# On the homogenization problem by means of surface integral equations

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**Abstract**

In this paper we present a new formulation of the homogenization problem based on surface integral equations. The homogenization is based on the excitation of the structure with a macroscopic source [1]. There is, however, a difference with respect to previous works, being related to the spatial distribution of the excitation currents. In our formulation the whole response of the system to the excitation is included in the definition of the effective permittivity, which accounts for spatial dispersion phenomena, and we prove that the homogenization problem can be reduced to the solution of a system of surface integral equations.

## 1. Introduction

When characterizing a metamaterial as a continuum medium, a homogenization process is needed. Needless to say, it is very convenient to have such a description to ease theoretical modeling, thus avoiding the computation of the full microscopic problem. Homogenization consists of the inference of the macroscopic properties of the medium from the response of a basic cell which, periodically repeated, builds up the metamaterial. This is a challenging issue, and several attemps to tackle it have appeared in the literature (for a review, see, e.g. [2]). Among them, only a few [1, 3] include the possibility of strong spatial dispersion effects. However, these may be very relevant effects [4], non negligible for certain metamaterials even in the extremely-long-wavelength limit [5]. Thus, although some features related to non-locality can be included in a local model, as is the case of gyrotropy for weakly spatially dispersive media, a complete description of non-local effects is very desirable when extracting the effective properties of metamaterials. In the present work, we present a homogenization scheme to obtain the non-local effective permittivity of metamaterials composed by inclusions of arbitrary shape and electromagnetic properties periodically arranged in a lattice. In particular, we allow for the possibility of studying metamaterials with magnetic inclusions and/or host medium, i.e., such that $\mu \neq 1$.

## 2. Theoretical formulation

Let us assume that we know the geometry and material parameters (local and frequency dispersive) of a given body occupying a volume $V$ (enclosed by the surface $\Gamma$). We assume also that we fill the space $\mathbf{R}^3$

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by periodically arranging identical copies of that given body in a lattice, with unit cell $\Omega$ defined by the primitive vectors $\mathbf{a}_i$ ($i = 1, 2, 3$) and with volume $V_{cell}$, and the volume exterior to them $\tilde{V}$ with a host medium whose electromagnetic properties are also known. We consider an external current $\mathbf{j}_{ext}$ flowing only in the volume $\tilde{V}$. It will, obviously, generate a response on the whole system. The macroscopic properties in the long-wavelength limit can then be computed from suitable spatial averaging of the microscopic fields distribution generated under such excitation. Following [1], for a given pair $(\omega, \mathbf{k})$, the macroscopic spatially dispersive permittivity, $\bar{\bar{\epsilon}}_{\text{eff}}(\omega, \mathbf{k})$, will be computed by exciting the system with an external current of the form $\mathbf{j}_{ext} = \mathbf{j}_{e,av} e^{i\mathbf{k}\cdot\mathbf{r}}$, the amplitude $\mathbf{j}_{e,av}$ being a constant vector. Since we want to compute the whole matrix $\bar{\bar{\epsilon}}_{\text{eff}}$, three linearly independent vectors $\mathbf{j}_{e,av}$ must be chosen.

It is well known that for a given microscopic field, $\mathbf{E}(\mathbf{r})$, the averaging procedure that preserves the form of Maxwell's equations is any of the form $\mathbf{E}_{macro}(\mathbf{r}) = \int \mathbf{E}(\mathbf{r} - \mathbf{r}') f(\mathbf{r}') d^3\mathbf{r}'$. In our work we will adopt the equivalent to ideal low pass filtering, thus taking a test function such that:

$$\tilde{f}(\mathbf{k}) = \begin{cases} 1 & : \mathbf{k} \in \text{B.Z.} \\ 0 & : \mathbf{k} \notin \text{B.Z.} \end{cases}$$

which filters all spatial oscillations on the order of the unit-cell size. It is easy to prove that, if the microscopic field is a Bloch mode asociated with $\mathbf{k}$, which is ensured by the periodic character of the system and by an excitation current of the form $\mathbf{j}_{ext} = \mathbf{j}_{e,av} e^{i\mathbf{kr}}$, then the macroscopic field takes the form of a plane-wave with wavevector $\mathbf{k}$ and amplitude $\mathbf{E}_{av} = (1/V_{cell}) \int_\Omega \mathbf{E}(\mathbf{r}) e^{-i\mathbf{kr}} d^3\mathbf{r}$.

