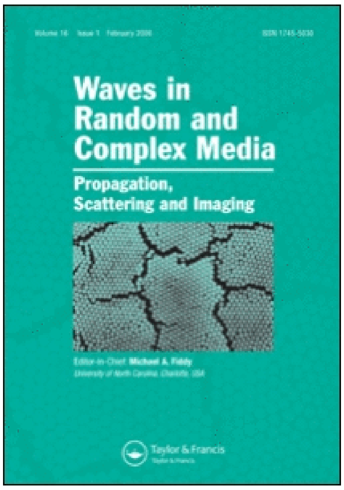

Waves in Random and Complex Media
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t716100762

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Online Publication Date: 01 November 2007

To cite this Article Guenneau, S., Zolla, F. and Nicolet, A.(2007)'Homogenization of 3D finite photonic crystals with heterogeneous permittivity and permeability',Waves in Random and Complex Media,17:4,653 — 697

To link to this Article: DOI: 10.1080/17455030701607013

URL: http://dx.doi.org/10.1080/17455030701607013

Waves in Random and Complex Media
Vol. 17, No. 4, November 2007, 653–697

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Homogenization of 3D finite photonic crystals with heterogeneous permittivity and permeability

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(Received 21 February 2007; in final form 26 July 2007)

We consider a heterogeneous magneto-dielectric photonic crystal and derive the so-called 'homogenized Maxwell system' via the multi-scale method and provide *ad hoc* proofs for the convergence of the electromagnetic field towards the homogeneous one using the notion of two-scale convergence. The homogenized medium is described by anisotropic matrices of permittivity and permeability, deduced from the resolution of two annex problems of electrostatic type on a periodic cell. Noteworthily, this asymptotic analysis also covers the case of photonic crystals with non-cuboidal periodic cells. We solve numerically the associated system of partial differential equations with a method of fictitious charges and a finite element method (FEM) in order to exhibit the matrices of effective permittivity and permeability for given magneto-dielectric periodic composites. We then compare our results in the 2D case against some Fourier expansion approach and provide duality relations in the case of magneto-dielectric checkerboards. We further compute some low-frequency eigenmodes of a photonic crystal fiber with metallic outer boundary and compare them with the eigenmodes of a corresponding effective anisotropic waveguide, thanks to the FEM. Finally, we derive the effective properties of a 3D photonic crystal both through classical homogenization (solving numerically two decoupled annex problems) and Bloch wave homogenization. In the case of spherical inclusions, the latter approach amounts to evaluating the slope of the first band around the origin on a Bloch diagram which we compute using finite edge elements.

1. Introduction

In a sense, every material can be considered as a composite, though the individual ingredients may consist of atoms and molecules. The original objective in defining a permittivity, ε, and a permeability, μ, was to present a homogeneous view of the electromagnetic properties of a medium: this natural homogenization gives mesoscopic effective properties by averaging a microscopic arrangement of atoms. It is only a small step to replace the atoms of the previous microscopic structure by some mesoscopic inclusions. In crystallography, experiments provide some evidence that one can still average the electromagnetic properties of the mesoscopic structures, and define an effective permittivity ε_{eff}, and an effective permeability, μ_{eff}: this second averaging process is called artificial homogenization. In what follows, we consider this meso-macro homogenization process using rigorous mathematical tools of limit analysis. However, we will concentrate here on periodic structures called 'photonic crystals', although these tools can be generalized to the study of some very interesting and unusual

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Waves in Random and Complex Media
ISSN: 1745-5030 (print), 1745-5049 (online)
http://www.tandf.co.uk/journals
DOI: 10.1080/17455030701607013

phenomena arising in the recently discovered 'photonic quasi-crystals' [1]. We model the periodic structures by a unit cell Y_η of characteristic dimensions η ($Y_\eta = [0, \eta[^3$). The content of the cell will define the effective response of the macroscopic finite structure. Clearly, there must be some restrictions on the dimensions of the cell Y_η. If we are concerned about the response of the composite structure to an electromagnetic radiation of frequency ω, the conditions should be $\eta \ll \lambda = \frac{2\pi c_0}{\omega}$, where c_0 denotes the speed of light. If such conditions were not obeyed, there would be the possibility that the internal structure of the medium could diffract as well as refract radiation. This so-called long wavelength limit assumption ensures that the electromagnetic wave is too myopic to detect the internal structure and in this *limit* an effective permittivity and permeability is a valid concept. In this paper, we will discuss how the diffracted field can be related to ε_{eff} and μ_{eff}.

In the last decade, advances have been made towards a better understanding of photonic crystals (PC). Such remarkable structures prohibit the propagation of light, or allow it only in certain directions at certain frequencies, or localize light in specified areas (PC with defaults). These materials, which affords us complete control on light propagation, result when a small block of dielectric material is repeated in space. The optical properties of such photonic crystals depend on the geometry of the crystal lattice [2–9]. PC are periodic devices which induce 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–Pérot filters, and distributed feedback lasers. All of these devices employ low-loss dielectrics that are periodic in one dimension, and are therefore called one-dimensional photonic crystals. However, while such mirrors are tremendously useful, their reflecting properties depend greatly upon the frequency of the incident wave in conjunction with its incidence. In practice, one wishes to reflect light of any polarization at any angle (complete photonic band gap) for some frequency range. This could be achieved with certain structures with periodicity in three dimensions. Such a three-dimensional photonic crystal has been engineered by Yablonovitch in 1987 [10]. The recent thrust in this area is partly fueled by advances in theoretical techniques, based on Fourier and multipole expansions in the vector electromagnetic Maxwell equations [11–14], which allow non prohibiting computations. This plane wave expansion method is by far the most popular theoretical tool employed for studying the photonic band gap problems. 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 [15]. Following the work of G. Bouchitté, D. Felbacq and R. Petit [16–19], we adapt these classical methods to electromagnetism for 'three-dimensional finite periodic' structures.

Throughout this paper, we consider a magneto-dielectric structure either illuminated by a monochromatic wave or within which such a wave propagates. Our main assumption is that the wavelength λ is large in comparison with typical heterogeneity sizes, i.e. with the period η of the medium. Using these hypotheses, our goal is to replace the photonic crystal by an equivalent homogeneous structure having analogous electromagnetic properties. Thanks to our formalism, we can treat 3D crystals of arbitrary shape Ω_f described by a piecewise continuous complex matrix valued permittivity and permeability for scattering problems. We need to further assume that these matrices are hermitian for spectral problems (this excludes at a stroke absorptive media).

Such hypotheses cover the physical domains of application. In the sequel, we will pay special attention to the case where the permittivity and permeability are piecewise constant functions. Such functions describe the 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 the basic cells; for instance, this allows us to study compact cubic structures such as face-centered cubic and simple cubic ones (figure 1) or the well-known 'Yablonovite' [20].

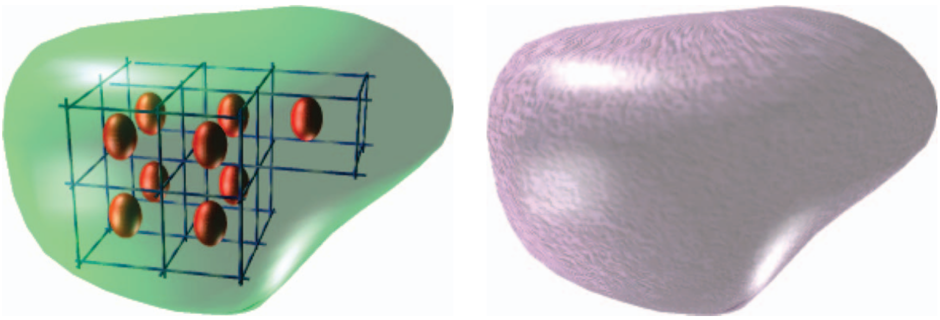

Figure 1. Homogenization of a photonic crystal made of ellipsoidal scatterers (right figure). The grid of dotted lines defines a virtual 'scaffolding' Ω_η of the whole obstacle Ω_f. For the sake of simplicity, we give an example with η near to 1, i.e. with a small number of rather big scatterers (here 5). 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 to 0). The result of the process of homogenization is a finite homogeneous anisotropic object (left figure).

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 a homogeneous material with an effective permittivity and permeability.

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: one used by most 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. This is a perfectly valid point of view: at first glance, the incident field seems to be confined within the complement of the overall space (of zero measure!) which suggests that the boundary of the crystal is not taken into account. In fact, the contribution of the boundary of the scattering obstacle appears in the behavior of so-called lattice sums near the origin of the reciprocal space, as one would expect from a low frequency analysis using a Fourier method. Also, the advantage of this method is that it gives some information for every size of wavelength: one can therefore deduce some effective properties for a photonic crystal even in the resonance domain, what may lead to anomalous dispersion [21]. We will make use of this Bloch wave homogenization in the sequel, yet restricting ourselves to low frequencies. For a high frequency analysis, we refer the reader to [22].

Now, if we consider that the obstacle and the wavelength remain fixed, while the size of scatterers goes to zero and their number goes to infinity, it is then quite intuitive that the boundary of the obstacle has an influence in this limit, and one can still speak of incident wave. This homogenization process is different from the first one (the crystal does not cover the whole space), but the results it provides are identical, as we shall rigorously prove.

Homogenization techniques used in this paper, namely the multiple scale and the Bloch wave methods, allow us to study structures of practical interest, for wavelengths large compared to the size of the scatterers of the obstacle. With the former approach we achieve mathematical proofs by using the so-called two-scale convergence [23]. We derive that the effective permittivity and permeability of the homogeneous object depend upon local problems arising in a basic cell of the crystal lattice (direct space). With the latter approach (Bloch wave homogenization) these quantities are deduced from problems taking place in the first Brillouin zone (reciprocal space). This work is an extension of our previous work on homogenization of 3D dielectric PC [24] (2000) and [25] (2004). Its material was first presented at the IUTAM symposium held in Liverpool in July 2002 [26]. In the case of vanishing filling ratio of a set of parallel metallic fibers, D. Felbacq and G. Bouchitté performed the homogenization of both 2D scalar TE and TM cases in 1997 [19] and vector coupled case in 2006 [27]. Last, but not least, K. Cherednichenko *et al.* looked at non-local effects in the homogenization of a periodic set of highly anisotropic fibers in 2006 [28].

Let us now outline the plan of the paper. In sections 2 and 3, we present the asymptotic derivation of homogenized scattering problems for periodic structures and their justification via two-scale convergence. In section 4, we look at corresponding spectral problems in the homogenization of heterogeneous cavities and waveguides. The material of these first sections is based upon the PhD thesis of S. Guenneau in 2001 [1], except for the subsection 4.3 which describes a Bloch wave approach of homogenization of 3D magneto-dielectric photonic crystals based upon the work by Bao Ke-Da *et al.* in 2000 [29]. In the year 2001, N. Wellander published an independent derivation for the homogenization of the scattering problem described in sections 2 and 3 [30]. We note that Wellander's asymptotic approach involves some ansatz for both electric and magnetic fields making use of the four Maxwell equations. Although this approach shortens the derivation of the homogenization result, it cannot handle the spectral problem. Moreover, it assumes some stronger hypotheses on the regularity of the electromagnetic field: in the present study, we merely assume that either the electric or the magnetic field is locally square integrable, not both of them. In section 5, we then present some numerical results for 2D and 3D photonic crystals (with elliptical and spherical inclusions). We also investigate properties of magneto-dielectric checkerboards, thereby extending our earlier work [31]. We finally look at effective properties of photonic crystal waveguides.

The asymptotic analysis carried out in our paper allows us to homogenize a 3D magneto-dielectric PC with a metallic boundary $\partial\Omega_f$ (asymptotic analysis of a spectral problem). Zhikov, Birman and Suslina have independently developed a general approach for such effective problems. The former author has adapted the notion of two-scale convergence to sequences of operators' resolvent [32]. The latter authors used the spectral perturbation theory for operator-valued functions admitting an analytic factorization [33]. It is worth noting that Allaire and Conca have introduced a notion of Bloch wave homogenization technique which, unlike the classical homogenization method, characterizes a renormalized limit of the spectrum (denoted by Bloch spectrum), which consists of sequences of eigenvalues of the order of the square of the medium period η^2 [34]. A natural extension of our study is to look for high frequency vibrations of a heterogeneous metallic magneto-dielectric cavity which may result in a limit spectrum consisting of a band spectrum (or Bloch spectrum, associated with photonic band gaps) and a boundary layer spectrum associated with modes whose support concentrate near the metallic outer boundary (surface waves). In the simpler case of a heterogeneous dielectric PC with no boundary (a Torus), the analysis has been performed in [22].

To conclude this introduction, although there is a vast amount of literature on homogenization theory as applied to problems of electromagnetism [15, 30, 33, 35–47], to the best of our knowledge the material presented in this paper is original. In the context of interferometric experiments, one will be concerned with the phase change of an electromagnetic wave as it crosses the composite material. In this latter context, homogenization using the Bloch theorem in the long wavelength limit seems to be more appropriate and can be carried out in a rigorous mathematical fashion [48]. Such a Bloch wave homogenization was performed in the low frequency regime for an infinite array of 3D dielectric spherical inclusions by Bao Ke-Da *et al.* [29] using the Rayleigh method. It has been further extended to fully anisotropic infinite periodic dielectric crystals in the high frequency regime in [22]. Here, we provide a plethora of homogenization results covering a wide range of 2D and 3D magneto-dielectric PCF (including fully anisotropic ones). Noteworthily, our analysis covers the case of periodic

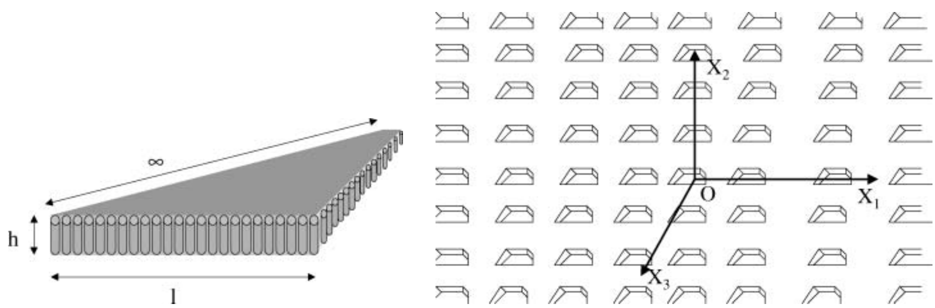

Figure 2. Band of finite parallel rods seen a 3D photonic crystal infinite in one direction (left figure). Bi-grating seen as a 3D photonic crystal bounded in the x_3 axis (right figure).

structures in other orthogonal coordinates systems (such as polar and spherical ones) and even non-orthogonal coordinate systems. In these cases, our formulas should be applied *mutatis mutandis* replacing ε and μ by the proper tensors involving the curvilinear metric of space attached to the (non-cubic) array (see for instance [49] for a comprehensive presentation of Maxwell's equation undergoing geometric transforms).

2. Set-up of the problem of diffraction

From now on, assuming a time dependance 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 physical. The first approach is a geometrical description of the obstacle, which lies in a fixed domain Ω_f not necessarily simply connected. Furthermore, although our study only deals with the bounded case, it remains relevant for Ω_f infinite in one (figure 2 left) or two directions (figure 2 right). In such cases, one just has to adapt the study with 'ad hoc' outgoing wave conditions (as for gratings, the reader may refer to [50]).

The second approach (a physical one) describes the optical characteristics of the material illuminated 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, $\mathbf{i} = (i_1, i_2, i_3)$ 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 designate by $\eta(\tau_i Y)$ the homothety on $\tau_i Y$ of ratio η: thus we form a box of size η and centre $\eta\mathbf{i}$ (figure 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 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 (figure 1). 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, denote the measure (volume) of Ω_η and 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

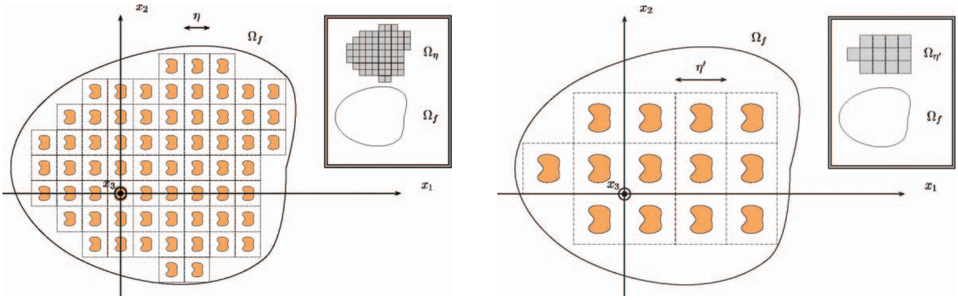

Figure 3. The fixed set Ω_f with two 'scaffolding' $\Omega_{\eta'}$ and Ω_η with $\eta < \eta'$ in the 2D case.

by its relative permittivity $\varepsilon_r^B(\mathbf{x})$ and permeability $\mu_r^B(\mathbf{x})$:

$$\forall \mathbf{x} \in \mathbb{R}^3,\ \varepsilon_{\mathbf{r}}^{\mathbf{B}}(\mathbf{x}) = \mathbf{1} - \chi_{\mathbf{Y}} + \chi_{\mathbf{Y}}\tilde{\varepsilon}_{\mathbf{r}}(\mathbf{x}),\ \mu_{\mathbf{r}}^{\mathbf{B}}(\mathbf{x}) = \mathbf{1} - \chi_{\mathbf{Y}} + \chi_{\mathbf{Y}}\tilde{\mu}_{\mathbf{r}}(\mathbf{x}),$$

with χ_Y the characteristic function of Y (i.e. $\chi_Y = 1$ when $x \in Y$ and $\chi_Y = 0$ elsewhere). Here, $\tilde{\varepsilon}_r(\mathbf{x})$ and $\tilde{\mu}_r(\mathbf{x})$ are two given piecewise continuous complex valued functions, which denote the relative permittivity and permeability 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 3D 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 $F_\eta = (E_\eta, H_\eta)$, corresponding to the field generated by the N_η SB when they are illuminated by a given incident monochromatic wave of wavelength λ: $F_i = (E_i, H_i)$. 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, $\varepsilon_r^{B_\eta}(\mathbf{x}) = \varepsilon_{\mathbf{r}}^{\mathbf{B}}(\frac{\mathbf{x}}{\eta})$ and $\mu_r^{B_\eta}(\mathbf{x}) = \mu_{\mathbf{r}}^{\mathbf{B}}(\frac{\mathbf{x}}{\eta})$, where ε_r^B and μ_r^B are two Y-periodic complex valued functions in Ω_f such that $0 \leq arg(\varepsilon_r^B) < \pi$, i.e. $\Re e(i\varepsilon_r^B) \geq 0$ (resp. for μ). Hence, unlike most of the articles dealing with solid state physics, we do not assume periodicity of ε_r^B and μ_r^B in the overall space $\mathbb{R}^3$.

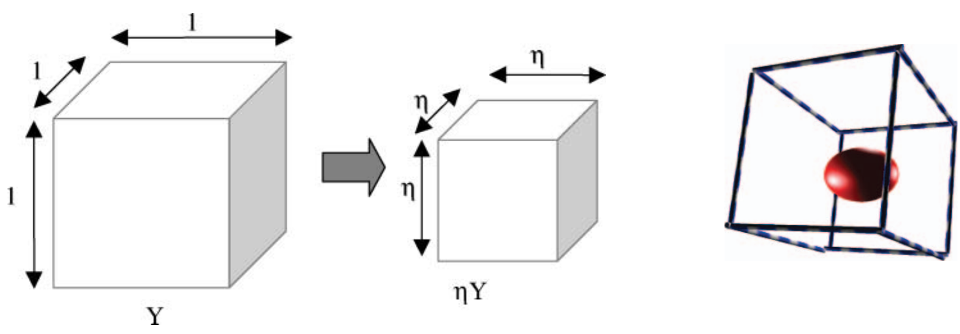

Figure 4. The elementary cell of the photonic crystal is the homothety on a unit cell of ratio η (left). Basic cell Y with an ellipsoidal scatterer (right).

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

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

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 and μ_r^B, these functions can be seen as two Y-periodic functions of the y variable (which continuously depends on its variable $\mathbf{x}$). Therefore, we can introduce $(\mathbf{E}_\eta^d, \mathbf{H}_\eta^d)$ the diffracted field (which only makes sense outside the structure) deduced from the incident field $(\mathbf{E}^i, \mathbf{H}^i)$ illuminating the structure by $(\mathbf{E}_\eta^d, \mathbf{H}_\eta^d) = (\mathbf{E}_\eta, \mathbf{H}_\eta) - (\mathbf{E}^i, \mathbf{H}^i)$. It is worth noting that we can rigorously define the diffracted field, since 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:

$$(\mathcal{P}_\eta) \begin{cases} \mathrm{curl}\mathbf{E}_\eta + i\omega\mu_0\mu_\eta\mathbf{H}_\eta = 0 & \text{(1a)} \\ \mathrm{curl}\mathbf{H}_\eta - i\omega\varepsilon_0\varepsilon_\eta\mathbf{E}_\eta = 0 & \text{(1b)} \\ \mathbf{H}_\eta^d = O\left(\dfrac{1}{\mid \mathbf{x} \mid}\right), \mathbf{E}_\eta^d = O\left(\dfrac{1}{\mid \mathbf{x} \mid}\right) & \text{(1c)} \\ k_0\mathbf{E}_\eta^d + \omega\mu\left(\dfrac{\mathbf{x}}{\mid \mathbf{x} \mid} \wedge \mathbf{H}_\eta^d\right) = o\left(\dfrac{1}{\mid \mathbf{x} \mid}\right) & \text{(1d)} \end{cases}$$

where (1c–1d) denote the outgoing wave conditions of Silver–Müller type, which play a fundamental role by insuring existence and uniqueness of the solution of $(\mathcal{P}_\eta)$: the uniqueness is due to the fact that if $(\mathbf{E}_\eta^d, \mathbf{H}_\eta^d)$ is null, then (1c) and (1d) ensure that for a given open subset Ω strictly including Ω_η ($\varepsilon_\eta(x) = \mu_\eta(x) = 1$ in $\mathbb{R}^3 \setminus \bar{\Omega}$)

$$\mathcal{R}e \int_{\partial\Omega} (\mathbf{E}_\eta \wedge \bar{\mathbf{H}}_\eta) \cdot \frac{x}{\mathbf{x}} ds \geq 0 \tag{2}$$

with equality in 2 if and only if $(\mathbf{E}_\eta, \mathbf{H}_\eta) = 0$ in $\mathbb{R}^3 \setminus \bar{\Omega}$ (for existence, see e.g. [51]).

