Computation of the Effective Parameters of Metamaterials Using a Finite-Difference Frequency-Domain Method

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Abstract — In a recent work, we have introduced a nonlocal homogenization method to extract the dielectric function of periodic structured materials formed by dielectric and metallic inclusions of arbitrary shape. Here, we report a Finite-Difference Frequency-Domain (FDFD) implementation of the nonlocal homogenization method.

I. Introduction

The interest in structured materials with electromagnetic properties not readily available in nature has grown significantly in the last decade. Such materials (known as metamaterials) may interact with electromagnetic waves in a controlled and desired way, hence opening a whole new road of exciting possibilities such as imaging not limited by diffraction [1] or the realization of very compact waveguides with subwavelength mode sizes [2-3]. During recent years it has been shown that by structuring conventional materials, so that the geometry of the inclusions and their spatial arrangement is chosen judiciously, it may be possible to synthesize novel media with unconventional properties, such as simultaneously negative permittivity and permeability [4], permittivity near zero [5], or extreme anisotropy [6]. Even though these concepts and ideas are today widely accepted and understood, the extraction of the effective parameters of metamaterials remains a matter of active research since the typical homogenization methods [7] are not completely general and unambiguous, and may fail near resonances or in presence of spatial dispersion.

Recently, our group has introduced a systematic and general homogenization method to extract the effective parameters of composite media [8]. Unlike previous works, which invariably assume that the electrodynamics of the material can be described in terms of an effective permittivity and permeability (or more generally in terms of a bianisotropic model), the method introduced in [8] describes the metamaterial in terms of a nonlocal dielectric function, i.e. in terms of a spatially dispersive model. A material with spatial dispersion is characterized by the fact that the polarizability acquired by the inclusions does not depend exclusively on the local electric field in the immediate vicinity of the particle, but may depend ultimately on the electric field in the whole crystal. The advantage of such approach is that it is completely general, and allows modeling arbitrary composite materials, even in the presence of nonlocal effects. Moreover, in Ref. [8] it was demonstrated that the conventional local parameters (permittivity and permeability) may be obtained (if they have physical meaning) directly from the nonlocal dielectric function through a relatively simple procedure.

In Ref. [8] we have shown how the dielectric function of a structured material may be numerically computed using the Method of Moments (MoM). Even though such procedure is completely general, it is well known that the MoM is mostly adequate for the characterization of metallic structures, being not so efficient in the analysis of dielectric structures, where finite difference methods are generally much more versatile and powerful.

The goal of this paper is to apply the finite difference frequency domain (FDFD) [9] method to solve numerically the homogenization problem formulated in Ref. [8], and extract the effective parameters of periodic dielectric materials made of nonmagnetic dielectric inclusions with arbitrary shapes.

In this work we assume that the fields are monochromatic and with time dependence $e^{j\omega t}$.

II. Homogenization using the FDFD method

A. The homogenization method

The method proposed in [8] permits the extraction of the effective parameters of a generic periodic composite material formed by nonmagnetic dielectric or metallic inclusions. The permittivity ε_r may be a complex number and depend on frequency. The unit cell Ω of a hypothetical metamaterial is shown in Fig. 1.

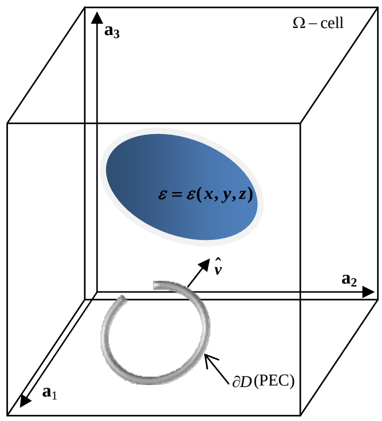

Fig. 1. Unit cell of a generic metamaterial with a dielectric inclusion and a PEC inclusion.

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The dielectric crystal is obtained by translating the unit cell along the primitive vectors $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_3$, which define the periodicity of the system.

