding section leads to the good homogenized problem, and in what sense. In other words, the diffraction problem $\mathcal{P}_\eta$ being well posed for a given η, in what sense does it converges to an homogenized problem, and is it still a diffraction problem at the limit?

Let us first assume that, for physical reasons, the electromagnetic field of each problem $\mathcal{P}_\eta$, namely $\mathbf{F}_\eta = (\mathbf{E}_\eta, \mathbf{H}_\eta)$ is locally of finite energy. In mathematical terms, it means that for all η, $\mathbf{F}_\eta$ is locally square integrable, that is to say that:

$$\forall \eta > 0 \ , \ \exists M_\eta > 0 \ , \ \int_{\Omega_f} \mid \mathbf{E}_\eta \mid^2 dx + \int_{\Omega_f} \mid \mathbf{H}_\eta \mid^2 dx \leq M_\eta$$

The following proof, based upon this hypothesis, is rather subtle and proceeds in two steps: in step 1, we assume $(\mathbf{H}_\eta)$ to be uniformly bounded in $L^2(\Omega_f)$, we deduce some important results allowing us notably to determine completely the limit function H_0. In step 2, assuming $\mathbf{H}_\eta$'s boundedness in $L^2(\Omega_f)$ for a given η, using a *reductio ad absurdum* method and theoretical results obtained in step 1, we prove that $(\mathbf{H}_\eta)$ is actually uniformly bounded in $L^2(\Omega_f)$. This paper being intended to physicists, we just report here the essential points of the step 1 of the proof. If necessary, the reader may get further details on the step 2 in the reference [2].

Let us make the hypothesis that $(\mathbf{H}_\eta)$ is uniformly bounded in $L^2(\Omega_f)$.

At this point, let us note that we have more information on the magnetic field $\mathbf{H}_\eta$ than on the electric one. Indeed, in our case the permeability is a constant function, which implies that $\mathrm{div}\mathbf{H}_\eta = 0$.

Thanks to the compactness properties of $H(\mathrm{curl}, \Omega_{\mathrm{f}})$ analogous to the ones of $H^1(\Omega_f)$ [25], and due to the unicity of the solution of the homogenized problem [25], it turns out that rigorous, but tedious mathematical computations not reported here (article in preparation with G. Bouchitté) show that $\|\mathbf{H}_\eta - \mathbf{H}_{hom}\|_{L^2(\Omega_f)} \overset{\eta\to 0}{\longrightarrow} 0$ and $\|\mathbf{H}_{\eta|\partial\Omega_f} - \mathbf{H}_{hom|\partial\Omega_f}\|_{L^2(\partial\Omega_f)} \overset{\eta\to 0}{\longrightarrow} 0$.

Hence, we "control" the kind of convergence of the normal and tangential components of the magnetic field $\mathbf{H}_\eta$ on $\partial\Omega_f$ and we find these **two fundamental results**:

$$\|\mathbf{H}_\eta \wedge n_{|\partial\Omega_f} - \mathbf{H}_{hom} \wedge n_{|\partial\Omega_f}\|_{L^2(\partial\Omega_f)} \overset{\eta\to 0}{\longrightarrow} 0.$$

$$\|\mathbf{H}_\eta \cdot n_{|\partial\Omega_f} - \mathbf{H}_{hom} \cdot n_{|\partial\Omega_f}\|_{L^2(\partial\Omega_f)} \overset{\eta\to 0}{\longrightarrow} 0.$$

Nevertheless, one cannot hope to get such a convergence for the sequence $(\mathbf{E}_\eta)$ (the divergence of $\mathbf{H}_\eta$ is null, unlike the one of $\mathbf{E}_\eta$, which implies strong oscillations for the gradient of the electric field $\mathbf{E}_\eta$).

Hence, if we want to keep control on the convergence of the electromagnetic diffracted field, (the trace of $\mathbf{E}_\eta$ appears in the Stratton-Chu formula), we have to place the rest of our study outside the obstacle, where the divergence of $\mathbf{E}_\eta$ is null.

Proof of the convergence in $\mathbb{R}^3 \setminus \bar{\Omega}_f$:

Let us remark that the fields $\mathbf{E}_\eta$ and $\mathbf{H}_\eta$ play a symmetric role outside the obstacle Ω_f. Thus, let us take a ball B_r of radius $r > 0$ strictly including Ω_f (Fig. 10). Thanks to the nullity of its divergence, $\mathbf{F}_\eta = (\mathbf{E}_\eta, \mathbf{H}_\eta)$ is solution of the Helmholtz vectorial equation $\Delta\mathbf{F}_\eta + k_0^2\mathbf{F}_\eta = 0$ for $|\, x \,| > r$, which assures us of the analycity of $\mathbf{F}_\eta$ in $\mathbb{R}^3 \setminus \bar{B}_r$.

