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Wave propagation retrieval method for chiral metamaterials

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Abstract: In this paper we present the wave propagation method for the retrieving of effective properties of media with circularly polarized eigenwaves, in particularly for chiral metamaterials. The method is applied for thick slabs and provides bulk effective parameters. Its strong sides are the absence of artificial branches of the refractive index and simplicity in implementation. We prove the validity of the method on three case studies of homogeneous magnetized plasma, bi-cross and U-shaped metamaterials.

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1. Introduction

Chiral metamaterials (MTMs) attract a lot of attention nowadays due to their promising properties. They can be used to achieve giant optical activity [1–3], large or/and broadband circular dichroism [4–6] and even negative index of refraction [7–12]. Effective parameters (EPs) introduction is a common approach to describe the electromagnetic properties of MTMs; therefore it is of crucial importance to have a proper tool for correct EPs restoration.

Usually effective parameters of chiral metamaterials are retrieved with a method based on inversion of reflection and transmission spectra [13–15], so we will refer to it as the standard method (SM). The main problem of the SM is multi-branching and it arises when the real part of the refractive index \( n \) is retrieved. Different branches of \( n \) can be very close to each other thus creating difficulties in choosing the correct refractive index. The SM is applicable only to thin MTM slabs consisting of few MTM monolayers as it relies on the transmission simulations. In a thick slab transmission can be at the noise level that distorts the restored parameters severely. At the same time few layers of MTM often do not show bulk effective parameters [16]. In conclusion, the SM is ambiguous since effective parameters and reflection/transmission spectra are not in biunique correspondence.

Recently, we have proposed the wave propagation retrieval method (WPRM) [17] for unambiguous restoration of EPs of bulk MTMs with linearly polarized eigenwaves. In this work we extend the WPRM on the case of media whose eigenwaves are circularly polarized. We therefore show the possibility of using this method for an important class of media, the chiral MTMs. To distinguish this extension from the conventional WPRM we will refer to it as WPRMC. As the problem of ambiguity is not really an issue for the impedance restoration but rather for the refractive indices, in this paper we will present the refractive indices retrieval only. Impedance retrieval is a conventional routine procedure identical to that described in [17]. We use case studies of a homogeneous gyrotropic medium, bi-cross MTM and U-shaped MTM, all having eigenmodes as right-circular polarized (RCP) and left-circular polarized (LCP) waves. These examples serve to illustrate the WPRMC capabilities.

2. Wave propagation retrieval methodology

The main idea behind the WPRM is to retrieve the EPs from the cell-averaged electric field \( E \) dependence on the coordinate for the wave propagation in a thick (quasi-semi-infinite) metamaterial slab [17]. In this case we can neglect the reflection of the wave from the rear interface and consider only the wave propagating in the forward direction.

Let us consider a linearly \( x \)-polarized wave propagating along the \( z \)-axis in vacuum:

\[
E_{\text{LP}} = (1, 0, 0) \exp(i k_0 z) + \frac{1}{2} [ (1, i, 0) \exp(i k_R z) + (1, -i, 0) \exp(i k_L z) ].
\]

(1)

It normally impinges onto the flat interface of an isotropic chiral material with the RCP and LCP eigenwaves:

\[
E_{\text{RCP}} = (1, i, 0) \exp(i k_R z), \quad E_{\text{LCP}} = (1, -i, 0) \exp(i k_L z),
\]

(2)

where \( k_0 \) is the vacuum wavenumber, \( n_R \) and \( n_L \) are the RCP and LCP refractive indices correspondingly. The linear polarized wave can be decomposed in a sum of RCP and LCP waves as read in formula (1).

The RCP and LCP have equal Fresnel’s transmission coefficients \( t_R = t_L = t \), so the electric field of the wave inside the chiral material is:

\[
E = \frac{1}{2} t (E_{\text{RCP}} + E_{\text{LCP}}),
\]

(3)
\[ E_x = \frac{1}{i} t \left( \exp(ik_x n_R z) + \exp(ik_x n_L z) \right), \quad (4) \]
\[ E_y = \frac{1}{i} t \left( \exp(ik_y n_R z) - \exp(ik_y n_L z) \right). \quad (5) \]