The objective of the method is to calculate the nonlocal dielectric function $\overline{\overline{\varepsilon}}_{eff} = \overline{\overline{\varepsilon}}_{eff}(\omega,\mathbf{k})$ of the metamaterial, where ω is the angular frequency and $\mathbf{k} = (k_x, k_y, k_z)$ is the wave vector. The possible dependence of $\overline{\overline{\varepsilon}}_{eff}$ on the wave vector $\mathbf{k}$ results from hypothetical spatial dispersion effects, which may exist in relevant metamaterials [10], even for very low frequencies [11-12]. As discussed in the Introduction, it may be advantageous to extract $\overline{\overline{\varepsilon}}_{eff}(\omega,\mathbf{k})$ instead of the parameters implicit in the bianisotropic constitutive relations [13] since the latter formalism is less general, and because there is no systematic method to compute the effective parameters associated with the bianisotropic model.

In order to compute the unknown dielectric function, the structure is excited with a periodic external distribution of electric current $\mathbf{J}_e$. It is assumed that $\mathbf{J}_e$ has the Floquet property, i.e., $\mathbf{J}_e e^{j\mathbf{k}.\mathbf{r}}$ is periodic along the crystal. Consequently, the excited microscopic electric and induction fields ($\mathbf{E}$, $\mathbf{B}$) have also the Floquet property. The fields $\mathbf{E}$ and $\mathbf{B}$ verify the frequency domain Maxwell equations,

$$\nabla \times \mathbf{E} = -j\omega\mathbf{B} \tag{1a}$$

$$\nabla \times \frac{\mathbf{B}}{\mu_0} = \mathbf{J}_e + \mathbf{J}_d + j\omega\varepsilon_0\mathbf{E}\,. \tag{1b}$$

where $\mathbf{J}_d = \varepsilon_0(\varepsilon_r - 1)j\omega\mathbf{E}$ is the induced current relative to the host medium, which, without loss of generality, is assumed vacuum.

In order to homogenize the structure, we introduce the average macroscopic fields $\mathbf{E}_{\text{av}}$ and $\mathbf{B}_{\text{av}}$:

$$\mathbf{E}_{\text{av}} = \frac{1}{\text{Vcell}}\int_{\Omega} \mathbf{E}(\mathbf{r})e^{+j\mathbf{k}.\mathbf{r}}d^3\mathbf{r}\,,\ \mathbf{B}_{\text{av}} = \frac{1}{\text{Vcell}}\int_{\Omega} \mathbf{B}(\mathbf{r})e^{+j\mathbf{k}.\mathbf{r}}d^3\mathbf{r}\,.$$

The macroscopic fields verify the following relations:

$$\begin{gathered} -\mathbf{k}\times\mathbf{E}_{\text{av}} + \omega\mathbf{B}_{\text{av}} = 0 \\ \omega(\varepsilon_0\mathbf{E}_{\text{av}} + \mathbf{P}_g) + \mathbf{k}\times\frac{\mathbf{B}_{\text{av}}}{\mu_0} = -\omega\mathbf{P}_e \end{gathered} \tag{2}$$

where $\mathbf{P}_e = \frac{1}{\text{V}_{\text{cell}}\,j\omega}\int_{\Omega} \mathbf{J}_e e^{+j\mathbf{k}.\mathbf{r}}d^3\mathbf{r}$ is the applied polarization vector and $\mathbf{P}_g$ is the generalized induced polarization vector,

$$\mathbf{P}_g = \frac{1}{\text{V}_{\text{cell}}\,j\omega}\int_{\Omega} \mathbf{J}_d e^{+j\mathbf{k}.\mathbf{r}}d^3\mathbf{r}\,. \tag{3}$$

The system of equations (2) shows that the dielectric function $\overline{\overline{\varepsilon}}_{eff}(\omega,\mathbf{k})$ must be defined consistently with the relation:

$$\overline{\overline{\varepsilon}}_{eff}(\omega,\mathbf{k}).\mathbf{E}_{\text{av}} = \varepsilon_0\mathbf{E}_{\text{av}} + \mathbf{P}_g\,, \tag{4}$$

