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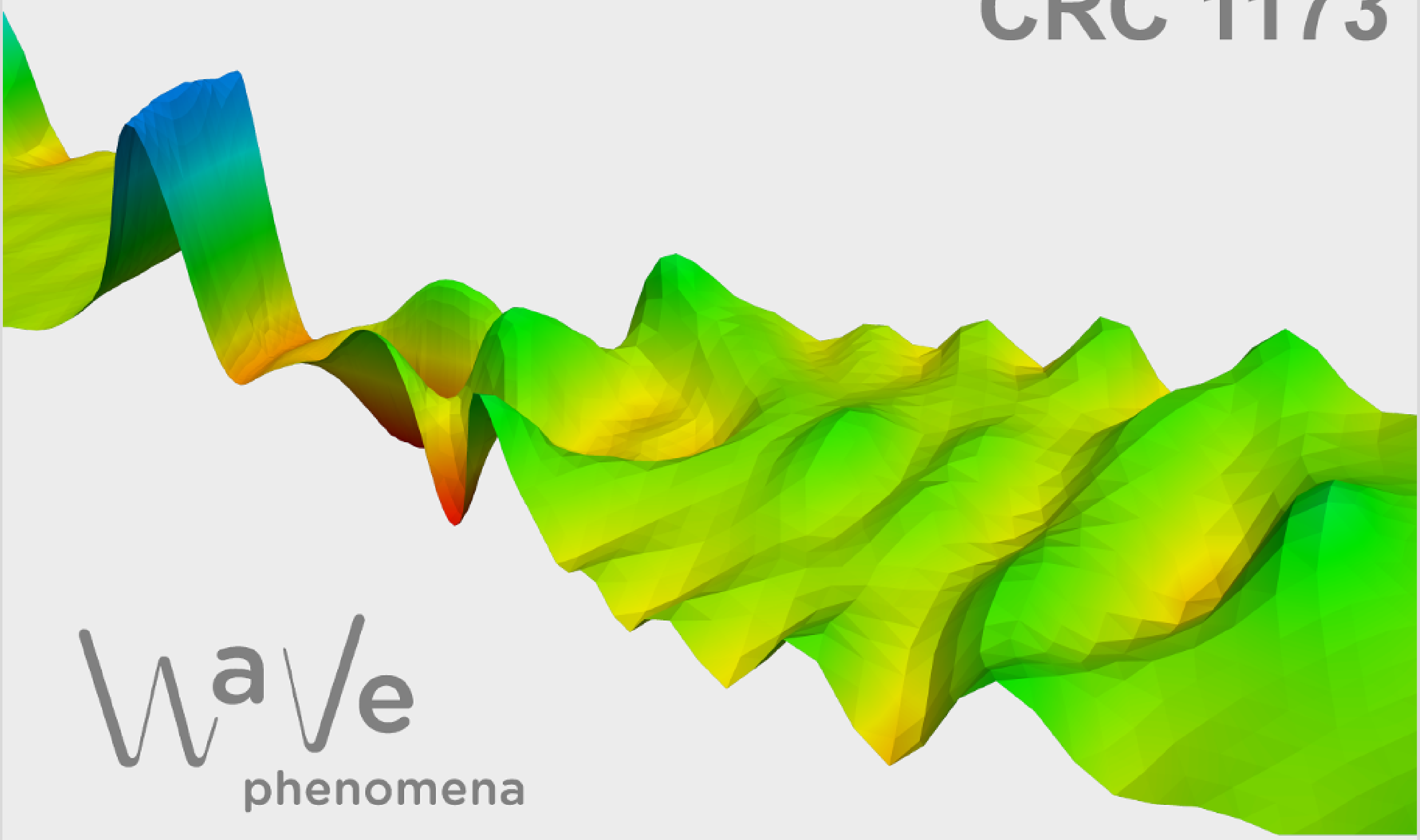

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Higher order constitutive relations and interface conditions for metamaterials with strong spatial dispersion

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Abstract

To characterize electromagnetic metamaterials at the level of an effective medium, nonlocal constitutive relations are required. In the most general sense, this is feasible using a response function that is convolved with the electric field to express the electric displacement field. Even though this is a neat concept, it bears little practical use. Therefore, frequently the response function is approximated using a polynomial function. While in the past explicit constitutive relations were derived that considered only some lowest order terms, we develop here a general framework that considers an arbitrary higher number of terms. It constitutes, therefore, the best possible approximation to the initially considered response function. The reason for the previously self-imposed restriction to only a few lowest order terms in the expansion has been the unavailability of the necessary interface conditions with which these nonlocal constitutive relations have to be equipped. Otherwise one could not make practical use of them. Therefore, besides the introduction of such higher order nonlocal constitutive relations, it is at the heart of contribution to derive the necessary interface conditions to pave the way for the practical use of these advanced material laws.

Keywords: metamaterials, Maxwell equations, nonlocal constitutive relations, strong spatial dispersion, Taylor approximation, interface conditions, weak formulation

1 Introduction

The study of wave phenomena based on the propagation of electromagnetic fields in different materials requires to take into consideration the properties of these materials when solving Maxwell's equations. These material properties are expressed by constitutive relations. In electrodynamics, constitutive relations are given in the most general sense by

$$\begin{aligned}\boldsymbol{\mathcal{D}}(\mathbf{r},t) &= \boldsymbol{\mathcal{E}}(\mathbf{r},t) + \mathbf{P}[\boldsymbol{\mathcal{E}},\boldsymbol{\mathcal{B}}](\mathbf{r},t),\\ \boldsymbol{\mathcal{H}}(\mathbf{r},t) &= \boldsymbol{\mathcal{B}}(\mathbf{r},t) - \mathbf{M}[\boldsymbol{\mathcal{B}},\boldsymbol{\mathcal{E}}](\mathbf{r},t),\end{aligned}$$

where $\boldsymbol{\mathcal{E}}(\mathbf{r},t)$ and $\boldsymbol{\mathcal{B}}(\mathbf{r},t)$ are the electric field and the magnetic induction, and $\boldsymbol{\mathcal{D}}(\mathbf{r},t)$ and $\boldsymbol{\mathcal{H}}(\mathbf{r},t)$ are auxiliary fields called the electric displacement and the magnetic field, respectively. $\mathbf{P}[\cdot,\cdot](\mathbf{r},t)$ and $\mathbf{M}[\cdot,\cdot](\mathbf{r},t)$ are the electric polarization and the magnetization. They capture the actual response of the materials at stake. Both quantities are induced by the electric field and the magnetic induction. It is not possible within the realm of electrodynamics to get access to the exact functionality of the polarization/magnetization on the fields [1]. That requires usually some sort of quantum treatment either in the context of chemistry or solid state physics, for example.