Of course, equations (1a) and (1b) 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 $\mathbb{R}^3$. The radiation conditions are relevant in $C^\infty(\mathbb{R}^3 \setminus \bar{\Omega}_\eta)$. That is to say, $\mathbf{E}_\eta$ and $\mathbf{H}_\eta$ are continuous, as all their derivatives outside the obstacle (this is a consequence of the Helmholtz equation arising outside the obstacle, which induces analyticity 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:

$$(\mathcal{P}_\eta^E) \begin{cases} \mathrm{curl}\left(\mu_\eta{}^{-1}\,\mathrm{curl}\,\mathbf{E}_\eta\right) - k_0^2\varepsilon_\eta\mathbf{E}_\eta = 0 & \text{(3a)} \\ \mathbf{E}_\eta^d = O\left(\dfrac{1}{\mid \mathbf{x} \mid}\right) & \text{(3b)} \\ \dfrac{\mathbf{x}}{\mid \mathbf{x} \mid} \wedge \mathrm{curl}\,\mathbf{E}_\eta^d + ik\mathbf{E}_\eta^d = o\left(\dfrac{1}{\mid \mathbf{x} \mid}\right) & \text{(3c)} \end{cases}$$

$$
(\mathcal{P}_\eta^H)\begin{cases}
\operatorname{curl}\left(\varepsilon_\eta{}^{-1}\operatorname{curl}\mathbf{H}_\eta\right) - k_0^2\mu_\eta\mathbf{H}_\eta = 0 & \text{(4a)}\\[1ex]
\mathbf{H}_\eta^d = O\left(\dfrac{1}{\mid\mathbf{x}\mid}\right) & \text{(4b)}\\[1ex]
\dfrac{\mathbf{x}}{\mid\mathbf{x}\mid}\wedge\operatorname{curl}\mathbf{H}_\eta^d + ik\mathbf{H}_\eta^d = o\left(\dfrac{1}{\mid\mathbf{x}\mid}\right) & \text{(4c)}
\end{cases}
$$

At this point, let us note a fundamental difference with our previous work on homogenization of dielectric PCF [24] in which it appeared much more difficult to perform the study of the problem $(\mathcal{P}_\eta^E)$ than the one of the problem $(\mathcal{P}_\eta^H)$, since μ was a constant function equal to μ_0 unlike ε_η. The magnetic field $\mathbf{H}_\eta$ was divergence free, in contrast with the Electric field for which $\operatorname{div}\mathbf{E}_\eta$ behaves like $\frac{1}{\eta}$. Indeed, taking the divergence in the second equation in $(\mathcal{P}_\eta)$, we obtain $\operatorname{div}(\varepsilon_\eta\mathbf{E}_\eta) = 0$ which implies that $\operatorname{div}\mathbf{E}_\eta = -\frac{\nabla\varepsilon_\eta}{\varepsilon_\eta}\mathbf{E}_\eta \sim -\frac{\nabla_y\varepsilon}{\eta\varepsilon}\mathbf{E}_\eta$. 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 [24] we exclusively dealt with $(\mathcal{P}_\eta^H)$. Here, the Maxwell system is completely symmetric and the same difficulty occurs for the magnetic field $\mathbf{H}_\eta$. We arbitrarily choose the magnetic field as the variable (this is more convenient to make some comparisons with results established in [1]), but all this study holds for the electric field *mutatis mutandis*. Thus, taking into account that $\mathbf{E}_\eta = \frac{i}{\omega\varepsilon_0\varepsilon_\eta}\operatorname{curl}\mathbf{H}_\eta$, 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 section, let us emphasize that in this paper, we explain in which sense the field $\mathbf{H}_\eta$ tends to a field $\mathbf{H}_{\text{hom}}$, solution of the so-called homogenized diffraction problem $(\mathcal{P}_{\text{hom}}^H)$, whose resolution leads to two annex problems of electrostatic types that are discussed in full details and solved numerically.

3. Homogenized Maxwell system for the scattering problem

In this section, we use the multiple-scale method to homogenize a 3D structure filled with a periodic arrangement of magneto-dielectric inclusions. More precisely, using a multi-scale expansion technique applied to a scattering problem, we prove that a 3D finite crystal behaves as if it were homogeneous, when the period becomes very small in regard with a fixed wavelength. We show that the homogeneous medium is actually anisotropic, and we derive the expression of its tensors of permittivity and permeability from the calculus of six scalar periodic potentials, solutions of two systems of partial differential equations of electrostatic type.

3.1 *Main homogenization results for cubic basic cells*

Let $\mathbf{H}_\eta$ be a sequence of locally square integrable functions on $\mathbb{R}^3$ solutions of

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

where $\tilde{\varepsilon}^{-1}(\mathbf{x}, \frac{\mathbf{x}}{\eta})$ and $\tilde{\mu}^{-1}(\mathbf{x}, \frac{\mathbf{x}}{\eta})$, respectively, denote the relative permittivity and permeability of the media.

We suppose that $\mathbf{H}_\eta$, solution of the problem $(\mathcal{P}_\eta^{\mathbf{H}})$ has a two-scale expansion of the form:

$$\forall \mathbf{x} \in \Omega_f, \mathbf{H}_\eta(\mathbf{x}) = \mathbf{H}_0\left(\mathbf{x}, \frac{\mathbf{x}}{\eta}\right) + \eta \mathbf{H}_1\left(\mathbf{x}, \frac{\mathbf{x}}{\eta}\right) + \eta^2 \mathbf{H}_2\left(\mathbf{x}, \frac{\mathbf{x}}{\eta}\right) + \cdots \tag{5}$$

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 $\mathbf{H}_0$, a rougher approximation to $\mathbf{H}_\eta$. 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 still makes sense in neighborhood of 0. If the above expansion is relevant, we can state the following fundamental result:

THEOREM 3.1 (*Homogenized Maxwell's system for a diffracting obstacle*) *When η tends to zero, $\mathbf{H}_\eta$ solution of the problem $(\mathcal{P}_\eta^{\mathbf{H}})$, converges weakly in $L^2(\Omega_f)$ to the average of the first term of its asymptotic expansion on the basic cell Y, namely $\mathbf{H}_{\text{hom}}(\mathbf{x}) = \int_Y H_0(\mathbf{x}, \mathbf{y})\, d\mathbf{y}$, which is the unique solution of the following problem $(\mathcal{P}_{\text{hom}}^{\mathbf{H}})$:*

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

with

$$\begin{cases} [\varepsilon_{\text{hom}}](\mathbf{x}) = \langle \tilde{\varepsilon}(\mathbf{x}, \mathbf{y})(I - \nabla_{\mathbf{y}} \mathbf{V}_Y(\mathbf{y})) \rangle_Y & , in\ \Omega_f \\ [\varepsilon_{\text{hom}}](\mathbf{x}) = I & , in\ \Omega_f^c \end{cases} \tag{6}$$

and

$$\begin{cases} [\mu_{\text{hom}}](\mathbf{x}) = \langle \tilde{\mu}(\mathbf{x}, \mathbf{y})(I - \nabla_{\mathbf{y}} \mathbf{W}_Y(\mathbf{y})) \rangle_Y & , in\ \Omega_f \\ [\mu_{\text{hom}}](\mathbf{x}) = I & , in\ \Omega_f^c \end{cases} \tag{7}$$

Here, $\langle f \rangle_Y$ is the average of f in Y (i.e. $\int_Y f(x, y) dy$). Furthermore, $\tilde{\varepsilon}(\mathbf{x}, \mathbf{y})$ and $\tilde{\mu}(\mathbf{x}, \mathbf{y})$ respectively denote

$$\tilde{\varepsilon}(\mathbf{x}, \mathbf{y}) = \begin{cases} 1 & , \ if\ \mathbf{x} \in \Omega_f^c \\ \varepsilon_r^B(\mathbf{y}) & , \ if\ \mathbf{x} \in \Omega_f \end{cases} \tag{8}$$

and

$$\tilde{\mu}(\mathbf{x}, \mathbf{y}) = \begin{cases} 1 & , \ if\ \mathbf{x} \in \Omega_f^c \\ \mu_r^B(\mathbf{y}) & , \ if\ \mathbf{x} \in \Omega_f \end{cases} \tag{9}$$

Besides, $\mathbf{V}_Y = (V_1, V_2, V_3)$ and $\mathbf{W}_Y = (W_1, W_2, W_3)$, where V_j, $j \in \{1, 2, 3\}$ and W_j, $j \in \{1, 2, 3\}$, are the unique solutions in $H_\sharp^1(Y)/\mathbb{R}$ of one of the six following problems $(\mathcal{K}_j)$ and $(\mathcal{M}_j)$ of electrostatic type:

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

and

$$(\mathcal{M}_j) : -\mathrm{div}_{\mathbf{y}}\left[\mu_r^B(\mathbf{y})(\nabla_{\mathbf{y}}(W_j(\mathbf{y}) - y_j))\right] = 0,\ j \in \{1, 2, 3\}$$

As η tends to zero, we can replace the isotropic heterogeneous magneto-dielectric diffracting obstacle of shape Ω_η, by a homogeneous obstacle of shape Ω_f with anisotropic permittivity and permeability given by what follows:

COROLLARY 3.2 (*Developed form for effective permittivity and permeability*) *The relative permittivity and permeability matrices arising in the homogenized problem* ($\mathcal{P}^{\mathbf{H}}_{\mathrm{hom}}$) *are equal to*:

$$[\varepsilon_{\mathrm{hom}}] = \begin{pmatrix} \langle \varepsilon_r^B(\mathbf{y})\rangle_Y & 0 & 0 \\ 0 & \langle \varepsilon_r^B(\mathbf{y})\rangle_Y & 0 \\ 0 & 0 & \langle \varepsilon_r^B(\mathbf{y})\rangle_Y \end{pmatrix} - \begin{pmatrix} \varphi_{11} & \varphi_{12} & \varphi_{13} \\ \varphi_{21} & \varphi_{22} & \varphi_{23} \\ \varphi_{31} & \varphi_{32} & \varphi_{33} \end{pmatrix}$$

and

$$[\mu_{\mathrm{hom}}] = \begin{pmatrix} \langle \mu_r^B(\mathbf{y})\rangle_Y & 0 & 0 \\ 0 & \langle \mu_r^B(\mathbf{y})\rangle_Y & 0 \\ 0 & 0 & \langle \mu_r^B(\mathbf{y})\rangle_Y \end{pmatrix} - \begin{pmatrix} \psi_{11} & \psi_{12} & \psi_{13} \\ \psi_{21} & \psi_{22} & \psi_{23} \\ \psi_{31} & \psi_{32} & \psi_{33} \end{pmatrix},$$

where φ_{ij} *and* ψ_{ij} *represent corrective terms defined by*:

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

and

$$\forall i, j \in \{1, 2, 3\}, \psi_{ij} = \left\langle \mu_r^B \frac{\partial W_j}{\partial y_i} \right\rangle_Y = \left\langle \mu_r^B \frac{\partial W_i}{\partial y_j} \right\rangle_Y = -\left\langle \mu_r^B \nabla W_i \cdot \nabla W_j \right\rangle_Y.$$

Here, the brackets denote averaging over Y. *Furthermore,* V_j *and* W_j *are the unique solutions in* $H^1_\sharp(Y)/\mathbb{R}$ *of the six partial differential equations* $\mathcal{K}_j$ *and* $\mathcal{M}_j$. *Hence, thanks to the symmetry of the matrices with entries* $\varphi_{ij} = \varphi_{ji}$ *and* $\psi_{ij} = \psi_{ji}$, *the homogenized permittivity and permeability are given by the knowledge of twelve terms* φ_{ij} *and* ψ_{ij}, *depending upon the resolution of six annex problems* ($\mathcal{K}_j$) *and* ($\mathcal{M}_j$).

Proof Since $\nabla_y \mathbf{V}_Y$ denotes the Jacobian matrix $\frac{\partial V_j}{\partial y_i}$ of $\mathbf{V}_Y$, $[\varepsilon_{\mathrm{hom}}]$ clearly derives from the equation of the theorem. Also, multiplying $\mathrm{div}_y(\varepsilon \nabla_y(V_i - y_i))$ by V_j, $j \in \{1, 2, 3\}$, and integrating by parts over the basic cell Y leads to:

$$\left\langle \varepsilon_r^B(\mathbf{y})(\nabla_y(V_i - y_i)) \cdot \nabla V_j \right\rangle_Y = 0.$$

Therefore, we get the equality:

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

Hence, we derive that $\varphi_{ij} = \varphi_{ji}$. As for the matrix of effective permeability, one can reproduce this derivation where μ_R^B, W_i and ψ_{ij} stand for ε_R^B, V_i and φ_{ij}.

3.2 *Homogenization result applied to non-cuboidal basic cells*

We now want to adapt Theorem 3.1 to the case of photonic crystals displaying other types of periodicity *e.g.* multiply-coated cylinders and spheres showing a periodicity along their radial direction respectively in polar and spherical coordinates. One way to do this is to adopt a covariant approach of Maxwell's equations, see for instance [49].

For this, let us consider a map from a co-ordinate system $\{u, v, w\}$ to the co-ordinate system $\{x_1, x_2, x_3\}$ given by the transformation characterized by $x_1(u, v, w)$, $x_2(u, v, w)$ and $x_3(u, v, w)$. We emphasize the fact that it is the transformed domain and co-ordinate system that are mapped onto the initial domain with Cartesian coordinates, and not the opposite. The transformation of the differentials is given by

$$\begin{cases} dx_1 = \dfrac{\partial x_1}{\partial u}du + \dfrac{\partial x_1}{\partial v}dv + \dfrac{\partial x_1}{\partial w}dw \\ dx_2 = \dfrac{\partial x_2}{\partial u}du + \dfrac{\partial x_2}{\partial v}dv + \dfrac{\partial x_2}{\partial w}dw \\ dx_3 = \dfrac{\partial x_3}{\partial u}du + \dfrac{\partial x_3}{\partial v}dv + \dfrac{\partial x_3}{\partial w}dw \end{cases} \tag{10}$$

This change of co-ordinates is characterized by the Jacobian of the transformation:

$$\mathbf{J}_{xu} = \frac{\partial(x_1, x_2, x_3)}{\partial(u, v, w)} = \begin{pmatrix} \dfrac{\partial x_1}{\partial u} & \dfrac{\partial x_1}{\partial v} & \dfrac{\partial x_1}{\partial w} \\ \dfrac{\partial x_2}{\partial u} & \dfrac{\partial x_2}{\partial v} & \dfrac{\partial x_2}{\partial w} \\ \dfrac{\partial x_3}{\partial u} & \dfrac{\partial x_3}{\partial v} & \dfrac{\partial x_3}{\partial w} \end{pmatrix}, \tag{11}$$

and the transformation of the differentials is given by

$$\begin{pmatrix} dx_1 \\ dx_2 \\ dx_3 \end{pmatrix} = \mathbf{J}_{xu} \begin{pmatrix} du \\ dv \\ dw \end{pmatrix}. \tag{12}$$

In electromagnetism, this change of coordinates amounts to replacing the different materials (often homogeneous and isotropic, which corresponds to the case of scalar piecewise constant permittivities and permeabilities) by equivalent inhomogeneous anisotropic materials described by a transformation matrix $\mathbf{T}$ (metric tensor) [49]. On a geometric point of view, the matrix $\mathbf{T}$

$$\mathbf{T} = \frac{\mathbf{J}^T\mathbf{J}}{det(\mathbf{J})}, \tag{13}$$

is a representation of the metric tensor.

In order to apply our Theorem 3.1 to photonic crystals with non cuboidal basic cell, the only thing to do in the transformed coordinates is to replace the materials (often homogeneous and isotropic) by equivalent ones that are inhomogeneous (their characteristics are no longer piecewise constant but merely depend on u, v, w co-ordinates) and anisotropic ones (tensorial nature). More precisely, this amounts to taking

$$\underline{\underline{\varepsilon'_\eta}} = \varepsilon_\eta \mathbf{T}^{-1} \text{ and } \underline{\underline{\mu'_\eta}} = \mu_\eta \mathbf{T}^{-1}, \tag{14}$$

in equation (4a) of $(\mathcal{P}_\eta^{\mathbf{H}})$, so that the main Theorem 3.1 applies *mutatis mutandis* by replacing ε_r^B and μ_r^B by $\underline{\underline{\varepsilon_r^{B'}}} = \varepsilon_r^B \mathbf{T}^{-1}$ and $\underline{\underline{\mu_r^{B'}}} = \mu_r^B \mathbf{T}^{-1}$.

Remark 1 In the case of orthogonal systems of coordinates (such as polar and spherical ones), the transformation matrix **T** is diagonal, thus the corollary 3.2 is still applicable. For non-orthogonal systems of coordinates, **T** has non-vanishing off diagonal entries and can also be non-symmetric: the homogenization of a photonic crystal consisting of a large assembly of spherical scatterers arranged within an oblique array leads to artificial anisotropy, unlike for a cubic array.

3.3 *Comments on the limit analysis*

3.3.1 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 a notion of two-scale convergence [23] for the convergence of the field in the photonic crystal together with considerations on the convergence of the diffracted field outside the photonic crystal. This method has been successfully applied, among others, by G. Bouchitté and R. Petit in the electromagnetic theory of gratings [16, 17] and by G. Bouchitté and D. Felbacq in the case of a 2D finite photonic crystal [52]. Let us briefly outline this mathematical justification.

The multi-scale method which relies on the boundedness of the asymptotic terms of the expansion (5), risks being mathematically unsound, and hence leading to untrue equations. Nevertheless, in our case, the multiple-scale method gives the good form of the homogenized equation: in case of dielectric media, this method has been successfully applied to various problems [15]. It remains to get the same results using the two-scale convergence relying on the following result due to G. Allaire [23]:

THEOREM 3.3 (*Two-scale convergence, Allaire*) *Let* Ω *be a bounded open subset of* $\mathbb{R}^3$ *and* (u_η) *be a bounded sequence in* $[L^2(\Omega)]^3$. *Then there exists* η_k *tending towards* 0 (*as k tends to infinity*) *and there exists a function* $u_0(x, y)$ *in* $[L^2(\Omega \times Y)]^3$ (*Y-periodic in y*) *such that for every* φ *in* $[L^2(\Omega, C_\sharp(Y))]^3$ (*such functions* φ *are said to be admissible*)

$$\lim_{k \longmapsto +\infty} \int_\Omega u_{\eta_k}(x) \cdot \varphi\left(x, \frac{x}{\eta_k}\right) dx = \iint_{\Omega \times Y} u_0(x, y) \cdot \varphi(x, y) dx dy. \tag{15}$$

Definition 3.4 A sequence (u_η) in $L^2(\Omega)$ satisfying (15) is said to two-scale weakly converge to a limit u_0 and we note $u_\eta \rightharpoonup\!\!\rightharpoonup u_0$.

Dealing with variational formulations, one has to take the limit in the product of bounded sequences of oscillating functions. To ensure a convergence in the sense of distributions of such sequences, we need to introduce the notion of strong two-scale convergence [23]:

Definition 3.5 (u_η) in $L^2(\Omega)$ strongly two-scale converge to $u_0(x, y) \in L^2_\sharp(\Omega \times Y)$ – and we note $u_\eta \twoheadrightarrow u_0(x, y)$ – if

$$\lim_{\eta \to 0} \int_\Omega |\, u_\eta \,|^2 \, dx = \iint_{\Omega \times Y} |u_0(x, y)|^2 \, dx dy.$$

The two-scale convergence 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. 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 $\|\mathbf{H}_\eta - (\mathbf{H}_{\text{hom}} + \eta\mathbf{C}_1)\|_{H^1(\text{curl},\Omega_f)} \to 0$. In other words, this expression converges to 0 for the Hilbert L^2 norm of the field and for the L^2 norm of its rotational. Roughly speaking, the corrector $\mathbf{C}_1$ is given for correcting strong oscillations near the macroscopic obstacle of shape Ω_f. It is very important in numerical computation since it gives a convergence criterion. This problem has been solved by Wellander [30] who proved that $\|\mathbf{H}_\eta - (\mathbf{H}_0(x, \frac{x}{\eta}) + \eta\mathbf{H}_1(x, \frac{x}{\eta}))\|_{H^1(\text{curl},\Omega_f)} \to 0$, if H_0, H_1 and their rotationals are admissible functions (in the 2D electromagnetic case, in transverse electric polarization, the proof is straightforwardly deduced from that of [23] given for the diffusion equation). Also, when $\text{div}(H_\eta)$ or $\text{div}(E_\eta) = 0$, the corrector type result holds in $H^1(\Omega_f)$: it is well-known, in functional analysis [51], that the Hilbert space $H^1(\Omega_f)$ has got a behavior close to $H^1(\text{curl}, \Omega_f)$'s provided one gets some control on the divergence in $L^2(\Omega_f)$ norm and on the trace on $\partial\Omega_f$. That is to say that the vectorial aspect of the diffraction by 3D 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 2D case [19].