In particular, it should be clear from Eq. (4) that one can determine the dielectric function for fixed $(\omega,\mathbf{k})$ provided $\mathbf{P}_g$ is known for three independent vectors $\mathbf{E}_{\text{av}}$. Hence, it is possible to compute the unknown dielectric function following the algorithm described next. To begin with, one selects three different distributions for the applied current $\mathbf{J}_e$ (ω and $\mathbf{k}$ are fixed) such that the corresponding average fields $\mathbf{E}_{\text{av}}$ form an independent set of vectors in the three dimensional space. Next, for each distribution of current, the source driven electromagnetic problem (1) is numerically solved to obtain the microscopic fields. Finally, using the calculated microscopic fields, $\mathbf{E}_{\text{av}}$ and $\mathbf{P}_g$ are computed and $\overline{\overline{\varepsilon}}_{eff}$ is obtained using Eq. (4). The described approach has the important property that $\overline{\overline{\varepsilon}}_{eff}$ is computed from the solution of a source-driven problem. Unlike other methods relying on the band structure of the periodic material, this permits to determine the effective parameters of the metamaterial, even when the frequency of interest lies in a complete band gap, or when the inclusions are lossy.

B. FDFD method

In order to solve the source-driven problem (1) we employ a widely used FDFD method based on the Yee's-mesh [14]. In the finite differences (FD) method, the unit cell Ω is divided into many rectangular grids. The FD method is excellent to model devices with a complex geometry or structures of finite size.

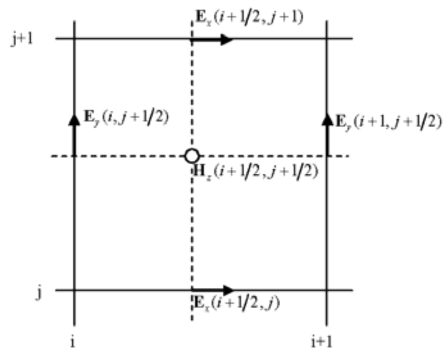

Fig. 2. 2D Yee's mesh for the homogenization of 2D periodic metamaterials. (TE modes' mesh).(After Ref. [9])

For simplicity, in the following we will assume that the geometry of the problem is intrinsically two-dimensional (axis of symmetry is along z) and that the electromagnetic waves are transverse electric (TE^z). Hence, in our case, the numerical problem to be solved assumes the following form from Eq. (1):

$$\begin{cases} \dfrac{\partial^2 E_y}{\partial x \partial y} - \dfrac{\partial^2 E_x}{\partial_y^2} - \text{k}_0^2\varepsilon_r E_x = -j\eta_0 J_{e,x} \\ \dfrac{\partial^2 E_x}{\partial x \partial y} - \dfrac{\partial^2 E_y}{\partial_x^2} - \text{k}_0^2\varepsilon_r E_y = -j\eta_0 J_{e,y} \end{cases}. \tag{5}$$

In the above system, E_x, E_y, $J_{e,x}$ and $J_{e,y}$ are the microscopic fields and applied current densities along the x and y coordinates, respectively. k_0 is the wavenumber in free-space and η_0 the impedance of free space. Finally, ε_r represents the relative electric permittivity of each considered point on the structure. The transverse plane of the unit cell is then discretized using Yee's mesh for the TE mode as shown in Fig. 2.