By simple algebraic manipulations, from Eq. (4) and (5) we derive
\[ n_R = -\frac{i}{k_0} \frac{\Delta \ln(E_x - iE_y)}{\Delta z}, \quad (6) \]
\[ n_L = -\frac{i}{k_0} \frac{\Delta \ln(E_x + iE_y)}{\Delta z}. \quad (7) \]

These formulas are essential for the WPRMC. In practice, the electric field is highly inhomogeneous inside the MTM unit cell, so we should use the volume averaged field. Bloch impedance \( Z_B \) (see the relevant discussion in review [18]) is retrieved unambiguously from the single reflection \( R \) on the vacuum–chiral MTM interface \( Z_B = (1 + R)/(1 - R) \). Other EPs can be restored in the following conventional way: refractive index \( n = (n_R + n_L)/2 \), chirality \( \kappa = (n_R - n_L)/2 \).

Strictly speaking, the complex logarithm in Eqs. (6) and (7) is a multivalued function, so we can find the values of \( \ln(E_x \pm iE_y) \) with accuracy up to \( \pm 2\pi m \), where \( m \) is an integer. In order to apply a linear fit while using Eqs. (6) and (7), the dependence of \( \Re[\ln(E_x \pm E_y)] \) on the unit cells coordinates \( z_{UC} \) should be made continuous. If the metamaterial is quasi-homogeneous the difference of the wave phase between neighboring unit cells should be less than \( \pi/2 \), thus aforementioned continuity is easy to persuade.

The constraints of the WPRMC are the same as of the WPRM for linearly polarized waves [17]. First, a metamaterial slab should be thick enough to prevent the reflection from the rear interface and standing wave formation. We found less than 1% error for the WPRM when \(-45 < n' k_0 d < 45 \) and \( 5 < n'' k_0 d < 56 \), where \( d \) is the slab thickness. For the case of low absorption, one can always increase \( d \). Another option is to use a time-domain method and to terminate the simulation when the excitation pulse reaches the rear interface of the slab. Second, the accuracy of the simulations should be sufficient to observe the linear dependence of \( \ln(E_x \pm E_y) \) on the coordinate \( z \), for that the electric field doesn’t have to drop down to the noise level within less than three unit cells.

### 3. Case studies

To check the validity of the WPRMC and illustrate its application we consider 3 case studies: 1) homogeneous gyrotropic medium, 2) bi-cross MTM and 3) U-shaped MTM. Commercial software CST Microwave Studio [19] was used in simulations. Simulations were performed in the frequency domain with open boundary conditions in the direction of propagation and periodic boundary conditions in the lateral directions.

#### 3.1 Homogeneous magnetized plasma

The main criteria for the WPRMC employment is that eigenwaves of the material are RCP and LCP waves, so this means that WPRMC is applicable to any material having circularly polarized eigenwaves. As a first example we chose homogeneous plasma magnetized along the direction of the wave propagation \( z \). We should note that such medium is not a chiral medium, but its effective refractive index can be calculated analytically, so it is a reliable reference. Its permittivity tensor is \( \varepsilon = \begin{bmatrix} \varepsilon_1, \varepsilon_2, 0 \end{bmatrix}, \begin{bmatrix} -i \varepsilon_2, \varepsilon_1, 0 \end{bmatrix}, (0, 0, \varepsilon_3) \]
\[
\varepsilon_1 = \varepsilon_\infty - \frac{\omega_p^2 (\omega + i \omega_{COL}) / \omega}{(\omega + i \omega_{COL})^2 - \omega_c^2}, \quad \varepsilon_2 = \frac{-\omega_p^2 \omega_c / \omega}{(\omega + i \omega_{COL})^2 - \omega_c^2}, \quad \text{and} \quad \varepsilon_3 = \varepsilon_\infty - \frac{\omega_p^2}{\omega(\omega + i \omega_{COL})}.
\]

The eigenwaves are RCP and LCP with refractive indices \( n_R = (\varepsilon_1 + \varepsilon_2)^{1/2} \) and \( n_L = (\varepsilon_1 - \varepsilon_2)^{1/2} \) [20]. For the simulations we chose plasma frequency \( \omega_p = 1.0 \times 10^{15} \, \text{s}^{-1} \), cyclotron and collision frequencies \( \omega_c = \omega_{COL} = 3.8 \times 10^{14} \, \text{s}^{-1} \) and \( \varepsilon_\infty = 3 \). For the simulation the slab of the plasma medium was divided into 100 layers. The WPRMC restores EPs in perfect agreement with the analytical ones (Fig. 1).

