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TIME-DEPENDENT ELECTROMAGNETIC WAVES IN A CAVITY

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Abstract. The electromagnetic initial-boundary value problem for a cavity enclosed by perfectly conducting walls is considered. The cavity medium is defined by its permittivity and permeability which vary continuously in space. The electromagnetic field comes from a source in the cavity. The field is described by a magnetic vector potential \mathbf{A} satisfying a wave equation with initial-boundary conditions. This description through \mathbf{A} is rigorously shown to give a unique solution of the problem and is the starting point for numerical computations. A Chebyshev collocation solver has been implemented for a cubic cavity, and it has been compared to a standard finite element solver. The results obtained are consistent while the collocation solver performs substantially faster. Some time histories and spectra are computed.

Keywords: time-dependent electromagnetic field, cavity, vector and scalar potentials, Lorenz gauge, Chebyshev collocation

MSC 2010: 78A25, 35Q60, 65M70

1. INTRODUCTION

This paper is devoted to Maxwell's equations from an analytical as well as a computational viewpoint. We deal with the description of the electromagnetic field in terms of the scalar and vector potentials φ and \mathbf{A} of the Lorenz gauge. We show rigorously that the electromagnetic field can be described by \mathbf{A} alone and that \mathbf{A} is the unique solution to an initial-boundary value problem for a certain wave equation. The purpose of the research reported here is on the one hand to establish rigorous results about \mathbf{A} and, on the other hand, to devise a feasible numerical method for the computation of \mathbf{A} and hence of the electromagnetic field. We emphasize that the method developed in this paper is suitable for rather smooth fields in space x

and time t . For regular data and a cubic cavity, we give numerical evidence that the proposed method is fast and efficient.

1.1. Maxwell's equations and the Lorenz gauge

The mathematical formulation of the electromagnetic phenomena considered in this paper starts from Faraday's and Ampere's laws, i.e.,

$$(1) \quad \frac{\partial \mathbf{B}}{\partial t} + \nabla \times (\varepsilon^{-1} \mathbf{D}) = 0 \quad \text{in } (0, T) \times \Omega,$$

$$(2) \quad \frac{\partial \mathbf{D}}{\partial t} - \nabla \times (\mu^{-1} \mathbf{B}) = -\mathbf{J} \quad \text{in } (0, T) \times \Omega,$$

supplemented with the boundary and initial conditions

$$(3) \quad \mathbf{n} \times \mathbf{D} = 0 \quad \text{on } (0, T) \times \partial\Omega,$$

$$(4) \quad \mathbf{B}|_{t=0} = \mathbf{B}_0 \quad \text{and} \quad \mathbf{D}|_{t=0} = \mathbf{D}_0 \quad \text{in } \Omega.$$

Here T is the length of the considered time interval, and initially $t = 0$. Equations (1)–(2) are to be understood in the setting of Sobolev space-valued functions of time t in the sense made precise in Section 2.

The problem is set in a bounded, simply connected, open subset Ω of \mathbb{R}^3 with a Lipschitz boundary $\partial\Omega$, whose unit outward normal vector is denoted by \mathbf{n} . Moreover, the complement of $\overline{\Omega}$ is connected. To rule out singular phenomena, we also assume

$$(5) \quad \text{either } \Omega \text{ is a convex polyhedron or } \partial\Omega \text{ is of class } C^{1,1}.$$

These conditions on the region ensure, in particular, the following regularity property: If $f \in L^2(\Omega)$ and $u \in H_0^1(\Omega)$ is the solution of Poisson's equation $-\Delta u = f$ vanishing on $\partial\Omega$, then $u \in H^2(\Omega)$; see e.g. [3]. They are also vital for the existence and uniqueness of potentials [3].

The region Ω is occupied by a medium with variable permittivity ε and permeability μ . Thus $\mathbf{D}(t, x) = \varepsilon(x)\mathbf{E}(t, x)$ and $\mathbf{B}(t, x) = \mu(x)\mathbf{H}(t, x)$ are the constitutive relations between the fields. We assume that $\varepsilon(x)$ and $\mu(x)$ are from $C^3(\overline{\Omega})$ and such that

$$(6) \quad \varepsilon(x), \mu(x) \geq c_0 > 0 \quad \text{for all } x \in \Omega,$$

for some constant c_0 .

