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Exact Modelling of a Finite Sample of Metamaterial

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Abstract: Metamaterials are electromagnetically complex structures. In this contribution we present a technique that allows for a detailed analysis of a finite sample of metamaterial incorporating all electromagnetic interactions. To this end we use a full-wave T-matrix formalism. To accelerate the simulations we use the Stable Plane Wave Multilevel Fast Multipole Method. We also present a direct method to dervive the effective material parameters from the T-matrix of a spherical sample of metamaterial.

Keywords: metamaterials, fast multipole methods

1. Introduction

Metamaterials consist of a large number of constituents embedded in a host medium. Each constituent can have a complex structure and e.g. consist of printed ring resonators and dipoles. When considering a finite piece of metamaterial one is interested in the overall effective medium parameters of this piece. These effective parameters are usually estimated from the polarizabilities of a constituent using homogenization formulas such as Maxwell-Garnett or Bruggeman [2].

In this paper we want to use another approach. We aim at performing a full-wave numerical simulation of a finite sample of metamaterial and then derive the effective parameters from these scattering simulations by comparison with a homogeneous sample of material with the same geometry. In this way all the electromagnetic interactions are taken into account. This approach allows us to check the validity of the homogenization formulas. Such formulas fail when the density of the constituents become high and these formulas also assume a material of infinite extent. This also means that the dependence of the geometry of the sample on the effective parameters only can be estimated using a full-wave simulation.

To solve the scattering problem we will use the T-matrix approach [1]. We will first determine the T-matrix of each constituent and then considering the interactions between all the T-matrices. If there are N constituents, and if each T-matrix contains M^2 elements then this requires the solution of a linear system of NM unknowns. Since N will be large it is not possible to use a direct or even an iterative solution of this system. The constituents are small compared to wavelength, although the sample can be several wavelengths in size. This means that the numerical problem is at the same time a low- and high-frequency problem. The solution of the linear system can be accelerated using a multilevel fast multipole technique but this technique needs to be valid for high as wel as low frequencies. For this purpose we opted the use of the Stable Plane Wave Method as derived by [3]. In this way it becomes possible to obtain a computational and memory complexity of $O(NM)$. We also use an acceleration to convert multipoles into evanescent plane waves as has been derived recently in [4].

To derive the effective parameters of a metamaterial we will consider a spherical sample. From the T-matrix of the individual constituents we can derive the T-matrix of the entire sample using the Stable Plane Wave Method. Then we compare this T-matrix with the T-matrix of a homogeneous sphere to identify the effective material paramaters. It turns out this can be done in a very elegant way using a recurrence relation of Bessel functions.

2. Analysis

The examples will consider a spherical sample consisting of spherical inclusions. Spherical inclusions have an analytical T-matrix. We will show the validity of the Maxwell-Garnett and Bruggeman formula and show the possibility to derive a negative index material for an example proposed in [5]. First we determine the T-matrix of the constituents of the metamaterial. This starts from the illumination of the constituent by incoming fields of the following forms

$$\mathbf{E}_{lm}^{inc,1}(\mathbf{r}) = \frac{\hat{\mathbf{L}}\left[j_l(kr)Y_{lm}(\mathbf{r})\right]}{\sqrt{l(l+1)}} \qquad \mathbf{E}_{lm}^{inc,2}(\mathbf{r}) = \frac{1}{k}\nabla\times\mathbf{E}_{lm}^{inc,1}(\mathbf{r}), \tag{1}$$

where k is the wavenumber, $Y_{lm}(\mathbf{r})$ are the scalar spherical harmonics and where $\hat{\mathbf{L}}$ is the angular momentum operator

$$\hat{\mathbf{L}} = -j\mathbf{r}\times\nabla = j\left[\mathbf{e}_\theta\frac{1}{\sin\theta}\frac{d}{d\theta} - \mathbf{e}_\phi\frac{d}{d\phi}\right]. \tag{2}$$

The resulting scattered fields can be decomposed into functions similar to (1), but with spherical Hankel functions instead of spherical Bessel functions. The coefficients arising in this decomposition can be interpreted as entries of the T-matrix of the constituent. All scattering information of the constituent is contained in the T-matrix.

In the next step the T-matrix of the entire spherical sample is determined. This is done using the Stable Plane Wave Method as developed in [3]. We will not go into the details of this multilevel fast multipole technique but suffice to say that the method remains stable at low frequencies by also incorporating evanscent plane waves in addition to propagating plane waves. In the desaggregation and aggregation steps it is necessary to transform the vectorial spherical harmonics expansion of the T-matrix into plane waves. For the evanscent plane waves this requires 6 different expansions along the $\pm x$-, $\pm y$- and the $\pm z$-axis. Recently [4] a new method was derived to reduce the workload of this process by a factor of 6.