In order to discretize the electric field derivatives in Eq. (5), the following formulas proposed in [15] are used:

$$\frac{\partial^2 E_y}{\partial x} = \frac{E_y(i+1,j)-2E_y(i,j)+E_y(i-1,j)}{(\Delta x)^2} \quad (6a)$$

$$\frac{\partial^2 E_y}{\partial x \partial y} = \frac{E_y(i+1,j)-E_y(i,j)-E_y(i+1,j-1)+E_y(i,j-1)}{\Delta x \Delta y} \quad (6b)$$

$$\frac{\partial^2 E_x}{\partial y} = \frac{E_x(i,j+1)-2E_x(i,j)+E_x(i,j-1)}{(\Delta y)^2} \quad (6c)$$

$$\frac{\partial^2 E_x}{\partial x \partial y} = \frac{E_x(i,j+1)-E_x(i,j)-E_x(i-1,j+1)+E_x(i-1,j)}{\Delta x \Delta y}, \quad (6d)$$

where Δx and Δy is the grid spacing in the x- and y-directions, respectively. For periodic structures, for a grid with $N+1$ nodes in each side of a unit cell, there are $2N^2$ FD equations and $2N^2$ unknowns. When a given node is situated at the boundary of the unit cell, some of the adjacent nodes are out of the unit cell but they can be "brought back" using the periodic boundary conditions,

$$\Phi(x+\mathrm{a}, \mathrm{y}+\mathrm{b}) = e^{-jk_x \mathrm{a} - jk_y \mathrm{b}}\Phi(x,\mathrm{y}). \quad (7)$$

Here, $\Phi(x,y)$ represents a generic field component, k_x, a, k_y and b are the wave vector components and lattice constants along the x- and y-directions, respectively.

Substituting Eq. (6) into Eq. (5) and taking into account the Floquet boundary conditions (7), it is possible to numerically solve the source-driven problem formulated in Sec. II A, and in this way to extract the unknown dielectric function.

III. NUMERICAL RESULTS

A. Validation of the FDFD method

In order to validate the FDFD method, initially we computed the dielectric function of a one dimensional metamaterial (Fig. 3) formed by a periodic stack of dielectric slabs normal to the *y*-direction. The numerically extracted results were then compared with theoretical results derived from the exact analytical solution of the homogenization problem.

The unit cell of the periodic structure has a single horizontal dielectric inclusion with permittivity $\varepsilon_r = 3.0$, as shown in Fig. 3a. We studied in-plane propagation with polarization TE^z. The homogenized material is anisotropic with principal directions along the coordinate axes. The calculated effective permittivity along the principal axes is represented in Fig. 3d as a function of frequency for $\mathbf{k}=0$. The effective parameters are nearly independent of frequency, and match well the theoretical ones, obtained from the analytical solution of the homogenization problem.

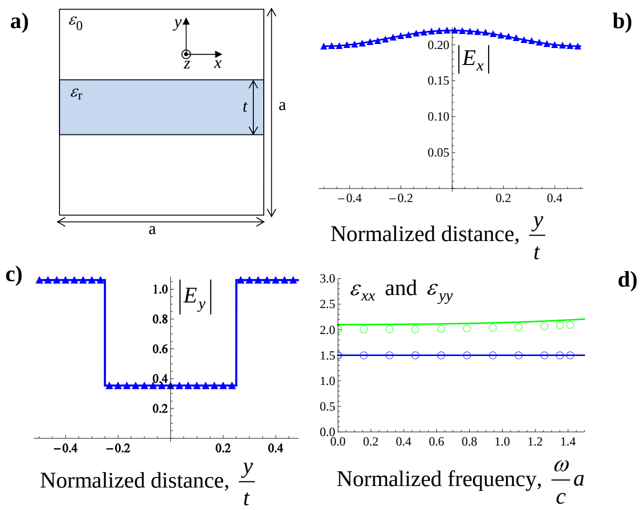

Fig. 3. (a): geometry of the unit cell, representing a metamaterial formed by a periodic stack of dielectric slabs. The inclusion has a permittivity $\varepsilon_r = 3.0$ and thickness $t = 0.5\mathrm{a}$. (b) and (c): amplitude of the electrical field as a function of y for a fixed x, when the current source is directed along x and y, respectively. The discrete triangles in (b) and (c) correspond to the values extracted with the FDFD method and the solid lines are the theoretical values. (d): the green and blue solid curves represent the extracted ε_{xx} and ε_{yy}, respectively, as function of frequency. The discrete circles in (d) represent the results calculated analytically.