The link between the homogenization problem in the open bounded set Ω_f with the diffraction problem lies in the following remarkable properties of the vectorial Helmholtz equation $\mathbf{\Delta}\mathbf{F}_\eta + k^2\mathbf{F}_\eta = 0$, which can be derived as a particular case of a Schwartz's theorem [23] (it is a hypo-elliptical operator):

If $\mathbf{F}_\eta$ converges to $\mathbf{F}_0$ in $\mathcal{D}'(B_r \setminus \bar{\Omega}_f)$, then $\mathbf{F}_0$ obviously satisfies the same equation and is thereby infinitely differentiable. Moreover, $\mathbf{F}_\eta$ converges uniformly to $\mathbf{F}_0$ on compact (closed and bounded) subsets of $B_r \setminus \bar{\Omega}_f$ and all derivatives of $\mathbf{F}_\eta$ converge uniformly to the associated derivatives of $\mathbf{F}_0$.

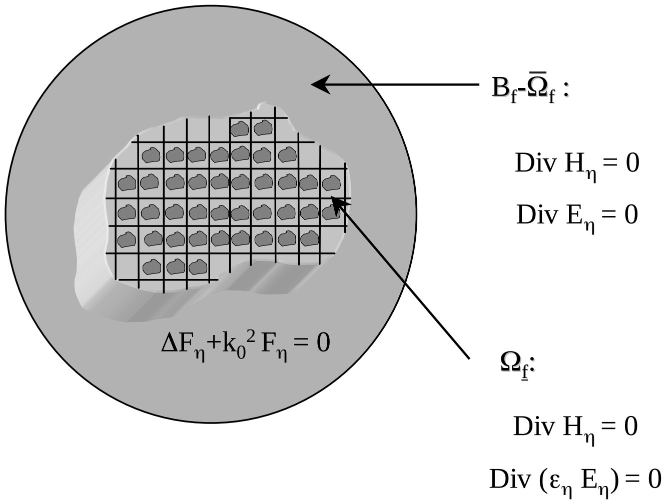

Figure 10. Link between the convergence of the field in the bounded obstacle and the one of the diffracted field in the overall space.

By the knowledge of the tangential trace of $\mathbf{F}_\eta$, for $|\mathbf{x}| = r$, we can explain the diffracted field $\mathbf{F}_\eta^d$ by using the Stratton-Chu formula:

$$\begin{cases} \mathbf{E}_\eta^d(\mathbf{x}) = i\omega\mu_0 \displaystyle\int_{|\mathbf{y}|=r} \mathbf{G}(\mathbf{x}-\mathbf{y}) \left(\frac{\mathbf{y}}{r} \wedge \mathbf{H}_\eta^d(\mathbf{y})\right) \, ds \\ \qquad\qquad + \displaystyle\int_{|\mathbf{y}|=r} \bigtriangledown\mathbf{G}(\mathbf{x}-\mathbf{y}) \left(\frac{\mathbf{y}}{r} \wedge \mathbf{E}_\eta^d(\mathbf{y})\right) \, ds \\ \mathbf{H}_\eta^d(\mathbf{x}) = -i\omega\varepsilon_0 \displaystyle\int_{|\mathbf{y}|=r} \mathbf{G}(\mathbf{x}-\mathbf{y}) \left(\frac{\mathbf{y}}{r} \wedge \mathbf{E}_\eta^d(\mathbf{y})\right) \, ds \\ \qquad\qquad + \displaystyle\int_{|\mathbf{y}|=r} \bigtriangledown\mathbf{G}(\mathbf{x}-\mathbf{y}) \left(\frac{\mathbf{y}}{r} \wedge \mathbf{H}_\eta^d(\mathbf{y})\right) \, ds \end{cases}$$

with the Green's function $\mathbf{G}(\mathbf{x}) = \dfrac{1}{4\pi} \dfrac{e^{ik_0|\mathbf{x}|}}{|\mathbf{x}|}$.