We have for our periodic system two sets of Maxwell's equations, one for the volume $\tilde{V}$, which will contain the external current, and another for the volumes $V_j$ of the inclusions, where no external current is present. It is straightforward to obtain the wave equations that the electric and magnetic fields must satisfy in each region, with inhomogeneous terms, $\mathbf{F}_{e,h}$, that are proportional to $\mathbf{j}_{ext}$ for $\mathbf{E}$ and to $\nabla \times \mathbf{j}_{ext}$ for $\mathbf{H}$. These equations, together with the equation for the Green's function associated with the operator $\mathbf{L} = -\epsilon\mu\frac{\omega^2}{c^2} + \nabla \times \nabla$, upon applying Green's theorem in vectorial form to the quantity $\mathbf{E} \cdot \mathbf{L}\bar{\bar{G}} - \bar{\bar{G}} \cdot \mathbf{L}\mathbf{E}$, will allow us to reduce the computation of the microscopic fields to the solution of a system of surface integral equations.

## 3. Surface Integral Equations

Let us consider, for simplicity, that our system is composed by inclusions invariant along $z$-axis and periodically arranged in the $xy$-plane with primitive vectors $\mathbf{a}_i$ ($i = 1, 2$). Let's consider also two polarizations: (i) electric field directed along $z$ ($s$-polarization or TE), (ii) magnetic field along $z$ ($p$-polarization or TM). Due to the specific geometry of the problem, no depolarization effects take place. Let $\psi = E_z = E$ ($= H_z = H$) represent the only non-zero component of the $\mathbf{E}$ ($\mathbf{H}$) field in $s$-($p$-) polarization. Then it's well known that applying Green's theorem to the quantity $\mathbf{E} \cdot \mathbf{L}\bar{\bar{G}} - \bar{\bar{G}} \cdot \mathbf{L}\mathbf{E}$ in an arbitrary volume $V'$, which is identified either with one of the volumes $V_j$ or with $\tilde{V}$ gives rise to the following equations, obtained upon considering the following cases [6]:

$$\psi^{in}(\mathbf{r}^<) = -\frac{1}{4\pi} \int_{\Gamma_j^-} [\psi^{in}(\mathbf{R_j}) \frac{\partial G_j^{in}(\mathbf{r}^<, \mathbf{R_j})}{\partial N_j} - G_j^{in}(\mathbf{r}^<, \mathbf{R_j}) \frac{\partial \psi^{in}(\mathbf{R_j})}{\partial N_j}] dS, \quad \texttt{if } \mathbf{r} \in V_j \texttt{ and } \mathbf{r}' \to \Gamma_j^- \quad (1)$$

$$0 = -\frac{1}{4\pi} \int_{\Gamma_j^-} [\psi^{in}(\mathbf{R_j}) \frac{\partial G_j^{in}(\mathbf{r}^>, \mathbf{R_j})}{\partial N_j} - G_j^{in}(\mathbf{r}^>, \mathbf{R_j}) \frac{\partial \psi^{in}(\mathbf{R_j})}{\partial N_j}] dS, \quad \texttt{if } \mathbf{r} \in \tilde{V} \texttt{ and } \mathbf{r}' \to \Gamma_j^- \quad (2)$$

$$\psi^{out}(\mathbf{r}^>) = \psi^{(s)}(\mathbf{r}^>) + \frac{1}{4\pi} \sum_j \int_{\Gamma_j^+} [\psi^{out}(\mathbf{R_j}) \frac{\partial G_j^{out}(\mathbf{r}^>, \mathbf{R_j})}{\partial N_j} - G_j^{out}(\mathbf{r}^>, \mathbf{R_j}) \frac{\partial \psi^{out}(\mathbf{R_j})}{\partial N_j}] dS,$$
$$\texttt{if } \mathbf{r} \in \tilde{V} \texttt{ and } \mathbf{r}' \to \Gamma_j^+ \quad (3)$$

