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Anomalous homogeneous behaviour of metallic photonic crystals

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Abstract. We study the diffractive properties of metallic photonic crystals in the homogenization regime. It is shown that for a $H\|$ polarized field, the metallic crystal has an anomalous behaviour: it behaves like an artificial dielectric material with a current on its boundary. Numerical computations are given showing the practical use of the theoretical results.

In this paper, our aim is to study the scattering properties of a set of parallel infinitely conducting fibres in the low-frequency regime. Such a structure may model, for instance, a metallic photonic crystal [1–3], a device that is the subject of many studies principally because it has a gap starting from zero frequency up to a plasma frequency [4–10], at least for $E\|$ polarized fields (electric field parallel to the axis of the fibres). The homogeneous study of such structures is aimed at providing a homogeneous medium possessing equivalent diffractive properties [9–17]. In a preceding paper [9], we gave some rigorous results concerning the homogeneous properties of both dielectric and metallic photonic crystal for both cases of polarization. We emphasize here the case of $H\|$ polarization (magnetic field parallel to the fibres), for which the homogeneous behaviour of a metallic crystal is anomalous; indeed it cannot be written as a classical diffraction problem. The structure is made of circular perfectly conducting scatterers that are periodically settled in a domain Ω of the plane, in the following way. First, we define an elementary cell $Y = [0, 1[^2$ (with coordinates (x_1, x_2)), in which we set a scatterer T (the size of Y is to be expressed in terms of wavelength units). We denote as θ the filling ratio of cell Y, which is the area measure of T. Then for a given scaling parameter $\eta > 0$, we fill up Ω with cells ηY containing a scatterer ηT. This way, Ω contains $N_\eta \simeq \frac{|\Omega|}{\eta^2}$ scatterers. When this structure is illuminated by an incident field u^i under $H\|$ polarization, it gives rise to a scattered field u_η verifying the Helmholtz equation outside the fibres and a Neumann condition on the fibres. Our aim is to describe the limit of u_η as η tends to zero (the size of cell ηT is thus very small compared with the wavelength). By means of homogenization analysis (see [10–12] for an introduction to this subject with an emphasis on electrostatics and electromagnetics), it may be shown that u_η converges, as η tends to zero, towards a function u_0, which satisfies

$$\begin{aligned} &\Delta u_0 + k_0^2 u_0 = 0 \qquad \text{outside} \quad \Omega \\ &\Delta u_0 + k_0^2 \varepsilon_h u_0 = 0 \qquad \text{inside} \quad \Omega \\ &u_0 - u^i \text{ satisfies a radiation condition} \end{aligned} \tag{1}$$

where

$$\varepsilon_h = \frac{1-\theta}{1-\theta+\chi} \tag{2}$$

is the homogenized relative permittivity (in general, when the cross section of the rods is not circular the homogenized medium is anisotropic). The coefficient χ is defined as $\chi = \int_{Y \setminus T} \frac{\partial w}{\partial x_2}\, \mathrm{d}x_2$, where w is the unique Y-periodic function with zero mean, verifying the so-called auxiliary problem:

$$\begin{aligned} -\Delta w &= 0 \qquad \text{in} \quad Y \setminus T \\ \frac{\partial w}{\partial n} &= -n_{x_1} \qquad \text{on} \quad \partial T \end{aligned} \tag{3}$$

where n_{x_1} is the x_1-component of the outer normal of ∂T (note that we would obtain the same result by inverting x_2 and x_1, because of the symmetry of the problem). Here we have given a very 'fuzzy' statement, since when one is considering the convergence of a sequence of functions, one should precise the topology for which the sequence converges. Without going into details, we can say that u_η converges uniformly towards u_0 on every compact domain outside Ω, but it converges only in quadratic mean towards u_0 inside Ω (it does not converge pointwise inside Ω).

Now, equations (1), (2) are not sufficient to completely define the limit field. Indeed, it is necessary to precise the transmission conditions. This is where the behaviour is anomalous as the new transmission conditions through $\partial\Omega$ take the following form:

$$\begin{aligned} u^- &= (1-\theta)u^+ \\ \frac{1}{\varepsilon_h}\left(\frac{\partial u}{\partial n}\right)^- &= \left(\frac{\partial u}{\partial n}\right)^+ . \end{aligned} \tag{4}$$

The notations f^+ and f^- denote, respectively, the exterior and interior trace of f on the boundary of Ω.