To be able to work, and while considering natural materials with a density of roughly 10^{23} atoms per cubic-centimeter, a simple averaging of the charge dynamics implies to neglect any spatial details of the actual material on the atomic scale and to consider it merely as a homogeneous medium. Then, the polarization and magnetization in some spatial coordinate depend exclusively on the electric field and the magnetic induction at the very same spatial location. This leads to what is called a local constitutive relation. As the magnetic response at optical frequencies of all natural materials is negligible, it suffices to consider only the response in the polarization thanks to the electric field. If the material is non-centro symmetric, effects associated to an electro-magnetic coupling can be observed that requires to consider the possibility to induce a polarization (magnetization) by a magnetic induction (electric field). The associated constitutive relations are those of a bi-anisotropic material and, basically, they are as complicated as it can get with natural materials.

But such local constitutive relations are not sufficient to describe the response of mesoscopic artificial materials such as Metamaterials (MMs). MMs are designed to control the light propagation in a way inaccessible with natural materials. By carefully tailoring the magnetic and electric response, novel applications can be perceived such as cloaking devices, super lenses, and others. For further information, we refer the reader to the following references list which is not exhaustive due to the big research activity in this field [4–11]. MMs consist of subwavelength inclusions called meta-atoms, mostly arranged in a periodic way. As MMs are usually made form non-magnetic materials, already the magnetic response needs to be induced by the external electric field. On simple grounds, it can be explained by the induction of ring-type currents in metallic or dielectric structures, that is driven into resonance. These ring type currents are associated to a magnetic dipole moment that lends the material at the effective level its magnetic response. Local constitutive relations can describe such materials at the effective level, but now we have to consider also a magnetic response in terms of a magnetic permeability. This, nevertheless, is only possible when the period of the meta-atoms' arrangement is much smaller than the wavelength of light (see for instance [12–14]). Unfortunately, this requirement contrasts with the desire to get a strong magnetic response, which asks for larger ring-like structures. Therefore, for most MMs their period and the operational wavelength are in the same order of magnitude. This questions the applicability of local constitutive relations as light starts to probe the spatial details of the underlying mesoscopic material. This implies that the optical response cannot be fully described with local constitutive relations.

Instead, retaining nonlocal properties in the effective description of MMs captures more accurately their properties than ordinary local constitutive relations. The efficiency of the nonlocal approach was shown through the research of several groups, for example, but not limited to, we cite [15–18, 22]. A major characteristics of nonlocality is that the induced response depends on the electric field and magnetic induction at the same spatial locations as well as on the fields at points located in a surrounding neighborhood. Besides the dependency on the fields, their gradients are also involved when writing the constitutive relations. The later notion is usually called strong spatial dispersion (SSD) (cf. [23, 24]), which is of crucial importance in this paper. Previously, SSD was considered when homogenizing MMs. This holds particularly for the non-asymptotic homogenization that does not require taking the limit to zero of the unit-cells' arrangement period (see, e.g., [17, 19–22, 25]).

A question of major importance for science is how to come up with these constitutive relations that can be used to describe MMs at the effective level. Moreover, it not just suffices to postulate them, but they always have to be equipped with the necessary interface conditions to render Maxwell's equations solvable. Our contribution here is dedicated to this problem.

In general, MMs are made from nonmagnetic materials as mentioned above. For time harmonic fields, this property is expressed by a trivial relation between the magnetic field $\mathbf{H}(\mathbf{r},\omega)$ and magnetic induction $\mathbf{B}(\mathbf{r},\omega)$. Therefore, the nonlocal constitutive relations concentrate on the link between the electric displacement $\mathbf{D}(\mathbf{r},\omega)$ and the electric field $\mathbf{E}(\mathbf{r},\omega)$. In its most comprehensive description, this relation is expressed through a convolution between a nonlocal response function $\mathbf{R}(\mathbf{r}-,\omega)$ and the electric field. Here, the response function provides the exact description. Please note, it is already written for a homogenous medium, as can be seen on the translational invariance. However, while being a useful concept, the practical application is rather negligible. First of all, an exact expression of $\mathbf{R}(\mathbf{r}-,\omega)$ for a given material is unknown and, moreover, even if their would be useful expression, we wouldn't be able to use it because at an interface its evaluation is not known.

To overcome this issue has prompted researchers to propose several polynomial approximations to the response function, that are in general of Taylor- or Padé-types, see for instance [22, 25–27]. It is well known that the considered order in the approximation determines its accuracy. Retaining only the lowest order term gives rise to a local constitutive relation where only a permittivity appears. To explain the appearance of an artificial magnetism, a second order term needs to considered [27]. Such an artificial magnetism can be expressed as a local constitutive relation using a suitable gauge transformation. However, as the artificial magnetism is indeed caused by nonlocality, one speaks here of a weak spatial dispersion (WSD). This also serves to distinguishes it from strong spatial dispersion (SSD), where a higher number of terms in the expansion are retained to form constitutive relations. A first order term actually can explain the effects of electro-magnetic coupling, but such odd order terms do not need to be considered for materials with an inversion symmetry as we do here. To improve the precision in the non-local constitutive relations, a fourth order approximations were proposed either by truncating the Taylor polynomials as in [22, 28], or by considering fractional functions in [25]. Due to the nature of the Maxwell equations and under some special considerations, these two different approaches coincide, up to multiplication with the wave number, and give the following constitutive relation

$$\mathbf{D}(\mathbf{r},\omega) = \varepsilon(\omega)\mathbf{E}(\mathbf{r},\omega) + \nabla\times\alpha(\omega)\nabla\times\mathbf{E}(\mathbf{r},\omega) + \nabla\times\nabla\times(\gamma(\omega)\nabla\times\nabla\times)\mathbf{E}(\mathbf{r},\omega),$$

for $\varepsilon(\omega)$, $\alpha(\omega)$, and $\gamma(\omega)$ being the effective material parameters. A detailed explanation of the physical meaning of these parameters can be found in [25]. Here, it is important to mention that considerable improvement of the quality of the resulting models were remarked when describing the optical response of an actual MM. This fact can be seen by measuring the difference between the reflection and transmission coefficients resulting from the proposed approximate models and those obtained numerically by fully solving the Maxwell system by the Fourier Modal Method (FMM) (cf. [29]) for a given MM.

Being motivated by the previous results, and instead of increasing the approximation with further two degrees, i.e., up to the sixth order, we suggest here, for the first time, to write an approximate nonlocal response function up to any given order. Notably, we consider a Taylor polynomial truncated at the order $2N$, for N being a positive integer. Please note, here as well, we consider only inversion symmetric MMs where odd order terms vanish [30, 31].