Let us now 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 electromagnetic energy. In mathematical terms, it means that for all η, $\mathbf{F}_\eta$ is locally square integrable, that is to say that: $\forall\eta > 0, \exists M_\eta > 0$, $\int_{\Omega_f} \varepsilon_\eta | \mathbf{E}_\eta |^2 dx + \int_{\Omega_f} \mu_\eta | \mathbf{H}_\eta |^2 dx \leq M_\eta$ (ε_η and μ_η are coercive and bounded). The proof of the convergence of the diffracted field, 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 $L^2(\Omega_f)$ and we state some result allowing us notably to determine completely the limit function H_0 (as given heuristically in the previous section by the multi-scale method) thanks to the two-scale convergence. In step 2, we consider a radius $R > 0$ and a ball Ω of $\mathbb{R}^3$ such that $\Omega := \{| x | < R\}$ satisfies $\bar{\Omega}_f \subset \Omega$ (Ω strictly includes the diffracting object of shape Ω_f). Then, assuming $\mathbf{H}_\eta$'s boundedness in $L^2(\Omega)$ for a given η, using a *reductio ad absurdum* method and theoretical results obtained in step 1, we deduce that $(\mathbf{H}_\eta)$ is actually uniformly bounded in $L^2(\Omega)$. In the sequel, we will just prove two lemmas, namely a result of two-scale convergence with *adequate* assumptions to be used in step 1, and a result of boundedness for the electromagnetic field to perform the second step of the proof. The reader can find any further details in the original work by Bouchitté and Petit [16,17] or in our previous paper about the homogenization of 3D dielectric PC [24].

3.3.2 Convergence of permittivity, permeability and refractive index. It is worth noting that we cannot expect any nice convergence for the sequences of permittivities and permeabilities ε_η and μ_η. Indeed, ε_η and μ_η are proportional to the identity matrix, hence characterize an isotropic magneto-dielectric medium, unlike their limits which characterize a medium with anisotropic matrices of permittivity and permeability (although their product $\varepsilon_\eta\mu_\eta$ which defines the refractive index, may remain proportional to the identity). It is a typical difficulty encountered in many homogenization problems (ε_η and μ_η are just bounded which implies bad convergence properties for $\mathbf{F}_\eta = (\mathbf{E}_\eta, \mathbf{H}_\eta) \sim (\varepsilon_\eta \,\text{curl}\, \mathbf{H}_\eta, \mu_\eta \,\text{curl}\, \mathbf{E}_\eta)$). Hence, there is no hope to get control on the convergence of the diffracted field, by means of volume integral equations. Furthermore, we note that bodies of various permittivity and permeability can verify $\varepsilon_{\text{eff}}\mu_{\text{eff}} = \alpha Id$, and one has thus to define a class of equivalence for such heterogeneous structures, which behave in the same way for the long wavelengths, although they are quite different structures: similarly to the well-known lack of uniqueness of the solution to inverse problems, the homogenized diffracted field can be associated to various effective structures. Also, since μ_{eff} can be close to 0 (μ_η can be chosen strictly lower than 1), the effective refractive index can be arbitrarily close to 0, giving rise to astonishing properties as was shown by Pendry *et al*. [53].

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. 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 $\mathbf{F}_{\text{hom}}$ is still solution of a diffraction problem. This can be done, thanks to the Stratton–Chu formula (SC), 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 3D finite structures: the divergence of the sequences of electric-fields and magnetic-fields goes to infinity, hence we cannot easily keep controlling $\mathbf{F}_{\eta|\partial\Omega_f}$. Therefore, we consider a ball Ω strictly including the diffracting obstacle Ω_f. By the knowledge of the convergence of the diffracted field on the boundary of the ball $\partial\Omega$, we deduce the convergence of the diffracted field outside the obstacle Ω_f, thanks to the Stratton–Chu formula (SC). Let us recall that there is no alternative way to achieve the proof by means of volume integral equations. Unlike physicists of solid state physics who 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 (one has to estimate the so-called boundary layer).

4. Homogenization of spectral problems for heterogeneous cavities and waveguides

Although the mathematical and physical natures of scattering and spectral problems look intimately different, we can take benefit of the asymptotic study carried out in the third section to look at effective properties of a 3D structure with an infinite conducting boundary filled with a periodic arrangement of magneto-dielectric inclusions. This leads to the uneasy questions of the connections between on one hand the classical homogenization theory [15, 23, 41] dealing with fast oscillating periodic functions (or more generally functions of fast and slow variables) and on the other hand the so-called Bloch wave homogenization introduced in various mathematical frameworks [29, 34, 48] which relies essentially on the theorem of Bloch wave decomposition (phase-shift assumption for waves propagating in heterogeneous periodic media). Although the question of how wave is propagating at low frequencies in an 'infinite periodic' medium [48] seems intimately connected with the properties of an incident wave to an analogous 'finite periodic' structure in the low frequency regime (being understood that no concentration effect occurs on the macroscopic boundary of the finite structure), one has to precise in which sense to analyse the effective properties in this particular context.

In this section, we will first adopt the point of view of multi-scale method (heuristic version of two-scale convergence) and then make use of the Rayleigh method (a heuristical version of Bloch wave homogenization introduced by Allaire and Conca). We will not prove the convergence results as we do in the appendix for section 3, since they are already well covered in the aforementioned literature. Nevertheless, we think it may be useful to recall the classical results on the homogenization of spectral problems. Let us consider differential operators of the form

$$\mathcal{A}_\eta = b(\mathbf{D})^* g\left(\frac{\mathbf{x}}{\eta}\right) b(\mathbf{D}),\ \eta > 0 \tag{16}$$

where $b(\mathbf{D}) \in \mathcal{L}(L^2(\mathbb{R}^d;\mathbb{C}^m))$ with constant coefficients and g is a bounded invertible periodic function. Here, $*$ denotes the adjoint of an operator. The homogenization theory (see [41]) amounts to looking at the convergence for the resolvent of $\mathcal{A}_\eta$ (in a suitable sense)

$$\left(b(\mathbf{D})^* g\left(\frac{\mathbf{x}}{\eta}\right) b(\mathbf{D}) + \mathbf{I}\right)^{-1} \to \left(b(\mathbf{D})^* g^0 b(\mathbf{D}) + \mathbf{I}\right)^{-1}, \tag{17}$$

when η tends to 0. The constant matrix g^0 associated with the homogenized medium is usually called effective matrix. In [33], Birman and Suslina identify this matrix g^0 by considering the spectral decomposition of the family of operators $\mathcal{A}_\eta$ in a neighborhood of the origin (hence, they do not pass to the limit). Their approach is related to the Bloch decomposition proposed by C. Conca and M. Vanninathan [43]. In our case, we consider the limit of the resolvent with g function of slow and fast variables (i.e. $g(\mathbf{x}, \frac{\mathbf{x}}{\eta})$): this function is only periodic in its second variable. This allows us to take into account the finite size of the photonic crystal (thanks to the slow variable $\mathbf{x}$). Also, our Maxwell operator involves two oscillating (matrix) functions $\varepsilon(\mathbf{x}, \frac{\mathbf{x}}{\eta})$ and $\mu(\mathbf{x}, \frac{\mathbf{x}}{\eta})$, which make its form more general than that of $\mathcal{A}_\eta$. In [32] Zhikov proves the mathematical results for such a two-scale convergence of operators' resolvent in the case of the wave equation in porous media. In the present case, the sequence of operators is uniformly elliptic and compact, hence the strong convergence in classical operator norm.

4.1 *Homogenization of a cavity problem*

We are looking for electromagnetic vibrations of a metallic cavity of shape Ω_f containing a heterogeneous magneto-dielectric periodic medium of period η when η tends towards 0. In the harmonic regime, this amounts to looking for eigenfrequencies $\omega \in \mathbb{R}^+$ and their associated electromagnetic eigenmodes $(\mathbf{E}_\eta, \mathbf{H}_\eta)$ in $L^2(\Omega_f, \mathbb{C}^3) \times L^2(\Omega_f, \mathbb{C}^3)$, $(\mathbf{E}_\eta, \mathbf{H}_\eta) \not\equiv (0, 0)$, such that

$$(\mathcal{S}P_\eta)\begin{cases} \operatorname{curl}\mathbf{E}_\eta + i\omega\mu_0\mu_\eta\mathbf{H}_\eta = 0, \text{ in } \Omega_f & (18a)\\ \operatorname{curl}\mathbf{H}_\eta - i\omega\varepsilon_0\varepsilon_\eta\mathbf{E}_\eta = 0, \text{ in } \Omega_f & (18b)\\ n\wedge\mathbf{H}_\eta = \mathbf{J}_\eta, \text{ on } \partial\Omega_f & (18c)\\ n\wedge\mathbf{E}_\eta = 0, \text{ on } \partial\Omega_f & (18d)\end{cases}$$

where $\mathbf{J}_\eta$ is a surface current with support on the metallic boundary $\partial\Omega_f$, ε_0, μ_0, are the permittivity and permeability of *vacuum* and $\varepsilon_\eta = \varepsilon(\frac{x}{\eta})$, $\mu_\eta = \mu(\frac{x}{\eta})$, where $\varepsilon(y)$ and $\mu(y)$ are Y-periodic *real* functions (or hermitian matrices) to ensure the self-adjointness of the Maxwell operator (see below).

Since the tangential trace $n\wedge\mathbf{H}_\eta$ of the magnetic field $\mathbf{H}_\eta$ on the boundary $\partial\Omega_f$ is an unknown of the spectral problem, we choose an electric field formulation: we are therefore looking for $(\Lambda_\eta, E_\eta) \in \mathbb{R}^+ \times [H^1(\operatorname{curl}, \Omega_f, \varepsilon_\eta dx)]^3$, $\mathbf{E}_\eta \not\equiv 0$, such that

$$\left(\mathcal{S}P_\eta^E\right)\begin{cases} \varepsilon\left(\frac{x}{\eta}\right)^{-1}\operatorname{curl}\left(\mu\left(\frac{x}{\eta}\right)^{-1}\operatorname{curl}\mathbf{E}_\eta\right) = \frac{1}{\Lambda_\eta}\mathbf{E}_\eta, \quad \text{in } \Omega_f & (19a)\\ n\wedge\mathbf{E}_\eta = 0, \quad \text{on } \partial\Omega_f & (19b)\end{cases}$$

where ε_η and μ_η satisfy the usual coercivity and boundedness properties to ensure the uniform ellipticity of the corresponding sequence of Maxwell operators. Since ε_η and μ_η are real oscillating functions (or hermitian matrices), we cannot handle absorptive materials (we require the self-adjointness of the operators), unlike for the corresponding scattering problem in Theorem 3.1.

Looking for the spectrum of $(\mathcal{S}P_\eta^E)$ amounts to characterizing the spectrum of the Green operator (resolvent) S_η defined for all $f \in [L^2(\Omega_f, \varepsilon_\eta dx)]^3$ by $S_\eta f = u_\eta$ where u_η is the unique solution (via Lax–Milgram lemma) in $H(\mathrm{curl}, \Omega_f, \varepsilon_\eta dx)$ of

$$\varepsilon_\eta^{-1}\,\mathrm{curl}\left(\mu_\eta^{-1}\,\mathrm{curl}\, u_\eta\right) = f \quad \text{in } \Omega_f, n \wedge u_\eta = 0 \quad \text{on } \partial\Omega_f. \tag{20}$$

Since Ω_f is bounded, S_η is compact self-adjoint $\mathcal{L}([L^2(\Omega_f, \varepsilon_\eta dx)]^3)$. The self-adjointness follows from the boundary condition together with the Green formula applied in $H(\mathrm{curl}, \Omega_f, \varepsilon_\eta dx)$, and the compactness derives from Rellich lemma: $S_\eta f = u_\eta \in H(\mathrm{curl}, \Omega_f, \varepsilon_\eta dx) \cap H(\mathrm{div}, \Omega_f, \varepsilon_\eta dx) \hookrightarrow [L^2(\Omega_f, \varepsilon_\eta dx)]^3 \hookrightarrow [L^2(\Omega_f, dx)]^3$. We note σ_η the spectrum of the operator associated with (20) which consists of a countable sequence of eigenvalues tending towards 0 and such that $\sigma_\eta = \{0\} \cup \bigcup_{k\geq 1}\{\Lambda_\eta^k\}$ [34]. Besides, to each eigenvalue Λ_η^k, one can associate an eigenfunction $u_\eta^k \in [L^2(\Omega_f, \varepsilon_\eta dx)]^3$ such that $\|u_\eta^k\|_{L^2(\Omega_f,\varepsilon_\eta dx)} = 1$. Moreover, the family $\{u_\eta^k\}_{k\geq 1}$ is an orthonormal basis of $[L^2(\Omega_f, \varepsilon_\eta dx)]^3$ [34]. The spectral asymptotic analysis consists in studying the convergence of the discrete spectrum σ_η, when η tends towards 0. The limit spectrum turns out to be also discrete, hence we are dealing here with a pointwise convergence of spectra. This is evident since we are dealing with a sequence of uniformly compact operators. We note that in the case of a high-frequency analysis (eigenvalues on the order of η^2), this is no longer the case: the limit spectrum may contain both continuous and discrete parts, as shown by Allaire and Conca for the scalar wave equation [34], and Cherednichenko and Guenneau for the vector Maxwell operator [22].

We can now state our basic theorem on the spectral asymptotic analysis of a heterogeneous cavity (classical homogenization at a fixed frequency):

THEOREM 4.1 (*Homogenized Maxwell's operator for a closed cavity*) *When η tends to zero, the sequence of bounded self-adjoint operators S_η in $\mathcal{L}([L^2(\Omega_f, \varepsilon_\eta dx)]^3) \hookrightarrow \mathcal{L}([L^2(\Omega_f, dx)]^3)$ (associated with $\mathcal{S}P_\eta^E$) strongly converges in operators norm to a limit operator S defined for every $f \in [L^2(\Omega_f, [\varepsilon_{\mathrm{hom}}]dx)]^3 \hookrightarrow [L^2(\Omega_f, dx)]^3$ by $Sf = \mathbf{E}_{\mathrm{hom}}$ where $\mathbf{E}_{\mathrm{hom}}$ are the non-zero eigenfields in $H(\mathrm{curl}, \Omega, [\varepsilon_{\mathrm{hom}}]dx)$ associated with the countable set of real positive eigenvalues Λ_{hom} of the following homogenized spectral problem*:

$$\left(\mathcal{S}P_{\mathrm{hom}}^{\mathbf{E}}\right) = \begin{cases} [\varepsilon_{\mathrm{hom}}]^{-1}\mathrm{curl}([\mu_{\mathrm{hom}}]^{-1}\mathrm{curl}\,\mathbf{E}_{\mathrm{hom}}(\mathbf{x})) = \frac{1}{\Lambda_{\mathrm{hom}}}\mathbf{E}_{\mathrm{hom}}(\mathbf{x}), & \text{in } \Omega_f, \\ n \wedge \mathbf{E}_{\mathrm{hom}}(\mathbf{x}) = 0, \quad \text{on } \partial\Omega_f, \end{cases} \tag{21}$$

where the effective permittivity and permeability $[\varepsilon_{\mathrm{hom}}]$ and $[\mu_{\mathrm{hom}}]$ are symmetric bounded coercive matrices respectively given by

$$[\varepsilon_{\mathrm{hom}}]\xi \cdot \xi = \min_{\Phi \in H_\sharp^1(Y)} \int_Y \varepsilon(y)(\xi + \nabla_y \Phi(y)) \cdot (\xi + \nabla \Phi(y))\, dy, \forall \xi \in \mathbb{R}^3, \tag{22}$$

and

$$[\mu_{\mathrm{hom}}]\xi \cdot \xi = \min_{\Psi \in H_\sharp^1(Y)} \int_Y \mu(y)(\xi + \nabla_y \Psi(y)) \cdot (\xi + \nabla \Psi(y))\, dy, \quad \forall \xi \in \mathbb{R}^3. \tag{23}$$

Also, when $\eta \to 0$, σ_η converges (in a pointwise sense) to σ_{hom}, spectrum associated with the limit operator $Sf = \mathbf{E}_{\mathrm{hom}}$.

Proof Since S_η is a sequence of uniformly compact resolvent operators, S is itself a compact self-adjoint operator and its spectrum σ_{hom} is discrete. More precisely, $\sigma = \{0\} \bigcup \bigcup_{k \geq 1} \Lambda^k_{\text{hom}}$ the eigenvalues being ordered in decreasing order and $\lim_{k \longmapsto +\infty} \Lambda^k_{\text{hom}} = 0$. From the Courant–Fischer min–max lemma, it follows that $\forall k \geq 1$, $\lim_{\eta \longmapsto 0} {\Lambda_\eta}^k = \Lambda^k_{\text{hom}}$ (see [34] for the scalar wave equation).

4.2 *Homogenization of metallic magneto-dielectric waveguides*

In this section, we are looking for out-of-plane propagating modes (oblique incidence, i.e. $(\mathbf{E}, \mathbf{H})(x_1, x_2, x_3) = (\mathbf{E}(x_1, x_2), \mathbf{H}(x_1, x_2))e^{i\gamma x_3}$, with $\gamma \geq 0$ the propagation constant. We consider the case of a metallic waveguide of constant cross-section Ω_f (open bounded subset of $\mathbb{R}^2$) filled with a periodic assembly of dielectric rods for the large wavelengths.

In waveguide theory, it is customary to develop the electric field $\mathbf{E}(x_1, x_2)$ in its transverse and longitudinal components $\mathbf{E_t}(x_1, x_2)$ and $E_l(x_1, x_2)$:

$$\mathbf{E}(x_1, x_2) = \mathbf{E_t}(x_1, x_2) + E_l(x_1, x_2)\mathbf{e}_3. \tag{24}$$

We then define its transverse gradient, divergence and curl as

$$\begin{aligned} \nabla_{\mathbf{t}} E_l(x_1, x_2) &= \frac{\partial E_l}{\partial x_1}\mathbf{e}_1 + \frac{\partial E_l}{\partial x_2}\mathbf{e}_2 \\ \text{div}_{\mathbf{t}}(E_{t,1}\mathbf{e}_1 + E_{t,2}\mathbf{e}_2) &= \frac{\partial E_{t,1}}{\partial x_1} + \frac{\partial E_{t,2}}{\partial x_2} \\ \text{curl}_{\mathbf{t}}(E_{t,1}\mathbf{e}_1 + E_{t,2}\mathbf{e}_2) &= \frac{\partial E_{t,2}}{\partial x_1} - \frac{\partial E_{t,1}}{\partial x_2}. \end{aligned} \tag{25}$$

It is also convenient to define the operators curl_γ and div_γ as per:

$$\begin{aligned} \text{div}_\gamma \mathbf{E} &= \frac{\partial E_{t,1}}{\partial x_1} + \frac{\partial E_{t,2}}{\partial x_2} + i\gamma H_l = \text{div}_{\mathbf{t}} E_t + i\gamma E_l \\ \text{curl}_\gamma \mathbf{E} &= \left(\frac{\partial E_l}{\partial x_2} - i\gamma E_{t,2}\right)\mathbf{e}_1 + \left(i\gamma H_{t,1} - \frac{\partial E_l}{\partial x_1}\right)\mathbf{e}_2 + \left(\frac{\partial E_{t,2}}{\partial x_2} - \frac{\partial E_{t,1}}{\partial y}\right)\mathbf{e}_3 \\ &= \text{curl}_{\mathbf{t}} E_t \mathbf{e}_3 + (\nabla_{\mathbf{t}} E_l - i\gamma \mathbf{E_t}) \times \mathbf{e}_3. \end{aligned} \tag{26}$$

The problem depends upon two positive real parameters: the small parameter η characterizing the distance between inclusions (tending to zero), and the fixed propagating constant γ. Since the tangential trace $n \wedge \mathbf{H}_\eta$ of the magnetic field $\mathbf{H}_\eta$ on the boundary $\partial\Omega_f$ is an unknown of the spectral problem, we choose an electric field formulation: we are therefore looking for $(\gamma, \Lambda_\eta, E_\eta) \in \mathbb{R}^+ \times \mathbb{R}^+ \times [H^1(\text{curl}, \Omega_f, \varepsilon_\eta dx)]^3$, $\mathbf{E}_\eta \not\equiv 0$, such that

$$\mathcal{P}^{\mathbf{E}}_\eta \begin{cases} {\varepsilon_\eta}^{-1}\big(\text{curl}_\gamma\, {\mu_\eta}^{-1}\, \text{curl}_\gamma \mathbf{E}_\eta(\mathbf{x})\big) = \dfrac{1}{\Lambda_\eta} E_\eta(\mathbf{x}) & \text{in } \Omega_f, \\ n \wedge \mathbf{E}_\eta = 0 & \text{on } \partial\Omega_f, \end{cases} \tag{27}$$

where ε_η and μ_η are real valued functions such that $M \geq \varepsilon_\eta, \mu_\eta \geq m > 0$. The operator associated with this problem has a compact resolvent. Its spectrum is a discrete set of isolated eigenvalues belonging to $[\frac{\gamma^2}{\varepsilon_\eta \mu_\eta}; +\infty[$.

