Homogenization of 3D finite chiral photonic crystals
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Abstract

We homogenize Maxwell’s equations for Drude-Born-Fedorov chiral crystals, using the multi-scale technique. We find that the homogenized material is described by dispersive anisotropic effective matrices, derived from frequency dependent coupled auxiliary problems. For low frequencies, these matrices may not be positive definite.

Key words: Multi-scale method, Homogenization, Meta-materials

PACS:

1. Introduction

Between 1996 and 1999, the British physicist John Pendry published a series of papers giving rise to a new class of composite structures (christened metamaterials) which exhibit low plasmon frequency (arrays of thin straight wires) and artificial magnetism (split ring resonators) in the low frequency regime (homogenization domain). When combined, these two structures may exhibit negative refractive index as was chiefly demonstrated by David Smith and others in the microwave regime. Recently, John Pendry proposed a new route to negative refraction through arrays of chiral inclusions of helicoidal shape [1]: Backward waves can propagate in composite structures with positive optical parameters provided that one of the constituent materials is chiral. This may open new vistas for negative refraction phenomena in the optical region via homogenized chiral media (the characteristic dimensions in the composite structure are much smaller than the wavelength). This is the main motivation for the present analysis of effective properties of finite periodic chiral structures.

2. Homogenization setting

In this paper, we consider the diffraction problem of a monochromatic wave incident on a heterogeneous chiral body, when its wavelength is large compared to the typical heterogeneity size, but possibly in resonance with the overall finite structure. To model this, let us introduce a unit cell $Y = [0; 1]^3$ whose homothety $\eta Y$ is repeated periodically within a fixed bounded domain $\Omega$. When $\eta$ tends to zero, $\Omega$ is filled by with an increasing number of very tiny cells, so that it looks homogeneous. We also define the relative permittivity and permeability and the chiral inductance at every point $x \in \mathbb{R}^3$ by $\chi_\eta(x) = \tilde{\chi}(x, \eta)$, $\chi \in \{ \varepsilon, \mu, \beta \}$ with

$$\tilde{\chi}(x, y) = \begin{cases} \chi(y), & \text{if } x \in \Omega, \\ 1 & \text{for } \chi = \varepsilon, \mu, \text{ if } x \in \mathbb{R}^3 \setminus \bar{\Omega}, \\ 0 & \text{for } \chi = \beta, \text{ if } x \in \mathbb{R}^3 \setminus \bar{\Omega}. \end{cases}$$

The electromagnetic field $(E_\eta, H_\eta)$ satisfies so-called Drude-Born-Fedorov equations within the chiral body:

$$\begin{cases} \nabla \times E_\eta = i \omega \mu_0 \mu_\eta (H_\eta + \beta \eta \nabla \times H_\eta), \\ \nabla \times H_\eta = -i \omega \varepsilon_0 \varepsilon_\eta (E_\eta + \beta \eta \nabla \times E_\eta), \quad (1) \end{cases}$$

where $\omega$ is the frequency, $\varepsilon_0 \mu_0 = c^2$, $c$ being the speed of light in vacuum. The ellipticity and boundedness of the operator are ensured by the following assumptions: $0 < m \leq \varepsilon, \mu, \leq M$ and $0 \leq \beta < 1$. The diffraction problem admits a unique solution under proper outgoing wave conditions [2].

In fact, the smaller the typical heterogeneity size $\eta$, the faster the modulus of the electromagnetic field $(E_\eta, H_\eta)$ oscillates. Hence, we suppose that it can be approximated by a two-scale expansion of the form:

$$E_\eta(x) = \sum_{k=0}^{\infty} \eta^k E_k(x, \frac{x}{\eta}), \quad H_\eta(x) = \sum_{k=0}^{\infty} \eta^k H_k(x, \frac{x}{\eta}), \quad (2)$$
where \( \mathbf{E}_\eta, \mathbf{H}_\eta : \mathbb{R}^3 \times Y \rightarrow \mathbb{C}^3 \) are smooth functions of 6 variables, independent of \( \eta \), such that \( \forall x \in \Omega, \mathbf{E}_x(x, \cdot) \) and \( \mathbf{H}_x(x, \cdot) \) are \( Y \)-periodic.

Our goal is to characterize the diffracted field when \( \eta \) tends to 0.

### 3. Homogenization result

To identify the limit problem, we introduce the rescaled operator
\[
\nabla = \nabla_x + \frac{1}{\eta} \nabla_y ,
\tag{3}
\]
where \( x \) denotes the macroscopic (slow) variable and \( y \) denotes the microscopic (fast) variable.

Substituting (2) and (3) in (1) and collecting the terms sitting in front of same powers of \( \eta \) we obtain the following homogenized Drude-Born-Fedorov equations:
\[
\begin{aligned}
\nabla_x \times \mathbf{E}_{\text{hom}} &= i \omega y_0 [\mu_{\text{hom}}] (\mathbf{H}_{\text{hom}} \\
&+ [\beta_{\text{hom}}] \nabla_x \times \mathbf{H}_{\text{hom}}) , \\
\nabla_x \times \mathbf{H}_{\text{hom}} &= - i \omega y_0 [\epsilon_{\text{hom}}] (\mathbf{E}_{\text{hom}} \\
&+ [\beta_{\text{hom}}] \nabla_x \times \mathbf{E}_{\text{hom}}) .
\end{aligned}
\tag{4}
\]