To characterize the light propagation in an infinitely extended medium, one usually solves the dispersion relation. It expresses the functional dependency of the components of the wave vector on the frequency of a time-harmonic plane wave. Frankly spoken, this is one equation for four paramaters. It can be solved by fixing three of them and the fourth has to be chosen to satisfy this dispersion relation. Quite frequently, the frequency and two wave vector components that are transverse to some principal propagation direction are the fixed quantities. Fore a medium with WSD, one can notice that only a single longitudinal wave vector component exists. It expresses that for a given transverse wave vector and frequency, only a single plane wave is excited. A particular feature of SSD now is the presence of additional modes [32]. It implies that for a given transverse wave vector and frequency, multiple plane waves are excited. To determine their amplitudes, for example when excited from a semi-infinite half space of vacuum, additional interface conditions are required to fix their amplitudes [33]. These additional interface conditions have to supplement always the constitutive relation in order to make use of them. We highlight that the number of these additional interface conditions depends on the approximation order of the nonlocal constitutive relation. Therefore, the second important contribution in the present paper is the rigorous derivation of all required interface conditions. For this purpose, we use the weak formulation approach. To make easy use of these interface conditions in some concrete situations, notably when writing the Fresnel coefficients by means of numerical tools, we propose a compact formula for most of them by defining an operator with an index that depends on the approximation order.

This paper is structured as follows. In Sec. 2, we set all the notations we use throughout this investigation. In Sec. 3, we recall the Maxwell equations and set the geometry of the domain in which the light propagates. We recall as well the local constitutive relations and explain their limit in the case of MMs. The alternative nonlocal constitutive relations are precised in Sec. 4. The higher order Taylor approximation for the nonlocal response function is also written explicitly. In Sec. 5, we write the wave-like Maxwell equation in the generalized sense by means of the approximate nonlocal constitutive relation. We precise as well the effective coefficients in the entire space. For the purpose of the derivation of all interface conditions, we write the physical model from which we start; it is obtained by writing the Maxwell equations in the weak sense. In Sec. 6, we derive the interface conditions and write them in compact formulas. Notably, we use the Kronecker delta and a general operator applied on the trace of the electric field on the surface separating vacuum to MM. The rigorous proof for deriving these interface conditions requires the use of certain auxiliary functions, that are given in 6.1. Some concluding remarks are drawn at the end of the paper.

2 Notations

We introduce some notations that will be used throughout the paper. Below, Ω is an *open* domain in $\mathbb{R}^n$.

- By $\mathbf{r} = (x, y, z)$ we denote points in $\mathbb{R}^3$ (spatial variable), by $\omega \in \mathbb{R}_+$ we denote the time frequency.
- $\mathbb{R}^3_+ := \{\mathbf{r} \in \mathbb{R}^3 : \ z > 0\}$, $\mathbb{R}^3_- := \{\mathbf{r} \in \mathbb{R}^3 : \ z < 0\}$, $\Gamma = \{\mathbf{r} \in \mathbb{R}^3 : \ z = 0\}$. They denote the different half-spaces above and below the interface Γ we consider.
- $\nabla\times$ is the curl with respect to $\mathbf{r}$.
- $(\mathrm{i}\mathbf{k}\times)^m := \underbrace{\mathrm{i}\mathbf{k}\times\mathrm{i}\mathbf{k}\times\ldots\mathrm{i}\mathbf{k}\times}_{m \text{ times}}, \quad (\nabla\times)^m := \underbrace{\nabla\times\nabla\times\ldots\nabla\times}_{m \text{ times}}.$
- $^{\mathrm{T}}$ is the operation of transposition.
- $\mathbf{n} = (0, 0, 1)^{\mathrm{T}}$ is the unit normal vector on Γ.
- $\mathsf{C}^m(\Omega)$, $m \leq \infty$, is the space of functions with continuous derivatives up to order m on Ω.
- $\mathsf{C}^m(\overline{\Omega})$, $m \leq \infty$, is the space of all restrictions of functions in $\mathsf{C}^m(\mathbb{R}^n)$ to $\overline{\Omega}$.
- $\mathsf{C}^m_0(\Omega)$ is the space of functions $f \in \mathsf{C}^m(\Omega)$ having compact support in Ω (i.e., $\mathrm{supp}(f) := \overline{\{x : \ f(x) \neq 0\}}$ is a compact set contained in Ω).
- $\mathsf{L}^2(\Omega)$ is the space of measurable functions $\Psi : \Omega \to \mathbb{C}$ satisfying $\int\limits_{\Omega} |\Psi(\mathbf{r})|^2 \, \mathrm{d}\mathbf{r} < \infty$.

- $\mathbf{C}^m(\Omega)$ (resp. $\mathbf{C}^m(\overline{\Omega})$, $\mathbf{C}_0^m(\Omega)$, $\mathbf{L}^2(\Omega)$) is the space of vector-functions $\mathbf{\Phi} : \Omega \to \mathbb{C}^3$ with components being in $\mathsf{C}^m(\Omega)$ (resp. $\mathsf{C}^m(\overline{\Omega})$, $\mathsf{C}_0^m(\Omega)$, $\mathsf{L}^2(\Omega)$).

- $\mathsf{L}^2_{\text{loc}}(\Omega)$ (resp. $\mathbf{L}^2_{\text{loc}}(\Omega)$) is the space of scalar (resp. vector-valued) functions belonging to $\mathsf{L}^2(\widehat{\Omega})$ (resp. $\mathbf{L}^2(\widehat{\Omega})$) for each subdomain $\widehat{\Omega} \subset \Omega$, such that $\overline{\widehat{\Omega}} \subset \Omega$ is compact.

- I is the identity (3×3)-matrix .

3 Maxwell's equations

In the present research, the propagation of light is assumed to take place in $\mathbb{R}^3$. The upper-half space $\mathbb{R}^3_+$ is occupied by vacuum and the lower-half space $\mathbb{R}^3_-$ is occupied by a MM. We suppose that the MM is made from non-magnetic media. The interface separating the upper-half space to the lower-half space is denoted by Γ. The unit normal vector $\mathbf{n}$ is directed outward from the MM (see Figure 1). For the sake of simplicity, we assume that the electromagnetic MM we are

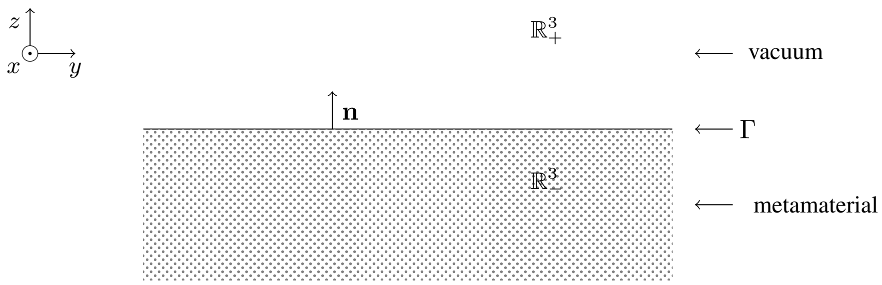

Figure 1: Illustration of the domain in which the light propagates, the upper-half space is occupied by vacuum and the lower-half space is occupied by a MM. The surface separating the two half-spaces is denoted Γ. The normal $\mathbf{n}$ is outward directed from the homogenized MM.

considering is centro-symmetric. A classical example of such structure, which is usually utilized in the literature, is the Fishnet MM (see, e.g., [27]).

