Surface mesoscopic effects in finite metamaterials

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Abstract: While the effective medium treatment of unbounded metamaterials appears to be well established and firmly proven, related phenomena in finite structures have not received sufficient attention. We report on mesoscopic effects associated with the boundaries of finite discrete metamaterial samples, which can invalidate an effective medium description. We show how to avoid such effects by proper choice of boundary configuration. As all metamaterial implementations are naturally finite, we are confident that our findings are crucial for future metamaterial research.

OCIS codes: (160.3918) Metamaterials; (260.2065) Effective medium theory.

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1. Introduction

Metamaterials — artificial media engineered with various structural units which play the role of atoms — have been in the focus of active research for more than a decade. One of the milestones in understanding metamaterial properties is the effective medium theory (EMT), which aims to describe metamaterials in terms of effective parameters: permittivity and permeability [1]. In particular, EMT has been essential for the lattices of split-ring-resonators (SRRs) — the key structure for obtaining an artificial magnetic response [2]. Approaches for determining the effective permeability of bulk SRR-metamaterials were attempted prior to metamaterials outburst [3]. Subsequently, fruitful theoretical procedures were developed to account for mutual interaction [4], bianisotropy [5], magnetoinductive waves [6] and their interaction with the electromagnetic spectrum [7, 8], spatial dispersion [8–10], mutual interaction between the electric and magnetic subsystems [11], specificity of boundary conditions [12, 13], arbitrary geometry of elements [14], multipole expansion [15], disorder [16, 17] and noise [18].

However, effective medium theories, in principle, consider unbounded lattices, whereas all practical metamaterials are of finite size. For conventional materials, it is well known [13, 19, 20] that at the boundaries a transition layer is formed, with properties different from those of the bulk (see the historical introduction in [13] for a detailed background). For large samples, however, transition layer does not significantly affect the overall macroscopic properties, and only manifests itself under specific conditions such as strongly oblique incidence, with surface modes not affecting the bulk considerably. But metamaterials are often constructed with a much fewer number of elements than reasonable pieces of conventional materials, so a comparison to atomic clusters might be more appropriate. At the same time, internal structure of metamaterials is often more complex than that of natural materials, in a sense that metamaterial elements may be quite densely arranged, be of different types or form geometrically independent sublattices [21]. This raises an issue of pronounced surface and spatial resonances which may appear in finite structures even in a quasi-static regime [22, 23].

For metamaterial slabs, having a finite size in one dimension (and the same applies to the small samples placed inside a waveguide, which is equivalent to a system infinite in transverse

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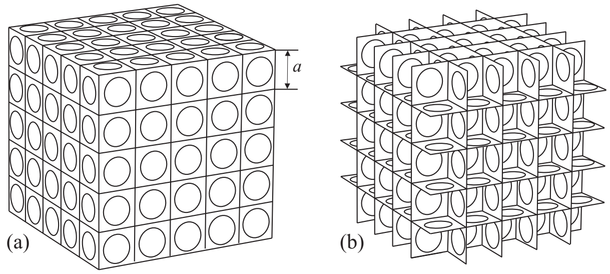

Fig. 1. Scheme of a symmetric finite cube with discrete structure, showing two options of surface configuration (for the same unit cell in the bulk): "flat" geometry (a) and "ragged" geometry (b). Note that the actual number of elements is not necessarily reflected here.

direction), bulk effective parameters can be, with certain precautions, extracted from transmission and reflection characteristics [24, 25] (see e.g. [26, 27] for a recent update on the methodology). On this way, it is known that the effective properties extracted for the slabs of finite thickness quickly converge to the EMT predictions when the number of unit cells across the slab increases, and for most structures with low spatial dispersion a thickness of a few unit cells is sufficient to yield the bulk properties.

In this paper, we address the most general case of practical relevance: metamaterials with finite size in all three dimensions, observed in free space. We will analyse whether such metamaterials can be described with EMT parameters, and what are the requirements for such a description to be valid. It turns out that while for a slab of metamaterial a few unit cells across the slab are sufficient for EMT to work well, for the finite size in 3D it may be not sufficient to take several unit cells in each direction, and that a dramatic effect is caused by the ambiguity in the boundary structure (see Fig. 1).

