Inherent noncausal features in the Maxwell-Garnett homogenization of metamaterials

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Abstract

We explain the noncausal features that arise in the homogenization of metamaterial arrays using standard point-dipole approximations. We are able to relate these noncausal features to the approximations commonly used in Maxwell-Garnett homogenization approaches, and we show that these anomalous effects may become particularly significant for the important case of densely packed metamaterial arrays.

1. Introduction

Metamaterials are usually characterized by an anomalous electromagnetic response originating from the collective wave interaction with a large number of inclusions operating near resonance [1]. A variety of homogenization techniques have been put forward to conveniently describe this response using a limited number of effective constitutive parameters, such as bulk permittivity and permeability (see, e.g., [2]-[6]), as is commonly done for natural materials and mixtures. The most common homogenization approaches, like those of Maxwell-Garnett and Clausius-Mossotti [4],[7]-[8], conform to the way macroscopic wave interactions are described in natural materials, and are usually based on approximating the response of the inclusions with their dipole moments. Although quasi-static approximations may be safely applied to natural materials and mixtures within these homogenization techniques [4],[8], in metamaterials more rigorous dynamic models have been put forward that can precisely capture the resonant response of the inclusions within the dipolar limit [3],[7]. In the following, we will prove that a rigorous Maxwell-Garnett homogenization method based on approximating the unit cell response with its dipole moment inherently introduces noncausal features. Only a full-wave solution of the boundary-value problem associated with the unit cell may restore the properly causal response of the system. We discuss the nature of these artifacts in metamaterial homogenization and their specific relevance in the case of more densely packed metamaterial arrays.

2. Maxwell-Garnett approach and noncausality

Using a standard Maxwell-Garnett homogenization approach to describe the electric response of a metamaterial array with a cubic lattice, the effective electric susceptibility is given by the well known formula [7]

$$\chi_{eff}(\omega) = \frac{1}{d^3\left(\alpha_e^{-1} - C_{int}\right)}, \tag{1}$$

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where α_e is the electric polarizability of the inclusions forming the array, d is the array period, and C_{int} is the interaction constant describing the lattice coupling. Clausius-Mossotti approaches [4] usually approximate the inclusion polarizability and the interaction constant with their well-known quasi-static expressions

$$\alpha_e \simeq 4\pi a^3 \frac{\varepsilon - \varepsilon_0}{\varepsilon + 2\varepsilon_0}, \qquad C_{int} \simeq \frac{d^{-3}}{3}, \tag{2}$$

predicting a quasi-static susceptibility response that is usually very accurate for natural materials and mixtures. In metamaterials, however, the coupling among inclusions and the array density are usually much larger than in natural materials, making these approximations too coarse. Therefore, more accurate homogenization approaches, considering retardation effects, are usually required [2]-[6]. Exact dynamic expressions for the inclusion polarizability and the interaction constant are available and they have been used to calculate the susceptibility response of metamaterials in a more rigorous and self-consistent way. It should be noted that the exact expression of C_{int} depends not only on frequency, but also on the guided wave number β describing the propagation along the array, as a symptom of possible spatial dispersion effects near the metamaterial resonances.

In general, as proven in [7], the imaginary parts of α_e^{-1} and C_{int} exactly cancel each other in the denominator of Eq. (1) for lossless inclusions, ensuring that the susceptibility is purely real. In other words, passivity and power conservation are generally satisfied by the dynamic expression of Eq. (1). However, the causality requirement for which the partial derivative $\partial\chi_{eff} / \partial\omega$ (for fixed β) is strictly positive in the lossless scenario may be violated in some metamaterial geometries, as in some examples studied in Ref. [5]. Consider, for instance, the effective permittivity $\varepsilon_{eff} = \varepsilon_0\left(1+\chi_{eff}\right)$ of a periodic array of dielectric spheres with relative permittivity $\varepsilon_r = 3$ and radius $a = 0.45d$. Its frequency dispersion is shown in Fig. 1(a) as the dashed pink line, after adding some negligible losses distributed uniformly across the frequency spectrum. Its slope in the range $k_0 d < 4$ (with $k_0 = \omega / c$) is negative, violating the causality requirements stemming from the Kramers-Kronig relations in transparent media.