![Fig. 1. (Color online). Theoretical (black line) and restored with WPRMC (red circles) refractive indices for RCP and LCP for the homogeneous magnetized plasma: (a) Re(\(n_R\)), (b) Re(\(n_L\)), (c) Im(\(n_R\)), (d) Im(\(n_L\)).](image)

### 3.2 Bi-cross metamaterial

As the second example we investigated a slightly modified bi-cross metamaterial [21], that is a chiral metamaterial for the optical range. The geometrical parameters are indicated in Fig. 2. The crosses in the bi-cross are connected in the middle with a cylindrical conducting rod. The bi-cross material is silver, which is approximated as the Drude metal with plasma frequency \( \omega_p = 1.37 \times 10^{16} \, \text{s}^{-1} \) and collision frequency \( \omega_{COL} = 8.5 \times 10^{13} \, \text{s}^{-1} \) [22]. The silver structure is embedded into silica (refractive index \( n = 1.44 \)).

In this case we lack the analytical results. Therefore WPRMC results are challenged against the ones, obtained by the standard method [15] as a reference. As we have already emphasized in the Introduction the EPs of few MTM layers are not the same as the bulk EPs so we do not anticipate the coincidence of the SM and WPRMC results. We have in mind rather the convergence of the SM results to WPRMC with the increasing thickness of the slab.

Indeed, the effective refractive indices converge very fast with the increase of the number of MTM layers (slab thickness) (Fig. 3). The effective properties of 3 layers are similar to the bulk ones restored with WPRMC from simulations of the 36 layers-thick structure.
To further illustrate the restoration procedure we plotted the logarithm of the electric field amplitude dependence on the distance (layer number) inside the MTM slab (Fig. 4) for two different cases. At frequency 110 THz (Fig. 4a) the RCP and LCP waves have small absorption, but the MTM exhibits strong circular dichroism. We clearly see the standing wave after the layer number 20, so for retrieving we should use data points before that. At frequency 150 THz (Fig. 4b) absorption of both modes is high (and equal). We observe linear behavior of the field until the 19th layer then the wave amplitude is reaching the noise level. In this case, the last part should be excluded when applying Eqs. (6) and (7) for restoration.
3.3 U-shaped metamaterial

To test our method in the microwave range we chose the recently published U-shaped metamaterial design [23]. The original paper presents the structure consisting of only two layers of MTM, so we stacked multiple layers for the WPRMC application (Fig. 5a). All the geometrical and material parameters were taken as in [23]. U-shaped resonators in each layer are 90 degrees rotated around their centers with respect to the preceding layer.

As we see from Fig. 5b and 5c, the effective properties change dramatically with the increasing thickness. One bi-layer of the U-shaped MTM shows pronounced negative values of the refractive index real part. For two bi-layers the refractive index is just slightly negative and further it becomes progressively positive for a thick structure (24 bi-layers). We explain this behavior as the result of strong interaction between meta-atoms in the adjacent layers, similar to the one described recently in [24]. Such interaction leads to mutual annihilation of total response finishing with a rather mitigated resonance. It is encouraging that correspondingly the absorption is much smaller than that of a single bi-layer (Fig. 5d and 5e). We suspect that the strong coupling between meta-atoms can represent a problem for the construction of bulk MTM on the basis of most of the proposed chiral MTMs designs. However, this is worth a special investigation that is beyond the scope of this paper.

4. Conclusion

In this paper we presented the wave propagation retrieval method for chiral metamaterials. However, the WPRMC is suitable to retrieve bulk effective parameters of any kind of materials with RCP and LCP eigenwaves. The method’s validity is verified on the case studies of homogeneous magnetized plasma and bi-cross chiral MTMs. We also analyzed the case of U-shaped MTMs possessing extremely poor convergence of effective parameters with the slab thickness. In such case the WPRMC provides important information on the bulk effective properties which are difficult or even impossible to obtain by the standard method with the few layers structures. Our method is straightforward in implementation and restores effective properties unambiguously. All this make the WPRMC a useful tool in chiral MTMs research.

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