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Abstract

Isotropic chiral media can be modeled in many ways. We use an unbiased homogenization technique to compute effective material parameters for a composite material with microstructure consisting of spirals, and then compare the results with three models: Tellegen, Post, and Drude-Born-Fedorov. Only the DBF model can fit the data, but requires a modification, so that the influence of the curl of the fields is different for the electric and the magnetic field, respectively.

1 Introduction

Chiral materials are challenging from a modelling point of view. The typical realization is the classical one by Lindman [1, 2], who took a lot of metal coils, all wound the same way, and embedded them in an isolating material. The result was a material which had different propagation properties for left and right hand circularly polarized waves, respectively. The same effect can be observed for visible light in sugar solutions, attributed to the chirality of the sugar molecule.

From a modelling point of view, the challenge lies in the fact that the chiral effect has to do with wave propagation, but most homogenization methods are only defined in the limit where the inclusions are infinitely small compared to the wavelength, meaning the fields can be considered quasi-static near the inclusions and the chiral effects cannot be observed. In recent years, new homogenization formalisms have been proposed that can take a finite scale difference into account, with sufficient mathematical rigor [3, 4]. In this paper, we study the outcome of this homogenization technique when applied to a microstructure similar to Lindman's original experiment. It is demonstrated that among the available model's in the literature, a modification of the Drude-Born-Fedorov model fits the computed data very closely.

2 Dispersion relations

Our model problem is periodic, and we present in this section some notation and general results for periodic media. The first step in describing periodic media is to define a unit cell U and a lattice basis $\boldsymbol{a}_1$, $\boldsymbol{a}_2$, and $\boldsymbol{a}_3$, such that the periodic material can be constructed by translating the unit cell by lattice vectors $\boldsymbol{x}_{\boldsymbol{n}} = n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2 + n_3\boldsymbol{a}_3$, where n_1, n_2, and n_3 are integers. Once this is done, a reciprocal unit cell U' and basis vectors $\boldsymbol{b}_1$, $\boldsymbol{b}_2$, $\boldsymbol{b}_3$ for the reciprocal lattice can be defined, such that $\boldsymbol{a}_i \cdot \boldsymbol{b}_j = 2\pi\delta_{ij}$. The reciprocal unit cell U' is often called the first Brillouin zone. Using the Floquet-Bloch representation an arbitrary square integrable field $\boldsymbol{E}(\boldsymbol{x})$ can be written [3, 5, 6],

$$\boldsymbol{E}(\boldsymbol{x}) = \frac{1}{|U'|}\int_{U'} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}\widetilde{\boldsymbol{E}}(\boldsymbol{x},\boldsymbol{k})\,\mathrm{d}\boldsymbol{k} \tag{1}$$

The field $\widetilde{\boldsymbol{E}}(\boldsymbol{x},\boldsymbol{k})$ is called the Bloch amplitude, and is U-periodic in $\boldsymbol{x}$ whereas the field $\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}\widetilde{\boldsymbol{E}}(\boldsymbol{x},\boldsymbol{k})$ is U'-periodic in $\boldsymbol{k}$. A typical effect when using this representation is the transformation of the nabla operator, $\nabla \to \nabla + \mathrm{i}\boldsymbol{k}$, when acting on the Bloch amplitude. It is shown in [3], that the following eigenvalue problem provides the relevant information of the problem when the material consists of only real permittivity $\boldsymbol{\epsilon}(\boldsymbol{x})$ and real permeability $\boldsymbol{\mu}(\boldsymbol{x})$, which are assumed U-periodic:

$$\begin{pmatrix} \mathbf{0} & -(\nabla + \mathrm{i}\boldsymbol{k}) \times \mathbf{I} \\ (\nabla + \mathrm{i}\boldsymbol{k}) \times \mathbf{I} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \widetilde{\boldsymbol{E}}_n \\ \widetilde{\boldsymbol{H}}_n \end{pmatrix} = \mathrm{i}\omega_n \begin{pmatrix} \boldsymbol{\epsilon}(\boldsymbol{x}) & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\mu}(\boldsymbol{x}) \end{pmatrix} \begin{pmatrix} \widetilde{\boldsymbol{E}}_n \\ \widetilde{\boldsymbol{H}}_n \end{pmatrix} \tag{2}$$

	Tellegen	Post	Drude-Born-Fedorov
$\boldsymbol{D} =$	$\epsilon_{\mathrm{T}}\boldsymbol{E} + \zeta\boldsymbol{H}$	$\epsilon_{\mathrm{P}}\boldsymbol{E} + \mathrm{i}\xi\boldsymbol{B}$	$\epsilon(\boldsymbol{E} + \beta\nabla\times\boldsymbol{E})$
$\boldsymbol{B} =$	$\mu_{\mathrm{T}}\boldsymbol{H} - \zeta\boldsymbol{E}$	$\mu_{\mathrm{P}}(\boldsymbol{H} - \mathrm{i}\xi\boldsymbol{E})$	$\mu(\boldsymbol{H} + \beta\nabla\times\boldsymbol{H})$