In the absence of external charges and currents, the harmonic Maxwell's equations describing the propagation of light in a material are given by

$$\nabla \times \mathbf{E}(\mathbf{r},\omega) - \mathrm{i}k_0\mathbf{B}(\mathbf{r},\omega) = 0, \qquad \nabla \cdot \mathbf{B}(\mathbf{r},\omega) = 0, \tag{1a}$$

$$\nabla \times \mathbf{H}(\mathbf{r},\omega) + \mathrm{i}k_0\mathbf{D}(\mathbf{r},\omega) = 0, \qquad \nabla \cdot \mathbf{D}(\mathbf{r},\omega) = 0. \tag{1b}$$

The four fields appearing here depend on the position $\mathbf{r}$ and the frequency ω in $\mathbb{R}^3 \times \mathbb{R}_+ \longrightarrow \mathbb{C}^3$. Here, k_0 refers to the wavenumber of the external monochromatic light, it is given by the relation $k_0 = \dfrac{\omega}{c}$, such that c refers to the speed of light.

In order to fully define the Maxwell system within the considered domain, we should provide the interface conditions defined on the surface Γ. They can be derived by means of the relations between the electromagnetic fields $(\mathbf{E}, \mathbf{H})$ and the electromagnetic inductions $(\mathbf{B}, \mathbf{D})$. These relations represent the constitutive relations when considering the MM at the effective level.

For local and homogeneous materials, the fields $\mathbf{D}$ and $\mathbf{H}$ depend linearly on the macroscopic fields $\mathbf{E}$ and $\mathbf{B}$ as follows

$$\mathbf{D}(\mathbf{r},\omega) = \mathbf{E}(\mathbf{r},\omega) + \mathbf{P}[\mathbf{E},\mathbf{B}](\mathbf{r},\omega), \tag{2a}$$

$$\mathbf{H}(\mathbf{r},\omega) = \mathbf{B}(\mathbf{r},\omega) - \mathbf{M}[\mathbf{B},\mathbf{E}](\mathbf{r},\omega), \tag{2b}$$

here, $\mathbf{P}$ and $\mathbf{M}$ represent, respectively, the polarization and magnetization. We can see clearly that they depend on $\mathbf{E}$ and $\mathbf{B}$ at the same spatial location $\mathbf{r}$. We emphasize explicitly that this local dependency leads to what we call local constitutive relations, and all relations which are of nonlocal character, such as convolution, do not make part of this kind of material laws. Furthermore, for materials with central symmetry the polarization $\mathbf{P}$ does not depend on $\mathbf{B}$ and the magnetization $\mathbf{M}$ does not depend on $\mathbf{E}$. This fact can be expressed by the absence of electromagnetic cross-coupling. Then, we can write simply the polarization and magnetization as follows: $\mathbf{P}[\mathbf{E}](\mathbf{r},\omega)$ and $\mathbf{M}[\mathbf{B}](\mathbf{r},\omega)$. Moreover, basically non-magnetic materials have a null magnetization, i.e., $\mathbf{M} \equiv 0$. Please note, such constitutive relation correspond to the usual realm of classical macroscopic electrodynamics when considering natural materials (see for instance [1]).

For such local constitutive relations (2), the interface conditions on the surface Γ are given by the continuity of the tangential components of the electromagnetic fields, i.e.,

$$[\mathbf{E} \times \mathbf{n}] \,|_\Gamma = 0, \qquad [\mathbf{H} \times \mathbf{n}] \,|_\Gamma = 0. \tag{3}$$

These interface conditions are enough for defining the propagating modes in mediums with WSD but not for mediums with SSD such as MMs. However, such local constitutive relation combined with such ordinary interface conditions are insufficient for MMs. They require nonlocal constitutive relations that are considered in the next section.

4 Non-local constitutive relations

Under the assumption that the considered MMs are non magnetic, we assume all the time a linear relation between the magnetic induction and the magnetic field as $\mathbf{H} = \mathbf{B}$. Nonlocal effects are present in the response tensor linking the electric field to the electric displacement. Notably, when considering the response of MMs to an exiting electric field at a given point $\mathbf{r}$, the response is affected by the electric field also from distant points $\mathbf{r}'$, which are located in a certain spatial domain around the observation point $\mathbf{r}$. At the effective level, the material law describing this nonlocal effect can be written in the real apace in the following general form

$$\mathbf{D}(\mathbf{r}, \omega) = \int_{\mathbb{R}^3} \mathbf{R}(\mathbf{r} - \mathbf{r}', \omega)\mathbf{E}(\mathbf{r}', \omega) \, \mathrm{d}\mathbf{r}', \tag{4}$$

which is a convolution of the response function $\mathbf{R}(\mathbf{r}-, \omega)$ with the exciting electric field $\mathbf{E}$. In the case where the response kernel $\mathbf{R}(\mathbf{r}-, \omega)$ holds distributional terms, mathematically it is more accurate to write the nonlocal constitutive relation (4) in the form of a distributional action as follows:

$$\mathbf{D}(\mathbf{r}, \omega) = \langle \, \mathbf{R}(\mathbf{r} - \cdot, \omega), \mathbf{E}(\cdot, \omega) \, \rangle \, . \tag{5}$$

Usually, there exist no explicit formula for the response $\mathbf{R}(\mathbf{r}-, \omega)$. Therefore, it is practically relevant to simplify it. We start by writing (4) in the spatial frequency space

$$\widehat{\mathbf{D}}(\mathbf{k}, \omega) = \widehat{\mathbf{R}}(\mathbf{k}, \omega)\widehat{\mathbf{E}}(\mathbf{k}, \omega), \tag{6}$$

where $\widehat{\mathbf{R}}(\mathbf{k}, \omega)$ is the spatial Fourier transform of $\mathbf{R}(\mathbf{r}, \omega)$, and the same for the other fields in (4). In the literature, several approximations for the unknown function $\widehat{\mathbf{R}}(\mathbf{k}, \omega)$ have been considered (see, e.g., [22, 25, 27]). The most advanced ones are up to the fourth order. Namely, a Taylor approximation truncated at the fourth order (see [22]) and a Padé-like approximations (see [25]) were considered. The latter one is written by means of rational functions, i.e., the quotient of two polynomials of order two. Both approaches seem to be different, but due to the nature of the Maxwell equations they coincide in some cases. This is why in the present research we consider a general Taylor approximate response function $\widehat{\mathbf{R}}(\mathbf{k}, \omega)$ which is valid at any order, given by

$$\widehat{\mathbf{R}}(\mathbf{k}, \omega) = \varepsilon(\omega) + \sum_{n=1}^{N} \sum_{m=0}^{2n} (-\mathrm{i}\mathbf{k}\times)^m \alpha_{n,m}(\omega)(-\mathrm{i}\mathbf{k}\times)^{2n-m}. \tag{7}$$

The material parameters ε and $\alpha_{n,m}$ are $\mathbb{C}^{3\times 3}$ anisotropic diagonal matrices with smooth and bounded entries depending on the frequency ω.