Moreover, the given charge density ϱ and current density \mathbf{J} are subject to the conservation law

$$(7) \quad \frac{\partial \varrho}{\partial t} + \nabla \cdot \mathbf{J} = 0.$$

The initial fields \mathbf{B}_0 and \mathbf{D}_0 are prescribed and fulfil the conditions

$$(8) \quad \nabla \cdot \mathbf{D}_0 = \varrho_0 \text{ in } \Omega, \text{ where } \varrho_0(x) = \varrho(0, x), \quad \text{and} \quad \mathbf{n} \times \mathbf{D}_0 = 0 \text{ on } \partial\Omega,$$

as well as

$$(9) \quad \nabla \cdot \mathbf{B}_0 = 0 \text{ in } \Omega \quad \text{and} \quad \mathbf{n} \cdot \mathbf{B}_0 = 0 \quad \text{on } \partial\Omega.$$

The electromagnetic cavity field is described analytically and computed numerically using the electromagnetic potentials \mathbf{A} and φ of the Lorenz gauge, i.e.,

$$(10) \quad \mathbf{B} = \nabla \times \mathbf{A},$$

$$(11) \quad \mathbf{E} = -\nabla \varphi - \mathbf{A}_t,$$

$$(12) \quad \varepsilon \mu \varphi_t + \nabla \cdot \mathbf{A} = 0.$$

The paper revolves around the fact that the vector potential satisfies the wave equation

$$(13) \quad \varepsilon(\nabla((\varepsilon\mu)^{-1}\nabla \cdot \mathbf{A}) - \mathbf{A}_{tt}) - \nabla \times (\mu^{-1}\nabla \times \mathbf{A}) = -\mathbf{J}.$$

In order to supplement (13) with correct initial conditions we choose \mathbf{A}_0 so that $\mathbf{B}_0 = \nabla \times \mathbf{A}_0$ and $\nabla \cdot \mathbf{A}_0 = 0$ in Ω as well as $\mathbf{n} \times \mathbf{A}_0 = 0$ on $\partial\Omega$ (under certain conditions, this can be done in a unique way). We require $\mathbf{A}(0) = \mathbf{A}_0$ and note that $\mathbf{A}_t(0) = -\mathbf{E}(0) = -\varepsilon^{-1}\mathbf{D}_0$ since $\varphi(0) = 0$ is assumed. Moreover, $\mathbf{n} \times \mathbf{A}(t)$ and $\nabla \cdot \mathbf{A}(t)$ are required to vanish on the boundary $\partial\Omega$ at every instant t . It turns out that the resulting initial-boundary value problem is well-posed. Consequently, the electromagnetic field can be obtained from the unique solution \mathbf{A} alone through (10)–(12). As already mentioned, the mathematical justification of this program constitutes one part of this paper.

1.2. Outline

The contribution of this paper is twofold. The first half of the paper deals with the analytical problems. In Lemma 1 the well-posedness of the electromagnetic Cauchy problem is recalled. Conditions are given which guarantee a suitable degree of regularity of the field for the success of our approach. The main analytical results are presented in Theorems 1–4. Theorem 1 furnishes the existence of the potentials \mathbf{A}

and φ in the Lorenz gauge, with respect to which (10)–(12) hold. Theorems 2 and 3 characterize \mathbf{A} as the unique solution of the initial-boundary value problem sketched above. The main analytical results are summarized in Theorem 4.

Secondly, for a cubic cavity, \mathbf{A} is computed numerically by a Chebyshev collocation approximation of (13); the trapezoidal rule is used for time integration. It is shown that the collocation solver is consistent with and much faster than a standard FEM solver and that Maxwell's equations are fulfilled. In addition, the computed time histories of (13) confirm that the method is time stable and yields reasonable eigenfrequencies.

2. MATHEMATICAL ANALYSIS

We start now with mathematical justification of our approach. It is based on semigroup theory for evolution equations, Sobolev spaces, and the vector analysis of [3].

