Anti-Resonant Response of Resonant Inclusions?

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Abstract

When retrieving the material parameters of a metamaterial with resonant inclusions, the expected Lorentz-like resonance in one parameter typically yields an unexpected and unphysical so-called antiresonance in the other effective parameter. Using a simple model problem with plasmonic cylinders, we discuss some explanations for the antiresonance-problem and argue that the fundamental reason is that the assumed homogeneous model with sharp boundaries is insufficient when the retrieval fails to produce physically reasonable results. Some promising paths towards a better model are also briefly discussed.

1 Introduction

The most popular way to obtain the material parameters of different metamaterial realizations seems to be the classical Nicolson–Ross–Weir (NRW) method, or S-parameter retrieval, as described in [1]. Briefly, the method is based on measuring or simulating the reflection and transmission (i.e., S-parameters S_{11} and S_{21}) for a plane wave normally incident on a slab of the proposed metamaterial. Thereafter, the effective permittivity ε_{eff} and effective permeability μ_{eff} are calculated based on the assumption that the slab can be accurately described as a homogeneous material with these parameters. There is a certain ambiguity in choosing the correct branch of a complex $\log(\cdot)$ or $\arccos(\cdot)$, as thoroughly discussed in [2], but otherwise there should not be any problems with the retrieved parameters—provided that the assumed model is a good approximation of the actual structure.

However, in many cases the reported material parameters seem unreasonable. The perhaps most troublesome artefact is the so-called antiresonance in either ε_{eff} or μ_{eff}, which is observed when the other parameter (μ_{eff} or ε_{eff}, respectively) has a strong and expected Lorentz-like resonance. One of the first papers trying to explain the antiresonance effect was [3], which got some strongly opposing comments. The explanation given in [3] and later elaborated in [4] is that the effect is due to the periodicity of the material, in combination with the fact that the unit cell is not vanishingly small compared with the wavelength. The periodicity cannot, however, be the only explanation since qualitatively similar antiresonances have been reported using the measured data for a disordered high permittivity composite in [5]. More recently, it has even been suggested that the antiresonances are purely due to numerical errors in simulations [6].

It seems obvious that the simple homogeneous model with ordinary ε_{eff} and μ_{eff} is not well founded if (one of) the obtained parameters violate the fundamental requirements of passivity and causality. A thorough review of the problems and pitfalls of metamaterial homogenization can be found in [7, 8], where the author also presents a refined model including surface layers and a procedure for obtaining a set of physically more reasonable material parameters. Many authors also mention (weak) spatial dispersion as the reason why the simple model fails, and recently a reasonably straightforward model for this spatial dispersion has been presented in [9].

In this presentation, we use an example with plasmonic cylinders in air to show that the antiresonance-problem can be demonstrated with a geometrically simple and computationally cheap benchmark problem. Using the obtained numerical results, we discuss the merits of the different explanations for the so-called antiresonances and also point out some other problems related to the S-parameter retrieval.

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2 Numerical Example

As a synthetic but representative benchmark problem, we consider the 2D geometry shown in Figure 1, where the composite consists of five layers of circular cylinders in a square lattice in air. The permittivity of the cylinders is given by the Drude model

$$\varepsilon(\omega) = 1 - \frac{\omega_{\mathrm{p}}^2}{\omega^2 - j\omega\nu}, \qquad \nu = \omega_{\mathrm{p}}/100 \tag{1}$$

and the cylinders occupy an area fraction $p = 1/10$ of a quadratic unit cell with side length a. Using a 2D version of the Maxwell Garnett formula, we get the quasistatic effective permittivity

$$\varepsilon_{\mathrm{eff}}(\omega) = 1 - \frac{\omega_{\mathrm{p,eff}}^2}{\omega^2 - \omega_{0,\mathrm{eff}}^2 - j\omega\nu}, \qquad \begin{cases} \omega_{\mathrm{p,eff}} = \omega_{\mathrm{p}}\sqrt{p} = 0.316\,\omega_{\mathrm{p}}, \\ \omega_{0,\mathrm{eff}} = \omega_{\mathrm{p}}\sqrt{(1-p)/2} = 0.671\,\omega_{\mathrm{p}}. \end{cases} \tag{2}$$

This Lorentz model is very accurate for the corresponding infinite lattice in the quasistatic limit since the chosen area fraction is small. One important reason for choosing this 2D and geometrically simple model problem is that the S-parameters can be simulated with excellent numerical accuracy.

We have computed the S-parameters for the frequency range $0.55 < \omega/\omega_{\mathrm{p}} < 0.85$, different electrical sizes of the unit cell $a/\lambda_{\mathrm{p}} = a\,\omega_p/(2\pi c_0)$, different incidence angles, and also different number of layers using Comsol Multiphysics 3.5a. Figure 2 shows what happens if we assume the simple isotropic model with $\varepsilon_{\mathrm{eff}}$ and μ_{eff} and retrieve the effective parameters using normal incidence ($\varphi_0 = 0$) and the usual formulas, choosing the branch so that the retrieved refractive index is as continuous as possible. The retrieved $\varepsilon_{\mathrm{eff}}$ exhibits an expected Lorentz-like resonance that converges towards the quasistatic prediction, but a typical antiresonance appears in the retrieved μ_{eff}.