We can state the following homogenization result:

Theorem 4.2 (*Homogenized Maxwell's operator for a closed waveguide*) *When η tends to zero, $\mathbf{E}_\eta$ eigensolution of the problem ($\mathcal{P}^{\mathbf{E}}_\eta$), converges (for the norm of energy on*

Ω_f) to the eigensolution $\mathbf{E}_{\text{hom}}$ of the spectral problem ($\mathcal{P}^{\mathbf{E}}_{\text{hom}}$) defined as follows: look for $(\gamma, \Lambda_{\text{hom}}, \mathbf{E}_{\text{hom}}) \in \mathbb{R}^+ \times \mathbb{R}^+ \times [H^1(\text{curl}, \Omega, \varepsilon_{\text{hom}} dx)]^3$, $\mathbf{E}_{\text{hom}} \not\equiv 0$, *such that*

$$\mathcal{P}^{\mathbf{E}}_{\text{hom}} \begin{cases} [\varepsilon_{\text{hom}}]^{-1}\text{curl}_\gamma [\mu_{\text{hom}}]^{-1}\text{curl}_\gamma\, \mathbf{E}_{\text{hom}}(\mathbf{x}) = \frac{1}{\Lambda_{\text{hom}}}\mathbf{E}_{\text{hom}}(\mathbf{x}) & \text{in } \Omega \\ n \wedge \mathbf{E}_{\text{hom}} = 0 & \text{on } \partial\Omega. \end{cases} \tag{28}$$

The relative permittivity and permeability matrices for the effective waveguide are equal to:

$$\chi_{\text{hom}} = \begin{pmatrix} \langle \chi_r^B(\mathbf{y})\rangle_Y & 0 & 0 \\ 0 & \langle \chi_r^B(\mathbf{y})\rangle_Y & 0 \\ 0 & 0 & \langle \chi_r^B(\mathbf{y})\rangle_Y \end{pmatrix} - \begin{pmatrix} \varphi_{11}^\chi & \varphi_{12}^\chi & 0 \\ \varphi_{21}^\chi & \varphi_{22}^\chi & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{29}$$

where $\chi \in \{\varepsilon, \mu\}$ and φ_{ij}^χ represent corrective terms defined by:

$$\forall i, j \in \{1, 2\}, \varphi_{ij}^\chi = \left\langle \chi_r^B \frac{\partial V_j^\chi}{\partial y_i} \right\rangle_Y = \left\langle \chi_r^B \frac{\partial V_i^\chi}{\partial y_j} \right\rangle_Y = -\left\langle \chi_r^B\, \nabla V_i^\chi \cdot \nabla V_j^\chi \right\rangle_Y,$$

the brackets denoting averaging over Y. Furthermore, V_j^χ are the unique solutions in $H^1_\sharp(Y)/\mathbb{R}$ of the four partial differential equations:

$$-\text{div}_{t,\mathbf{y}}\left[\chi_r^B(\mathbf{y})\left(\nabla_{t,\mathbf{y}}(V_j^\chi(\mathbf{y}) - y_j)\right)\right] = 0,\ j \in \{1, 2\},\ \chi \in \{\varepsilon, \mu\}.$$

Hence, thanks to the symmetry of the right matrix in (29) *with entries $\varphi_{ij}^\chi = \varphi_{ji}^\chi$, the homogenized permittivity and permeability are fully described by the knowledge of the six terms φ_{ij}^χ, $i, j \in \{1, 2\}, i \geq j, \chi \in \{\varepsilon, \mu\}$.*

Remark 1 We have actually a strong convergence (in operator norm) for the sequence of uniformly compact resolvent operators associated with $\mathcal{P}^{\mathbf{E}}_\eta$ and thus a pointwise convergence for the sequence of corresponding spectra as in Theorem 4.1. The resolvent operator associated with $\mathcal{P}^{\mathbf{E}}_{\text{hom}}$ is therefore compact and its spectrum is discrete.

To conclude this paragraph, we note that our homogenization results do not cover the important case of a periodic assembly of vanishing fibers. For the transverse case, we refer the reader to the work by Felbacq and Bouchitté [19], and for the oblique case to the paper by Poulton *et al.* [54]. In this latter case, the oblique parameter γ makes the problem singularly perturbed (suggesting non-commuting limits): it is not obvious to retrieve the homogenization results in [19] simply by taking the limit $\gamma \to 0$.

4.3 *Multi-scale method versus Bloch wave homogenization*

In Theorem 3.1, we have assumed that if $\{\mathbf{E}_\eta\}_{\eta>0}$, satisfies certain limit conditions on the boundary $\partial\Omega_f$ of the cavity, in addition to the equation $A_\eta \mathbf{E}_\eta = f$ in Ω_f, then the $H(\text{curl}, \Omega_f, \varepsilon_\eta dx)$ bound on $\{\mathbf{E}_\eta\}$ was a consequence of ellipticity and the Poincaré inequality. In the present section, $\Omega_f = \mathbb{R}^3$ is unbounded, then there is no estimate on $\{\mathbf{E}_\eta\}$ in $H(\text{curl}, \mathbb{R}^3, \varepsilon_\eta dx)$ because the Poincaré inequality is not available (note that if we consider $A_\eta + Id$ instead of A_η, then the bound in $H(\text{curl}, \mathbb{R}^3, \varepsilon_\eta dx)$ is automatic). The natural question which arises is to know what happens to periodic oscillations in Fourier space. To this end, we denote by ξ and ζ the variables dual to x and y in Fourier space. Since the Fourier transform of a function depending on x/η is a function of $\eta\xi$, we have the relation $\xi = \eta\zeta$. This indicates that the fast oscillations in the medium give place to the slow variable ζ. Further, if we replace each derivative $\partial/\partial x_j$ as is usual in Fourier analysis, by ξ_j, which is equal to $\eta^{-1}\zeta_j$, we see that we accumulate negative powers of η. The original difficulty arising from products of weakly convergent sequences is therefore transformed to dealing with slow variations combined with singularities in the Fourier space. The passage to the limit in the homogenization process requires now certain regularity of the dominant Bloch eigenvalue and of the corresponding eigenmode in a neighborhood of the origin: the homogenized matrix is given by the Hessian of this dominant Bloch eigenvalue at the origin. In the 2D case, it was numerically shown that the two approaches (classical homogenization together with finite elements versus Bloch wave homogenization via a multipole method) give the same numerical results for elliptical dielectric inclusions [31].

In the sequel, we want to discuss these connections with respect to the work by Bao Keda *et al.* [29]. This multipole expansion is essentially based on the so-called Rayleigh identity, which contains within it all the information on Bloch waves, solutions of Helmholtz equations, propagating in a homogeneous medium (in that case, there are no bands in the spectrum). From the derivation of a scattering matrix associated with boundary conditions for the electromagnetic field across the interface between the two-media, and the Rayleigh identity, one can derive some effective properties in the long-wavelength limit, which are graphically interpreted as the slope of the dispersion curves going through the origin, i.e. the limit when the modulus of the Bloch vector $\mathbf{k}_{\text{Bloch}}$ (which lies within the first Brillouin zone $]0; 2\pi[^3$) tends to zero along with the eigenfrequency. In the classical book by Bensoussan, Lions and Papanicolaou (1978) [15], a lemma states that when it exists, the tensor

$$\varepsilon^{-1}_{\text{hom},pq} = \frac{1}{2}\frac{\partial^2\omega_{12}}{\partial\mathbf{k}_{\text{Bloch},p}\,\partial\mathbf{k}_{\text{Bloch},q}}(0),$$

defines the effective mass tensor of the first band which is generated by eigenfrequencies ω_1 for various values of the Bloch vector $\mathbf{k}_{\text{Bloch}}$. The work by McPhedran *et al.* (1996) [48] which establishes the first dynamic correction to the Lorentz–Lorenz formula by using the Rayleigh identity should thus provide consistent numerical results with our approach. We are going to show that the analytical formulae derived with the Rayleigh method in the quasi-static limit are consistent with that of the multi-scale method.

If we consider a 3D periodic two-phase medium with spherical inclusions, our results give also some information on the corresponding effective properties of the material derived as a limit case of the multipole expansion (long-wavelength and dilute composite): the propagation of electromagnetic waves in triply periodic lattices of magneto-dielectric spheres can be represented in terms of Debye potentials and leads to a generalized Rayleigh identity. It must be noticed that this procedure leads to an eigenvalue problem formulation that enables one to construct both low-frequency curves (giving rise to effective properties) and high-order dispersion curves. The philosophy of this method is connected to the 'Bloch wave homogenization' theory co-developed by G. Allaire and C. Conca [34]: these methods are dual in the Fourier sense discussed above. For the sake of completeness, in the sequel we adapt the homogenization result of Bao Keda *et al.* [29] derived in the long-wavelength limit for a cubic array of dielectric spheres thanks to the multipole expansion, to the case of magneto-dielectric spheres.

The solution of the Maxwell equations can be expressed in terms of two-scalar functions (v and w), called Debye potentials (see Van Bladel [55]), as follows:

$$\mathbf{E}(\mathbf{r}) = i\omega\mu(\mathbf{r})\,\mathrm{curl}\{f(\mathbf{r})w(\mathbf{r})\} + \mathrm{curl}\,\mathrm{curl}\{f(\mathbf{r})v(\mathbf{r})\}, \tag{30}$$

$$\mathbf{H}(\mathbf{r}) = -i\omega\varepsilon(\mathbf{r})\,\mathrm{curl}\{f(\mathbf{r})v(\mathbf{r})\} + \mathrm{curl}\,\mathrm{curl}\{f(\mathbf{r})w(\mathbf{r})\}, \tag{31}$$

where ω represents the frequency of the wave, $\mathbf{r} = \mathbf{x}/\mid \mathbf{x} \mid$ and ε and μ are piecewise constant functions, which take value ε^i and μ^i inside the sphere and ε^e and μ^e otherwise.

Following Bao Keda *et al.* [29], the Debye potentials v and w satisfy Helmholtz equations in each homogeneous medium. If u represent either v or w, we have

$$(\Delta + \nu^2\tau^2k^2)u^{(i)}(\mathbf{r}) = 0, \tag{32}$$

in the inclusions (ν and τ denoting respectively the scaled relative permittivity $\varepsilon_r^i/\varepsilon_r^e$ and the scaled relative permeability μ_r^i/μ_r^e), and

$$(\Delta + k^2)u^{(e)}(\mathbf{r}) = 0, \tag{33}$$

outside the inclusions.

The spectral problem is well-specified if the Debye potentials satisfy *adequate* boundary conditions at the surface of the spheres (derived from the continuity of the tangential components of the fields [55]) together with quasi-periodicity (or Floquet–Bloch) conditions

$$u(\mathbf{r} + \mathbf{R}_p) = v(r)e^{i\mathbf{k}_{\mathrm{Bloch}}\cdot\mathbf{R}_p}, \tag{34}$$

where $\mathbf{k}_{\mathrm{Bloch}}$ is known as the Bloch wave-vector and $\mathbf{R}_p = p_1\mathbf{a}^{(1)} + p_2\mathbf{a}^{(2)} + p_3\mathbf{a}^{(2)}$ is the vector attached to the nodes $(p_1, p_2) \in \mathbb{Z}^2$ of the lattice of translations vectors $\mathbf{a}^{(1)}$ and $\mathbf{a}^{(2)}$, which form the basis for the lattice as a whole.

Setting $\mathbf{f}(\mathbf{r}) = \mathbf{R} - \mathbf{R}_p$ in the unit cell centred about $\mathbf{R}_p$, (30) and (31) reduce to classical expressions used in the Mie theory [55]. Moreover, by means of the Debye potentials we can classify fields in E-type (or transverse magnetic), when only the electric field has a component along $\mathbf{r}$ ($w = 0$) and M-type (or transverse electric) when only the magnetic field has a component along $\mathbf{r}$ ($v = 0$). In each case we use a multipole expansion of the corresponding Debye potentials v and w in the vicinity of the sphere ($r =\mid \mathbf{r} \mid= r_c$) located at the origin. In the inclusions, we have

$$u = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} c_{lm}^{\alpha} J_l(kr)Z_{lm}(\theta, \varphi), \tag{35}$$

where u denotes v if $\alpha = E$ and w if $\alpha = M$; here, J_l and Y_l represent spherical Bessel functions and Z_{lm} are spherical harmonics. Besides, θ and φ are the usual angular variables in spherical coordinates. Similarly, we get the following expansion between the inclusions:

$$u = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} \left\{a_{lm}^{\alpha} J_l(kr) + b_{lm}^{\alpha} Y_l(kr)\right\} Z_{lm}(\theta, \varphi). \tag{36}$$

On the interface boundary $\{r = r_c\}$ we prescribe the conditions of the continuity of the Debye potential and of the normalized flux. According to the choice of polarization, two types of boundary conditions are possible:

$$u^{(e)} = u^{(i)} \text{ and } \frac{\partial \mu^{(e)}}{\partial r} = \frac{1}{\xi}\frac{\partial \mu^{(i)}}{\partial r} \tag{37}$$

In transverse magnetic polarization (E-type) we have the boundary conditions (37) with $u = v$ and $\xi = 1/\tau^2$, whereas in transverse electric polarization M(-type), $u = w$ and ξ should be $1/\nu^2$. Using multipole expansions (35)–(36), we are led to

$$c_{ml}^{\alpha} J_m\big(k^{(i)}r_c\big) = a_{ml}^{\alpha} J_m\big(k^{(e)}r_c\big) + b_{ml}^{\alpha} Y_m\big(k^{(e)}r_c\big), \tag{38}$$

$$\xi c_{ml}^{\alpha} J_m'\big(k^{(i)}r_c\big) = a_{ml}^{\alpha} J_m'\big(k^{(e)}r_c\big) + b_{ml}^{\alpha} Y_m'\big(k^{(e)}r_c\big), \tag{39}$$

where ξ stands for $\frac{1}{\nu^2}$ if $\alpha = E$ and $\frac{1}{\tau^2}$ if $\alpha = M$; also, $k^{(e)} = \nu\tau k$ and $k^{(e)} = k$. Eliminating c_m we find

$$a^{\alpha}_{ml} = -M^{\alpha\alpha}_{m} b^{\alpha}_{ml}, \tag{40}$$

where

$$M^{\alpha\alpha}_{m} = \frac{\xi^{-1} J_m\big(k^{(i)} r_c\big) Y'_m\big(k^{(e)} r_c\big) - J'_m\big(k^{(i)} r_c\big) Y_m\big(k^{(e)} r_c\big)}{\xi^{-1} J_m\big(k^{(i)} r_c\big) J'_m\big(k^{(e)} r_c\big) - J'_m\big(k^{(i)} r_c\big) J_m\big(k^{(e)} r_c\big)}. \tag{41}$$

This so-called **M** matrix is block diagonal ($M^{(EM)}_l = M^{(ME)}_l = 0$).

Because the Debye potentials are quasi-periodic and obey the Helmholtz equation, we obtain the following Rayleigh identities

$$a^{\alpha}_{lm} = \sum_{l',m'} \sigma_{lm,l'm'} b^{\alpha}_{l',m'}, \quad \forall \alpha \in \{E, M\}, \tag{42}$$

where expressions $\sigma_{lm,l'm'}$ depend on the so-called lattice sums [29, 56]:

$$S^{Y}_{lm}(k^e, \mathbf{k}_{\mathrm{Bloch}}) = \sum_{p \in \mathbb{Z}^3 \setminus (0,0,0)} Y_l(k^e R_p) Z^{*}_{lm}(\theta_p, \varphi_p) e^{i\Phi_q l + i\mathbf{k}_{\mathrm{Bloch}} \cdot R_p}. \tag{43}$$

Therefore the Rayleigh system for the triply periodic structure has the form:

$$\sum_{l',m'} \left\{ M^{\alpha\alpha}_{l} \delta_{ll'} \delta_{mm'} + \sum_{l''=|l-l'|}^{l+l'} S^{Y}_{l'',m-m'}\big(k^{(e)}, \mathbf{k}_{\mathrm{Bloch}}\big) A^{l'',m-m'}_{lm,l'm'} \right\} B^{\alpha}_{l'm'} = 0, \tag{44}$$

for every $\alpha \in \{E, M\}$. Here $S^{Y}_{l'',m-m'}(k^{(e)}, \mathbf{k}_{\mathrm{Bloch}})$ are the dynamic lattice sums and $A^{l'',m-m'}_{lm,l'm'}$ can be expressed in terms of Clebsch–Gordan coefficients for the vector coupling of angular momenta l and l'.

Furthermore, we want to truncate this infinite algebraic system to the dipole order ($-1 \le l, l', m, m' \le 1$) and take the quasi-static limit when k_{Bloch} tends towards 0, as does k with $k = \alpha k_{\mathrm{Bloch}}$.

Now, we assume that α has the following expansion

$$\alpha = \alpha_0 + \alpha_2 (k_{\mathrm{Bloch}} d)^2 + O(k_{\mathrm{Bloch}} d)^4. \tag{45}$$

Here, α_0 and α_2 are quantities we seek to determine: α_0 is related to an equivalent (phase) refractive index for the array, since the change of phase across the unit cell is given by

$$\Delta\Phi = k_{\mathrm{Bloch}} d = N_{\mathrm{eff}} k^{(e)}_{\perp} d. \tag{46}$$

Taking into account the following series expansions for small $k^{(e)}$ [29]

$$M^{\alpha\alpha}_{0} \sim \frac{1}{(\xi^{-1} - 1) k r_c}, \quad \forall \alpha \in \{E, M\}, \tag{47}$$

where $\xi = 1/\tau^2$ in transverse magnetic polarization (E-type), whereas for transverse electric polarization M(-type) ξ should be $1/\nu^2$. For the lattice sums, one finds the following leading order asymptotics [29, 56]

$$S^{Y}_{0,0} \sim -\frac{\sqrt{4\pi}}{\alpha(1-\alpha^2)} \frac{1}{k^3_{\mathrm{Bloch}}}, \; S^{Y}_{1,m} \sim -\frac{4\pi Z_{1,m}(\theta_0, \varphi_0)}{\alpha^2(1-\alpha^2)} \frac{1}{k^3_{\mathrm{Bloch}}}, \tag{48}$$

$$S^{Y}_{2,m} \sim \frac{4\pi Z_{2,m}(\theta_0, \varphi_0)}{\alpha^2(1-\alpha^2)} \frac{1}{k^3_{\mathrm{Bloch}}} - \frac{3}{(\alpha k_{\mathrm{Bloch}})^3} S_{2,m}. \tag{49}$$

Denoting the area fraction of the spheres f by $f = \frac{4\pi r_c^3}{3d^3}$ and collecting the terms of the same order of k_{Bloch} in the dipole approximation of (44) one gets two equations of Clausius–Mossotti type

$$\varepsilon_{\text{eff}}^0 = \frac{\nu + 2f}{\nu - f}, \quad \mu_{\text{eff}}^0 = \frac{\tau + 2f}{\tau - f}, \tag{50}$$

which can both be deduced by an electrostatic argument involving a Lorentz cavity [57]. Also, multiplying these two expressions, we get

$$\left(N_{\text{eff}}^0\right)^2 = \varepsilon_{\text{eff}}^0 \mu_{\text{eff}}^0 = \left(\frac{\nu + 2f}{\nu - f}\right)\left(\frac{\tau + 2f}{\tau - f}\right). \tag{51}$$

This formula calls for two few remarks.

Firstly, the decoupling between effective permittivity and permeability is in agreement with our results of section 2. Secondly, we note that in the 2D case, $2f$ should be replaced by f, where $f = \pi r_c^2/d^2$. Therefore, if the dielectric contrast and the magnetic contrast across the interface boundary are chosen such that $\nu = \tau^{-1}$ or $\nu = -\tau$, the effective refractive index is that of the vacuum. This suggests that when ν is replaced by $-\nu$ (resp. τ by $-\tau$), ε_{eff} is replaced by $1/\varepsilon_{\text{eff}}$ (resp. μ_{eff} with $1/\mu_{\text{eff}}$). In the 2D case, this is in accordance with Keller's theorem [58] (1964). In 1970, Dykhne, using the fact that a divergence-free field in 2D when rotated locally at each point by 90 degrees produces a curl-free field and vice versa, could generalize Keller's result to isotropic multiphase and polycrystalline media [59]. Zolla and Guenneau noticed that it still holds true for 2D media described by bounded, symmetric and coercive tensors of permittivity [31]. In the 3D case, there is no such simplification (there is no equivalent to the checkerboard problem in 3D): this is caused by the fact that the symmetry of the problem appeals to compose by two rotations of 90 degrees in 3D, but they do not commute (taking $\nu = -2\tau$ does not simplify the Clausius–Mossotti expression).