Table 1: Three different possible descriptions of isotropic chiral media, see [7, pp. 15–16] and [8].

where $\boldsymbol{x} \in U$ and $\boldsymbol{k} \in U'$. When the unit cell contains a PEC region Ω (such as the coils in Lindman's experiment), the problem is modified so that only space vectors outside the PEC region, $\boldsymbol{x} \in U \setminus \Omega$, are considered. We also require the boundary condition that electric fields tangential to the surface of Ω are zero, *i.e.*, $\hat{\boldsymbol{n}} \times \widetilde{\boldsymbol{E}} = \boldsymbol{0}$ where $\hat{\boldsymbol{n}}$ is the normal to $\partial\Omega$. The same conclusions can then be made for the PEC case as when the entire unit cell is filled with finite material parameters $\boldsymbol{\epsilon}(\boldsymbol{x})$ and $\boldsymbol{\mu}(\boldsymbol{x})$.

It is shown in [3] that the eigenvalue problem (2) is well posed, and the solutions can be used as a basis in a properly defined function space for Maxwell's equations. The eigenvalues ω_n are real, and form a nondecreasing sequence

$$0 \leq \omega_1^2 \leq \omega_2^2 \leq \cdots \tag{3}$$

Since $\boldsymbol{k} \in U'$ is a free parameter, the eigenvalue problem (2) defines ω_n as a function of $\boldsymbol{k}$, which is the dispersion relation $\omega_n = W_n(\boldsymbol{k})$.

3 Calculation of effective material parameters

In [3, 4], it is shown that a periodic heterogeneous material can be replaced by a homogeneous, effective material when the wavelength is large enough. More precisely, the condition can be written as

$$2\pi\frac{a}{\lambda_0} < \frac{\pi - 1}{\|\boldsymbol{\epsilon}(\cdot)/\epsilon_0 - 1\| + 1} \tag{4}$$

for non-magnetic media, where λ_0 is the vacuum wavelength, ϵ_0 is the permittivity of vacuum, and a is the length of the unit cell. Note that this does not require the unit cell to be infinitely small compared to the vacuum wavelength. For a fixed $\boldsymbol{k} \in U'$, the effective material parameters can be expressed in terms of the mean values of the eigenvectors corresponding to the four eigenvalues with smallest absolute value. The relation defining the parameters is

$$\begin{pmatrix} \langle\widetilde{\boldsymbol{D}}\rangle \\ \langle\widetilde{\boldsymbol{B}}\rangle \end{pmatrix} = \begin{pmatrix} \boldsymbol{\epsilon}_{\mathrm{eff}} & \boldsymbol{\xi}_{\mathrm{eff}} \\ \boldsymbol{\zeta}_{\mathrm{eff}} & \boldsymbol{\mu}_{\mathrm{eff}} \end{pmatrix} \begin{pmatrix} \langle\widetilde{\boldsymbol{E}}\rangle \\ \langle\widetilde{\boldsymbol{H}}\rangle \end{pmatrix} \tag{5}$$

where $\langle\widetilde{\boldsymbol{D}}\rangle$ denotes the mean value of the Bloch amplitude of the electric flux density over the unit cell U. The explicit formula for the effective material parameters in terms of the first four modes is

$$\begin{pmatrix} \boldsymbol{\epsilon}_{\mathrm{eff}} & \boldsymbol{\xi}_{\mathrm{eff}} \\ \boldsymbol{\zeta}_{\mathrm{eff}} & \boldsymbol{\mu}_{\mathrm{eff}} \end{pmatrix} = \sum_{n=1}^{4} \frac{\begin{pmatrix} \langle\boldsymbol{\epsilon}\cdot\widetilde{\boldsymbol{E}}_n\rangle \\ \langle\boldsymbol{\mu}\cdot\widetilde{\boldsymbol{H}}_n\rangle \end{pmatrix} \begin{pmatrix} \langle\boldsymbol{\epsilon}\cdot\widetilde{\boldsymbol{E}}_n\rangle^* \\ \langle\boldsymbol{\mu}\cdot\widetilde{\boldsymbol{H}}_n\rangle^* \end{pmatrix}}{\langle\boldsymbol{\epsilon}\cdot\widetilde{\boldsymbol{E}}_n\rangle^*\cdot\langle\widetilde{\boldsymbol{E}}_n\rangle + \langle\boldsymbol{\mu}\cdot\widetilde{\boldsymbol{H}}_n\rangle^*\cdot\langle\widetilde{\boldsymbol{H}}_n\rangle} \tag{6}$$

where the nominator should be understood as a dyadic product. The parameters $\boldsymbol{\xi}_{\mathrm{eff}}$ and $\boldsymbol{\zeta}_{\mathrm{eff}}$ model the possible direct coupling between electric and magnetic fields in the constitutive relation. The point of the method which is sketched here, is that by solving equation (2) and computing the right hand side of (6), we can compute the effective material matrices without assuming any particular model for the effective material. Thus, we can use this unbiased method to study which theoretical model is best suited for a particular microstructure.