In the final step the T-matrix of the entire sample is matched to the analytical T-matrix of an homogeneous sphere. This T-matrix is diagonal and the diagonal elements are given by

$$T_{l,m}^1 = -\frac{Z_i\frac{\mathcal{J}_l(k_oa)}{j_l(k_oa)} - Z_o\frac{\mathcal{J}_l(k_ia)}{j_l(k_ia)}}{Z_i\frac{\mathcal{H}_l^{(2)}(k_oa)}{j_l(k_oa)} - Z_o\frac{\mathcal{J}_l(k_ia)}{j_l(k_ia)}\frac{h_l^{(2)}(k_oa)}{j_l(k_oa)}}, \tag{3}$$

$$T_{l,m}^2 = -\frac{Z_o\frac{\mathcal{J}_l(k_oa)}{j_l(k_oa)} - Z_i\frac{\mathcal{J}_l(k_ia)}{j_l(k_ia)}}{Z_o\frac{\mathcal{H}_l^{(2)}(k_oa)}{j_l(k_oa)} - Z_i\frac{\mathcal{J}_l(k_ia)}{j_l(k_ia)}\frac{h_l^{(2)}(k_oa)}{j_l(k_oa)}}. \tag{4}$$

Here, $\mathcal{J}_l(x) = \frac{1}{x}\frac{d}{dx}\left[xj_l(x)\right]$ and $\mathcal{H}_l^{(2)}(x) = \frac{1}{x}\frac{d}{dx}\left[xh_l^{(2)}(x)\right]$. The unknowns are Z_i and k_i, the impedance and wavenumber inside the sphere. The left hand sides of both of these equations are known as are the radius of the piece of metamaterial and the parameters of the surrounding host medium. Therefore these equations can be solved for the two quantities $\frac{Z_o}{Z_i}$ (thus yielding Z_i) and $A_l = \frac{\mathcal{J}_l(k_ia)}{j_l(k_ia)}$. From the latter, a unique value for k_ia is not easily found, but since this

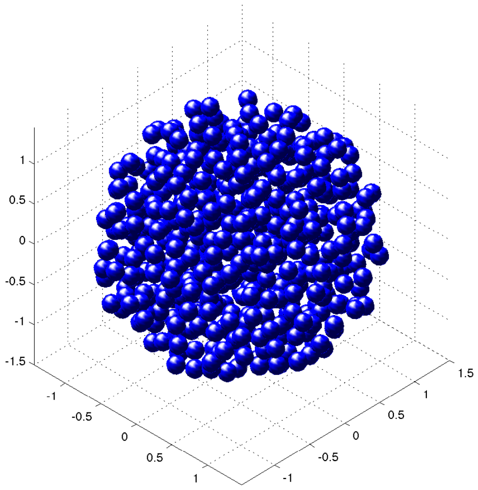

Figure 1: A spherical sample with 500 spheres.

quantity is known for a whole series of l, the recurrences of the Bessel functions can be used to obtain the following quadratic equation which can be solved easily

$$-\left(\frac{l+1}{k_i a}\right)^2 + (A_l - A_{l+1})\frac{l+1}{k_i a} + A_l A_{l+1} + 1 = 0. \tag{5}$$

Determining which one of the two roots to choose is done by calculating these roots for various l and checking which one is consistent.

3. Numerical example

As an example we consider a spherical sample with radius $R = 1.477m$ at a frequency of $25MHz$, hence the spheres have a diameter of about one quarter of a wavelength in free space. The host medium has a relative permittivity $\epsilon_r = -1.5 + j$ and a relative permeability $\mu_r = 2.0 + 1.2j$. In the host medium spheres with a radius of $r = 0.1m$ are embedded. These spheres have a relative permittivity $\epsilon_r = -6 + 0.9j$ and a relative permeability $\mu_r = 1.5 + 0.2j$. By varying the number of spheres we vary the volume fraction of the inclusions. To obtain high volume fractions we invert the medium by interchanging the material parameters of the spheres and the host medium. Figure 1 shows a volume fraction of 16% obtained by randomly placing 500 spheres in the spherical host medium.

Figures 2 and 3 respectively show the real and imaginary part of the effective relative permittivity. The result predicted in [5] using the Bruggeman homogenization formula (indicated as ”Mackey” on the figures)are also shown as well as the results of the Maxwell-Garnett formula. As can be seen the Maxwell-Garnett formula is more accurate than the Bruggeman formula. Similar conclusions can be drawn from the real and imaginary part of the effective permeability as shown in Figures 4 and 5.