We can take the limit over η in this expression, thanks to the uniform convergence of $\mathbf{F}_\eta$ (and thus of its traces) on every compact subset of $\mathbb{R}^3 \setminus \bar{B}_r$, to get:

$$\begin{cases} \mathbf{E}^d_{hom}(\mathbf{x}) = i\omega\mu_0 \displaystyle\int_{|\mathbf{y}|=r} \mathbf{G}(\mathbf{x}-\mathbf{y}) \left(\frac{\mathbf{y}}{r} \wedge \mathbf{H}^d_{hom}(\mathbf{y})\right) \, ds \\ \qquad + \displaystyle\int_{|\mathbf{y}|=r} \bigtriangledown \mathbf{G}(\mathbf{x}-\mathbf{y}) \left(\frac{\mathbf{y}}{r} \wedge \mathbf{E}^d_{hom}(\mathbf{y})\right) \, ds \\ \mathbf{H}^d_{hom}(\mathbf{x}) = -i\omega\varepsilon_0 \displaystyle\int_{|\mathbf{y}|=r} \mathbf{G}(\mathbf{x}-\mathbf{y}) \left(\frac{\mathbf{y}}{r} \wedge \mathbf{E}^d_{hom}(\mathbf{y})\right) \, ds \\ \qquad + \displaystyle\int_{|\mathbf{y}|=r} \bigtriangledown \mathbf{G}(\mathbf{x}-\mathbf{y}) \left(\frac{\mathbf{y}}{r} \wedge \mathbf{H}^d_{hom}(\mathbf{y})\right) \, ds \end{cases}$$

Applying the Cauchy-Schwarz inequality leads us to:

$$\begin{aligned} | \mathbf{H}^d_{hom} - \mathbf{H}^d_\eta | \leq \|\mathbf{H}^d_{hom} - \mathbf{H}^d_\eta\|_{L^2(\partial B_r)} \|\mathbf{G}\|_{L^2(\partial B_r)} \\ + \|\mathbf{E}^d_{hom} - \mathbf{E}^d_\eta\|_{L^2(\partial B_r)} \|\mathbf{G}\|_{L^2(\partial B_r)} \end{aligned}$$

$\mathbf{H}^d_\eta$ and $\mathbf{E}^d_\eta$ playing a symetric role, we denote by $\|\mathbf{F}^d_\eta\|_{L^2(\partial B_r)}$ the norm $\|\mathbf{E}^d_\eta\|_{L^2(\partial B_r)} + \|\mathbf{H}^d_\eta\|_{L^2(\partial B_r)}$ induced by the cartesian product of the Hilbert trace spaces $L^2(\partial B_r)$. Taking the max of the regular function $\mathbf{G}$ over every compact subset K of $\mathbb{R}^3 \setminus \bar{B}_r$ assures us of the existence of a positive constant (depending on the measure of K) such that:

$$\sup_{\mathbf{x} \in K} | \mathbf{F}^d_{hom} - \mathbf{F}^d_\eta | \leq C_K \|\mathbf{F}^d_{hom} - \mathbf{F}^d_\eta\|_{L^2(\partial B_r)}$$

Thereby, we can deduce the uniform convergence of $\mathbf{F}_\eta$ towards $\mathbf{F}_{hom}$ on every compact subset of $\mathbb{R}^3 \setminus \bar{\Omega}_f$.

Remark on the convergence of the permittivity

It is worth noting that we cannot expect a nice convergence for the sequence of permittivities ε_η. Indeed, ε_η is proportional to the identity matrix, hence characterizes an isotropic medium, unlike its limit which characterizes an anisotropic medium. It is a typical difficulty encountered in many homogenization problems (ε_η is just bounded which implies bad convergence properties for $\varepsilon_\eta \mathrm{curl} \mathrm{H}_\eta$). Hence, there is no hope to get control on the convergence of the diffracted field, by means of volume integral equations [26].

In fact, it is to be understood that in both mathematical and physical aspects in homogenization of diffraction, the good parameter is the diffracted field. Hence, our goal is to show in what sense does the electromagnetic field $\mathbf{F}_\eta = (\mathbf{E}_\eta, \mathbf{H}_\eta)$ converge towards the first term of its asymptotic expansion, and to be more precise to verify that the limit field $\mathbf{F}_{hom}$ is still solution of a diffraction problem. This can be done, thanks to the Stratton-Chu formula, which assures that we only have to control the restriction of the electromagnetic field on the boundary of the lit body to keep control on the field in the overall space. Here is the main difficulty of the homogenization of diffraction of three-dimensional finite structures: the divergence of the sequence of electric-fields goes to infinity, hence we cannot easily keep controlling $\mathbf{F}_{\eta|\partial\Omega_f}$. Therefore, we consider a ball strictly including the obstacle. By the knowledge of the convergence of the diffracted field on the boundary of the ball, we deduce the convergence of the diffracted field outside the obstacle, thanks to the Stratton-Chu formula. Let us recall that there is no alternative way to achieve the proof by means of volume integral equations [26].

To conclude this paragraph, we want to point out that the main problem of homogenization of diffraction comes from the strong oscillations of the electromagnetic field near the interior boundary of the obstacle. Mathematically speaking, unlike physicists of solid state physics which consider an obstacle whose boundary is going to infinity, we deal with global problems: the boundary of the obstacle remaining fixed, its influence is still sensible at the limit.

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