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Additional Boundary Conditions for Spatially Dispersive Media

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Abstract

In this paper we give a review of the current state in the investigations of spatially dispersive media and, especially, of the problems involving interface boundaries between such media.

1. Introduction

Natural and artificial media are dispersive (though rather weakly sometimes). We know two types of dispersion: temporal dispersion and spatial dispersion. Temporal dispersion results in different electromagnetic properties of media at different frequencies. This phenomenon occurs due to inertiality and (or) resonance behaviour of the medium polarization response. The effects of temporal dispersion are well known and investigated. No specific knowledge of the electromagnetic properties of media boundaries is needed to account for temporal dispersion. Mathematically, dispersion of this kind is described by frequency dependence of the medium material parameters.

Spatial dispersion is often more complicated to study. One of the reasons of that is difficulty in studying interfaces between media. Here the medium response is spatially nonlocal. This fact results in more complicated material relations and the increased complexity gives us differential equations for the fields having higher order than the usual ones. Hence, to solve a boundary value problem for a spatially dispersive medium we should use some additional boundary conditions.

Most of the results for spatially dispersive media were obtained for materials with the first-order spatial dispersion called reciprocal bianisotropic media. The theory shows that for the first-order spatial dispersion we can find such a form of the constitutive relations that no additional boundary conditions are necessary. The problem of the additional boundary conditions has been considered in the literature (e.g., [1, 2, 3]), but no general method for obtaining additional boundary conditions is available. Moreover, this question still causes conceptual problems, see recent paper [5] where the very necessity of additional boundary conditions is negated.

2. Theoretical Description of Spatially Dispersive Media

From the point of view of macroscopic electrodynamics the spatial dispersion phenomenon can be described by two main approaches. The first one deals with integral operators and the second one uses spatial derivatives of the fields. These approaches mostly lead to similar results especially when Fourier space-transformed field equations are used. In such a case the set of the Maxwell equations together with the material relations for a spatially dispersive medium is reduced to a dispersion equation from which the propagation factors of the medium eigenwaves can be found. Here the spatial dispersion shows itself by appearance of new dispersion branches of eigenwaves.

Till today there is some misunderstanding in the macroscopic theory of the constitutive relations and the boundary conditions for spatially dispersive media. Different authors use different forms of relations to describe media of the same type. In non-magnetic media all the polarization effects can be described only with the help of the averaged electric polarization current in the medium. Using this method (valid also as a model of higher-order dispersion effects), one writes

$$\mathbf{D}'(\omega,\mathbf{k}) = \overline{\overline{\varepsilon}}'(\omega,\mathbf{k})\cdot\mathbf{E}(\omega,\mathbf{k}), \qquad \mathbf{B}(\omega,\mathbf{k}) = \mu_0\mathbf{H}'(\omega,\mathbf{k}) \tag{1}$$

Here $\overline{\overline{\varepsilon}}'(\omega,\mathbf{k})$ takes into account magnetoelectric interaction and induced magnetism in the medium. On the other hand, phenomenologically considering non-magnetic media with first-order spatial dispersion, the relations can be written in a symmetric way with no explicit dependence on the wave vector:

$$\begin{aligned} \mathbf{D}(\omega) &= \overline{\overline{\varepsilon}}(\omega)\cdot\mathbf{E}(\omega) + \overline{\overline{\kappa}}(\omega)\cdot\mathbf{H}(\omega) \\ \mathbf{B}(\omega) &= -\overline{\overline{\kappa}}^T(\omega)\cdot\mathbf{E}(\omega) + \overline{\overline{\mu}}(\omega)\cdot\mathbf{H}(\omega) \end{aligned} \tag{2}$$

It is often asked: which form of the constitutive relations is "more correct": symmetric (2) or nonsymmetric (1)? The answer is that both are correct[1] but only with appropriate boundary conditions.