3 Discussion

The antiresonance in the retrieved effective permeability μ_{eff} violates passivity and causality, which is obviously not physically reasonable. This suggests that either the retrieval algorithm or the assumed homogeneous model is inaccurate. The results are quite smooth and robust with respect to various adjustments to the simulation-parameters, and thus simple numerical inaccuracy does not seem like a good explanation.

In addition to the antiresonance in μ_{eff}, the retrieved results are disturbed by weaker Fabry–Pérot resonances, which occur when the effective thickness of the slab is an integer multiple of one half wavelength. These appear, interestingly, as positive resonances in μ_{eff} and negative resonances in $\varepsilon_{\mathrm{eff}}$, although the latter are almost invisible in magnitude compared with the expected Lorentz resonance in $\varepsilon_{\mathrm{eff}}$. This problem is related to the instability in retrieving the effective impedance from S-parameters, as discussed for instance in [10]. One straightforward way to get rid of the Fabry–Pérot resonances would be to *a priori* assume that $\mu_{\mathrm{eff}} \equiv 1$ and retrieve $\varepsilon_{\mathrm{eff}} = n^2$, which at the same time would eliminate the infamous antiresonance problem. This is a reasonable approximation if the unit cell is small enough, and it gives the passive and causal effective material parameters shown in Figure 3. However, the drawback is that the obtained $\varepsilon_{\mathrm{eff}}$ with $\mu_{\mathrm{eff}} \equiv 1$ does not predict the reflection and transmission very accurately.

We obviously need more material parameters if the one-parameter model $\varepsilon_{\mathrm{eff}} = n^2$ is not sufficiently accurate, but the most popular model with homogeneous $\varepsilon_{\mathrm{eff}}$ and μ_{eff} does not seem appropriate. Looking at the main resonance–antiresonance pairs in Figure 3 it seems that the electric resonance gives some kind of effective magnetic response, but this magnetoelectric effect should not be forced into μ_{eff}. It is not, however, immediately obvious how this (weak) magnetoelectric coupling should be modeled using some kind of material parameters. At the moment, we are investigating the recently proposed model [9] for arbitrary plane-wave fields $e^{-j\mathbf{k}\cdot\mathbf{r}}$

$$\mathbf{D} = \varepsilon_{\mathrm{eff}}\mathbf{E} - \kappa_{\mathrm{eff}}\mathbf{k}\times\mathbf{H}, \qquad \mathbf{B} = \mu_{\mathrm{eff}}\mathbf{H} + \kappa_{\mathrm{eff}}\mathbf{k}\times\mathbf{E}. \tag{3}$$

This model with (weak) spatial dispersion is promising and reasonably simple with only three scalar parameters, but the algorithm for retrieving these parameters from simulated or measured S-parameters is still under development.

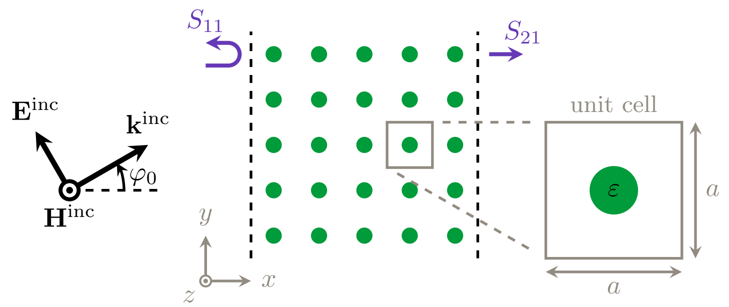

Figure 1: Geometry of the model problem with five layers of plasmonic cylinders in free space and an incident TM-polarized plane-wave.