5. Numerical implementation

5.1 *Numerical illustration in 2D*

5.1.1 TM polarization deduced from the 3D case. In the sequel we seek to determine the coefficients of the tensor of effective permittivity $[\varepsilon_{\text{hom}}]$ in 2D case (this procedure repeats *mutatis mutandis* for the effective permeability $[\mu_{\text{hom}}]$). More precisely, Ω_f is invariant itself with respect to the third component and we look at the particular case of TM polarization, i.e. $\mathbf{H} = u(x_1, x_2)\mathbf{e}_3$. When ε does not depend on the third component namely $\varepsilon(\mathbf{y}) = \varepsilon(y_1, y_2)$ we get from the annex problem $(\mathcal{K}_j)$

$$[\varepsilon_{\text{hom}}] = \begin{pmatrix} [A_{\text{hom}}] & \begin{matrix} 0 \\ 0 \end{matrix} \\ 0\ 0 & \langle \varepsilon \rangle_{Y^2} \end{pmatrix},$$

where $Y^2 =]0; 1[^2$ and $[A_{\text{hom}}]$ is the 2×2 matrix given by:

$$[A_{\text{hom}}] = \begin{pmatrix} \langle \varepsilon \rangle_{Y^2} - \langle \varepsilon \partial_1 V_1 \rangle_{Y^2} & -\langle \varepsilon \partial_1 V_2 \rangle_{Y^2} \\ -\langle \varepsilon \partial_2 V_1 \rangle_{Y^2} & \langle \varepsilon \rangle_{Y^2} - \langle \varepsilon \partial_2 V_2 \rangle_{Y^2} \end{pmatrix},$$

and V_j, $j \in \{1, 2\}$, is the unique solution in $H_\sharp^1(Y^2)/\mathbb{R}$ of

$$(\mathcal{K}_j) : \operatorname{div}[\varepsilon(\mathbf{y})(\nabla(V_j(\mathbf{y}) - y_j))] = 0.$$

Multiplying $\mathrm{div}_y(\varepsilon\,\nabla_y(V_i - y_i))$ by V_j in $(\mathcal{P}_j)$, $j \in \{1, 2\}$, and integrating by parts over the basic cell Y^2 leads to the weak formulation:

$$\langle \varepsilon(\mathbf{y})(\nabla_y(V_i - y_i)) \cdot \nabla V_j \rangle_{Y^2} = 0. \tag{52}$$

To get the corresponding variational equation from the annex problem $(\mathcal{M}_j)$, one has to replace ε by μ in $(\mathcal{K}_j)$. In the discrete formulation the basic cell is meshed with triangles and node elements are used for the scalar fields V_i:

$$V_i = \sum_k^n \beta_i^k w_k^n(x, y), \qquad \text{in } Y^2, \tag{53}$$

where β_i^k denotes the nodal value of the component V_i of the multi-scalar potential $\mathbf{V}$. Besides, w_k^n are basis functions of first order finite elements. The GetDP software [60] has been used to set up the finite element problem with some periodicity conditions imposed to the field on opposite sides of the basic cell Y. If we take ε as a piecewise constant function in (52), i.e. $\varepsilon = 4 + 3i$ in an elliptical inclusion (minor and major axes 0.3 and 0.4) and 1.25 elsewhere (*cf.* figure 5), $[\varepsilon_{\mathrm{hom}}]$ is

$$\begin{pmatrix} 1.9296204 + i0.2536979 & (-1-i)10^{-16} \\ (-44-2i)10^{-18} & 2.1127643 + i0.4618554 \end{pmatrix},$$

with $\langle \varepsilon \rangle_{Y^2} = 2.2867255 + i1.1309734$ (see figure 5 for the associated potentials V_1 and V_2). We note that the off-diagonal terms are not strictly null: this artificial anisotropy induced by the mesh of the structure indicates the order of magnitude of the numerical error. Also, these numerical results have been retrieved with the so-called method of fictitious charges based on an integral approach, which we discuss in the next paragraph (see also [31]). We found that the diagonal terms were accurate to the seven first significant figures (which are therefore reported above). The order of magnitude of the off diagonal terms was about the same in both methods.

5.1.2 TE polarization deduced from the 3D case.

We can also look at the case of TE polarization, i.e. $\mathbf{E} = u(x_1, x_2)\mathbf{e}_3$. When μ does not depend on the third component namely

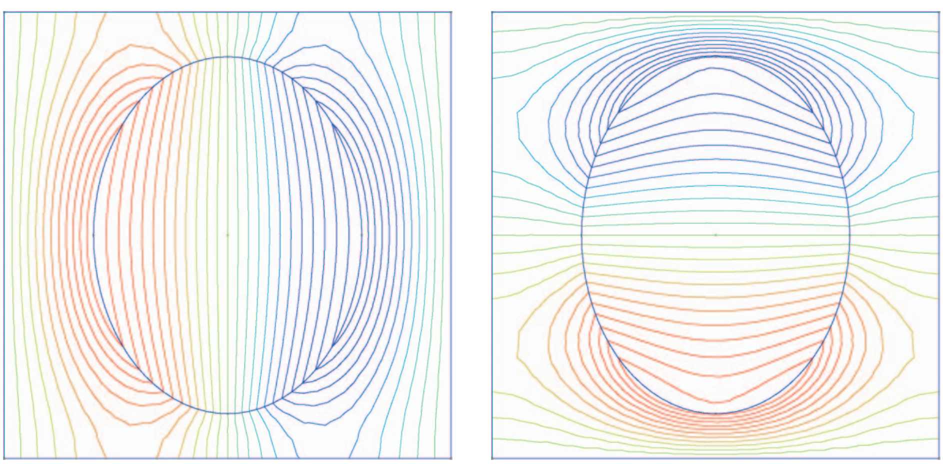

Figure 5. Potentials V_1 (left) and V_2 (right): the basic cell contains an elliptic inclusion ($\varepsilon = 4.0 + 3i$) with minor and major axes $a = 0.3$ and $b = 0.4$ in a silica matrix ($\varepsilon = 1.25$).

$\mu(\mathbf{y}) = \mu(y_1, y_2)$ we get from the annex problem $(\mathcal{M}_j)$

$$[\mu_{\text{hom}}] = \begin{pmatrix} [B_{\text{hom}}] & \begin{matrix} 0 \\ 0 \end{matrix} \\ 0\ 0 & \langle \mu \rangle_{Y^2} \end{pmatrix}$$

where $Y^2 =]0; 1[^2$ and $[B_{\text{hom}}]$ is the 2×2 matrix given by:

$$[B_{\text{hom}}] = \begin{pmatrix} \langle \mu \rangle_{Y^2} - \langle \mu \partial_1 W_1 \rangle_{Y^2} & -\langle \mu \partial_1 W_2 \rangle_{Y^2} \\ -\langle \mu \partial_2 W_1 \rangle_{Y^2} & \langle \mu \rangle_{Y^2} - \langle \mu \partial_2 W_2 \rangle_{Y^2} \end{pmatrix}$$

and W_j, $j \in \{1, 2\}$, is the unique solution in $H^1_\sharp(Y^2)/\mathbb{R}$ of

$$(\mathcal{M}_j) : \operatorname{div}[\mu(\mathbf{y})(\nabla(W_j(\mathbf{y}) - y_j))] = 0$$

5.1.3 Generalized Keller formulae. Let us now consider the TM field $\mathbf{H}_\eta = u_\eta(x_1, x_2)\mathbf{e}_3$, where u_η is the unique solution of the scalar wave equation:

$$\mu^{-1}\left(\mathbf{x}, \frac{\mathbf{x}}{\eta}\right) \operatorname{div}\left(\varepsilon^{-1}\left(\mathbf{x}, \frac{\mathbf{x}}{\eta}\right) \nabla u_\eta\right) + k_0^2 u_\eta = 0$$

with Sommerfeld radiation conditions

$$(\mathcal{SO}) : u^d_\eta = O(1/\sqrt{|\,\mathbf{x}\,|}), \quad \left(u^d_\eta - ik_0 \partial u^d_\eta / \partial x\right) = o(1/\sqrt{|\,\mathbf{x}\,|}).$$

When η tends to 0, u_η tends in $L^2_{loc}(\mathbb{R}^2)$ to $u = u(x_1, x_2)$ unique solution of

$$\langle \mu \rangle_{Y^2}{}^{-1} \operatorname{div}(A'_{\text{hom}} \nabla u) + k_0^2 u = 0$$

where the diffracted field u^d satisfies the radiation conditions $(\mathcal{SO})$ and where A'_{hom} is given by:

$$A'_{\text{hom}} = \begin{pmatrix} \langle \varepsilon^{-1} \rangle_{Y^2} - \langle \varepsilon^{-1} \partial_1 V'_1 \rangle_{Y^2} & -\langle \varepsilon^{-1} \partial_1 V'_2 \rangle_{Y^2} \\ -\langle \varepsilon^{-1} \partial_2 V'_1 \rangle_{Y^2} & \langle \varepsilon^{-1} \rangle_{Y^2} - \langle \varepsilon^{-1} \partial_2 V'_2 \rangle_{Y^2} \end{pmatrix}$$

with V'_j the unique solution in $H^1_\sharp(Y^2)/\mathbb{R}$ of

$$(\mathcal{N}_j) : \operatorname{div}[\varepsilon^{-1}(\mathbf{y})(\nabla(V'_j(\mathbf{y}) - y_j))] = 0$$

with $j \in \{1, 2\}$.

If we now consider the TE field $\mathbf{E}_\eta = u_\eta(x_1, x_2)\mathbf{e}_3$, where u_η is the unique solution of the scalar wave equation:

$$\varepsilon^{-1}\left(\mathbf{x}, \frac{\mathbf{x}}{\eta}\right) \operatorname{div}\left(\mu^{-1}\left(\mathbf{x}, \frac{\mathbf{x}}{\eta}\right) \nabla u_\eta\right) + k_0^2 u_\eta = 0$$

When η tends to 0, u_η tends in $L^2_{loc}(\mathbb{R}^2)$ to $u = u(x_1, x_2)$ unique solution of

$$\langle \varepsilon \rangle_{Y^2}{}^{-1} \operatorname{div}(B'_{\text{hom}} \nabla u) + k_0^2 u = 0$$

where the diffracted field u^d satisfies the radiation conditions $(\mathcal{SO})$ and where B'_{hom} is given by:

$$B'_{\text{hom}} = \begin{pmatrix} \langle \mu^{-1} \rangle_{Y^2} - \langle \mu^{-1} \partial_1 W'_1 \rangle_{Y^2} & -\langle \mu^{-1} \partial_1 W'_2 \rangle_{Y^2} \\ -\langle \mu^{-1} \partial_2 W'_1 \rangle_{Y^2} & \langle \mu^{-1} \rangle_{Y^2} - \langle \mu^{-1} \partial_2 W'_2 \rangle_{Y^2} \end{pmatrix}$$

with W'_j the unique solution in $H^1_\sharp(Y^2)/\mathbb{R}$ of

$$(\mathcal{P}_j) : \mathrm{div}[\mu^{-1}(\mathbf{y})(\nabla(W'_j(\mathbf{y}) - y_j))] = 0$$

with $j \in \{1, 2\}$.

We are facing a paradox: the annex problems $(\mathcal{K}_j)$ and $(\mathcal{M}_j)$ for TE polarization (respectively $(\mathcal{N}_j)$ and $(\mathcal{P}_j)$ for TM polarization) involve respectively the permittivity (TE case) and permeability (TM case) and their inverse. To explain this discrepancy, we establish the following subtle property:

PROPOSITION 5.1

$$\mu_{\mathrm{hom}}^{-1}\,\mathrm{curl}\left(\varepsilon_{\mathrm{hom}}^{-1}\,\mathrm{curl}(u(x_1,x_2)\mathbf{e}_3)\right) = -\langle\mu\rangle_{Y^2}^{-1}\,\mathrm{div}\left(R\left(\frac{\pi}{2}\right)A_{\mathrm{hom}}^{-1}R\left(-\frac{\pi}{2}\right)\nabla u\right)\mathbf{e}_3$$

$$\varepsilon_{\mathrm{hom}}^{-1}\,\mathrm{curl}\left(\mu_{\mathrm{hom}}^{-1}\,\mathrm{curl}(u(x_1,x_2)\mathbf{e}_3)\right) = -\langle\varepsilon\rangle_{Y^2}^{-1}\,\mathrm{div}\left(R\left(\frac{\pi}{2}\right)B_{\mathrm{hom}}^{-1}R\left(-\frac{\pi}{2}\right)\nabla u\right)\mathbf{e}_3$$

where $R(\pi/2)$ is the rotation matrix of angle $\pi/2$, namely:

$$R(\pi/2) = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

Proof

Let L and M be two symmetric matrices defined as

$$L = \begin{pmatrix} l_{11} & l & 0 \\ l & l_{22} & 0 \\ 0 & 0 & l_{33} \end{pmatrix} = \begin{pmatrix} \tilde{L} & 0 \\ 0 & l_{33} \end{pmatrix}, M = \begin{pmatrix} m_{11} & m & 0 \\ m & m_{22} & 0 \\ 0 & 0 & m_{33} \end{pmatrix} = \begin{pmatrix} \tilde{M} & 0 \\ 0 & m_{33} \end{pmatrix} \tag{54}$$

we get:

$$L\,\mathrm{curl}(M\,\mathrm{curl}(u(x_1,x_2)\mathbf{e}_3)) = -l_{33}\left(\frac{\partial}{\partial x_1}\left(m_{22}\frac{\partial u}{\partial x_1} - m\frac{\partial u}{\partial x_2}\right) + \frac{\partial}{\partial x_2}\left(m_{11}\frac{\partial u}{\partial x_2} - m\frac{\partial u}{\partial x_1}\right)\right)\mathbf{e}_3 \tag{55}$$

Furthermore, let M' be defined as

$$M' = \begin{pmatrix} m'_{11} & m'_{12} \\ m'_{21} & m'_{22} \end{pmatrix} \tag{56}$$

we have

$$L\,\mathrm{curl}(M\,\mathrm{curl}(u(x_1,x_2)\mathbf{e}_3)) = -l_{33}\,\mathrm{div}(M'\nabla u)\mathbf{e}_3$$

if and only if

$$m'_{11}\frac{\partial u}{\partial x_1} + m'_{12}\frac{\partial u}{\partial x_2} = m_{22}\frac{\partial u}{\partial x_1} - m\frac{\partial u}{\partial x_2}$$

$$m'_{21}\frac{\partial u}{\partial x_1} + m'_{22}\frac{\partial u}{\partial x_2} = m_{11}\frac{\partial u}{\partial x_2} - m\frac{\partial u}{\partial x_1}$$

which is true if $M' = R(\frac{\pi}{2})\tilde{M}R(-\frac{\pi}{2})$. As a conclusion the results found for TE and TM polarizations are consistent if and only if

$$A'_{\mathrm{hom}} = R\left(\frac{\pi}{2}\right)A_{\mathrm{hom}}^{-1}R\left(-\frac{\pi}{2}\right), B'_{\mathrm{hom}} = R\left(\frac{\pi}{2}\right)B_{\mathrm{hom}}^{-1}R\left(-\frac{\pi}{2}\right),$$

i.e.

$$A'_{\text{hom}} = \frac{A_{\text{hom}}}{\det(A_{\text{hom}})}, \quad B'_{\text{hom}} = \frac{A_{\text{hom}}}{\det(A_{\text{hom}})}.$$

This remarkable result can be straightforwardly proved with the following result [31].

LEMMA 5.1 *Let A_{hom} and A'_{hom} (respectively B_{hom} and B'_{hom}) be the homogenized matrices associated to v_j and v'_j (respectively w_j and w'_j), $j \in \{1, 2\}$, unique solutions in $H^1_\sharp(Y^2)/\mathbb{C}$ of the eight following problems:*

$$\operatorname{div}(a(\mathbf{y})\,\nabla(y_j + v_j(\mathbf{y}))) = 0, \quad \operatorname{div}(b(\mathbf{y})\,\nabla(y_j + w_j(\mathbf{y}))) = 0 \tag{57}$$

$$\operatorname{div}(a'(\mathbf{y})\,\nabla(y_j + v'_j(\mathbf{y}))) = 0, \quad \operatorname{div}(b'(\mathbf{y})\,\nabla(y_j + w'_j(\mathbf{y}))) = 0 \tag{58}$$

where $a' = a^{-1}$ and $b' = b^{-1}$. Then, we have:

$$A'_{\text{hom}} = \frac{A_{\text{hom}}}{\det(A_{\text{hom}})}, B'_{\text{hom}} = \frac{B_{\text{hom}}}{\det(B_{\text{hom}})}. \tag{59}$$

5.1.4 Two-phase media. Let Ω_f be a bounded photonic crystal filled with a periodic heterogeneous material with two optical indices $n_1 = \sqrt{\varepsilon_1\mu_1}$ and $n_2 = \sqrt{\varepsilon_2\mu_2}$. Thanks to the previous proposition, we can deduce from the computation of the effective 'refractive matrix' $N_{\text{hom}}([\varepsilon_1, \varepsilon_2]) = A_{\text{hom}}([\varepsilon_1, \varepsilon_2])B_{\text{hom}}([\mu_1, \mu_2])$ the effective 'refractive matrix' $N_{\text{hom}}([\varepsilon_2, \varepsilon_1]) = A_{\text{hom}}([\varepsilon_2, \varepsilon_1])B_{\text{hom}}([\mu_2, \mu_1])$ corresponding to the same structure with the reverse contrast. For this we use the following general property:

$$A_{\text{hom}}(\lambda\varepsilon) = \lambda A_{\text{hom}}(\varepsilon), B_{\text{hom}}(\lambda\mu) = \lambda B_{\text{hom}}(\mu) \quad \text{for any fixed } \lambda \text{ in } \mathbb{C}.$$

and the duality relation. Indeed, we have:

$$A_{\text{hom}}([\varepsilon_2, \varepsilon_1]) = \varepsilon_1\varepsilon_2 A_{\text{hom}}([\varepsilon_1^{-1}, \varepsilon_2^{-1}]), B_{\text{hom}}([\mu_2, \mu_1]) = \mu_1\mu_2 B_{\text{hom}}\left(\left[\mu_1^{-1}, \mu_2^{-1}\right]\right)$$

and then

$$\chi_{\text{hom}}([\xi_2, \xi_1]) = \frac{\xi_1\xi_2}{\det \chi_{\text{hom}}([\xi_1, \xi_2])}\chi_{\text{hom}}([\xi_1, \xi_2]), \forall(\chi, \xi) \in \{(A, \varepsilon), (B, \mu)\}$$

In particular for lossless dielectric materials, we have:

$$\chi_{\text{hom}}([\xi_1, \xi_2]) = R(\varphi)\begin{pmatrix} \xi_M & 0 \\ 0 & \xi_m \end{pmatrix} R(-\varphi), \forall(\chi, \xi) \in \{(A, \varepsilon), (B, \mu)\},$$

i.e.

$$A_{\text{hom}}([\varepsilon_1, \varepsilon_2])B_{\text{hom}}([\mu_1, \mu_2]) = R(\varphi)\begin{pmatrix} \varepsilon_M\mu_M & 0 \\ 0 & \varepsilon_m\mu_m \end{pmatrix} R(-\varphi)$$

where $R(\varphi)$ is the rotation matrix of angle φ and where $\varepsilon_M > \varepsilon_m$ (respectively $\mu_M > \mu_m$). The relation between the two matrices $A_{\text{hom}}([\varepsilon_1, \varepsilon_2])$ and $A_{\text{hom}}([\varepsilon_2, \varepsilon_1])$ (respectively $B_{\text{hom}}([\mu_1, \mu_2])$ and $B_{\text{hom}}([\mu_2, \mu_1])$) leads to the following property:

$$\chi_{\text{hom}}([\xi_2, \xi_1]) = R(\varphi)\begin{pmatrix} \xi'_M & 0 \\ 0 & \xi'_m \end{pmatrix} \quad R(-\varphi), \forall(\chi, \xi) \in \{(A, \varepsilon), (B, \mu)\},$$

i.e.

$$A_{\text{hom}}([\varepsilon_2, \varepsilon_1])B_{\text{hom}}([\mu_2, \mu_1]) = R(\varphi)\begin{pmatrix} \varepsilon'_M\mu'_M & 0 \\ 0 & \varepsilon'_m\mu'_m \end{pmatrix} R(-\varphi)$$

with $\varepsilon'_M\mu'_M = \frac{\varepsilon_1\varepsilon_2\mu_1\mu_2}{\varepsilon_m\mu_m}$ and $\varepsilon'_m\mu'_m = \frac{\varepsilon_1\varepsilon_2\mu_1\mu_2}{\varepsilon_M\mu_M}$ (note that $\varepsilon'_M\mu'_M > \varepsilon'_m\mu'_m$).

5.1.5 Checkerboards. The checkerboard problem is obviously a two-phase problem. Besides, for a square symmetry (it is the case for the checkerboard problem up to a translation) it can be easily proved that A_{hom} is equal to $R(\frac{\pi}{2})A_{\text{hom}}R(\frac{-\pi}{2})$ and consequently A_{hom} (respectively B_{hom}) is proportional to the identity matrix (the effective permittivity/permeability in TM/TE polarization is therefore isotropic):

$$\begin{aligned} A_{\text{hom}}([\varepsilon_1, \varepsilon_2]) &= A_{\text{hom}}([\varepsilon_2, \varepsilon_1]) = a_{\text{hom}}I, \\ B_{\text{hom}}([\mu_1, \mu_2]) &= B_{\text{hom}}([\mu_2, \mu_1]) = b_{\text{hom}}I. \end{aligned} \tag{60}$$

The previous result shows that:

$$A_{\text{hom}}([\varepsilon_1, \varepsilon_2])B_{\text{hom}}([\mu_1, \mu_2]) = \frac{\varepsilon_1\varepsilon_2\mu_1\mu_2 A_{\text{hom}}([\varepsilon_1, \varepsilon_2])B_{\text{hom}}([\mu_1, \mu_2])}{\det A_{\text{hom}}([\varepsilon_1, \varepsilon_2]) \det B_{\text{hom}}([\mu_1, \mu_2])},$$

and consequently

$$\det A_{\text{hom}}([\varepsilon_1, \varepsilon_2]) \det B_{\text{hom}}([\mu_1, \mu_2]) = a_{\text{hom}}^2 b_{\text{hom}}^2 = \varepsilon_1\varepsilon_2\mu_1\mu_2.$$

Finally we generalize the result of Dykhne:

$$A_{\text{hom}}B_{\text{hom}} = B_{\text{hom}}A_{\text{hom}} = \sqrt{\varepsilon_1\varepsilon_2}\sqrt{\mu_1\mu_2}I\ . \tag{61}$$

A striking physical implication is to consider a two phase composite such that

$$\varepsilon_1 = \frac{C}{\mu_2}, \varepsilon_2 = \frac{1}{C\mu_1}, \tag{62}$$

where C is a positive constant. This implies that $\varepsilon_{\text{eff}}\mu_{\text{eff}} = 1$ and consequently the effective index is that of *vacuum*. This is physically reasonable, since there exist some materials with permeabilities $0 < \mu_1 < \mu_2 < 1$ (unlike their permittivities ε_1 and ε_2, which should always be greater than 1). This composite would be transparent for the waves of low frequency (no guiding properties).