Indeed, if vectors $\mathbf{E}$ and $\mathbf{B}$ are considered as defined by the Lorentz force, then $\mathbf{D}$ and $\mathbf{H}$ should be considered as auxiliary vectors. It is known that there is some freedom in the definition of $\mathbf{D}$ and $\mathbf{H}$. The Maxwell equations do not change under the following transformation with an arbitrary differentiable vector $\mathbf{T}$:

$$\mathbf{D} = \mathbf{D}' + \nabla\times\mathbf{T}, \qquad \mathbf{H} = \mathbf{H}' + j\omega\mathbf{T} \tag{3}$$

It can be shown that if one properly finds the necessary form of vector $\mathbf{T}$, the two systems of the constitutive relations (1) and (2) can be converted one into the other.

We want to emphasize here that not only the constitutive relations change under transformation (3). The boundary conditions involving the auxiliary vectors should be transformed too. This fact is sometimes ignored and the same boundary conditions (the usual Maxwellian plus some additional phenomenological conditions if needed) are used together with different sets of the material relations of a medium. For media with weak spatial dispersion this problem is discussed in [4].

3. Boundary Conditions

From the above consideration one can see that the boundary conditions and the material relations are connected, i.e. for different approaches used to describe the response of a material the

[1] Sometimes in the literature relations (2) are "generalized" to include also dependence on the wave vector (or convolutions over space coordinate variables). Care should be exersised here because the cross terms in these relations already come from the Taylor expansion of a space convolution kernel. For modelling reciprocal media just one space convolution integral is enough to account for arbitrary spatial dispersion effects, as in (1). Note also that sometimes relations (2) are called *local* constitutive relations because they connect the field vectors at the same point in space. This can be misleading because these relations account for first-order spatial dispersion effects. In fact, first-order derivatives of the electric field are "hidden" here, as it is obvious from the Maxwell equations.

boundary conditions must be different. Following [2] we can write the boundary conditions for the tangential field components as

$$\mathbf{z}_0 \times (\mathbf{H}_2 - \mathbf{H}_1) = -j\omega \left\{ \int_{-\delta}^{-0} \Delta\mathbf{D}_1 \, dz + \int_{+0}^{+\delta} \Delta\mathbf{D}_2 \, dz \right\}, \qquad \mathbf{z}_0 \times (\mathbf{E}_2 - \mathbf{E}_1) = 0 \tag{4}$$

where $\mathbf{z}_0$ is the unit vector normal to the interface boundary directed from medium 1 to medium 2. Here the right-hand side of the relation for $\mathbf{H}$ represents the surface polarization current. This current can be calculated as follows. Authors of [2] propose to consider a model reflection problem. The problem assumes fast but continuous changing of the material parameters through the interface (we denote the character size of the transition region as δ). To solve such a problem no additional boundary conditions are necessary. One should make here some assumptions on how the medium parameters vary across the interface layer. If the problem is solved, we can then find the difference between the smooth and sharp interface models. In (4) that difference is represented by $\Delta\mathbf{D}_1$ and $\Delta\mathbf{D}_2$ which correspond to the first and the second media, respectively. More exactly, $\Delta\mathbf{D} = \mathbf{D}(z, \mathbf{E}) - \mathbf{D}^{(0)}(z, \mathbf{E}^{(0)})$ where $\mathbf{D}(z, \mathbf{E})$ is obtained from the smooth model and $\mathbf{D}^{(0)}(z, \mathbf{E}^{(0)})$ is given by the sharp model, i.e. by the constitutive relations supposed to be correct up to the interface boundary. It allows the authors of [2] to conclude that considering boundary value problems may lead to necessity in new material relations for the surface polarization current.

From the above consideration we see that the problem of boundary conditions is not so simple as it may seem at first sight. Even the relations corresponding to the usual Maxwellian boundary conditions happen to be much more complex in the spatially dispersive media. The difficulties become yet more significant when the number of the usual conditions is not enough and some additional relations should be used. How to find these additional conditions? How do they correlate with the material relations? May they be obtained from the field equations as the usual ones? There are many questions here.