After backward Fourier transform, the polynomial approximation (7) amounts to the following differential operator

$$\mathbf{R}(\mathrm{i}\nabla, \omega) = \varepsilon(\omega) + \sum_{n=1}^{N} \sum_{m=0}^{2n} (\nabla\times)^m \alpha_{n,m}(\omega)(\nabla\times)^{2n-m}. \tag{8}$$

Finally, the nonlocal constitutive relation describing the behavior of MMs in the real space is given by

$$\mathbf{D}(\mathbf{r}, \omega) = \varepsilon(\omega)\mathbf{E}(\mathbf{r}, \omega) + \sum_{n=1}^{N} \sum_{m=0}^{2n} (\nabla\times)^m \alpha_{n,m}(\nabla\times)^{2n-m}\mathbf{E}(\mathbf{r}, \omega). \tag{9}$$

How does this nonlocal material law affects the wave-like equation for the Maxwell system, that describes the electromagnetic response in medium with SSD, will be discussed in the next section.

5 Generalized solutions

We know that the material properties for the two half spaces are different. Notably, the upper half-space-vacuum is a medium with WSD governed by local constitutive relations; for which the relative permittivity ε is equal to one. The lower half-space-MM is a medium with SSD governed by a nonlocal constitutive relation; it is characterized by the effective electric permittivity ε and the parameters $\alpha_{n,m}$ for which we do not have a specific physical explanation until now. Therefore, in the entire space we can regroup the material laws as follows

$$\mathbf{D}(\mathbf{r},\omega) = \begin{cases} \mathbf{E}(\mathbf{r},\omega), & \text{in } \mathbb{R}_+, \\ \varepsilon(\omega)\mathbf{E}(\mathbf{r},\omega) + \sum_{n=1}^{N}\sum_{m=0}^{2n}(\nabla\times)^m\alpha_{n,m}(\nabla\times)^{2n-m}\mathbf{E}(\mathbf{r},\omega), & \text{in } \mathbb{R}_-. \end{cases} \tag{10}$$

We recall the wave-like equation for the Maxwell system, written for the electric field

$$\nabla\times\nabla\times\mathbf{E}(\mathbf{r},\omega) = k_0^2\mathbf{D}(\mathbf{r},\omega). \tag{11}$$

By substituting the constitutive relations (10) into (11), we can write the $\mathbf{E}$-formulation for the Maxwell equations formally as follows

$$\nabla\times\nabla\times\mathbf{E}(\mathbf{r},\omega) = k_0^2\widetilde{\varepsilon}\mathbf{E}(\mathbf{r},\omega) + k_0^2\sum_{n=1}^{N}\sum_{m=0}^{2n}(\nabla\times)^m\widetilde{\alpha}_{n,m}(\nabla\times)^{2n-m}\mathbf{E}(\mathbf{r},\omega). \tag{12}$$

The material parameters $\widetilde{\varepsilon}$ and $\widetilde{\alpha}_{n,m}$ are given by

$$\widetilde{\varepsilon} = \begin{cases} I, & z>0, \\ \varepsilon, & z<0, \end{cases} \qquad \widetilde{\alpha}_{n,m} = \begin{cases} 0, & z>0, \\ \alpha_{n,m}, & z<0, \end{cases}$$

such that ε and $\alpha_{n,m}$ are, as assumed in Sec. 4, $\mathbb{C}^{3\times3}$ anisotropic diagonal matrices with smooth and bounded entries that are depending on the frequency ω.

Due to the discontinuity of the matrix-functions $\widetilde{\varepsilon}$ and $\widetilde{\alpha}_{n,m}$, we are not allowed to regard the differential expression on the right-hand-side of the equation (12) in the classical sense. The natural idea is then to treat this equation in a suitable generalised (or weak) sense. Namely, being inspired by our previous contributions [22, 25], the vector-valued function $\mathbf{E}:\mathbb{R}^3\times\mathbb{R}_+\to\mathbb{C}^3$ is said to be *a weak (or generalized) solution* to the wave equation (12) if it meets the regularity properties

$$\mathbf{E}\in\mathbf{L}^2_{\text{loc}}(\mathbb{R}^3), \qquad \nabla\times\mathbf{E}\in\mathbf{L}^2_{\text{loc}}(\mathbb{R}^3), \qquad \text{and} \qquad \alpha_{n,m}(\nabla\times)^{2n-m}\mathbf{E}\in\mathbf{L}^2_{\text{loc}}(\mathbb{R}^3_-), \tag{13}$$

for $n=1,\cdots,N$ and $m=0,\cdots,2n$, and moreover, for each vector-valued function $\mathbf{\Phi}\in\mathbf{C}_0^\infty(\mathbb{R}^3)$ the following integral identity holds:

$$\int_{\mathbb{R}^3}(\nabla\times\mathbf{E})\cdot(\nabla\times\mathbf{\Phi})\,\mathrm{d}\mathbf{r} = k_0^2\int_{\mathbb{R}^3_+}\mathbf{E}\cdot\mathbf{\Phi}\,\mathrm{d}\mathbf{r} + k_0^2\int_{\mathbb{R}^3_-}\varepsilon\mathbf{E}\cdot\mathbf{\Phi}\,\mathrm{d}\mathbf{r} + k_0^2\sum_{n=1}^{N}\sum_{m=0}^{2n}\int_{\mathbb{R}^3_-}(\alpha_{n,m}(\nabla\times)^{2n-m}\mathbf{E})\cdot((\nabla\times)^m\mathbf{\Phi})\,\mathrm{d}\mathbf{r}. \tag{14}$$

In the following, we will always require additional regularity on the weak solutions to the equation (12), namely

$$\mathbf{E}_+\in\mathsf{C}^{2N}(\overline{\mathbb{R}^3_+}),\ \mathbf{E}_-\in\mathsf{C}^{2N}(\overline{\mathbb{R}^3_-}), \tag{15}$$

where $\mathbf{E}_\pm := \mathbf{E}\restriction_{\mathbb{R}^3_\pm}$. Apparently, these additional smoothness conditions are indeed satisfied if the material parameters ε and $\alpha_{n,m}$ are constant matrix-functions (at least in the case where the differential equation (17) below is elliptic). Note that the interface conditions we are going to derive in the next section under the additional assumption (15) also remain valid when only our conditions (13) are satisfied. But then they hold only in some generalized sense which needs the concept of traces; cf. [28] for more details.