Remark 1 In the case of a four-phase checkerboard structure, i.e. where the unit cell of periodicity is square and subdivided in four equal squares each having a different conductivity, a generalized Dykhne's formula (61) has been conjectured by Mortola and Steffe in 1985 [61] and independently derived by Craster and Obnosov [62] and Milton [63].

In our case, using the same arguments as above, we found that the effective properties of the four-phase magneto-dielectric checkerboard are given by two diagonal matrices, namely

$$A_{\text{hom}}([\varepsilon_1, \varepsilon_2, \varepsilon_3, \varepsilon_4]) = \sqrt{\frac{\varepsilon_1\varepsilon_2\varepsilon_3\varepsilon_4(1/\varepsilon_1 + 1/\varepsilon_2 + 1/\varepsilon_3 + 1/\varepsilon_4)}{\varepsilon_1 + \varepsilon_2 + \varepsilon_3 + \varepsilon_4}} \times \begin{pmatrix} \sqrt{\frac{(\varepsilon_1+\varepsilon_2)(\varepsilon_3+\varepsilon_4)}{(\varepsilon_1+\varepsilon_4)(\varepsilon_2+\varepsilon_3)}} & 0 \\ 0 & \sqrt{\frac{(\varepsilon_1+\varepsilon_4)(\varepsilon_2+\varepsilon_3)}{(\varepsilon_1+\varepsilon_2)(\varepsilon_3+\varepsilon_4)}} \end{pmatrix}$$

Table 1. Comparison of effective refractive index for a square array of dielectric cylinders of circular cross-section and permittivity 50 lying in air computed in [12] using Fourier expansions (N_{eff}) with N^*_{eff} given by the finite element method. The filling fraction $f = \pi r_c^2$ is increased whereas the number of triangles for the mesh remains constant (about 2500 triangles); in [12] the number of Fourier coefficients was also kept constant (corresponding to summation over 1812 reciprocal vectors of the square lattice). The computational time with the finite element software Getdp [60] is about 2 seconds on a 1 GHz PC with 128 Mb RAM.

f	ε Ref. [12]	εPresent work	ε^* Ref. [12]	ε^* Present work
0.1	1.239010	1.239007	40.354793	40.354791
0.2	1.511636	1.511634	33.076744	33.076741
0.3	1.971824	1.971821	25.357226	25.357223
0.4	2.644923	2.644921	18.904143	18.904141
0.5	7.071068	7.071066	7.071068	7.071065

and B_{hom} whose entries are deduced from that of A_{hom} simply by replacing ε_i by μ_i. The product of A_{hom} by B_{hom} (which commutes) then provides us with the Mortola–Steffe formula for magneto-dielectric four-phase checkerboards.

5.2 *Effective properties for oblique propagation*

In this section, we give some numerical results on the homogenization of a circular metallic waveguide made of a periodic arrangement of dielectric rods of elliptic cross-section of refractive index 2 embedded in a matrix of refractive index 1. We derive the tensor of effective permittivity from the resolution of the two annex problems of electrostatic type $\mathcal{K}_j$ (*cf.* Theorem 3.1), with the method of fictitious charges [31] (its dynamic analogue is the method of fictitious sources [64]). This method consists in representing the potential by an approximate potential created by two families of fictitious charges: the first ones are located in the scatterer S and they radiate in its complement $Y \setminus S$ in the periodic cell Y, and the second ones are located in $Y \setminus S$ and radiate in S. Each of these charges satisfies a Laplace equation in Y with periodic conditions and they are chosen such that the potential V_j verifies the boundary conditions that appears in the following system:

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

with

$$\varepsilon = \begin{cases} \varepsilon_{\text{scat}}, & \text{in } S \\ 1, & \text{in } Y \setminus \bar{S}. \end{cases}$$

Table 2. Same caption as table 1 except that the dielectric cylinders have now a permittivity 100.

f	ε Ref. [12]	ε Present work	ε^* Ref. [12]	ε^* Present work
0.1	1.249889	1.249887	80.007121	80.007120
0.2	1.569954	1.569952	63.696132	63.696131
0.3	2.000515	2.000512	49.987129	49.987127
0.4	2.935262	2.935259	34.068509	34.068507
0.5	10.000000	9.999999	10.000000	9.999999

$[f]_{\partial S}$ denotes the jump of f across the boundary ∂S, and n_j, $j \in \{1, 2\}$, denotes the projection on the axis e_j of a normal of ∂S.

Moreover, the calculus of the anisotropic permittivity can be simplified. Indeed it had been shown [24] that the coefficients $\varphi_{i,j}$ are given by the following simple integral:

$$\varphi_{i,j} = [\varepsilon]_{\partial S} \int_{\partial S} V_i n_j \, dl. \tag{63}$$

Let us remark that V_i is well defined on ∂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_i (which gives rise to numerical inaccuracy) to perform the calculus of the homogenized permittivity.

In figure 6, we compare the transverse electromagnetic field of a heterogeneous metallic waveguide made of a periodic arrangement of elliptic dielectric rods with that of its effective anisotropic waveguide, derived from the asymptotic analysis. We must solve an annex problem set in the basic cell $Y =]0;1[^2$ with the shape of the scatterer defined by the equation $\frac{y_1^2}{a^2} + \frac{y_2^2}{b^2} = 1$ with $a = 0.4$ and $b = 0.2$. Its permittivity is given by $\varepsilon_{\text{scat}} = 4$. The method of fictitious sources gives us

$$\varepsilon_{\text{hom}} = \begin{pmatrix} 1.39787 & 0 & 0 \\ 0 & 2.01435 & 0 \\ 0 & 0 & 4.769911 \end{pmatrix} \tag{64}$$

If we denote by $\varepsilon^{\text{hom}}_{\text{harm}}$ the harmonic mean of ε over the basic cell Y, we check that $\varepsilon^{\text{hom}}_{\text{harm}} = 1.30824 \le \varepsilon^{\text{hom}}_{1,1}, \varepsilon^{\text{hom}}_{2,2} \le \varepsilon^{\text{hom}}_{3,3} = \langle \varepsilon^{\text{hom}} \rangle_Y$, which is consistent in this canonical case with the theory of bounds [65]. An interesting case is that of a metallic inclusion within the basic cell Y: this induces an infinite value for $\varepsilon^{\text{hom}}_{3,3} = \langle \varepsilon^{\text{hom}} \rangle_Y$. We use the GetDP software [60] to model the anisotropic waveguide defined by the tensor of permittivity given above (see figure 6).

5.3 *Numerical illustration in 3D*

The possible formulations are identical to the ones of the resonant cavity problem [66] and as our purpose is to deal not only with dielectric but also with metallic inclusions, the electric field formulation is chosen. According to the Bloch theorem [67], our problem reduces to looking for Bloch waves solutions which are the solutions $\mathbf{E_k}$ that have the form:

$$\mathbf{E_k}(x, y, z) = e^{i\mathbf{k}\cdot\mathbf{r}} \mathbf{E}(x, y, z) = e^{i(k_x x + k_y y + k_z z)} \mathbf{E}(x, y, z) \tag{65}$$

where $\mathbf{k} = (k_x, k_y, k_z) \in \mathbb{R}^3$ is a parameter (the so-called Bloch vector or quasi-momentum in solid state physics) and $\mathbf{E}(x, y, z)$ is a periodic function on the unit cube Y.

In order to find Bloch modes with the finite element method, some changes have to be performed with respect to classical boundary value problems that will be named *Bloch conditions* [68]. The classical weighted residual is used

$$\mathcal{R}(\mathbf{E_k}, \mathbf{E'_k}) = \int_{Y\setminus\Omega_m} \text{curl}\,\mathbf{E_k} \cdot \overline{\text{curl}\,\mathbf{E'_k}} \, dxdy - \mu_0 \omega^2 \int_{Y\setminus\Omega_m} \varepsilon \mathbf{E_k} \cdot \overline{\mathbf{E'_k}} \, dxdy \tag{66}$$

where Ω_m are the perfectly conducting inclusions. For discretization, edge elements on a tetrahedral mesh are introduced. The constraint on the mesh is that opposite faces of the cube Y must have exactly the same surface triangular mesh. In the case of a periodic problem, unknowns (i.e. line integrals of $\mathbf{E_k}$) on corresponding edges are imposed to have the same value. In the case of a Bloch problem, equal values up to the phase factor given by (65) are imposed. Equations associated to corresponding edges have also to be combined, using

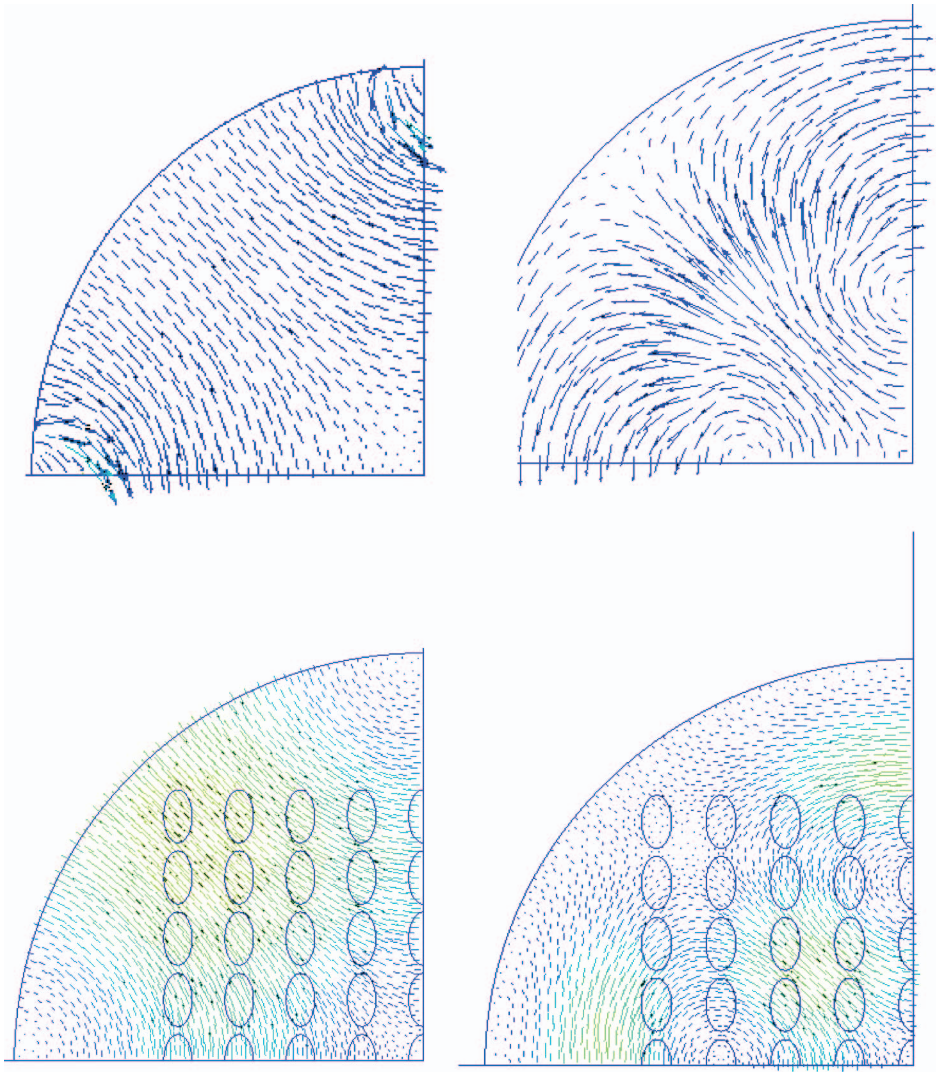

Figure 6. Comparison between the transverse electric fields TE_{21} and TE_{31} of a metallic PCF for a propagation constant $\gamma = 1\ \text{cm}^{-1}$ (wave numbers $k = 0.7707\ \text{cm}^{-1}$ and $k = 0.7607\ \text{cm}^{-1}$) with the ones of the homogenized anisotropic associated metallic waveguide for $\gamma = 1\ \text{cm}^{-1}$ ($k = 0.5478\ \text{cm}^{-1}$ and $k = 0.5201\ \text{cm}^{-1}$).

the complex conjugate of the phase factor [68]. Finally, a generalized eigenvalue problem involving large sparse Hermitian matrices is obtained. The eigenvalues correspond to feasible values of ω^2 for the given Bloch vector $\mathbf{k}$. Such a problem can be solved using a Lanczos algorithm, which permits to compute the largest eigenvalues. Since we are in fact interested in the smallest eigenvalues, the inverse of the matrix of the system must be used in the iterations. The inverse is never computed explicitly but the matrix–vector products are replaced by system solutions thanks to a GMRES method. The practical implementation of the model has been performed thanks to the *GetDP* software [60].

Our edge-element formulation for Bloch waves (65) also holds for dielectric inclusions, for this one has just to integrate over the whole cell Y in (66). An interesting issue is then to look at the effective properties of 3D dielectric photonic crystals by means of Bloch approach and

Table 3. Comparison of effective refractive index N_{eff} given by the Clausius–Mossotti formula, N^*_{eff} given by 'Bloch homogenization' and N^{**}_{eff} given by 'two-scale homogenization', for different values of the radius r_c of a spherical dielectric inclusion of permittivity 3 surrounded by air in a cubic unit cell.

r_c	N_{eff}	N^*_{eff}	N^{**}_{eff}
0.1	1.0020952	1.0020968	1.0022840
0.25	1.0329132	1.0332791	1.0374103
0.34	1.0836032	1.0875975	1.0950892
0.43	1.1724446	1.2157954	1.1977349

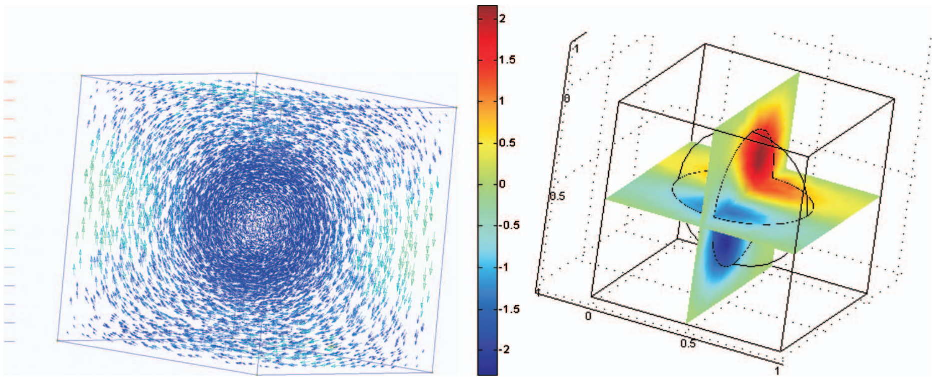

Figure 7. Quasi-periodic electric field in a basic cell of air containing a dielectric spherical inclusion of permittivity 3 whose radius $r_c = 0.34$ when the Bloch vector $\mathbf{k}_{\text{Bloch}} = (\pi/100, 0, 0)$ (left); First component V_1 of the periodic multi-scalar potential $\mathbf{V}_y$ for the same basic cell and inclusion (right).

to compare it with both two-scale homogenization and Clausius–Mossotti formula (50). If we consider a dielectric sphere of radius r_c and relative permittivity ε_r surrounded by air in a cubic basic cell $Y =]0;1[^3$, the Clausius–Mossotti formula [69] tells us that the effective refractive index should be $N_{\text{eff}} = \sqrt{\frac{\varepsilon_r+2f}{\varepsilon_r-f}}$ where $f = \frac{4\pi r_c^3}{3}$ is the volume fraction of the sphere. On the other hand, the effective index N_{eff} can be defined as the limit of $\frac{dk}{d\omega}$ when both the modulus of the Bloch vector k and ω tend to zero (note that in the case of an ellipsoidal inclusion, the previous limit is a tensor since it depends on the trajectory in the coordinates $\{\mathbf{k}, \omega\}$, i.e. the effective material is anisotropic). In our case, if we pick up a point corresponding to a particular Bloch vector in the neighborhood of the origin, say $\mathbf{k} = (0.01\pi, 0, 0)$, the associated lower frequency in the spectrum will provide us with N_{eff}. In the table above, we report the values for N_{eff} given by the Mossotti's formula, the ones provided by edge-element computations for Bloch electromagnetic waves and those derived from nodal-element computations for periodic electrostatic problems.

6. Conclusion

In this paper, we have achieved the homogenization of 2D and 3D finite photonic crystals described by coercive and bounded permittivity and permeability, which covers the range of physical applications from 2D-3D photonic crystals to photonic crystal fibers. We have discussed some new duality relations for magneto-dielectric materials in the long wavelength limit. We have also presented two very efficient numerical algorithms to illustrate our theoretical study: a method of fictitious charges and a finite element modeling. We have provided a comprehensive bibliography on related numerical and theoretical work: although some material on homogenization of other spectral problems with similar tools may be found in [33, 34], to the best of our knowledge, the theoretical results presented in this paper are new and would by no means intersect with existing ones in the classical literature on homogenization theory [15, 41] or most recent papers [30]. Our 2D numerical results are validated with previous work by Halevi *et al.* [12, 13]. In the general case, the effective properties provided in this paper for photonic crystal fibers and 3D photonic crystals have been checked with finite element models for heterogeneous waveguides and 3D periodic structures. Finally, we discuss the connections between the homogenization of scattering and spectral problems (finite/infinite photonic crystal structures).

Acknowledgements

This work was undertaken while the authors received fundings from the Franco-British Partnership Programme ALLIANCE (project PN 05.026). The authors want to thank Pr. A. B. Movchan and R. C. McPhedran for valuable discussions about singularly perturbed problems, duality results and the multipole method met in the homogenization of photonic crystals.

Appendix A: Multiple-scale expansion of $\mathbf{H}_\eta$

The main idea underlying our asymptotic analysis 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 illuminated periodic structure. In fact, the smaller the size η of the SB, the faster the modulus of the field $\mathbf{F}_\eta$ 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:

$$\mathbf{H}_\eta = \mathbf{H}_0\left(\mathbf{x}, \frac{\mathbf{x}}{\eta}\right) + \eta \mathbf{H}_1\left(\mathbf{x}, \frac{\mathbf{x}}{\eta}\right) + \cdots + \eta^N \mathbf{H}_N\left(\mathbf{x}, \frac{\mathbf{x}}{\eta}\right) + o(\eta^N), \tag{A1}$$

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 $\varepsilon_\eta(x) = \varepsilon_\sharp(\frac{x}{\eta})$ in the 'bounded periodic' structure.