For each volume fraction we only considered one realization of the medium. Nevertheless the simulated results show a very smooth behavior indicating that the medium really can be considered homogeneous. Using (5) we can derive the effective medium parameters also for various values of l. It turns out that our results are independent of l again confirming previous

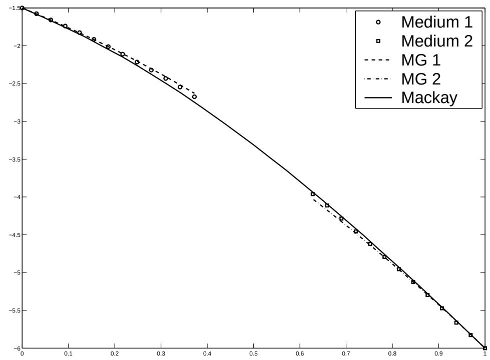

Figure 2: Real part of the effective permittivity.

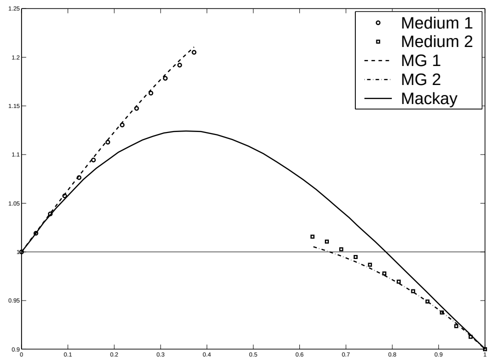

Figure 3: Imaginary part of the effective permittivity.

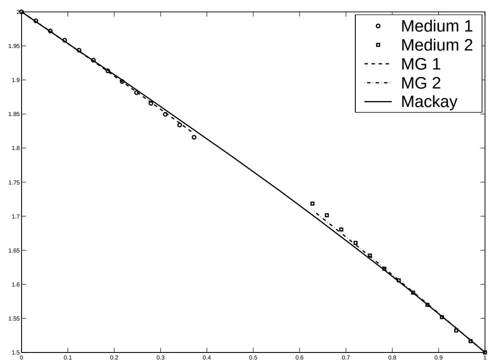

Figure 4: Real part of the effective permeability.

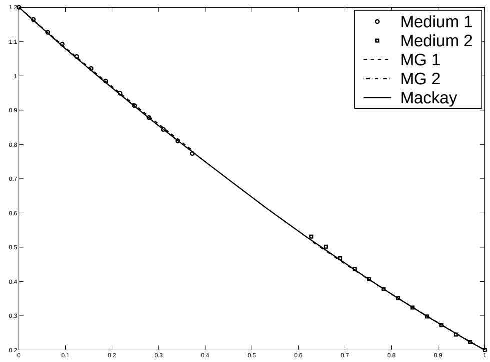

Figure 5: Imaginary part of the effective permeability.

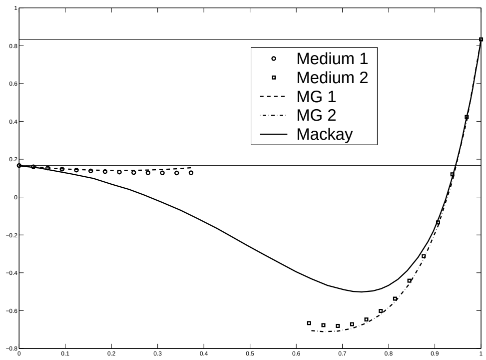

Figure 6: Negative phase velocity parameter.

conclusion. This conclusion will be less evident if one considers higher frequencies. Then the effective parameters will depend on the radius of the spherical example and different realizations will yield different effective parameters.

For the example considered here we also calculated the negative phase velocity parameter ρ_{NPV} given by [5]

$$\rho_{NPV} = \frac{\Re[\epsilon_{eff}]}{\Im[\epsilon_{eff}]} + \frac{\Re[\mu_{eff}]}{\Im[\mu_{eff}]}. \tag{6}$$

For a negative index medium this parameter has to be negative. The curve in Figure 6 indeed shows a region of volume fractions corresponding to a negative index medium.

4. Conclusions

It is shown that using a multilevel fast multipole method including evansecent and propagating plane waves such as the stable plane wave method allows for the accurate simulation of a finite piece of metamaterial. These simulations allow to check the validity of the homogenization assumption as well as of homogenization formulas. We also presented a new direct method to obtain the effective parameters from a spherical sample.

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