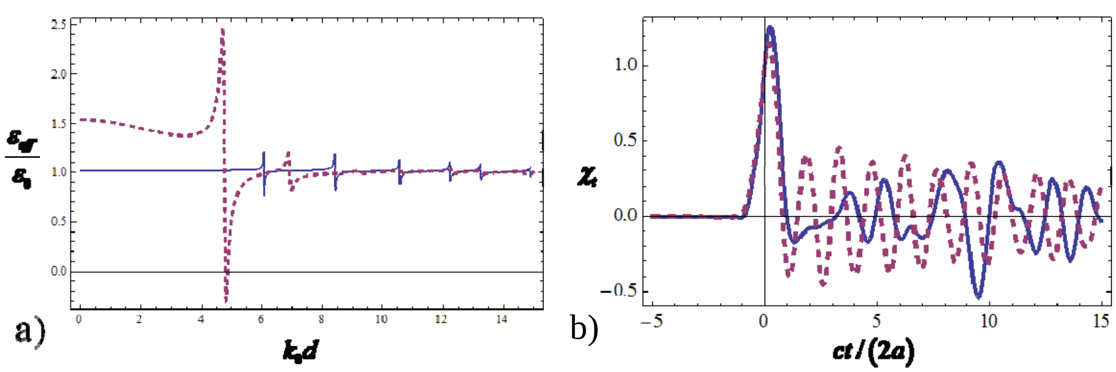

Fig. 1: (a) Effective permittivity, (b) normalized time response (arbitrary units), for a metamaterial array formed by dielectric spheres with relative permittivity $\varepsilon_r = 3$ and radius $a = 0.45d$ (dashed pink lines) and $a = 0.15d$ (solid blue lines).

For less dense arrays ($a = 0.15d$, blue solid line), this issue is corrected and the permittivity slope is positive in all transparent frequency regions. Fig. 1(b) shows the associated time responses, calculated as the inverse Fourier transform of Eq. (1). It is seen how both time responses, independent of the array density, present noncausal features starting near the instant $t = -2a / c$. We have rigorously proven [9] that this noncausal response is associated with the point-dipole approximations introduced in the derivation of Eq. (1). In particular, we have shown that the time response of the electric polarizability α_e of an arbitrary inclusion has a noncausal time response that starts at the precise instant $t = -2\delta / c$, where δ is the distance of the object surface from the origin of the reference system (usually the unit cell center) in the direction in which the wave hits the object. It is easy to understand the physical reason behind this noncausal response: although the dipole moment is evaluated at the center of the unit cell, and by definition the instant $t = 0$ corresponds to the moment in which the excitation hits this point, the inclusion interaction with the impinging wave starts when its surface is hit, at time $t = -\delta / c$ (for a sphere $\delta = a$). In addition, the scattered radiation has a time advance of another $t = -\delta / c$ compared to the dipolar radiation, since it originates from the inclusion surface, rather than from the center of the unit cell. The total time advance compared to an ideal dipole radiating at the origin is exactly $t = -2\delta / c$, consistent with the results in Fig. 1. The contribution of C_{int} in Eq. (1), also based on point-dipole approximations, may modify the instant at which the response starts, leaving unchanged its overall noncausal nature. This noncausality issue stems directly from the point-dipole approximations introduced in Eq. (1), and it is common to all periodic arrays. For $\delta \ll d$, the noncausal time advance becomes negligible with respect to the time delay introduced by the wave propagation across one unit cell and therefore the point-dipole approximation remains well suited for the homogenization of natural and artificial materials, as in the less dense array of Fig. 1 (blue solid line), which indeed shows a positive slope for the effective permittivity. The noncausality of Eq. (1) becomes relevant when the introduced time advance is comparable with the propagation across one unit cell, as for the more densely packed array in Fig. 1. In this situation, the point-dipole approximation considerably deviates from the first-principle definition of effective permittivity, which may be calculated using rigorous numerical methods [3] and proven to rigorously satisfy causality so as to exhibit positive slope and obey the Kramers-Kronig relations.

3. Conclusion

We have discussed here the noncausal effects introduced by the point-dipole approximations in standard Maxwell-Garnett homogenization approaches. These effects are particularly relevant in the case of densely packed arrays and metamaterials, for which the point-dipole approximation may not necessarily be applied to rigorously extract their effective permittivity response.

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