Indeed, a unit cell of the isotropic system shown in Fig. 1 contains three resonant loops non-symmetrically positioned with respect to the geometrical centre of the cell: three sides of the cube carry resonators, and the other three do not (as those resonators belong to the adjacent unit cells). This makes no difference in the middle of the structure. However, at the boundaries, overall symmetry of the sample can be achieved either by adding extra surface resonators on the three sides, Fig. 1(a), or, less trivially, by removing the unnecessary resonators on the opposite sides, Fig. 1(b). We will further refer to these methods of assembly as "flat" and "ragged".

We should note that early analysis [4] confirmed that anisotropic stacks of uniformly oriented SRRs (all having parallel axes), with about one thousand elements can be successfully described with EMT; however that structure has no ambiguity of the kind described above.

2. Results and discussion

We will now analyse metamaterial cubes with isotropic cubic unit cells, and having different surface geometry as discussed above, and compare their characteristics to those of homogeneous pieces of a bulk material with the corresponding effective parameters [8]. In order to avoid any complications related to spatial dispersion and fit well into the EMT domain, we study a system with deeply subwavelength and strongly interacting resonant current loops: $k_{\mathrm{res}}a \approx 0.02$ and $a/r_0 \approx 3.1$ (where k_{res} is the value of the free space wavenumber k_0 at resonance, a is the lattice constant and r_0 is the mean radius of the loop). A high quality factor of the resonators, $Q \approx 500$, has been chosen in order to present more illustrative results.

The finite size in all three directions does not permit a consistent study in terms of transmission characteristics, but there is a convenient macroscopic characteristic that can be attributed

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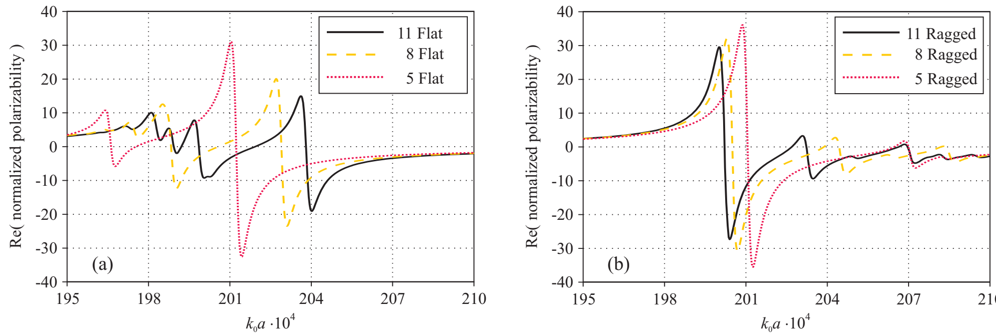

Fig. 2. Real part of the normalised polarisability (arbitrary units) of discrete cubes with 5, 8 or 11 layers of resonators in each direction, having either a "flat" geometry (a) or a "ragged" geometry (b).

to finite samples: normalised polarisability, i.e. the total magnetic moment of the sample per unit external magnetic field and per unit volume. For subwavelength objects made of a homogeneous isotropic medium, this quantity is a scalar independent of the size. To find the polarisability of our discrete cubes, we solved a system of circuit equations for coupled resonators [6, 28], assuming a uniform external magnetic field perpendicular to the face of the cube; note that taking all the mutual interactions into account is essential for such analysis. The total magnetic moment is then computed by summing the individual magnetic moments of each ring.

In Fig. 2, we compare the normalised polarisabilities of several metamaterial samples with various number of layers in each direction, calculated for either "flat" or "ragged" boundary. The normalised polarisability of the discrete cubes changes remarkably as the number of elements grows (unlike what we would expect for a homogeneous material), and it does not show a trend towards similarity between "flat" and "ragged" versions. However, the results obtained for the "ragged" geometry show more uniformity than those obtained for "flat" cubes.