It is easy to show that if $\mathbf{E}$ is a weak solution to the equation (12) and the properties (15) hold, then

$$\nabla\times\nabla\times\mathbf{E} = k_0^2\mathbf{E} \quad \text{in } \mathbb{R}^3_+, \tag{16}$$

$$\nabla\times\nabla\times\mathbf{E} = k_0^2\varepsilon\mathbf{E} + k_0^2\sum_{n=1}^{N}\sum_{m=0}^{2n}(\nabla\times)^m\alpha_{n,m}(\nabla\times)^{2n-m}\mathbf{E} \quad \text{in } \mathbb{R}^3_-. \tag{17}$$

Indeed, taking $\mathbf{\Phi}\in\mathbf{C}_0^\infty(\mathbb{R}^3_-)$ in (14) we get

$$\int_{\mathbb{R}^3_-}(\nabla\times\mathbf{E})\cdot(\nabla\times\mathbf{\Phi})\,\mathrm{d}\mathbf{r} = k_0^2\int_{\mathbb{R}^3_-}\varepsilon\mathbf{E}\cdot\mathbf{\Phi}\,\mathrm{d}\mathbf{r} + k_0^2\sum_{n=1}^{N}\sum_{m=0}^{2n}\int_{\mathbb{R}^3_-}\left(\alpha_{n,m}(\nabla\times)^{2n-m}\mathbf{E}\right)\cdot\left((\nabla\times)^m\mathbf{\Phi}\right)\,\mathrm{d}\mathbf{r}. \tag{18}$$

Integrating by parts and taking into account that $\mathbf{\Phi}$ vanishes in a neighborhood of Γ (thus no surface integrals over Γ appear) we deduce from (18)

$$\int_{\mathbb{R}^3_-} \left(\nabla \times \nabla \times \mathbf{E} - k_0^2 \varepsilon \mathbf{E} - k_0^2 \sum_{n=1}^{N} \sum_{m=0}^{2n} (\nabla \times)^m \alpha_{n,m} (\nabla \times)^{2n-m} \mathbf{E} \right) \cdot \mathbf{\Phi} \ \mathrm{d}\mathbf{r} = 0,$$

hence, taking into account the arbitrariness of $\mathbf{\Phi}$, we obtain (17). The proof of (16) is similar. Thus in both half-spaces weak solutions are also classical solutions provided smoothness assumptions (15) hold.

6 Derivation of interface conditions

Our main interest in the present research is to prove that if $\mathbf{E}$ is a generalized solution of the equation (12) and satisfies the regularity assumptions (15), then $\mathbf{E}$ satisfies the following interface conditions on Γ:

$$(\mathbf{E}_+ - \mathbf{E}_-) \times \mathbf{n} = 0, \tag{19a}$$

$$\delta_{k0} (\nabla \times \mathbf{E}_+ - \nabla \times \mathbf{E}_-) \times \mathbf{n} + \mathbb{L}_k \mathbf{E}_- \times \mathbf{n} = 0 \quad \text{for} \quad k \in \{0, ..., 2N-1\}, \tag{19b}$$

where δ_{k0} is the Kronecker delta (i.e., $\delta_{k0} = 1$ as $k = 0$ and $\delta_{k0} = 0$ as $k \neq 0$), the surface operator $\mathbb{L}_k$ acts on $\mathbf{E}_-$ as follows

$$\mathbb{L}_k \mathbf{E}_- = k_0^2 \sum_{n=\lceil \frac{k+1}{2} \rceil}^{N} \sum_{m=k+1}^{2n} (\nabla \times)^{m-(k+1)} \alpha_{n,m} (\nabla \times)^{2n-m} \mathbf{E}_-, \qquad k \in \{0, 1, ..., 2N-1\}. \tag{20}$$

We recall that $\lceil \cdot \rceil$ is the ceiling function, it maps $x \in \mathbb{R}$ to the least integer greater than or equal to x.

The $2N+1$ equations (19a), (19b) are not necessarily independent. A part of them may even read $0 = 0$, if some of the matrices $\alpha_{n,m}$ are zero. Hence, (19a), (19b) constitute at most $2N+1$ independent interface conditions. This set of interface conditions is complete in the following sense: if the vector-valued function $\mathbf{E}$ satisfies (15), solves (16) in $\mathbb{R}^3_+$, solves (17) in $\mathbb{R}^3_-$, and the interface conditions (19a)–(19b) are fulfilled, then $\mathbf{E}$ is a generalized solution to the wave equation (12); see Sec. 6.4.

We emphasize that the derivation of the interface conditions (19b), by means of the weak formulation approach, requires the use of some auxiliary functions. In the next sub-section, we will present the explicit formulas of these functions.

6.1 Auxiliary test functions

Recall that by $\mathbf{r} = (x, y, z)$ we denote points in $\mathbb{R}^3$. To justify the above interface conditions we will use special test-functions $\mathbf{\Phi}_n$ of the form

$$\mathbf{\Phi}_n(\mathbf{r}) = \left(\Phi_1(x,y) z^n \chi(z), \Phi_2(x,y) z^n \chi(z), 0 \right)^T, \quad n \geq 0, \tag{21}$$

where $\Phi_1, \Phi_2 \in \mathsf{C}_0^\infty(\mathbb{R}^2)$, $\chi \in \mathsf{C}_0^\infty(\mathbb{R})$ such that $\chi(z) = 1$ in a neighborhood of 0. Evidently,

$$\mathbf{\Phi}_n(\mathbf{r})|_\Gamma = \begin{cases} (\Phi_1, \Phi_2, 0)^T, & n = 0, \\ (0, 0, 0)^T, & n > 0. \end{cases} \tag{22}$$

Moreover, we briefly state a general formula of $(\nabla \times)^k \mathbf{\Phi}_n|_\Gamma$, for $k \leq n$. Induction yields:

$$(\nabla \times)^k \mathbf{\Phi}_n(\mathbf{r}) = \begin{pmatrix} \left(z^n \chi(z) \right)^{(k)} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}^k \begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix} \\ 0 \end{pmatrix} + \mathcal{R}_k.$$

Here, the remainder terms $\mathcal{R}_k$ depend linearly on the derivatives $\big(z^n\chi(z)\big)^{(j)}$ with $j < k \le n$. Since $\big(z^n\chi(z)\big)^{(j)}|_{z=0} = n!$ if $j = n$, and $= 0$ if $j < n$, we obtain

$$k = 1,\dots,2N-1: \qquad (\nabla\times)^k \mathbf{\Phi}_n(\mathbf{r})|_\Gamma = \begin{cases} \begin{pmatrix} n! \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}^k \begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix} \\ 0 \end{pmatrix}, & k = n, \\ \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, & k < n. \end{cases} \tag{23}$$

We highlight that when taking into consideration the parity of the order k, one can go further by giving explicit formulas for the multiplication constants in (23). They are represented through the 2×2 rotation matrix and their present formula is sufficient for the proof of the interface conditions (19b).