4 Different constitutive relations for chiral media

Throughout the years, at least three major models have been used for isotropic chiral materials, see Table 1. It can be shown that it is possible to transform the different models into each other. If sources are present, they may need to

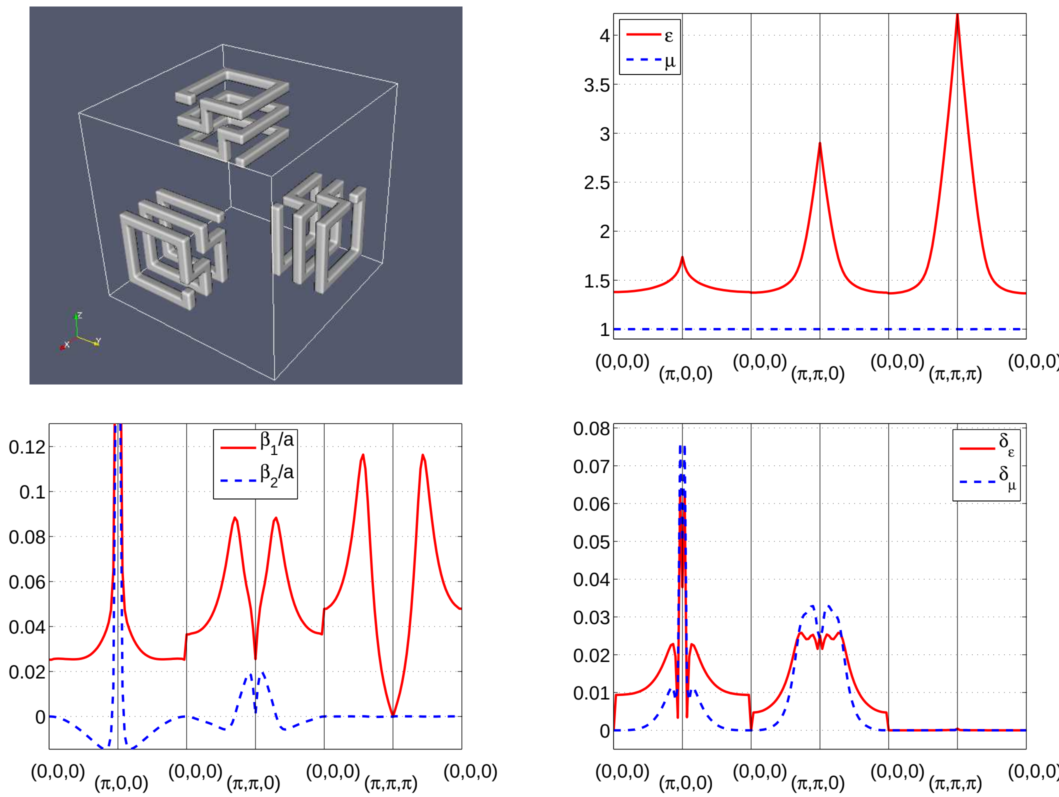

Figure 1: Spiral geometry and the effective ϵ/ϵ_0, μ/μ_0, β_1, and β_2 parameters, as well as the relative errors δ_ϵ and δ_μ. On the horizontal axis are different values of the normalized wave vector $\boldsymbol{k}a$ within the reciprocal unit cell $U' = [-\pi/a, \pi/a]^3$. The peaks for β_1 and β_2 close to $\boldsymbol{k}a = (\pi, 0, 0)$ have been truncated, the peak values are both $\beta_1 = \beta_2 = 0.7a$. The spirals were simulated using a permittivity of 100, making them numerically reasonably close to metal.

be transformed too. Using the results from the previous section, we now investigate if any of these models is close to what is computed by the unbiased method in (6). To start with, one can use symmetry arguments to prove that the magneto-electric coupling terms $\boldsymbol{\xi}_{\text{eff}}$ and $\boldsymbol{\zeta}_{\text{eff}}$ computed from (6) must be identically zero, if the microscopic material parameters $\boldsymbol{\epsilon}(\boldsymbol{x})$ and $\boldsymbol{\mu}(\boldsymbol{x})$ are real and symmetric. This leaves the Drude-Born-Fedorov model as the only candidate.