Further distinctions are revealed (Fig. 3) by comparing discrete cubes with an equivalent cube made of a homogeneous medium, with the permeability given by Eq. (13) of [8],

$$\mu = 1 + \frac{\gamma}{(k_{\text{res}}a)^2 \big/ (k_0 a)^2 - 1 - 2\varkappa_{\text{a}} - 4\varkappa_{\text{c}} - \gamma/3}, \qquad (1)$$

where $\gamma = 0.162$ is a coefficient related to the polarisability of a ring (determined by its geometry), $\varkappa_{\text{a}} = 0.0195$ and $\varkappa_{\text{c}} = -0.0173$ are inductive coupling coefficients to the axial and coplanar nearest neighbours; the numerical values specified here, correspond to the example used in our illustrations. Note that, although it is generally necessary to take more remote neighbours into account as well [4], for an unbounded cubic lattice taking only the nearest neighbours explicitly and then using Lorentz correction for farther neighbours [8] provides a sufficiently good accuracy. The polarisability of the homogeneous cube was found using the CST "Microwave Studio" commercial package. In order to avoid the appearance of multiple non-physical resonances, the edges and corners of the homogeneous cube must be rounded [29]. We have used a rounding radius corresponding to one half of the unit cell size of the discrete cubes. Such rounding leads to a minor difference between the simulation results for cubes of various absolute sizes, but this difference is very small in comparison with discrete cubes, and is not of a qualitative nature. Figure 3 shows that the polarisability of the "ragged" cube is significantly closer to that of the homogeneous cube, than the polarisability of the "flat" cube.

These results can be understood in view of the essential role of surface elements [13, 20], since they do not have the same surroundings as the elements in the bulk and form transition

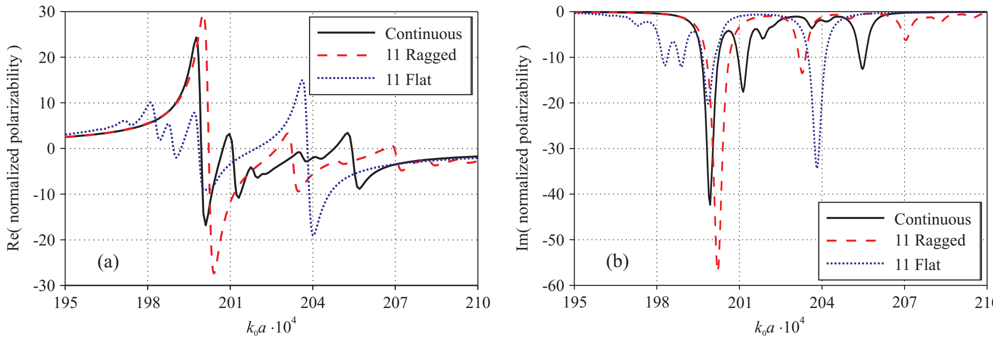

Fig. 3. Real (a) and imaginary (b) parts of the normalised polarisability (arbitrary units) of discrete cubes with 11 layers in each direction, having either a "flat" geometry (dashed lines) or "ragged" geometry (dotted lines), in comparison with the polarizability of a homogeneous cube (solid lines).

layers with different properties. Then the difference between a "flat" structure and a "ragged" structure can be qualitatively assessed by noting that the elements of a "flat" surface do not have 5 out of 14 nearest neighbours, as compared to fully immersed rings, while in "ragged" surfaces, only 3 of the nearest neighbours are absent. This suggests that the behaviour of the "ragged" cube should be closer to the behaviour of an unbounded piece.

Although the considered metamaterial samples are formed by hundreds or even thousands of elements, they still behave like mesoscopic systems. The reason for this is that the number of periods is relatively small, so the surface excitations do not sufficiently dissipate within the sample, making a consistent macroscopic field averaging unreliable. However, we can attempt to extract the effective permeability directly from the polarisability of our cubic samples, as these quantities must be related. For this purpose, we assume that the functional form of the polarisability of a cube is similar to that of a sphere $\alpha_o = 3(\mu-1)/(\mu+2)$. So, we formally express the polarisability of a cube as

$$\alpha = A \cdot (\mu - 1)/(\mu + C), \tag{2}$$

where A and C are real frequency-dependent coefficients (see Fig. 4 for an example of their functional form). But for a homogeneous cube we know both the permeability function μ given

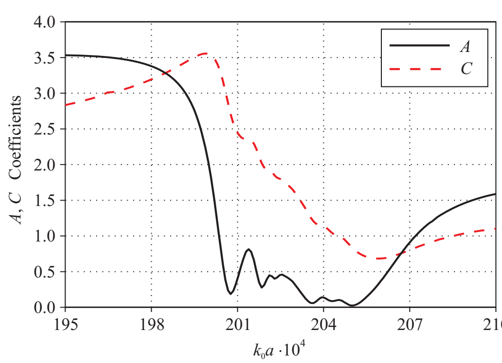

Fig. 4. Frequency dependence of the A and C coefficients calculated with Eq. (3) based on the effective permeability μ of a homogeneous cube Eq. (1) and its polarisability α, obtained from numerical simulations.