The panels (b) and (c). are drawn for $\mathrm{k}_0 a = 0.3\pi$, $\mathrm{k}_x = 0$ and $\mathrm{k}_y a = 0.8\pi$ and show the absolute value of the microscopic electrical field when the current source is directed along x, i.e., $\mathbf{J}_e = J_e \hat{\mathbf{u}}_x$, or along *y*, i.e. $\mathbf{J}_e = J_e \hat{\mathbf{u}}_y$, respectively. When $\mathrm{k}_x = 0$, E_x (E_y) vanishes when the current source is directed along y (x). Consistent with the boundary conditions at a dielectric interface, the ratio between E_y inside and outside the dielectric slab, is approximately equal to the ratio between the permittivities.

B. Extraction of the effective permittivity of a material formed by plasmonic particles

In a second example, we have computed the effective dielectric function of a metamaterial formed by square-shaped tilted plasmonic inclusions (with negative permittivity) arranged in a square lattice (Fig. 4) [16].

The extracted permittivity is shown in Fig. 4 as a function of the (negative) permittivity of the square-shaped inclusion. The quasi-static regime is assumed and losses are taken into account. Unlike the previous example, it is not possible to solve the homogenization problem analytically. It can be seen that the composite material may have an effective response quite distinct from those of its constituents, and that the effective permittivity of the structure may have several singularities. This irregular behavior is a consequence of the excitation of multiple quasi-static resonances, which are characteristic of plasmonic particles (surface plasmon resonances). In particular, the sharp corners of the plasmonic inclusion may cause a great enhancement of the electromagnetic field in their vicinity. It may be seen in Fig. 4 that when the corners of the inclusion are less rounded (blue line) the number and density of singularities increases.

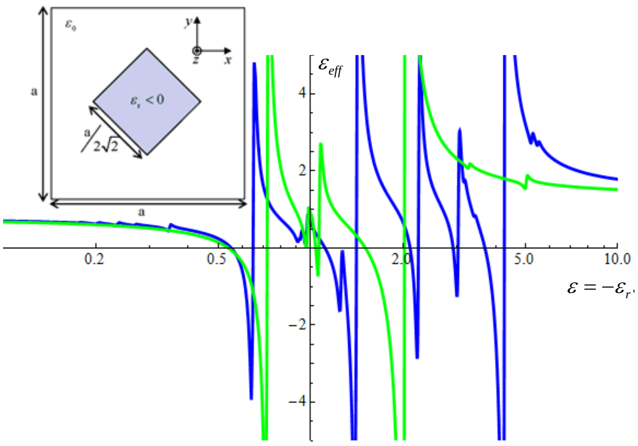

Fig 4. Real part of the effective quasi-static permittivity ε_{eff} as a function of the real part of the inclusion's permittivity ε_r', using different rounding R/a=0.16 (green curve), R/a=0.04 (blue curve) and small losses $\varepsilon_r'' = 0.01\varepsilon_r'$. R is the radius of the corners. The geometry of the unit cell of the two dimensional metamaterial is shown in the inset: the unit cell consists of a square-shaped inclusion with negative permittivity $\varepsilon_r = \varepsilon_r' - j\varepsilon_r''$ and sharp corners. The host material is air.

The described results are consistent with those obtained in Ref. [16] using a different homogenization approach. It was shown in [16] that when the inclusion has negative permittivity and an infinitely sharp wedge, the electromagnetic fields may have a very pathological behavior at the wedge, and, in the absence of loss, the stored energy may not be finite. These problems can be avoided by either rounding the corners of the sharp wedge, and possibly by adding loss to the material, as our results have also confirmed.

In conclusion, we have demonstrated that the FDFD may be an excellent solution to solve the homogenization problem formulated in Ref. [8], yielding very accurate results, and allowing for the computation of the effective parameters of metamaterial structures formed by dielectric inclusions with arbitrary shapes.

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