2.1. Prerequisites

In view of the lower bound (6), instead of the standard scalar product in the Hilbert space $\mathcal{H} = L^2(\Omega)^3 \times L^2(\Omega)^3$ one may use the following equivalent one:

$$(M, M^*)_{\mathcal{H}} = \int_{\Omega} (\mu(x)^{-1} \mathbf{B}(x) \cdot \mathbf{B}^*(x) + \varepsilon(x)^{-1} \mathbf{D}(x) \cdot \mathbf{D}^*(x)) dx$$

for $M = (\mathbf{B}, \mathbf{D})$ and $M^* = (\mathbf{B}^*, \mathbf{D}^*)$ in \mathcal{H} . We proceed to the operator \mathcal{A} defined by

$$\mathcal{A}\mathbf{U} = \mathcal{A}(\mathbf{B}, \mathbf{D}) = (\nabla \times (\varepsilon^{-1} \mathbf{D}), -\nabla \times (\mu^{-1} \mathbf{B})),$$

its domain being

$$\text{dom}(\mathcal{A}) = \{(\mathbf{B}, \mathbf{D}) \in \mathcal{H} : (\nabla \times (\varepsilon^{-1} \mathbf{D}), -\nabla \times (\mu^{-1} \mathbf{B})) \in \mathcal{H}; \mathbf{n} \times \mathbf{D} = 0 \text{ on } \partial\Omega\}.$$

The operator \mathcal{A} is naturally associated with (1)–(2). The curl operator $\nabla \times$ appearing in the definition of \mathcal{A} is understood in the sense of distributions (see e.g. [3, Chap. IX]) and is therefore well-defined. In generic terms, if $\mathbf{u} \in \mathcal{D}'(\Omega)^3$ is a distribution, then the partial derivative $D_j \mathbf{u} = \partial \mathbf{u} / \partial x_j$ is the distribution defined by

$$\langle D_j \mathbf{u}, \Phi \rangle = -\langle \mathbf{u}, D_j \Phi \rangle, \quad \forall \Phi \in \mathcal{D}(\Omega),$$

while the curl $\nabla \times \mathbf{u}$ is the distribution given by

$$\langle \nabla \times \mathbf{u}, \Phi \rangle = \langle \mathbf{u}, \nabla \times \Phi \rangle, \quad \forall \Phi \in \mathcal{D}(\Omega)^3.$$

Likewise, the gradient, divergence, Laplacian, etc., appearing in this paper, are defined in the sense of distributions.

Assuming $\mathbf{B}, \mathbf{D} \in L^2(\Omega)^3$, we note that $(\nabla \times (\varepsilon^{-1}\mathbf{D}), -\nabla \times (\mu^{-1}\mathbf{B})) \in \mathcal{H}$ exactly when $\nabla \times \mathbf{B}$ and $\nabla \times \mathbf{D}$ are in $L^2(\Omega)^3$, since ε, μ as well as $\varepsilon^{-1}, \mu^{-1}$ are smooth and positive on $\overline{\Omega}$. Recall that $\mathbf{D} \in L^2(\Omega)^3$ together with $\nabla \times \mathbf{D} \in L^2(\Omega)^3$ ensures that $\mathbf{n} \times \mathbf{D}$ on $\partial\Omega$ is defined in the trace sense [3, Chap. IX, Thm. 2]. Similarly, if \mathbf{B} and its divergence $\nabla \cdot \mathbf{B}$ both belong to $L^2(\Omega)$, then $\mathbf{n} \cdot \mathbf{B}|_{\partial\Omega}$ is defined in the sense of traces [3, Chap. IX, Thm. 1].

Remark 1. We refrain from systematically using the spaces $H(\text{curl}, \Omega)$ and $H(\text{div}, \Omega)$ extensively investigated in [3, Chap. IX]:

$$\begin{aligned} H(\text{curl}, \Omega) &= \{\mathbf{u} \in L^2(\Omega)^3 : \nabla \times \mathbf{u} \in L^2(\Omega)^3\}, \\ H(\text{div}, \Omega) &= \{\mathbf{u} \in L^2(\Omega)^3 : \nabla \cdot \mathbf{u} \in L^2(\Omega)\}. \end{aligned}$$