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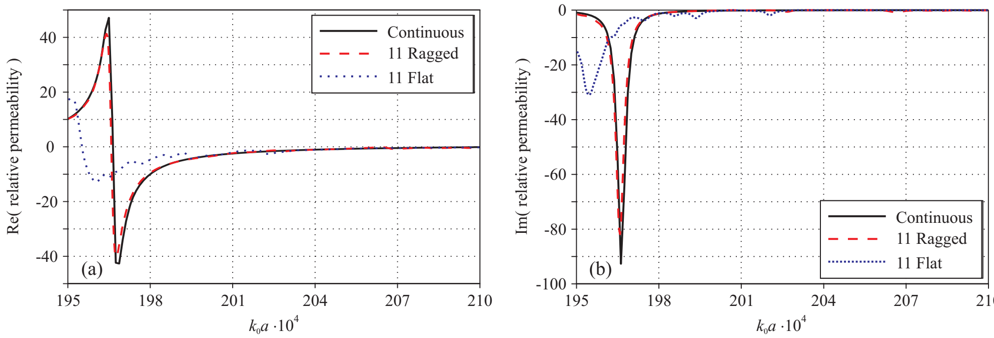

Fig. 5. A comparison between the permeability μ of a homogeneous cube (solid line) and the effective permeability $\mu^{\#}$ obtained for 11-layer discrete cubes with a "flat" geometry (dashed lines) or a "ragged" geometry (dotted lines); real (a) and imaginary (b) parts.

by Eq. (1), and the polarisability α (which was computed numerically and shown with solid lines in Fig. 3). Thus, we can uniquely calculate A and C (shown in Fig. 4) as

$$C = \frac{|\mu|^2 - \mathrm{Re}\,\mu - \dfrac{\mathrm{Re}\,\alpha}{\mathrm{Im}\,\alpha}\,\mathrm{Im}\,\mu}{1 - \mathrm{Re}\,\mu + \dfrac{\mathrm{Re}\,\alpha}{\mathrm{Im}\,\alpha}\,\mathrm{Im}\,\mu}, \qquad A = \frac{(\mathrm{Re}\,\mu + C)^2 + (\mathrm{Im}\,\mu)^2}{\mathrm{Im}\,\mu \cdot (C+1)}\,\mathrm{Im}\,\alpha. \tag{3}$$

Now, these A and C coefficients can be used to evaluate the effective permeability of discrete cubes from their polarisability $\alpha^{\#}$ which is available from our analysis (shown with the dashed and dotted lines in Fig. 3), using an inverse of equation (2):

$$\mu^{\#} = (A + C\alpha^{\#})/(A - \alpha^{\#}). \tag{4}$$

The result of this procedure is shown in Fig. 5: the curve corresponding to the "ragged" cube is very similar to the actual permeability of a homogeneous cube, unlike the curve of the "flat" cube. This result can be regarded as a strong argument in favour of the "ragged" configuration, in a sense that its effective permeability retrieved through the above procedure, matches the EMT prediction, whereas for the "flat" configuration such retrieval fails.

3. Conclusions

We have shown that the behaviour of finite metamaterial samples can deviate significantly from continuous medium expectations. We conclude that for isotropic SRR-metamaterials with up to several thousands of elements, the "ragged" boundary structure should be used for practical applications to permit a description in terms of the effective parameters of an unbounded metamaterial. We are confident that, for the size range in which most practical metamaterials fit, our results provide valuable information and design guidelines, allowing for to control the properties of finite metamaterial structures. Our results can be also of interest for the general theory of mesoscopic electromagnetic systems.

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