 

$$0 = \psi^{(s)}(\mathbf{r}^<) + \frac{1}{4\pi}\sum_j \int_{\Gamma_j^+} [\psi^{out}(\mathbf{R_j})\frac{\partial G_j^{out}(\mathbf{r}^<, \mathbf{R_j})}{\partial N_j} - G_j^{out}(\mathbf{r}^<, \mathbf{R_j})\frac{\partial \psi^{out}(\mathbf{R_j})}{\partial N_j}]dS,$$
$$\texttt{if } \mathbf{r} \in V_j \texttt{ and } \mathbf{r}' \to \Gamma_j^+ \qquad (4)$$

Here, $\mathbf{r}$ represents the observation point, $\mathbf{r}'$ represents the source point and $\mathbf{R} = \mathbf{r}'|_\Gamma$. Note that the equations are different whether the source point approaches the surface from the exterior ($\mathbf{r}' \to \Gamma_j^+$) or the interior ($\mathbf{r}' \to \Gamma_j^-$) of the inclusion. Note also that only the scalar Green's function, $G$, i.e., the field due to a single point source in a homogeneous dielectric, appears in the equations. Simplification with respect to the fully 3D case is only due to the specific geometry. The infinite summation over $j$ is taken over all the inclusions. $\psi_{s,p}^{(s)}$ represent the excitation field in the system, different for each polarization:

$$\psi_{s,p}^{(s)}(\mathbf{r}) = \int_{\tilde{V}} G^{(out)}(\mathbf{r}, \mathbf{r}')\mathbf{F}_{e,h}(\mathbf{r}')d^3\mathbf{r}' \qquad (5)$$

Equations (1)-(4) are, obviously, not independent. Only two of them are needed (we will use eqs.(3) and (2)) and will be consistently solved by taking the limit $\mathbf{r}^{><} \to \mathbf{r}|_\Gamma$. Upon making use of the Bloch's behaviour of the fields, i.e. $\psi(\mathbf{r} + \mathbf{t}) = e^{i\mathbf{kt}}\psi(\mathbf{r})$ with $\mathbf{t} = \sum c_i \mathbf{a}_i$ where $c_i \in \mathbf{Z}$, we can "bring back" the equations as to involve computations only in the unit cell by defining the periodic Green's function:

$$G_p(\mathbf{r}, \mathbf{R}) = \sum_{\mathbf{t}} e^{i\mathbf{kt}} G^{out}(\mathbf{r}, \mathbf{R} + \mathbf{t}) \qquad (6)$$

The same can be done with the excitation fields. It is then possible to make use of the continuity conditions for the fields and their derivatives on the surface in order to solve Eqs.(2) and (3) self-consistently. We end up with the system of integral equations to be solved for the magnetic (electric) field and its normal derivative on the surface for $p$-($s$-)polarization. Once we know these terms, the fields are known in every point of space, through eqs.(1)-(4). Therefore, defining a generalized averaged polarization vector consistently with [1] and with the fact that there is magnetization at the microscopic level, i.e.,

$$\mathbf{P}_{g,av} = \frac{1}{V_{cell}}\int_\Omega (\epsilon - \epsilon^{out})\mathbf{E}(\mathbf{r})e^{-i\mathbf{k}\cdot\mathbf{r}}d^3\mathbf{r} - \frac{1}{V_{cell}}\frac{\mathbf{k}}{\omega} \times \int_\Omega (\frac{\mu}{\mu^{out}} - 1)\mathbf{H}(\mathbf{r})e^{-i\mathbf{k}\cdot\mathbf{r}}d^3\mathbf{r}, \qquad (7)$$

we can find $\bar{\bar{\epsilon}}_{\text{eff}}(\omega, \mathbf{k})$ for every pair $(\omega, \mathbf{k})$, taking three lineraly independent $j_{e,av}$, and using the relation $(\bar{\bar{\epsilon}}_{\text{eff}} - \epsilon_0\bar{\bar{I}})\mathbf{E}_{av} = \mathbf{P}_{g,av}$. The local constitutive parameters can be computed from the derivatives of the nonlocal dielectric function with respect to the wave vector [1]. Numerical results will be presented and the formalism for the full 3D problem will be delineated.

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