Obviously, there is a current that appears on the boundary of Ω, and *the homogeneous problem is not that of a simple artificial dielectric*, since the magnetic field is not continuous through the boundary of Ω. It should be noted that this is the only case where such a situation occurs. In all other cases, that is for dielectric or metallic media illuminated by $E\|$ fields or dielectric media illuminated by $H\|$ fields, the homogeneous medium leads to a standard problem of diffraction [9]. From a physical point of view, let us remark that on the perfectly conducting fibres, the magnetic field induces turning currents; these micro-currents lead to a macroscopic current situated on the boundary of Ω when passing to the limit $\eta \to 0$.

Now there are two major problems that we should tackle. First, the homogeneous description of the medium is relevant if one is able to provide some sort of answer to the following question: under what hypothesis is it possible to replace a finite set of fibres by the homogeneous problem (1), (4)? That is, we hope that the homogeneous description will conveniently describe a practical situation with a reasonable value of the number of scatterers and for not too large wavelengths. In other words, though the mathematical analysis was performed for η tending to zero, we hope that the limit field u_0 will handle the case of small, but nonzero, values of η. The second problem is that of calculating the equivalent permittivity. Obviously, when dealing with a homogenization process, one wishes to get *in fine* a simpler problem than the one we started from. However, the auxiliary problem (3) is far from simple to deal with if one wishes to obtain precise numerical results; consequently the interest shown in the homogenized problem may be questionable. Although there is a large amount of literature devoted to this numerical problem [19–23], here we shall adopt another line of attack. The homogenized permittivity will be obtained by a direct computation relying on a rigorous theory

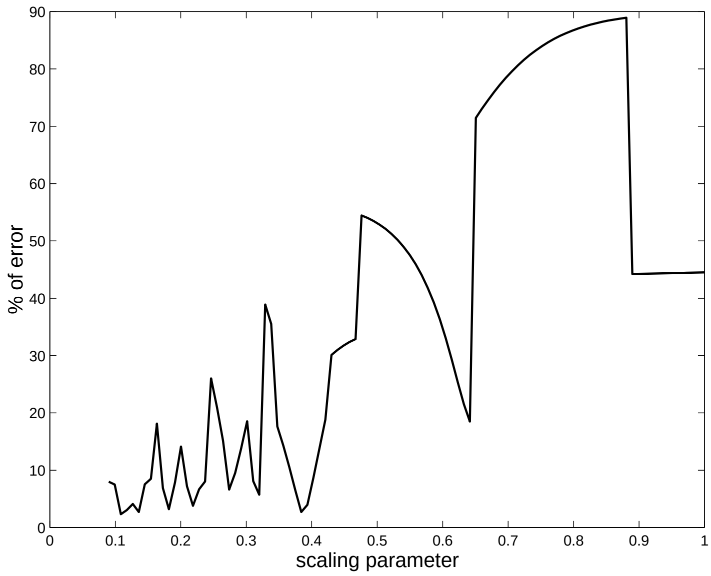

Figure 1. Minimal values of J for varying η ($\lambda = 2$, $r/\lambda = \frac{1}{16}$, $R/\lambda = \frac{1}{2}$).

of diffraction by a set of parallel rods [18], and by an optimization algorithm. For the numerical computations, we use a circular domain Ω (radius R) because it simplifies the optimization process, but the results extend to an arbitrarily shaped domain Ω as the homogenized problem only depends upon the geometry of the basic cell Y.

More precisely, we first compute the field $g_\eta(\varphi)$ diffracted at infinity by a set of N_η parallel infinitely conducting circular fibres (radius $\eta \times r$) for an incident monochromatic plane wave u^i under $H \parallel$ polarization with wavelength in vacuum λ (let us recall that $u_\eta - u^i \underset{\rho\to+\infty}{\sim} \frac{e^{ik\rho}}{\sqrt{k\rho}} g_\eta(\varphi)$, where$(\rho, \varphi)$ denote the usual polar coordinates and $k = \frac{2\pi}{\lambda}$). We want to find a couple $(\tilde{\varepsilon}_h, \tilde{\theta})$ such that the field $g_0(\varphi)$ diffracted at infinity by a cylinder of cross section Ω and relative permittivity $\tilde{\varepsilon}_h$, with the particular transmission conditions (4) (with parameter $\tilde{\theta}$), fits at best with $g_\eta(\varphi)$. We thus define a normalized cost function