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

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

where $f(\mathbf{x}, \mathbf{y})$ and $f(\mathbf{x}, \frac{\mathbf{x}}{\eta})$ are respectively locally square integrable functions of $\Omega_f \times \mathbb{R}^3 \longmapsto \mathbb{C}^3$ and $\Omega_f \longmapsto \mathbb{C}^3$ of finite energy. It is worth noting that R_η obeys the following rules of calculation:

PROPOSITION A.1 *(Properties of R_η)*

(i) *R_η is a 'distributive operator', that is to say that*

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

(ii) *Furthermore, we can define the action of the differential operator on the projector R_η by:*

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

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

Assuming that the expansion (A1) is relevant, we can state the following lemma:

LEMMA A.2 *The Maxwell operator $A_\eta = \mathrm{curl}\,\tilde{\varepsilon}_\eta^{-1}\,\mathrm{curl}$ associated to the problem $\mathcal{P}_\eta$ satisfies the following operator expansion $A_\eta = R_\eta\{\eta^{-2}A_{\mathbf{yy}} + \eta^{-1}A_{\mathbf{xy}} + \eta^0 A_{\mathbf{xx}}\} + o(1)$, where $A_{\mu,\nu}$ denotes the operator $\mathrm{curl}_\mu\,\tilde{\varepsilon}^{-1}(\mathbf{x},\mathbf{y})\,\mathrm{curl}_\nu$, the couple (μ,ν) being in $\{\mathbf{x},\mathbf{y}\}\times\{\mathbf{x},\mathbf{y}\}$. Besides, the asymptotic terms of A_η are solutions of:*

$$(\mathcal{S}_0)\begin{cases} A_{\mathbf{yy}}\mathbf{H}_0 = 0 & \text{(A2a)}\\ A_{\mathbf{yy}}\mathbf{H}_1 + A_{\mathbf{xy}}\mathbf{H}_0 + A_{\mathbf{yx}}\mathbf{H}_0 = 0 & \text{(A2b)}\\ A_{\mathbf{yy}}\mathbf{H}_2 + A_{\mathbf{xy}}\mathbf{H}_1 + A_{\mathbf{yx}}\mathbf{H}_1 + A_{\mathbf{xx}}\mathbf{H}_0 - k_0^2\tilde{\mu}(\mathbf{x},\mathbf{y})\mathbf{H}_0 = 0 & \text{(A2c)}\end{cases}$$

Proof With the help of the operator R_η, the equation (A1) can be rewritten in the form:

$$\mathbf{H}_\eta(\mathbf{x}) = R_\eta\left\{\sum_{j=0}^{N}\eta^j\mathbf{H}_j(\mathbf{x},\mathbf{y})\right\} + o(\eta^N). \tag{A3}$$

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

$$\frac{\partial}{\partial \mathbf{x}_i}\mathbf{H}_\eta(\mathbf{x}) = \left(R_\eta\frac{\partial}{\partial \mathbf{x}_i} + \frac{1}{\eta}R_\eta\frac{\partial}{\partial \mathbf{y}_i}\right)\left\{\sum_{j=0}^{N}\eta^j\mathbf{H}_j(\mathbf{x},\mathbf{y})\right\} + o(\eta^{N-1}). \tag{A4}$$

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

$$\begin{aligned}&\mathrm{curl}_\mathbf{x}((R_\eta\tilde{\varepsilon}^{-1}(\mathbf{x},\mathbf{y}))(\mathrm{curl}_\mathbf{x} R_\eta\mathbf{H}_j))\\ &= \mathrm{curl}_\mathbf{x}\left((R_\eta\tilde{\varepsilon}^{-1}(\mathbf{x},\mathbf{y}))\left(R_\eta\,\mathrm{curl}_\mathbf{x}\mathbf{H}_j + \tfrac{1}{\eta}R_\eta\,\mathrm{curl}_\mathbf{y}\mathbf{H}_j\right)\right)\end{aligned} \tag{A5}$$

Taking into account once more that $\mathrm{curl}_\mathbf{x}$ and R_η do not commute:

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

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:

$$\mathrm{curl}_\mathbf{x}(\tilde{\varepsilon}^{-1}\,\mathrm{curl}_\mathbf{x}(\mathbf{H}_0 + \eta\mathbf{H}_1)) + \frac{1}{\eta}\,\mathrm{curl}_\mathbf{x}(\tilde{\varepsilon}^{-1}\,\mathrm{curl}_\mathbf{y}(\mathbf{H}_0 + \eta\mathbf{H}_1))$$

$$
\begin{aligned}
&+\frac{1}{\eta}(\operatorname{curl}_{\mathbf{y}}\tilde{\varepsilon}^{-1}\operatorname{curl}_{\mathbf{x}}(\mathbf{H}_0+\eta\mathbf{H}_1))\\
&+\frac{1}{\eta}\operatorname{curl}_{\mathbf{y}}(\tilde{\varepsilon}^{-1}\operatorname{curl}_{\mathbf{y}}(\mathbf{H}_0+\eta\mathbf{H}_1+\eta^2\mathbf{H}_2))\\
&-k_0^2\tilde{\mu}(\mathbf{H}_0+\eta\mathbf{H}_1)+o(\eta)=0
\end{aligned}
$$

which leads to

$$
\begin{aligned}
\eta^{-2}A_{\mathbf{yy}}\mathbf{H}_0+\eta^{-1}(A_{\mathbf{yy}}\mathbf{H}_1+A_{\mathbf{xy}}\mathbf{H}_0+A_{\mathbf{yx}}\mathbf{H}_0)+\eta^0(A_{\mathbf{yy}}\mathbf{H}_2+A_{\mathbf{xy}}\mathbf{H}_1+A_{\mathbf{yx}}\mathbf{H}_1+A_{\mathbf{xx}}\mathbf{H}_0\\
-k_0^2\tilde{\mu}(\mathbf{x},\mathbf{y})\mathbf{H}_0)=o(\eta)
\end{aligned}
$$

In a neighborhood of $\eta=0$, we express the vanishing of the coefficients of successive powers of $\frac{1}{\eta}$ which leads to the system $(\mathcal{S}_0)$.

Let us rewrite the equation (A2a) of the previous system $(\mathcal{S}_0)$:

$$\operatorname{curl}_y(\tilde{\varepsilon}^{-1}(\mathbf{x},\mathbf{y})\operatorname{curl}_y\mathbf{H}_0)=0. \tag{A6}$$

The next step in the asymptotic expansion is to show the link between $(\mathbf{E}_0,\mathbf{H}_0)(\mathbf{x},\mathbf{y})$ and the so-called homogenized electromagnetic field $(\mathbf{E}_{\text{hom}},\mathbf{H}_{\text{hom}})(\mathbf{x})$.

LEMMA A.3 *Let, for fixed* $\mathbf{x}\in\Omega_f$, $\mathbf{H}_0$ *be a* Y *periodic function in* $\mathbf{y}$ *solution of equation (A2a), such that* $\operatorname{curl}_{\mathbf{y}}\mathbf{H}_0(x,.)\in H(\operatorname{curl},Y)$. *Then*

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

Proof Multiplying equation (A2a) in $\mathcal{S}_0$ by the conjugate of $\mathbf{H}_0^*$ of $\mathbf{H}_0$ and integrating over Y leads to:

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

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:

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

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

$$a.e.\mathbf{y}\in Y,\operatorname{curl}_{\mathbf{y}}\mathbf{H}_0(\mathbf{x},\mathbf{y})=0. \tag{A7}$$

From Lemma A.3, we can derive the following result.

LEMMA A.4 $\mathbf{H}_0$, *solution of the system* $\mathcal{S}_0$, *is such that*

$$\textit{For almost every } \mathbf{y} \textit{ in } Y,\ \operatorname{div}_y(\tilde{\mu}(\mathbf{x},\mathbf{y})\mathbf{H}_0(\mathbf{x},\mathbf{y}))=0.$$

Remark A1 In [24], we studied the homogenization of a 3D diffracting problem using the same multi-scale expansion method in the magnetic field formulation. We also deduced that

$\mathrm{curl}_y\, \mathbf{H_0}(\mathbf{x},\mathbf{y}) = 0$. Noting that $\mu = \mu_0$ (non magnetic medium) we knew that $\mathrm{div}_y\, \mathbf{H_0}(\mathbf{x},\mathbf{y}) = 0$, which is obviously no more the case. We therefore deduced that $\Delta_y \mathbf{H_0}(\mathbf{x},\mathbf{y}) = 0$, which ensured us that $\mathbf{H}_0$ did not depend on the microscopic variable $\mathbf{y}$. Consequently, $\mathbf{H}_0$ could be seen as a homogenized magnetic field $\mathbf{H}_{\mathrm{hom}}(\mathbf{x})$, i.e. $\mathbf{H_0}(\mathbf{x},\mathbf{y}) = \mathbf{H}_{\mathrm{hom}}(\mathbf{x})$. The main difference with [24] is thus that the first term $\mathbf{H_0}$ of the ansatz is here dependent of the microscopic $\mathbf{y}$ variable. The fact that in our current paper, the first order term $\mathbf{H_0}$ of the asymptotic expansion depends on the microscopic variable can be explained in terms of a singularly perturbed problem by writing (4a) as follows

$$\mu_\eta{}^{-1}\mathrm{curl}\left(\varepsilon_\eta{}^{-1}\,\mathrm{curl}\,\mathbf{H}_\eta\right) - k_0^2\mathbf{H}_\eta = 0 \tag{A8}$$

and can be thereby regarded as a problem of non commuting limits (see e.g. [70] for similar effects in high contrast doubly periodic structures).

Proof From equations (A2b) and (A7), we have:

$$\mathrm{curl}_{\mathbf{y}}(\tilde{\varepsilon}^{-1}(\mathbf{x},\mathbf{y})\,\mathrm{curl}_{\mathbf{x}}\,\mathbf{H}_0(\mathbf{x},\mathbf{y})) + \mathrm{curl}_{\mathbf{y}}(\tilde{\varepsilon}^{-1}(\mathbf{x},\mathbf{y})\,\mathrm{curl}_{\mathbf{y}}\,\mathbf{H}_1(\mathbf{x},\mathbf{y})) = 0 \tag{A9}$$

By applying $\mathrm{div}_{\mathbf{y}}$ to (A2c), we derive:

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

Since $\mathrm{div}_y\,\mathrm{curl}_x\, A(x,y) = -\,\mathrm{div}_x\,\mathrm{curl}_y\, A(x,y)$, this expression reduces to:

$$-\,\mathrm{div}_{\mathbf{x}}(\mathrm{curl}_{\mathbf{y}}(\tilde{\varepsilon}^{-1}\,\mathrm{curl}_{\mathbf{x}}\,\mathbf{H}_0) + \mathrm{curl}_{\mathbf{y}}\left(\tilde{\varepsilon}^{-1}\,\mathrm{curl}_{\mathbf{y}}\,\mathbf{H}_1)\right) + k_0^2\,\mathrm{div}_{\mathbf{y}}(\tilde{\mu}(\mathbf{x},\mathbf{y})\mathbf{H}_0) = 0.$$

Taking (A9) into account, we finally get the following formulation:

$$\mathrm{div}_{\mathbf{y}}(\tilde{\mu}(\mathbf{x},\mathbf{y})\mathbf{H}_0(\mathbf{x},\mathbf{y})) = 0.$$

We want to show some analogous properties for $\mathbf{E}_0$.

LEMMA A.5 *If we state* $\mathbf{E}_0$ *as follows:*

$$\mathbf{E}_0(\mathbf{x},\mathbf{y}) := \frac{i}{\omega\varepsilon_0}\tilde{\varepsilon}^{-1}(\mathbf{x},\mathbf{y})(\mathrm{curl}_{\mathbf{y}}\mathbf{H}_1(\mathbf{x},\mathbf{y}) + \mathrm{curl}_{\mathbf{x}}\mathbf{H}_0(\mathbf{x},\mathbf{y})), \tag{A10}$$

then we have the two following equations:

$$\mathrm{curl}_{\mathbf{y}}(\mathbf{E}_0(\mathbf{x},\mathbf{y})) = 0,\ \textit{and}\ \mathrm{div}_{\mathbf{y}}(\tilde{\varepsilon}\mathbf{E}_0(\mathbf{x},\mathbf{y})) = 0. \tag{A11}$$

Remark A2 The equation (A10) is just a definition, since it has not been proved that $\mathbf{E}_\eta$ were converging towards $\mathbf{E}_0$.

Proof The curl equation in (A11) derives straightforwardly from equation (A9) and the definition of $\mathbf{E}_0$. To prove the divergence equation in (A11), we start from the equation (A10) and we take its divergence in the $\mathbf{y}$ variable. Noting once more that $\mathrm{div}_y\,\mathrm{curl}_x\, A(x,y) = -\,\mathrm{div}_x\,\mathrm{curl}_y\, A(x,y)$, thanks to Lemma A.3 we get the desired equation.

The average of $\mathbf{E}_0$ on Y gives us a field independent of the microscopic variable, hence it seems legitimate to denote by $\mathbf{E}_{\mathrm{hom}}$ the following quantity:

$$\mathbf{E}_{\mathrm{hom}}(\mathbf{x}) := \langle\mathbf{E}_0\rangle_Y = \int_Y \mathbf{E}_0(\mathbf{x},\mathbf{y})\,d\mathbf{y}. \tag{A12}$$

With this definition we can state the following lemma:

LEMMA A.6 $\mathbf{E}_0$ *and* $\mathbf{E}_{\text{hom}}$ *are linked by the following relation:*

$$\mathbf{E}_0 = (I - \nabla_{\mathbf{y}} \mathbf{V}_Y)\mathbf{E}_{\text{hom}}, \tag{A13}$$

with $\mathbf{V}_Y = (V_1, V_2, V_3)$*, where* V_j*,* $j \in \{1, 2, 3\}$ *are the unique solutions in* $H^1_\sharp(Y)/\mathbb{R}$ *of one of the three following problems* $(\mathcal{K}_j)$ *of electrostatic type:*

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

Proof We firstly remark that $\text{curl}_{\mathbf{y}}(\mathbf{E}_0 - \mathbf{E}_{\text{hom}}) = 0$. In general, this merely implies that $\mathbf{E}_0 = \mathbf{E}_{\text{hom}}(\mathbf{x}) - \nabla_{\mathbf{y}} V(\mathbf{x}, \mathbf{y}) + \mathbf{E}_{\text{cohom}}(\mathbf{x})$, where $\mathbf{E}_{\text{cohom}}$ 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 $\tilde{Y}$. In our case, $\langle \mathbf{E}_0 \rangle_Y = \langle \mathbf{E}_{\text{hom}} \rangle_Y$ and $\langle \nabla_{\mathbf{y}} V \rangle_Y = 0$ which implies that $\mathbf{E}_{\text{cohom}} = 0$. Then, $\mathbf{E}_0 - \mathbf{E}_{\text{hom}}$ 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:

$$\mathbf{E}_0 = \mathbf{E}_{\text{hom}} - \nabla_{\mathbf{y}} V. \tag{A14}$$

It is worth noting that this deduction would not hold necessarily 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 [19].

Injecting (A14) in (A11), leads us to:

$$\text{div}_{\mathbf{y}}(\tilde{\varepsilon}(\mathbf{E}_{\text{hom}} - \nabla_{\mathbf{y}} V)) = 0. \tag{A15}$$

By linearity of the divergence, we can write that:

$$\begin{aligned} -\text{div}_{\mathbf{y}}(\tilde{\varepsilon}(\nabla_{\mathbf{y}} V)) &= -\text{div}_{\mathbf{y}}(\tilde{\varepsilon}\mathbf{E}_{\text{hom}}) = -\text{div}_{\mathbf{y}}\left(\tilde{\varepsilon}\sum_{j=1}^{3} \mathbf{E}_{\text{hom},j} e_j\right) \\ &= -\textstyle\sum_{j=1}^{3} \text{div}_{\mathbf{y}}(\tilde{\varepsilon}(\mathbf{x}, \mathbf{y})e_j)\mathbf{E}_{\text{hom},j}(\mathbf{x}). \end{aligned} \tag{A16}$$

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

$$(\mathcal{K}_j) : -\text{div}_{\mathbf{y}}(\tilde{\varepsilon}(\mathbf{x}, \mathbf{y})(\nabla_{\mathbf{y}} V_j - e_j)) = 0,\ j \in \{1, 2, 3\}, \tag{A17}$$

The variational form associated with this problem is sesquilinear, continue and coercive in the Hilbert space $H^1_\sharp(Y)/\mathbb{R}$, hence the Lax–Milgram lemma ensures 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 $(\mathcal{P}_\eta)$, $\text{div}_{\mathbf{y}}(\tilde{\varepsilon}(\mathbf{x}, \mathbf{y})e_j)$ 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 (A15) are given by the functions:

$$V(\mathbf{x}, \mathbf{y}) = \sum_{j=1}^{3} V_j(\mathbf{y}) E_{\text{hom},j}(\mathbf{x}) = \mathbf{V}_Y \cdot \mathbf{E}_{\text{hom}}, \tag{A18}$$

where $\mathbf{V}_Y = (V_1, V_2, V_3)$ and V_j respectively denote the multi-scalar potential of the basic cell and one of the scalar potentials associated with the density of charges $\text{div}_{\mathbf{y}}(\varepsilon(\mathbf{y})e_j)$. Before going further, it is worth noting that the problem $(\mathcal{K}_j)$ is of interest by itself. In the section 4, we solve it thanks to a finite element modeling with periodic conditions. We also solve the annex problem in the scalar case thanks to a method of fictitious charges, whose corresponding algorithm in the dynamic case is called method of fictitious sources [64].

From (A14) and (A18) we get that:

$$\mathbf{E}_0 = (I - \nabla_{\mathbf{y}} \mathbf{V}_Y)\mathbf{E}_{\text{hom}} \tag{A19}$$

where I denotes the identity matrix and $\nabla_{\mathbf{y}} \mathbf{V}_Y$ denotes the jacobian of $\mathbf{V}_Y$. That is to say that:

$$\mathbf{E}_0 = \left(I - \begin{bmatrix} \dfrac{\partial V_1}{\partial y_1} & \dfrac{\partial V_2}{\partial y_1} & \dfrac{\partial V_3}{\partial y_1} \\ \dfrac{\partial V_1}{\partial y_2} & \dfrac{\partial V_2}{\partial y_2} & \dfrac{\partial V_3}{\partial y_2} \\ \dfrac{\partial V_1}{\partial y_3} & \dfrac{\partial V_2}{\partial y_3} & \dfrac{\partial V_3}{\partial y_3} \end{bmatrix} \right) \mathbf{E}_{\text{hom}} \tag{A20}$$

We want now to precise the link between $\mathbf{E}_{\text{hom}}$ and the average $\mathbf{H}_{\text{hom}}$ of $\mathbf{H}_0(\mathbf{x}, \mathbf{y})$ over the basic cell Y.

More precisely, we will prove the lemma

LEMMA A.7 *If we state* $\mathbf{H}_{\text{hom}}(\mathbf{x}) = \langle \mathbf{H}_0 \rangle_Y = \int_Y \mathbf{H}_0(\mathbf{x}, \mathbf{y})\, d\mathbf{y}$ *then we have*

$$k_0^2 \int_Y \tilde{\mu}(\mathbf{x}, \mathbf{y})\mathbf{H}_0(\mathbf{x}, \mathbf{y})\, d\mathbf{y} + i\omega\varepsilon_0 \operatorname{curl} \mathbf{E}_{\text{hom}} = 0, \tag{A21}$$

where $\mathbf{H}_{\text{hom}}$ *and* $\mathbf{E}_{\text{hom}}$ *satisfy a homogenized Maxwell equation associated to an effective matrix of permittivity* $[\varepsilon_{\text{hom}}]$ *given as*

$$\begin{cases} \operatorname{curl}_{\mathbf{x}} \mathbf{H}_{\text{hom}}(\mathbf{x}) = -i\omega\varepsilon_0[\varepsilon_{\text{hom}}]\mathbf{E}_{\text{hom}} \\ [\varepsilon_{\text{hom}}] = \langle \tilde{\varepsilon}(I - \nabla_{\mathbf{y}} \mathbf{V}_Y) \rangle_Y. \end{cases} \tag{A22}$$

Proof From (A19) and (A10), we deduce that:

$$(I - \nabla_{\mathbf{y}} \mathbf{V}_Y)\mathbf{E}_{\text{hom}} = \frac{i}{\omega\varepsilon_0} \tilde{\varepsilon}^{-1}(\operatorname{curl}_{\mathbf{y}} \mathbf{H}_1 + \operatorname{curl}_{\mathbf{x}} \mathbf{H}_0(\mathbf{x}, \mathbf{y})).$$

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

$$\int_Y \operatorname{curl}_{\mathbf{y}} \mathbf{H}_1(\mathbf{x}, \mathbf{y})\, dy + \operatorname{curl}_{\mathbf{x}} \mathbf{H}_{\text{hom}}(\mathbf{x}) = -i\omega\varepsilon_0 \langle \tilde{\varepsilon}(I - \nabla_{\mathbf{y}} \mathbf{V}_Y) \rangle_Y \mathbf{E}_{\text{hom}}.$$

Thanks to the periodicity of $\mathbf{H}_1$ and due to the anti-periodicity of the outer normal $\mathbf{n}$ to ∂Y, by virtue of the Green formula, we have:

$$\int_Y \operatorname{curl}_{\mathbf{y}} \mathbf{H}_1(\mathbf{x}, \mathbf{y}) d\mathbf{y} = \int_{\partial Y} n \wedge \mathbf{H}_1 ds = 0.$$

Then, we are led to the homogenized Maxwell equation and its associated effective matrix of permittivity (A22).