Similarly to the case of ferro-magnetic photonic crystals [3] (for which \( \beta = 0 \) in (1)), the homogenized matrices \([\mu_{\text{hom}}], [\epsilon_{\text{hom}}]\) are deduced from two auxiliary problems arising on the basic cell \( \Omega \). But it turns out that they are now coupled and most importantly they do depend on the frequency \( \omega \) of the incoming wave. Indeed, the auxiliary problem takes the following form:
\[
\nabla_y \cdot \{ [M_{\beta,\omega}] (y) \nabla_y (V_x, W_y) \} = 0 ,
\tag{5}
\]
where
\[
[M_{\beta,\omega}] (y) = \begin{pmatrix}
\frac{\epsilon}{\Lambda} & \frac{i}{\omega} & \frac{\frac{\epsilon_0}{\mu_0} - 1 - \Lambda}{\beta \Lambda} \\
\frac{i}{\omega} & 1 - \Lambda & \frac{i \omega}{\epsilon_0 \mu_0} \\
\frac{\frac{\epsilon_0}{\mu_0} - 1 - \Lambda}{\beta \Lambda} & \frac{i \omega}{\epsilon_0 \mu_0} & \frac{\epsilon_0}{\mu_0}
\end{pmatrix} ,
\tag{6}
\]
with
\[
\Lambda = 1 - \omega^2 \beta^2 \epsilon \mu .
\tag{7}
\]

We note that for ferro-magnetic media \( \beta = 0 \), so that
\[
\Lambda = 1 , \quad (1 - \Lambda) / \beta = \omega^2 \beta \epsilon \mu = 0 .
\tag{8}
\]

Hence, one can see that off-diagonal entries of \([M_{\beta,\omega}]\) vanish in that case and we retrieve the result of [3].

We also note that
\[
\text{Det}([M_{\beta,\omega}]) = \sqrt{\frac{\epsilon_0}{\mu_0} / \Lambda^2 (\epsilon \mu - (1 - \Lambda) / \omega^2)}
\tag{9}
\]
which is positive since \( 0 \leq \beta < 1 \) (this is the case for chiral materials at hand [2]). Hence, from Lax-Milgram lemma there is a unique solution (up to an additive constant) to (5) in the space of periodic potentials of square integrable energy on \( Y \).

The homogenized matrices of permittivity and permeability are given by
\[
[\epsilon_{\text{hom}}] = \begin{pmatrix}
\frac{\epsilon_0}{\mu_0} & \frac{i \omega}{\epsilon_0 \mu_0} & \frac{\frac{\epsilon_0}{\mu_0} - 1 - \Lambda}{\beta \Lambda} \\
\frac{i \omega}{\epsilon_0 \mu_0} & 1 - \Lambda & \frac{i \omega}{\epsilon_0 \mu_0} \\
\frac{\frac{\epsilon_0}{\mu_0} - 1 - \Lambda}{\beta \Lambda} & \frac{i \omega}{\epsilon_0 \mu_0} & \frac{\epsilon_0}{\mu_0}
\end{pmatrix} ,
\tag{10}
\]
and
\[
[\mu_{\text{hom}}] = \begin{pmatrix}
\frac{\epsilon_0}{\mu_0} & \frac{i \omega}{\epsilon_0 \mu_0} & \frac{\frac{\epsilon_0}{\mu_0} - 1 - \Lambda}{\beta \Lambda} \\
\frac{i \omega}{\epsilon_0 \mu_0} & 1 - \Lambda & \frac{i \omega}{\epsilon_0 \mu_0} \\
\frac{\frac{\epsilon_0}{\mu_0} - 1 - \Lambda}{\beta \Lambda} & \frac{i \omega}{\epsilon_0 \mu_0} & \frac{\epsilon_0}{\mu_0}
\end{pmatrix} ,
\tag{11}
\]
with \( < . , . > = \int_\Omega \cdot dy \). We remark that these matrices describe dispersive media (they depend upon \( \omega \)): Interestingly, if \( \omega \) is small enough, \([\epsilon_{\text{hom}}]\) will become negative definite.

Finally, the homogenized matrix of chiral inductance can be expressed in two ways:
\[
[\beta_{\text{hom}}] = - [\epsilon_{\text{hom}}]^{-1} \begin{pmatrix}
\frac{\epsilon_0}{\mu_0} & \frac{i \omega}{\epsilon_0 \mu_0} & \frac{\frac{\epsilon_0}{\mu_0} - 1 - \Lambda}{\beta \Lambda} \\
\frac{i \omega}{\epsilon_0 \mu_0} & 1 - \Lambda & \frac{i \omega}{\epsilon_0 \mu_0} \\
\frac{\frac{\epsilon_0}{\mu_0} - 1 - \Lambda}{\beta \Lambda} & \frac{i \omega}{\epsilon_0 \mu_0} & \frac{\epsilon_0}{\mu_0}
\end{pmatrix} \begin{pmatrix}
\frac{\epsilon_0}{\mu_0} \\
\frac{i \omega}{\epsilon_0 \mu_0} \\
\frac{\frac{\epsilon_0}{\mu_0} - 1 - \Lambda}{\beta \Lambda}
\end{pmatrix} ,
\tag{12}
\]
where \( \{ \varepsilon, \mu \} \in \{ (\varepsilon, \mu), (\mu, \varepsilon) \} \). This makes an easily implementable consistency criterion to test convergence of a numerical algorithm.

### 4. Conclusion

The results obtained so far are only theoretical ones, but we are now investigating the numerical solutions of the auxiliary problems for realistic values of permittivity, permeability and chiral parameter thanks to finite elements modeling. We note that one can only prove a weak \( L^2(\Omega) \) convergence of \((H_y, E_y)\) towards the leading order term \((H_0, E_0)\) of the asymptotic expansion (2). This is because \((H_y, E_y)\) is not divergence free, a fact which was already reported for the homogenization of ferro-magnetic photonic crystals in [3]. For a proof of strong \( L^2(\Omega) \) convergence in the case of a dielectric (non-magnetic) photonic crystal, we refer the reader to [4].

### References