$$J = \sqrt{\frac{\int_0^{2\pi} |g_\eta(\varphi) - g_0(\varphi)|^2 \, d\varphi}{\int_0^{2\pi} |g_\eta(\varphi)|^2 \, d\varphi}} \tag{5}$$

and we use an optimization algorithm in order to minimize J (we use a Nelder–Mead-type simplex search method). We denote $\tilde{J}(\tilde{\varepsilon}_h, \tilde{\theta}) = \min J$. If the homogenization scheme is valid for given wavelength λ and scaling parameter η, then we should find numerically that $\theta \simeq \tilde{\theta}$, and that $\tilde{J}(\tilde{\varepsilon}_h, \tilde{\theta})$ is rather small (this point is indeed rather subjective). Moreover, if $\tilde{\theta}$ is near θ and $\tilde{J}(\tilde{\varepsilon}_h, \tilde{\theta})$ is small enough, then the numerical value $\tilde{\varepsilon}_h$ will be an approximate value of ε_h.

First, we want to know for which ratios η the homogenization scheme is valid. We take $\lambda = 2$, $r/\lambda = \frac{1}{16}$, $R/\lambda = \frac{1}{2}$ (recall that the side of the elementary cell Y is 1 in λ units) and we compute u_η for η varying between 0.1 and 1. The values of $\tilde{J}(\tilde{\varepsilon}_h, \tilde{\theta})$ are plotted as a percentage in figure 1. Clearly, here there is a converging process, and for values of η less than 0.15 ($\eta \times 1/\lambda < 0.075$) the relative error is less than 10%. Let us now study the homogenized parameters $\tilde{\varepsilon}_h$ and $\tilde{\theta}$. In order to avoid artefact effects, we perform another computation with $R/\lambda = 0.2$ and $\eta \times 1/\lambda = 0.025$, so that the homogenization regime is reached. We now use

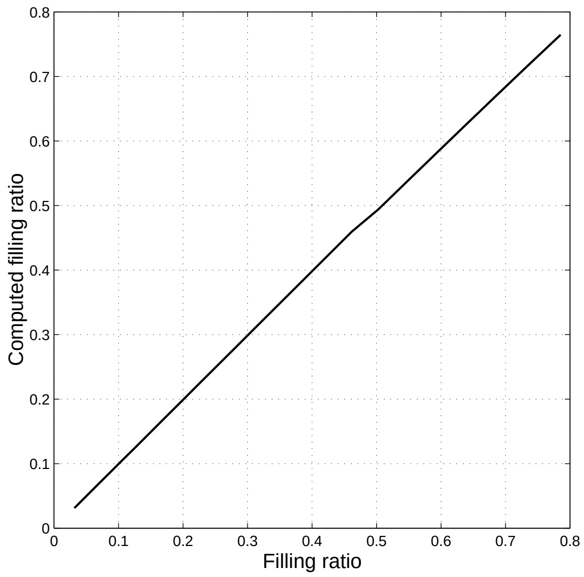

Figure 2. Comparison between the true filling ratio θ and the computed $\tilde{\theta}$, for varying θ ($R/\lambda = 0.2$, $\eta \times 1/\lambda = 0.025$).

the optimization scheme for θ varying between $\pi/100$ and $\pi/4$ (this last value is the maximum for circular fibres). We thus obtain $\tilde{\varepsilon}_h$ and $\tilde{\theta}$ as functions of θ. First we verify, see figure 2, that $\tilde{\theta} \simeq \theta$ (apart perhaps for the highest values of θ). On the other hand, in figure 3, the solid curve is a plot of the equivalent index $\tilde{n}_h = \sqrt{\tilde{\varepsilon}_h}$, obtained by the minimization of (5), which is an approximate value of $\sqrt{\varepsilon_h}$. This curve shows that the homogenized relative index depends almost linearly of the filling ratio θ. A numerical fitting procedure provides us with the following estimate:

$$\tilde{n}_h = 0.45 \times \theta + 1. \qquad (6)$$

The graph of this function is plotted as a dashed line in figure 3. It is perfectly understandable that the affine part of this equation should be equal to 1, as the case $\theta = 0$ corresponds to a void medium. Finally, it is quite simple to obtain the homogenized index from relation (6). Nevertheless, we have obtained this simple law through a particular numerical experiment ($\eta/\lambda = 0.025$, $R/\lambda = 0.2$) so that the generality of this formula needs to be checked. To do so, we plot the values of $\tilde{\varepsilon}_h$ (dashed curve in figure 4) and $\tilde{\theta}$ (dashdot line in figure 4) obtained from the first numerical experiment ($\lambda = 2$, $r/\lambda = \frac{1}{16}$, $R/\lambda = \frac{1}{2}$), as well as the actual value of θ (dotted straight line in figure 4, $\theta = \pi/64$), and the value of the equivalent permittivity (= 1.0447) predicted by (6) (solid straight line in figure 4). We see a clear convergence towards these values as $\eta \to 0$. Therefore, formula (6) appears to be rather general, so that it proves to be a good, and particularly simple way of solving the auxiliary problem (3). To complete these results, in figure 5 we have plotted the fields diffracted at infinity for both the set of fibres and the homogenized medium for $\eta = 0.1$. In that case the relative error defined in (5) is equal to 7%. One can see that there is a fair agreement between the two curves. Moreover, one may wonder about the near-field behaviour since we obtained our results by optimizing the field diffracted at infinity. Therefore, we have also plotted, see figure 6, the total exterior field for both problems on the boundary of Ω. We see that the agreement is also very good, so that

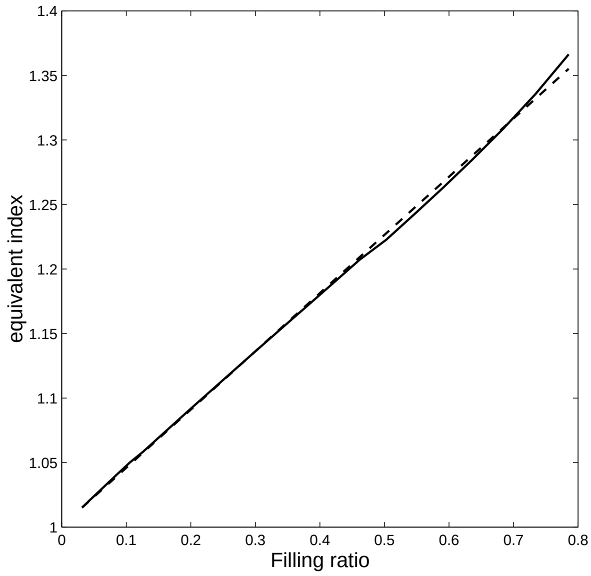

Figure 3. Fitting of the computed homogenized index $\tilde{n}_h$ as a function of θ (solid curve) by the affine law (6) (dashed line).

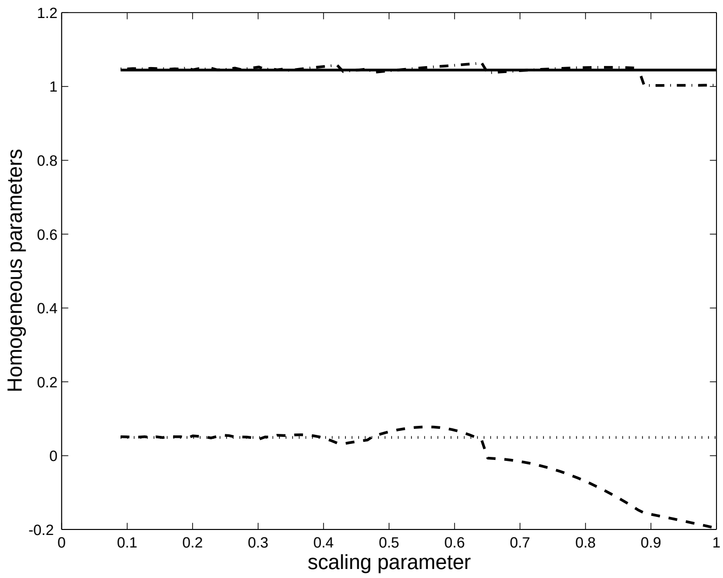

Figure 4. Convergence of the computed homogenized permittivity $\tilde{\varepsilon}_h$ and filling ratio $\tilde{\theta}$ for varying η ($\lambda = 2$, $r/\lambda = \frac{1}{16}$, $R/\lambda = \frac{1}{2}$).

the homogenized problem represents very well the true problem for both far and near fields.