These are Hilbert spaces for the norms

$$\begin{aligned} \|\mathbf{u}\|_{H(\text{curl}, \Omega)} &= (\|\mathbf{u}\|_{L^2(\Omega)^3}^2 + \|\nabla \times \mathbf{u}\|_{L^2(\Omega)^3}^2)^{1/2}, \\ \|\mathbf{u}\|_{H(\text{div}, \Omega)} &= (\|\mathbf{u}\|_{L^2(\Omega)^3}^2 + \|\nabla \cdot \mathbf{u}\|_{L^2(\Omega)}^2)^{1/2}, \end{aligned}$$

respectively. The trace theorem for $H(\text{curl}, \Omega)$ [3, Chap. IX, Thm. 2] states that the trace mapping $\mathbf{u} \mapsto \mathbf{n} \times \mathbf{u}|_{\partial\Omega}$ defined on $\mathcal{D}(\overline{\Omega})^3$ extends by continuity to a continuous linear mapping γ_τ from $H(\text{curl}, \Omega)$ into $H^{-1/2}(\partial\Omega)^3$. The accompanying trace theorem for $H(\text{div}, \Omega)$ [3, Chap. IX, Thm. 1] yields the existence of an extension of $\mathbf{u} \mapsto \mathbf{n} \cdot \mathbf{u}|_{\partial\Omega}$ to a continuous linear mapping γ_n from $H(\text{div}, \Omega)$ into $H^{-1/2}(\partial\Omega)^3$.

The fields $\mathbf{B}, \mathbf{D}, \mathbf{E}, \mathbf{H}$ are understood as functions mapping time t into Banach spaces (Sobolev spaces). For instance, \mathbf{B} is the mapping $t \mapsto \mathbf{B}(t)$ where $\mathbf{B}(t)$ belongs to a Sobolev space for each t and enjoys certain regularity as a function of t . We frequently apply the divergence and curl operators in the sense of distributions, e.g., the divergence $\nabla \cdot \mathbf{B}(t)$ is defined in $\mathcal{D}'(\Omega)$ for each fixed t .

Integrals with respect to time, of Banach space-valued integrands, are understood in the Bochner sense. We use interchangeably \mathbf{u}' , $d\mathbf{u}/dt$ and \mathbf{u}_t to denote the time derivative in the Banach-valued weak sense of \mathbf{u} where \mathbf{u} can be $\mathbf{B}, \mathbf{D}, \mathbf{E}$ or \mathbf{H} . In generic terms, let X be a Banach space and $\mathbf{u} \in L^1(0, T; X)$. We say that $\mathbf{v} \in L^1(0, T; X)$ is the *weak derivative* of \mathbf{u} , written $\mathbf{v} = \mathbf{u}' \equiv d\mathbf{u}/dt \equiv \mathbf{u}_t$, provided

$$\int_0^T \Phi'(t)\mathbf{u}(t) dt = - \int_0^T \Phi(t)\mathbf{v}(t) dt$$

for all scalar test functions $\Phi \in \mathcal{D}(0, T)$. The weak derivative of $\mathbf{u} \in L^1_{\text{loc}}(\mathbb{R}; X)$ is defined analogously. Of course, if \mathbf{u} happens to be smooth, say $\mathbf{u} \in C^1(\mathbb{R}; X)$, then

$$\lim_{h \rightarrow 0} \left\| \frac{\mathbf{u}(t+h) - \mathbf{u}(t)}{h} - \mathbf{u}'(t) \right\|_X = 0$$

for every $t \in \mathbb{R}$, and $t \mapsto \mathbf{u}'(t)$ is a continuous mapping from \mathbb{R} into X . In our applications, X is a Sobolev space. Let us derive a familiar calculus rule, which will be tacitly used in the sequel. To be definite, let $X = H^1(\Omega)$ and $\mathbf{u} \in C^1(\mathbb{R}; H^1(\Omega)^3)$ for the moment. Then the order of time and space differentiation may be interchanged, i.e., $D_j(\mathbf{u}'(t)) = (D_j\mathbf{u})'(t)$ where $D_j = \partial/\partial x_j$ in the sense of $\mathcal{D}'(\Omega)$. Indeed, from