It remains to give the equation verified by $\mathbf{H}_{\text{hom}}(\mathbf{x})$. Summing the equation (A2c) in the system $(\mathcal{S}_0)$ over Y, we derive that:

$$\begin{aligned} &- k_0^2 \int_Y \tilde{\mu}(\mathbf{x}, \mathbf{y})\mathbf{H}_0(\mathbf{x}, \mathbf{y})\, d\mathbf{y} + \int_Y \operatorname{curl}_{\mathbf{x}}(\tilde{\varepsilon}^{-1}(\operatorname{curl}_{\mathbf{x}} \mathbf{H}_0(\mathbf{x}, \mathbf{y})))\, d\mathbf{y} \\ &+ \int_Y \operatorname{curl}_{\mathbf{x}}(\tilde{\varepsilon}^{-1}(\operatorname{curl}_{\mathbf{y}} \mathbf{H}_1))\, d\mathbf{y} = 0 \end{aligned}$$

Taking into account (A10) and using the definition of $\mathbf{E}_{\text{hom}}$, we obtain:

$$k_0^2 \int_Y \tilde{\mu}(\mathbf{x}, \mathbf{y})\mathbf{H}_0(\mathbf{x}, \mathbf{y})\, d\mathbf{y} + i\omega\varepsilon_0 \operatorname{curl} \mathbf{E}_{\text{hom}} = 0$$

To conclude the proof of the theorem, we must express the first integrand in terms of $[\mu_{\text{hom}}]$ and $\mathbf{H}_{\text{hom}}$. From Lemmas A.3 and A.4, we know that:

$$\begin{cases} \operatorname{curl}_{\mathbf{y}}\big(\mathbf{H}_0(\mathbf{x}, \mathbf{y})\big) = 0 \\ \operatorname{div}_{\mathbf{y}}\big(\tilde{\mu}(\mathbf{x}, \mathbf{y})\mathbf{H}_0(\mathbf{x}, \mathbf{y})\big) = 0, \end{cases}$$

which is the counterpart of (A11) for the leading order term in the ansatz of the magnetic field. Therefore we can state the lemma

Lemma A.8 $\mathbf{H}_0$ *and* $\mathbf{H}_{\text{hom}}$ *are linked by the following relation:*

$$\mathbf{H}_0 = (I - \nabla_{\mathbf{y}} \mathbf{W}_Y)\mathbf{H}_{\text{hom}}, \tag{A23}$$

with $\mathbf{W}_Y = (W_1, W_2, W_3)$*, where* W_j, $j \in \{1, 2, 3\}$ *are the unique solutions in* $H^1_\sharp(Y)/\mathbb{R}$ *of one of the three following problems* $(\mathcal{M}_j)$ *of electrostatic type:*

$$(\mathcal{M}_j) : -\operatorname{div}_{\mathbf{y}}\big[\mu_r^B(\mathbf{y})\big(\nabla_{\mathbf{y}}(W_j(\mathbf{y}) - y_j)\big)\big] = 0,\ j \in \{1, 2, 3\}.$$

From (A23) and Lemma A.7, we deduce that:

$$k_0^2 \left(\int_Y \mu(\mathbf{x}, \mathbf{y})(I - \nabla_{\mathbf{y}} \mathbf{W}_Y)\, d\mathbf{y} \right) \mathbf{H}_{\text{hom}} + i\omega\varepsilon_0 \operatorname{curl} \mathbf{E}_{\text{hom}} = 0. \tag{27}$$

The homogenized equation then clearly follows from the system (A22):

$$\operatorname{curl}\left(\left[\varepsilon_{\text{hom}}^{-1}\right](\operatorname{curl} \mathbf{H}_{\text{hom}}(\mathbf{x}))\right) - k_0^2[\mu_{\text{hom}}]\mathbf{H}_{\text{hom}}(\mathbf{x}) = 0.$$

with the effective permittivity defined by:

$$[\varepsilon_{\text{hom}}] = \langle \tilde{\varepsilon}(\mathbf{x}, \mathbf{y})(I - \nabla_{\mathbf{y}} \mathbf{V}_Y) \rangle_Y,$$

and the effective permeability defined by:

$$[\mu_{\text{hom}}] = \langle \tilde{\mu}(\mathbf{x}, \mathbf{y})(I - \nabla_{\mathbf{y}} \mathbf{W}_Y) \rangle_Y.$$

Appendix B: Convergence of the diffracted field

Lemma B.1 *Let* Ω *be a smooth bounded open subset in* $\mathbb{R}^3$, (u_η) *a bounded sequence in* $[L^2(\Omega)]^3$ *such that for a given sequence of coercive and bounded symmetric matrices* μ_η

$$\begin{cases} \operatorname{div}(\mu_\eta u_\eta) = 0 \\ \sup\limits_\eta \displaystyle\int_\Omega \Big(|\, u_\eta\,|^2 + |\operatorname{curl} u_\eta\,|^2\Big) dx < +\infty \\ u_\eta \wedge n \text{ is bounded in } [H^{\frac{1}{2}}(\partial\Omega)]^3. \end{cases}$$

Then $\exists u_0 \in H(\mathrm{curl}, \Omega)$, $\exists u_1 \in L^2(\Omega, H^1_\sharp(\mathrm{curl}, Y))$ *and a subsequence (still denoted by* (u_η)*) such that:*

$$\begin{cases} u_\eta \rightharpoonup u_0(x,y) \\ \mathrm{curl}\, u_\eta \rightharpoonup \mathrm{curl}_x\, u_0(x,y) + \mathrm{curl}_y\, u_1(x,y) \\ \mathrm{div}(\mu_\eta u_\eta) \rightharpoonup \mathrm{div}_x(\mu_0(x,y)u_0(x,y)) + \mathrm{div}_y(u_1(x,y)) = 0 \\ \eta\, \mathrm{div}(u_\eta) \rightharpoonup \mathrm{div}_y(u_0(x,y)) \end{cases}$$

(for the sake of simplicity we denote by $\mu_0(x, y)$ *the limit of* μ_η*, assuming that there is no confusion in the present mathematical section with the value* $\mu_0 = 4.10^{-7}\pi N \cdot A^{-2}$ *of the permeability of vacuum).*

Remark B1 If μ_η is constant, $\mathrm{div}_x(u_0(x, y)) = 0$ in $L^2_\sharp(\Omega \times Y)$, i.e.

$$a.e.x \in \Omega, \mathrm{div}_y\, u_1(x,y) = 0 \tag{B1}$$

This implies

$$\nabla u_\eta \rightharpoonup \nabla_x\, u_0(x,y) + \nabla_y\, u_1(x,y) \tag{B2}$$

Noting that there is a constant $C > 0$ (which only depends upon the measure of Ω) such that [51]

$$\|u_\eta\|_{[H^1(\Omega)]^3} \le C\left\{\|u_\eta\|_{[L^2(\Omega)]^3} + \|\mathrm{curl}\, u_\eta\|_{[L^2(\Omega)]^3} + \|\mathrm{div}\, u_\eta\|_{[L^2(\Omega)]^3} + \|u_\eta \wedge n\|_{[H^{\frac{1}{2}}(\partial\Omega)]^3}\right\} \tag{B3}$$

we get

$$\sup_\eta \|u_\eta\|_{[H^1(\Omega)]^3} < +\infty \tag{B4}$$

and Rellich's lemma ensures us that $u_\eta \to u_0(x)$ strongly in $[L^2(\Omega)]^3$, thus (B2) implies that $\nabla u_\eta \rightharpoonup \nabla u_0(x) + \nabla_y\, u_1(x, y)$ (which is the classical result of G. Allaire [23]).

B.1 *Proof of Lemma B.1, first step:* $u_\eta \rightharpoonup u_0(x, y)$ *such that* $\mathrm{div}_y(\mu_0(x, y)u_0(x, y)) = 0$ *and* $\mathrm{curl}_y(u_0(x, y)) = 0$

(i) u_η and $\mathrm{div}(\mu_\eta u_\eta)$ are bounded in $[L^2(\Omega)]^3$ and $L^2(\Omega)$ and are therefore two-scale converging (up to a subsequence) to $u_0(x, y) \in [L^2(\Omega \times Y)]^3$ and $\chi_0 \in L^2(\Omega\times Y)$. Let $\varphi \in \mathcal{D}(\Omega; C^\infty_\sharp(Y))$ then

$$\lim_{\eta\longmapsto 0} \int_\Omega \mathrm{div}(\mu_\eta u_\eta)\varphi\left(x, \frac{x}{\eta}\right) dx = \iint_{\Omega\times Y} \chi_0(x,y) \cdot \varphi(x,y)\, dxdy \tag{B5}$$

Using the Green's formula, (B5) can be rewritten as $\iint_{\Omega\times Y} \chi_0(x, y)\varphi\ (x, y)\, dxdy = \lim_{\eta\longmapsto 0} I_\eta$ with

$$I_\eta = \left[-\int_\Omega \mu_\eta u_\eta \cdot (\nabla_x\, \varphi)\left(x, \frac{x}{\eta}\right) dx - \frac{1}{\eta}\int_\Omega \mu_\eta u_\eta \cdot (\nabla_y\, \varphi)\left(x, \frac{x}{\eta}\right) dx\right] \tag{B6}$$

Since I_η is bounded, we deduce from (B6) that

$$0 = \lim_{\eta\longmapsto 0} \eta I_\eta = \lim_{\eta\longmapsto 0}\left[-\int_\Omega \mu_\eta u_\eta \cdot (\nabla_y\, \varphi)\left(x, \frac{x}{\eta}\right) dx\right]. \tag{B7}$$

Taking the two-scale limit of $\mu_\eta u_\eta$ which is bounded in $L^2(\Omega)$, we get:

$$\iint_{\Omega\times Y} \mu_0(x,y)u_0(x,y)\cdot(\nabla_y\varphi)(x,y)\,dxdy = 0. \tag{B8}$$

In (B8) we choose the particular test function $\varphi(x,y)=\theta(x)\psi(y)$ where $\theta\in\mathcal{D}(\Omega)$ and $\psi\in C^\infty_\sharp(Y)$. We obtain the equation (valid for almost all $x\in\Omega$):

$$\mathrm{div}_y(\mu_0(x,y)u_0(x,y)) = 0 \text{ dans } \mathcal{D}'(Y). \tag{B9}$$

(ii) Similarly to (i), let u_η and $\mathrm{curl}(u_\eta)$ be bounded in $[L^2(\Omega)]^3$ and therefore two-scale converge (up to a subsequence) to $u_0(x,y)\in[L^2(\Omega\times Y)]^3$ and $\chi_1\in[L^2(\Omega\times Y)]^3$. Let $\varphi\in[\mathcal{D}(\Omega;C^\infty_\sharp(Y))]^3$ then

$$\lim_{\eta\longmapsto 0}\int_\Omega \mathrm{curl}(u_\eta)\cdot\varphi\left(x,\frac{x}{\eta}\right)\,dx = \iint_{\Omega\times Y}\chi_1(x,y)\cdot\varphi(x,y)\,dxdy. \tag{B10}$$

Applying the Green's formula, and taking the two scale-limit in the rescaled rotational $\mathrm{curl}\,\varphi(x,\frac{x}{\eta}) = (\mathrm{curl}_x\varphi)(x,\frac{x}{\eta}) + \frac{1}{\eta}(\mathrm{curl}_y\varphi)(x,\frac{x}{\eta})$, we obtain

$$\iint_{\Omega\times Y} u_0(x,y)\cdot(\mathrm{curl}_y\varphi)(x,y)\,dxdy = 0, \forall\varphi\in[\mathcal{D}(\Omega;C^\infty_\sharp(Y))]^3. \tag{B11}$$

Hence, the equation (valid for almost all $x\in\Omega$)

$$\mathrm{curl}_y(u_0(x,y)) = 0 \text{ in } [\mathcal{D}'(Y)]^3. \tag{B12}$$

B.2 Proof of Lemma B.1, second step: Identification of χ_0 given by (B5)

Let $\varphi\in\mathcal{D}(\Omega;C^\infty_\sharp(Y))$ be such that $\nabla_y\varphi=0$ and let us take the limit when $\eta\to 0$ in (B6). Integrating by parts, we deduce that $\forall\varphi\in\mathcal{D}(\Omega;C^\infty_\sharp(Y))$:

$$\iint_{\Omega\times Y}[\chi_0(x,y) - \mathrm{div}_x(\mu_0(x,y)u_0(x,y))]\varphi(x,y)\,dxdy = 0. \tag{B13}$$

Now, we localize in x: taking φ such that $\varphi(x,y)=\theta(x)\psi(y)$ with $\psi\in C^\infty_\sharp(Y)$ such that $\nabla_y\psi=0$ and $\theta\in\mathcal{D}(\Omega)$ in (B13), we get:

$$\text{a.e. } x\in\Omega,\ \int_Y\big(\chi_0(x,y) - \mathrm{div}_x(\mu_0(x,y)u_0(x,y))\big)\psi(y)\,dy = 0. \tag{B14}$$

We extend (B14) by density to every function $\psi\in L^2_\sharp(Y)$ such that $\nabla_y\psi=0$. To characterize the set of functions Ψ, we consider the following set

$$M = \{w\in L^2_\sharp(Y)\ |\ \exists v\in[H^1_\sharp(Y)]^3\ \mathrm{div}_y v = w\},$$

which is a closed subset of $L^2_\sharp(Y)$ and with an orthogonal characterized by

$$M^\perp = \{\psi\in L^2_\sharp(Y)\,\big|\,\nabla_y\psi = 0\}.$$

From (B14) we deduce that $\chi_0(x,.) - \mathrm{div}_x(\mu_0(x,.)u_0(x,.))\in M^{\perp\perp} = M$ (M is closed). Therefore, there exists $u_1(x,.)\in[H^1_\sharp(Y)]^3$ such that $\chi_0(x,.) = \mathrm{div}_x(\mu_0(x,.)u_0(x,.)) + \mathrm{div}_y u_1(x,.)$.

B.3 Proof of Lemma B.1, third step: The singularly perturbed limit $\mathrm{div}_y(u_0(x,y))$ of $\eta\,\mathrm{div}(u_\eta)$

u_η and $\eta\,\mathrm{div}(u_\eta)$ are bounded in $[L^2(\Omega)]^3$ and $L^2(\Omega)$ and are therefore two-scale converging (up to a subsequence) to $u_0(x,y) \in [L^2(\Omega \times Y)]^3$ and $\chi_1 \in L^2(\Omega \times Y)$. Let $\varphi \in \mathcal{D}(\Omega; C^\infty_\sharp(Y))$ then

$$\lim_{\eta \longmapsto 0} \int_\Omega \eta\,\mathrm{div}(u_\eta)\varphi\left(x, \frac{x}{\eta}\right) dx = \iint_{\Omega\times Y} \chi_1(x,y)\cdot\varphi(x,y)\,dxdy, \tag{B15}$$

(B15) can be rewritten as $\iint_{\Omega\times Y} \chi_1(x,y)\varphi(x,y)\,dxdy = \lim_{\eta\longmapsto 0} I_\eta$ with

$$I_\eta = \left[-\int_\Omega \eta u_\eta\cdot(\nabla_x\varphi)\left(x,\frac{x}{\eta}\right)dx - \int_\Omega u_\eta\cdot(\nabla_y\varphi)\left(x,\frac{x}{\eta}\right)dx\right]. \tag{B16}$$

Taking the two-scale limit of u_η which is bounded in $L^2(\Omega)$, we get:

$$\iint_{\Omega\times Y} \chi_1(x,y)\cdot\varphi(x,y)\,dxdy = -\iint_{\Omega\times Y} u_0(x,y)\cdot(\nabla_y\varphi)(x,y)\,dxdy. \tag{B17}$$

B.4 L^2 bounds on (E_η, H_η) and its curl

We now consider a radius $R > 0$ and a bounded subset Ω of $\mathbb{R}^3$ such that $\Omega := \{|\,x\,| < R\}$ satisfies $\bar{\Omega} \subset \Omega$.

LEMMA B.2 *Let (E_η, H_η) be a solution of $\mathcal{P}_\eta^{(E,H)}$ such that* $\sup_\eta \int_\Omega |\,H_\eta\,|^2 dx < +\infty$. *If ε_η and μ_η are lower and upper bounded on Ω, the sequences (E_η),* $(\mathrm{curl}\,E_\eta)$ *and* $(\mathrm{curl}\,H_\eta)$ *are bounded in* $[L^2(\Omega)]^3$.

Proof Thanks to (1a) and (1b) in $\mathcal{P}_\eta$, we just have to show that $\sup_\eta \int_\Omega |\,\mathrm{curl}\,H_\eta\,|^2 dx < +\infty$. Assuming that (H_η) is bounded in $[L^2(\Omega)]^3$, the equation (4a) of $\mathcal{P}_\eta^H$ ensures us that $(\mathrm{curl}(\frac{1}{\varepsilon_\eta(x)}\mathrm{curl}\,H_\eta))$ is also bounded in $[L^2(\Omega)]^3$. Multiplying (4a) by the test function φ_η in $[\mathcal{D}(\mathbb{R}^3)]^3$ and integrating over Ω leads us to:

$$\int_\Omega \mathrm{curl}\left(\frac{1}{\varepsilon_\eta(x)}\mathrm{curl}\,H_\eta\right)\cdot\varphi_\eta\,dx - k_0^2\int_\Omega \mu_\eta H_\eta\cdot\varphi_\eta\,dx = 0, \forall\varphi_\eta \in [\mathcal{D}(\mathbb{R}^3)]^3 \tag{B18}$$

Now, the Poynting identity ensures that for every test function φ_η in $[\mathcal{D}(\mathbb{R}^3)]^3$:

$$\int_\Omega \mathrm{curl}\left(\frac{1}{\varepsilon_\eta(x)}\mathrm{curl}H_\eta\right)\cdot\varphi_\eta\,dx = \int_\Omega \frac{1}{\varepsilon_\eta(x)}\mathrm{curl}H_\eta\cdot\mathrm{curl}\varphi_\eta\,dx + \int_\Omega \mathrm{div}\left(\frac{1}{\varepsilon_\eta(x)}\mathrm{curl}H_\eta\wedge\varphi_\eta\right)dx. \tag{B19}$$

Green's theorem applied to the sequence of functions $\psi_\eta(x) = \frac{1}{\varepsilon_\eta(x)}\mathrm{curl}H_\eta \wedge \varphi_\eta$ in $[L^2(\Omega)]^3$ whose divergence belongs to $L^2(\Omega)$ tells us that there exists a sequence $(\psi_\eta\cdot n)$ in $H^{-\frac{1}{2}}(\partial\Omega)$ such that:

$$\int_\Omega \mathrm{div}\,\psi_\eta\,dx = \langle\psi_\eta\cdot n\,,\,\mathbf{1}\rangle_{H^{-\frac{1}{2}}(\partial\Omega),H^{\frac{1}{2}}(\partial\Omega)} \tag{B20}$$

From (B19), we derive that for every test function φ_η in $[\mathcal{D}(\mathbb{R}^3)]^3$:

$$\int_\Omega \operatorname{curl}\left(\frac{1}{\varepsilon_\eta(x)}\operatorname{curl}H_\eta\right)\cdot\varphi_\eta\,dx = \int_\Omega \frac{1}{\varepsilon_\eta}\operatorname{curl}H_\eta\cdot\operatorname{curl}\varphi_\eta\,dx$$
$$-\left\langle (n\wedge\varphi_\eta)\cdot\left(\frac{1}{\varepsilon_\eta}\operatorname{curl}H_\eta\right),\mathbf{1}\right\rangle_{H^{-\frac{1}{2}}(\partial\Omega),H^{\frac{1}{2}}(\partial\Omega)} \quad \text{(B21)}$$

From (B18) it follows that for all φ_η in $[\mathcal{D}(\mathbb{R}^3)]^3$:

$$\begin{aligned}&\int_\Omega \frac{1}{\varepsilon_\eta(x)}\operatorname{curl}H_\eta\cdot\operatorname{curl}\varphi_\eta dx - k_0^2\int_\Omega \mu_\eta H_\eta\cdot\varphi_\eta dx\\ &= \langle\big(n\wedge\varphi_\eta\big)\cdot\big(\frac{1}{\varepsilon_\eta}\operatorname{curl}H_\eta\big),\ \mathbf{1}\rangle_{H^{-\frac{1}{2}}(\partial\Omega),H^{\frac{1}{2}}(\partial\Omega)}\end{aligned} \quad \text{(B22)}$$

We now note that $\varepsilon_\eta = 1$ on $\partial\Omega$. Thanks to the density of $[\mathcal{D}(\mathbb{R}^3)]^3$ in $[L^2(\mathbb{R}^3)]^3$, we can choose $\varphi_\eta = H_\eta$, and we are thus led to:

$$\begin{aligned}&\int_\Omega \frac{1}{\varepsilon_\eta(x)}|\operatorname{curl}H_\eta|^2 dx - k_0^2\int_\Omega \mu_\eta|H_\eta|^2 dx\\ &= \langle\big(n\wedge H_\eta\big)\cdot\operatorname{curl}H_\eta,\ \mathbf{1}\rangle_{H^{-\frac{1}{2}}(\partial\Omega),H^{\frac{1}{2}}(\partial\Omega)}\end{aligned} \quad \text{(B23)}$$

Since (H_η) converges weakly in $[L^2(\Omega)]^3$ and satisfies $\Delta H_\eta + k_0^2 H_\eta = 0$ in $\mathbb{R}^3\setminus\bar{\Omega}$, from the hypo-ellipticity of the Helmholtz operator, (H_η) extended to $[L^2(\mathbb{R}^3)]^3$ via Stratton–Chu formula

$$(SC)\begin{cases} E_\eta^d(x) = i\omega\mu_0\displaystyle\int_{|y|=r} G(x-y)\left(\frac{y}{r}\wedge H_\eta^d(y)\right)ds \\ \quad +\displaystyle\int_{|y|=r}\nabla G(x-y)\left(\frac{y}{r}\wedge E_\eta^d(y)\right)ds & \text{(B24a)}\\ H_\eta^d(x) = -i\omega\varepsilon_0\displaystyle\int_{|y|=r} G(x-y)\left(\frac{y}{r}\wedge E_\eta^d(y)\right)ds \\ \quad +\displaystyle\int_{|y|=r}\nabla G(x-y)\left(\frac{y}{r}\wedge H_\eta^d(y)\right)ds & \text{(B24b)}\end{cases}$$

where G is the Green's function $G(x) = \frac{1}{4\pi}\frac{e^{ik_0|x|}}{|x|}$ and $|x| > R$. The sequence (H_η) thus uniformly converges (as well as all its derivatives) on every compact $K\subset\mathbb{R}^3\setminus\bar{\Omega}$. Therefore, we deduce that:

$$\lim_{\eta\to 0}\langle(n\wedge H_\eta)\cdot\operatorname{curl}H_\eta,\ 1\rangle_{H^{-\frac{1}{2}}(\partial\Omega),H^{\frac{1}{2}}(\partial\Omega)} = \langle(n\wedge H_0)\cdot\operatorname{curl}H_0,\ \mathbf{1}\rangle_{H^{-\frac{1}{2}}(\partial\Omega),H^{\frac{1}{2}}(\partial\Omega)} \quad \text{(B25)}$$

Also, the integral $k_0^2\int_\Omega \mu_\eta(x)|H_\eta|^2 dx$ is bounded by hypothesis (μ_η is upper bounded). Taking the limit in (B23), we conclude that $\int_\Omega \frac{1}{\varepsilon_\eta(x)}|\operatorname{curl}H_\eta|^2 dx$ remains bounded. Besides, $\frac{1}{\varepsilon_\eta(x)}$ is lower bounded in Ω, hence the conclusion.

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