In summary, we have described the behaviour of metallic photonic crystal for $H\|$ polarization in the low-frequency domain. In this case, the photonic crystal behaves as a homogeneous dielectric medium with a current on its boundary. The given theoretical results

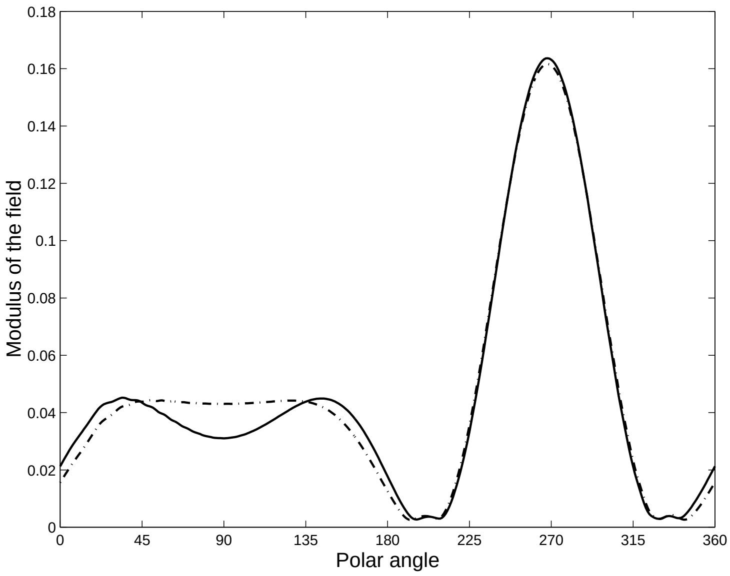

Figure 5. Comparison between the field diffracted at infinity by the set of fibres (solid curve) ($\lambda = 2$, $r/\lambda = \frac{1}{16}$, $R/\lambda = \frac{1}{2}$, $\eta = 0.1$) and the field diffracted at infinity by the homogenized medium (dashed curve) ($\varepsilon_h = 1.0447$, $\theta = \pi/64$).

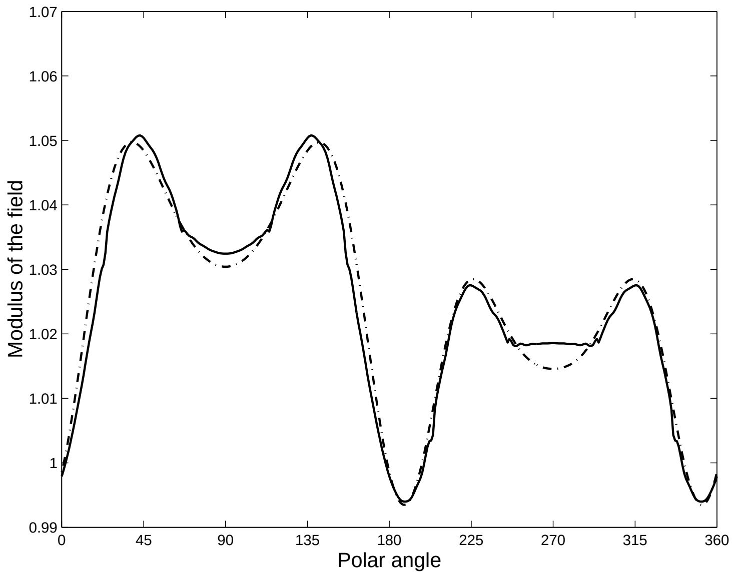

Figure 6. Modulus of the exterior field on $\partial\Omega$ for the set of fibres (solid curve) and for the homogenized medium (dashed curve) (same parameters as in figure 5).

come from a rigorous asymptotic study of the Maxwell equations, and their practical interest has been discussed numerically, by means of a rigorous theory of diffraction.

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