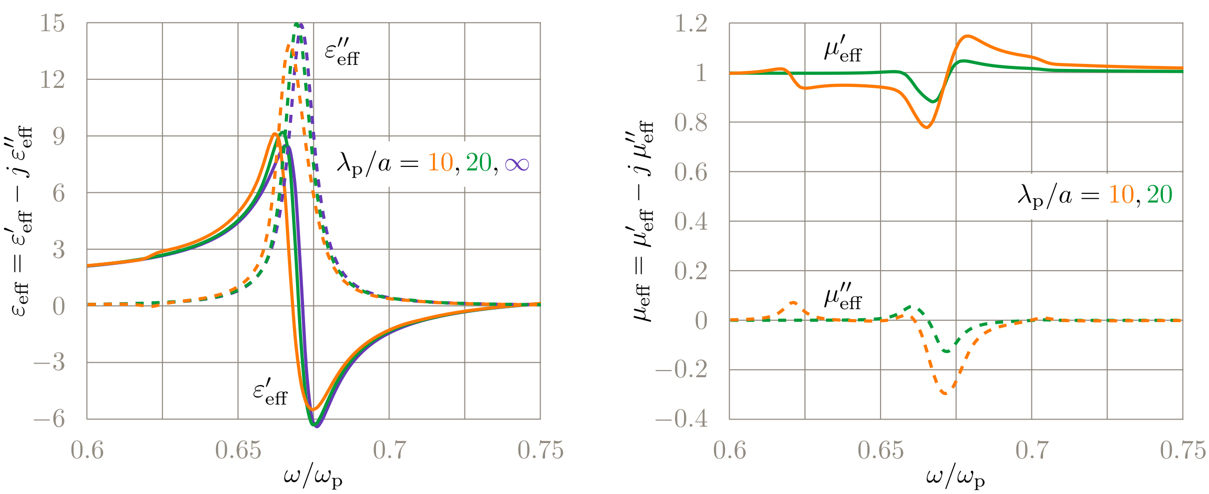

Figure 2: The retrieved permittivity (left) seems reasonable and converges towards the quasistatic result (∞) with smaller unit cells compared with the wavelength, but the retrieved permeability (right) is clearly unphysical. The overall μ_{eff} response is dominated by an apparent antiresonance at the frequency where $\varepsilon_{\mathrm{eff}}$ exhibits its expected Lorentz-like resonance. The additional much weaker resonances are due to Fabry–Pérot resonances in the slab.

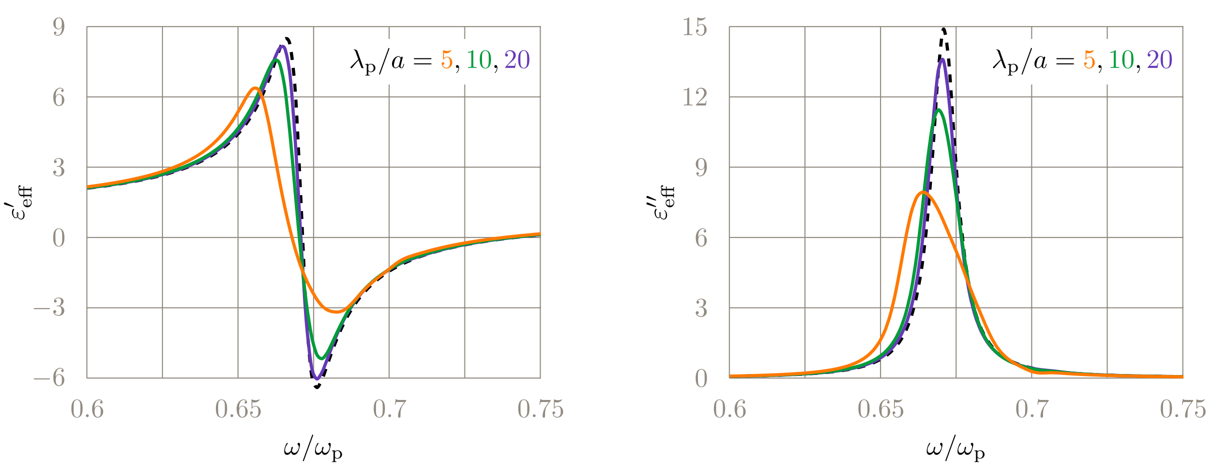

Figure 3: Assuming $\mu_{\mathrm{eff}} \equiv 1$ and retrieving the permittivity from the refractive index only gives a nice looking result, which converges towards the quasistatic estimate (dashed line).

In [9] the three effective parameters ε_{eff}, μ_{eff}, and κ_{eff}, are presented for infinite simple cubic lattices with spherical inclusions. Similar calculations could be done for circular inclusions in a square lattice, but the finite thickness of the slab in Figure 1 makes the situation more complicated. In addition to the problems related to Fabry–Pérot resonances, the interface between the slab and free space needs some extra consideration, as discussed in much more detail for instance in [7]. If we compute ε_{eff} for the current model problem by averaging the simulated fields over each unit cell, it seems that the first and last cells should have slightly different parameters from the rest, as in [11]. However, the effect of the surface layers seems quite small if we retrieve the (dubious) parameters ε_{eff} and μ_{eff} from S-parameters with different number of layers, and overall it is difficult to separate the surface or thickness effects from the bulk effects.

4 Conclusions

The modeling of a composite with resonant inclusions is not a straightforward exercise, and the retrieval of effective and physically reasonable material parameters from a slab of such a composite is even more challenging. Regardless of the underlying mechanism, it seems that the popular NRW-method always yields an unexpected antiresonance in μ_{eff} when ε_{eff} has an expected resonance, and vice versa. This is not physically reasonable, and the simple explanation is that the assumed homogeneous model with sharp and well defined boundaries fails to model the composite slab accurately enough. Instead of inventing dubious explanations why the antiresonant parameters could be useful anyway, we should find a better model without too many additional effective material parameters.

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