There is a chapter in [1] devoted to the considered problem. The authors of [1] try to find a general form of the boundary conditions. This form includes a set of unknown coefficients which could be then somehow found for particular cases. They propose to use the following form:

$$\mathbf{D} + \overline{\overline{\Gamma}} \cdot \mathbf{E} = 0 \tag{5}$$

Such a condition gives three additional scalar equations for the amplitudes of waves. If the number of new waves in a medium is greater than three, then some relations with space derivatives of the fields are needed. Also, here some questions arise: how does dyadic $\overline{\overline{\Gamma}}$ depend on $\mathbf{k}$ and ω? And how to specify the form of $\overline{\overline{\Gamma}}$? The authors of [1] claim that in general only the microscopic theory can give answers to such questions. However, considering the situation in the vicinity of an isolated exciton resonance, the form of $\overline{\overline{\Gamma}}$ can be specified as shown in [1].

Semiconductor is an example of a spatially dispersive medium. The dispersion effects exist there, for instance, due to charge diffusion. Phenomena of this kind at microwaves are considered in [3]. In presence of diffusion the macroscopic medium induced current can be represented as

$$\mathbf{J} = \sigma\mathbf{E} - \epsilon D \nabla(\nabla \cdot \mathbf{E}) \tag{6}$$

where D is the diffusion coefficient. Eq. (6) can be considered as a material relation for media with second-order spatial dispersion. Here the order of dispersion means the highest order of spatial derivatives of field presented in the relation. Second-order dispersion may lead to new eigenwaves in the medium and it can be necessary to use some additional boundary conditions there.

Authors of [3] give special attention to the boundary condition problem. They use an approach based on the uniqueness requirement. New form of the material relation requires to repeat the standard uniqueness development with new terms. Considering the difference between two possible solutions and writing down the Poynting theorem for the difference fields **E** and **H** they obtain:

$$\mathrm{Re}\int_S \{\mathbf{E}\times\mathbf{H}^* - \epsilon D\mathbf{E}(\nabla\cdot\mathbf{E}^*)\}\cdot d\mathbf{S} + \int_V \left\{\sigma|\mathbf{E}|^2 + \epsilon D|\nabla\cdot\mathbf{E}|^2\right\} dV = 0 \qquad (7)$$

From here one can see that some conditions on the normal component of the electric field or on the divergence of the electric field are required in addition to the usual boundary conditions. For a dielectric-semiconductor interface this condition reduces to vanishing of the normal component of the current **J** at the surface.

In a recent paper [5] entitled "Additional boundary conditions: an historical mistake" the author claims that no additional boundary conditions are needed at all. Let us consider his speculations in more details. The author starts from a scalar electric field wave equation

$$\frac{\partial^2 E(x,\omega)}{\partial x^2} + \frac{\omega^2}{c^2}\int_{-\infty}^{+\infty} dx'\epsilon(x-x',\omega)E(x',\omega) = s(x,\omega) \qquad (8)$$

Here sources $s(x,\omega)$ represent equivalent polarization in the transition region (an interface between free space and the medium is under investigation) induced additionally to that already considered in ϵ. These equivalent sources replace free-space volume and sources there, as in Huygens' principle. Next, the author assumes that the transition layer is negligibly thin compared to the wavelengths of all eigenmodes in the medium, and comes to the conclusion that the reflection problem has a unique solution with no need for additional boundary conditions. However, the thickness of the transition layer is comparable to the inhomogeneity scale of the medium. For example, for interfaces with regular crystals, the layer has thickness of a few periods of the lattice (for the theory of transition layers see e.g. [6] and references therein). Thus, the assumption that the transition layer is negligibly thin is in fact equivalent to the assumption that spatial dispersion effects in the medium can be neglected (because the inhomogeneity scale is very small compared to the wavelength). Naturally, no additional boundary conditions are needed in this case.

4. Conclusion

We see how many problems arise when we start to consider boundaries between spatially dispersive media. This area of science is very prospective to study and we hope that in the near future a more complete and logical theory of the boundary problems for spatially dispersive media will be developed.

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