Now, we can present the proof of deriving all interface conditions. We split it in the next two sub-sections.

6.2 Proof of the interface condition (19a)

The first interface condition is a well-known consequence of the conditions

$$\mathbf{E} \in \mathbf{L}^2_{\text{loc}}(\mathbb{R}^3), \qquad \nabla\times\mathbf{E} \in \mathbf{L}^2_{\text{loc}}(\mathbb{R}^3).$$

For convenience of the reader, we repeat here the arguments. The distributional definition of $\nabla\times\mathbf{E}$, for each $\mathbf{\Phi} \in \mathbf{C}_0^\infty(\mathbb{R}^3)$, is given by

$$\int_{\mathbb{R}^3} \mathbf{E}\cdot(\nabla\times\mathbf{\Phi})\,\mathrm{d}\mathbf{r} = \int_{\mathbb{R}^3} (\nabla\times\mathbf{E})\cdot\mathbf{\Phi}\,\mathrm{d}\mathbf{r}, \tag{24}$$

while integrating by parts in each half-space we get

$$\begin{aligned} \int_{\mathbb{R}^3} (\nabla\times\mathbf{E})\cdot\mathbf{\Phi}\,\mathrm{d}\mathbf{r} &= \int_{\mathbb{R}^3_-} (\nabla\times\mathbf{E})\cdot\mathbf{\Phi}\,\mathrm{d}\mathbf{r} + \int_{\mathbb{R}^3_+} (\nabla\times\mathbf{E})\cdot\mathbf{\Phi}\,\mathrm{d}\mathbf{r} \\ &= \int_{\mathbb{R}^3_-} \mathbf{E}\cdot(\nabla\times\mathbf{\Phi})\,\mathrm{d}\mathbf{r} + \int_{\mathbb{R}^3_+} \mathbf{E}\cdot(\nabla\times\mathbf{\Phi})\,\mathrm{d}\mathbf{r} + \int_\Gamma (\mathbf{E}_+\times\mathbf{n} - \mathbf{E}_-\times\mathbf{n})\cdot\mathbf{\Phi}\,\mathrm{d}s \\ &= \int_{\mathbb{R}^3} \mathbf{E}\cdot(\nabla\times\mathbf{\Phi})\,\mathrm{d}\mathbf{r} + \int_\Gamma (\mathbf{E}_+\times\mathbf{n} - \mathbf{E}_-\times\mathbf{n})\cdot\mathbf{\Phi}\,\mathrm{d}s. \end{aligned} \tag{25}$$

Here $\mathrm{d}s = \mathrm{d}x\,\mathrm{d}y$ is the area of the surface element on Γ. The first interface condition (19a) follows from (24)-(25) and the arbitrariness of $\mathbf{\Phi}$.

6.3 Proof of the interface condition (19b)

To justify the remaining interface conditions we represent the integral in the left-hand-side of (14) as a sum of two integrals, over $\mathbb{R}^3_+$ and $\mathbb{R}^3_-$. Then in each term in (14) we integrate by parts "shifting" all $(\nabla\times)-$derivatives from the test function $\mathbf{\Phi}$ to the electric field $\mathbf{E}$. As a result we get

$$\begin{aligned} &\int_{\mathbb{R}^3_+} \big((\nabla\times\nabla\times\mathbf{E}) - k_0^2\mathbf{E}\big)\cdot\mathbf{\Phi}\,\mathrm{d}\mathbf{r} + \int_{\mathbb{R}^3_-} \left((\nabla\times\nabla\times\mathbf{E}) - k_0^2\varepsilon\mathbf{E} - k_0^2\sum_{n=1}^{N}\sum_{m=0}^{2n}(\nabla\times)^m\alpha_{n,m}(\nabla\times)^{2n-m}\mathbf{E}\right)\cdot\mathbf{\Phi}\,\mathrm{d}\mathbf{r} \\ &= \int_\Gamma \big((\nabla\times\mathbf{E}_+ - \nabla\times\mathbf{E}_-)\times\mathbf{n}\big)\cdot\mathbf{\Phi}\,\mathrm{d}s + k_0^2\sum_{n=1}^{N}\sum_{m=1}^{2n}\sum_{k=0}^{m-1}\int_\Gamma \Big(\big((\nabla\times)^k\alpha_{n,m}(\nabla\times)^{2n-m}\mathbf{E}_-\big)\times\mathbf{n}\Big)\cdot(\nabla\times)^{m-k-1}\mathbf{\Phi}\,\mathrm{d}s. \end{aligned} \tag{26}$$

Please note that for $m = 0$ in the right-hand-side in (14), there will be no $(\nabla\times)-$derivatives to be shifted from the test function $\mathbf{\Phi}$ to the electric field $\mathbf{E}$. Therefore, the sum with respect to m for surface integrals in the right-hand-side in (26) starts from one and not zero as in the left-hand-side for volume integrals.

Moreover, the left-hand side in (26) vanishes due to (16)-(17), hence the right-hand-side vanishes too. Then, by changing the order of summation, we can write

$$\int_\Gamma \big((\nabla \times \mathbf{E}_+ - \nabla \times \mathbf{E}_-) \times \mathbf{n}\big) \cdot \mathbf{\Phi} \, \mathrm{d}s + \sum_{k=0}^{2N-1} \int_\Gamma (\mathbb{L}_k \mathbf{E}_- \times \mathbf{n}) \cdot (\nabla\times)^k \mathbf{\Phi} \, \mathrm{d}s = 0, \tag{27}$$

where the operators $\mathbb{L}_k$ are defined by (20). We explain a little bit more about how the changing of summations is made. When the index n takes its upper value N, then $m \leq 2N$ and $k \leq 2N-1$. It implies that we have always $n \geq \frac{k+1}{2}$. Here, we remark that the index n may have non-integer values when k is even. Furthermore, the lowest value that the index n may have is 1. Therefor, the use the ceiling function by writing $n \geq \lceil \frac{k+1}{2} \rceil$ allows to write the right lower bound in the new adopted summation order. Regarding the index m, since we have in (26) that $k \leq m-1$, then in the new order we have directly $m \geq k+1$.