Applying the Floquet-Bloch transformation to the electric part of the Drude-Born-Fedorov model implies (remember that in the effective model the material parameters are constants)

$$\widetilde{\boldsymbol{D}} = \epsilon(\widetilde{\boldsymbol{E}} + \beta(\nabla + \mathrm{i}\boldsymbol{k}) \times \widetilde{\boldsymbol{E}}) \quad \Longrightarrow \quad \langle \widetilde{\boldsymbol{D}} \rangle = \epsilon(\mathbf{I} + \beta \mathrm{i}\boldsymbol{k}\times) \langle \widetilde{\boldsymbol{E}} \rangle \tag{7}$$

where the equality for the mean values follow since the mean value of any derivative of a periodic field is zero, $\langle \nabla \times \widetilde{\boldsymbol{E}} \rangle = \mathbf{0}$. As a numerical test, spiral inclusions have been implemented in the program described in [9] as depicted in Figure 1. If we extend the Drude-Born-Fedorov model by allowing different β-factors for electric and magnetic field, respectively,

$$\langle \widetilde{\boldsymbol{D}} \rangle = \epsilon(\mathbf{I} + \beta_1 \mathrm{i}\boldsymbol{k}\times) \langle \widetilde{\boldsymbol{E}} \rangle \tag{8}$$

$$\langle \widetilde{\boldsymbol{B}} \rangle = \mu(\mathbf{I} + \beta_2 \mathrm{i}\boldsymbol{k}\times) \langle \widetilde{\boldsymbol{H}} \rangle \tag{9}$$

we see that this model can actually be used to represent any isotropic matrix, provided we only study components orthogonal to the propagation direction, *i.e.*, the components dealing with propagating waves. It is shown in [3] that the matrix computed from (6) is precisely such a matrix, and isotropy is provided by arranging the spirals in all coordinate directions as shown in Figure 1. The error in the parameter fit is computed as $\delta_\epsilon = \|\boldsymbol{\epsilon}'_{\text{eff}} - \boldsymbol{\epsilon}_{\text{eff}}\| \,/\, \|\boldsymbol{\epsilon}_{\text{eff}}\|$, where $\boldsymbol{\epsilon}'_{\text{eff}}$ is the effective permittivity as computed from the parametric model (8), and $\boldsymbol{\epsilon}_{\text{eff}}$ is computed from (6). The relative errors δ_ϵ and δ_μ in Figure 1 can be explained by the structure not being completely isotropic, since the spirals are slightly asymmetrical. When looking only at the chiral contribution, *i.e.*, the error in the imaginary part of $\boldsymbol{\epsilon}_{\text{eff}}$ and $\boldsymbol{\mu}_{\text{eff}}$, the error level drops to less than $3 \cdot 10^{-5}$ for both quantities and all $\boldsymbol{k}$. It is seen that we obtain

$$\beta_1 \to \beta_0 \neq 0 \quad \text{and} \quad \beta_2 \to 0 \quad \text{when} \quad |\boldsymbol{k}| \to 0 \tag{10}$$

The factor β_0 is in the order of $0.04a$, and depends on in which direction the origin is approached. This does not contradict the isotropy of the effective material, since this can only be required to be isotropic exactly at the origin $\boldsymbol{k} = \mathbf{0}$, since any $\boldsymbol{k} \neq \mathbf{0}$ implies there is a preferred direction (the propagation direction), and hence there is no reason for the material to be isotropic. The factor β_0 is multiplied with $\mathrm{i}\boldsymbol{k}\times$, which makes the chiral contribution go to zero as $|\boldsymbol{k}| \to 0$. This means that when the applied wavelength is very long compared to the unit cell ($\boldsymbol{k}a$ is small), the material is described by $\langle \widetilde{\boldsymbol{D}} \rangle = \epsilon_{\text{eff}}(\langle \widetilde{\boldsymbol{E}} \rangle + \beta_0 \mathrm{i}\boldsymbol{k} \times \langle \widetilde{\boldsymbol{E}} \rangle)$ and $\langle \widetilde{\boldsymbol{B}} \rangle = \mu_0 \langle \widetilde{\boldsymbol{H}} \rangle$, which is Born's original model [10]. Note that for wave vectors close to $\boldsymbol{k}a = (\pi, 0, 0)$ (and by symmetry also $(0, \pi, 0)$ and $(0, 0, \pi)$), the β_1 and β_2 factors are both large and equal, which is close to Fedorovs model.

5 Conclusions

We have applied an unbiased finite scale homogenization method to the problem of finding effective material parameters for an isotropic chiral microstructure. The result is that this kind of structure can be modelled with a modified Drude-Born-Fedorov model, with different couplings to the curl of the electric and magnetic field, respectively. For small frequencies, only the electric field contribute to the chiral effects in the consitutive relations, whereas the couplings are equal for higher frequencies. The couplings depend on the size and direction of the wave vector.

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