Now, we insert into (27) the test-function $\mathbf{\Phi} = \mathbf{\Phi}_{2N-1}$; recall that the functions $\mathbf{\Phi}_n$ are defined by (21). Taking into account (22)-(23) we conclude that the first integral in (27) vanishes, and also all terms with $k < 2N-1$ in the sum $\sum_{k=0}^{2N-1} \int_\Gamma (\dots) \, \mathrm{d}s$ are equal to zero. Thus, only the term with $k = 2N-1$ survives

$$\int_\Gamma (\mathbb{L}_{2N-1} \mathbf{E}_- \times \mathbf{n}) \cdot (\nabla\times)^{2N-1} \mathbf{\Phi} \, \mathrm{d}s = 0. \tag{28}$$

Due to (23), the tangential components of $(\nabla\times)^{2N-1}\mathbf{\Phi}|_\Gamma$ coincides with $\Phi_2, \ \Phi_1$, up to multiplication by the constants given through the following matrix: $(2N-1)! \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}^{2N-1}$.

From (28), the arbitrariness of Φ_1, Φ_2 implies

$$\mathbb{L}_{2N-1} \mathbf{E}_- \times \mathbf{n} = 0 \quad \text{on} \quad \Gamma. \tag{29}$$

On the next step we insert into (27) the test-function $\mathbf{\Phi} = \mathbf{\Phi}_{2N-2}$. Again, by virtue of (22)-(23), the first integral in (27) equals zero, also all terms with $k < 2N-2$ vanish. Moreover, due to (29) the term with $k = 2N-1$ vanishes too. Consequently,

$$\int_\Gamma (\mathbb{L}_{2N-2} \mathbf{E}_- \times \mathbf{n}) \cdot (\nabla\times)^{2N-2} \mathbf{\Phi} \, \mathrm{d}s = 0.$$

Once again, by (23) the tangential components of $(\nabla\times)^{2N-2}\mathbf{\Phi}|_\Gamma$ coincides with $\Phi_1, \ \Phi_2$, up to multiplication this time by the constants given through: $(2N-2)! \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}^{2N-2}$.

While $\Phi_1, \Phi_2 \in \mathsf{C}^\infty(\mathbb{R}^2)$ are arbitrary functions. Hence

$$\mathbb{L}_{2N-2} \mathbf{E}_- \times \mathbf{n} = 0 \quad \text{on} \quad \Gamma.$$

Repeating verbatim the above arguments (i.e., successively inserting into (27) the test-functions $\mathbf{\Phi}_{2N-3}$, $\mathbf{\Phi}_{2N-4}$, ..., $\mathbf{\Phi}_1$, $\mathbf{\Phi}_0$ and then using (22)-(23) and interface conditions established on the previous steps) we arrive at the rest of the interface conditions (19b).

We emphasize that previously starting from the definition of the weak formulation corresponding to the wave equation (12) and the regularities making the integrals in (14) well defined, we could derive all interface conditions. In order to complete the proof, we will check the opposite direction in next sub-section.

6.4 Proof of the completeness of interface conditions

The regularities

$$\mathbf{E} \in \mathbf{L}^2_{\mathrm{loc}}(\mathbb{R}^3) \quad \text{and} \quad \alpha_{n,m} (\nabla\times)^{2n-m} \mathbf{E} \in \mathbf{L}^2_{\mathrm{loc}}(\mathbb{R}^3_-),$$

for $n = 1, \cdots, N$ and $m = 1, \cdots, 2n$, follow from (15). The interface condition (19a) implies

$$\nabla \times \mathbf{E} \in \mathbf{L}^2_{\mathrm{loc}}(\mathbb{R}^3).$$

To obtain (14), we note that for an arbitrary function $\mathbf{\Phi} \in \mathbf{C}_0^\infty(\mathbb{R}^3)$ one has the following integral identity:

$$\int_{\mathbb{R}^3_+} \Big((\nabla \times \nabla \times \mathbf{E}) - k_0^2 \mathbf{E} \Big) \cdot \mathbf{\Phi} \, \mathrm{d}\mathbf{r}$$
$$+ \int_{\mathbb{R}^3_-} \Big(\nabla \times \nabla \times \mathbf{E} - k_0^2 \varepsilon \mathbf{E} - k_0^2 \sum_{n=1}^{N} \sum_{m=0}^{2n} (\nabla \times)^m \alpha_{n,m} (\nabla \times)^{2n-m} \mathbf{E} \Big) \cdot \mathbf{\Phi} \, \mathrm{d}\mathbf{r}$$
$$= \int_\Gamma \big((\nabla \times \mathbf{E}_+ - \nabla \times \mathbf{E}_-) \times \mathbf{n} \big) \cdot \mathbf{\Phi} \, \mathrm{d}s + \sum_{k=0}^{2N-1} \int_\Gamma (\mathbb{L}_k \mathbf{E}_- \times \mathbf{n}) \cdot (\nabla \times)^k \mathbf{\Phi} \, \mathrm{d}s$$
$$+ \int_{\mathbb{R}^3} (\nabla \times \mathbf{E}) \cdot (\nabla \times \mathbf{\Phi}) \, \mathrm{d}\mathbf{r} - k_0^2 \int_{\mathbb{R}^3_+} \mathbf{E} \cdot \mathbf{\Phi} \, \mathrm{d}\mathbf{r} - k_0^2 \int_{\mathbb{R}^3_-} \varepsilon \mathbf{E} \cdot \mathbf{\Phi} \, \mathrm{d}\mathbf{r}$$
$$- k_0^2 \sum_{n=1}^{N} \sum_{m=0}^{2n} \int_{\mathbb{R}^3_-} \big(\alpha_{n,m} (\nabla \times)^{2n-m} \mathbf{E} \big) \cdot \big((\nabla \times)^m \mathbf{\Phi} \big) \, \mathrm{d}\mathbf{r}. \quad (30)$$

Since the left-hand side of (30) vanishes due to (16)-(17), while the sum of the integrals over Γ vanishes due to (19b), we conclude that (30) implies (14).

7 Conclusion

In conclusion, while retaining nonlocal effects when describing the propagation of light in MMs, we depart from a nonlocal response function linking the electric displacement to the electric field. This function grants the exact description of the optical effects in MMs, without possessing an explicit formula. It is a long-standing dream of researchers revealing this exact characterization. To do this, motivated from previous investigations providing several approximations for the response function, we propose in this article a general Taylor approximation written for any given order; followed with a hierarchy of additional interface conditions written in only one compact indexed formula by means of the Kronecker delta and a general differential operator. The approach we follow is based on writing the wave-like Maxwell equation in a weak form. We do believe that the proposed models makes the realization of our main concern very close to be achieved. Moreover, the simplified formulas for the interface conditions will definitely facilitate the task for doing further research on this topic and make it more practical especially when using numerical tools.

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