$$\lim_{h \rightarrow 0} \left\| \frac{\mathbf{u}(t+h) - \mathbf{u}(t)}{h} - \mathbf{u}'(t) \right\|_{H^1(\Omega)^3} = 0$$

it follows that

$$\lim_{h \rightarrow 0} \left\| \frac{D_j\mathbf{u}(t+h) - D_j\mathbf{u}(t)}{h} - D_j\mathbf{u}'(t) \right\|_{L^2(\Omega)^3} = 0,$$

or in other words that $(D_j\mathbf{u})'(t) = D_j(\mathbf{u}'(t))$ where $D_j\mathbf{u} \in C^1(\mathbb{R}; L^2(\Omega)^3)$.

See e.g. [6], [13] for the use of Banach space-valued functions of time in the context of partial differential equations.

2.2. Classical solutions

As was proved in [5], $\text{dom}(\mathcal{A})$ is dense in \mathcal{H} and \mathcal{A} is skew-adjoint, i.e., $\text{dom}(\mathcal{A}^*) = \text{dom}(\mathcal{A})$ and \mathcal{A} is a graph closed operator with $\mathcal{A}^* = -\mathcal{A}$. Since \mathcal{A} is skew-adjoint, $i\mathcal{A}$ is self-adjoint. By Stone's theorem, \mathcal{A} is therefore the infinitesimal generator of a unique one-parameter group of unitary operators $G(t)$ (see e.g. [12, Thm. 10.8]). The Cauchy problem (1)–(4) may, under very weak assumptions on the data, be formulated as follows: Given $\mathbf{J} \in L^1(0, T; L^2(\Omega)^3)$ and $\mathbf{U}_0 = (\mathbf{B}_0, \mathbf{D}_0) \in \text{dom}(\mathcal{A})$, find $\mathbf{U}(t) = (\mathbf{B}(t), \mathbf{D}(t)) \in \text{dom}(\mathcal{A})$ satisfying (in a sense to be specified) the initial value problem

$$(14) \quad d\mathbf{U}(t)/dt + \mathcal{A}\mathbf{U}(t) = \mathbf{F}(t), \quad t \in (0, T); \quad \mathbf{U}(0) = \mathbf{U}_0$$

where $\mathbf{F}(t) = (0, -\mathbf{J}(t))$. By definition, the *mild solution* of (14) is

$$(15) \quad \mathbf{U}(t) = G(t)\mathbf{U}_0 + \int_0^t G(t-\tau)\mathbf{F}(\tau) d\tau.$$

By a *classical solution* $\mathbf{U}(t)$ of (14) we mean a function \mathbf{U} belonging to $C([0, T]; \mathcal{H}) \cap C^1((0, T); \mathcal{H})$, satisfying $\mathbf{U}(t) \in \text{dom}(\mathcal{A})$ and equation (14) for every $t \in (0, T)$, as

well as the initial condition $\mathbf{U}(0) = \mathbf{U}_0$. If \mathbf{U} is a classical solution, then \mathbf{U} is necessarily the mild solution (15), but the converse fails in general since the mild solution (15) may lack the required regularity (see e.g. [12, Chap. 4] or [4, Chap. XVII]). In particular, if it exists, the classical solution is unique.

It is well known [12, Cor. 4.2.5] that if $\mathbf{J} \in C^1([0, T]; L^2(\Omega)^3)$ and $\mathbf{U}_0 \in \text{dom}(\mathcal{A})$, then the mild solution is a classical solution. Below we assume at least $\mathbf{J} \in C^1(\mathbb{R}; L^2(\Omega)^3)$, which implies that the classical solution $\mathbf{U}(t)$ exists and can be extended to $t \in \mathbb{R}$, hence $\mathbf{U} \in C^1(\mathbb{R}; L^2(\Omega)^6)$. Recall that the classical solution, in particular, is such that $\mathbf{U}(t) = (\mathbf{B}(t), \mathbf{D}(t)) \in \text{dom}(\mathcal{A})$ for each $t \in \mathbb{R}$, which boils down to the conditions that, firstly, $\mathbf{D}(t)$ and $\mathbf{B}(t)$ along with their curls, understood in the distribution sense (i.e., in the sense of $\mathcal{D}'(\Omega)$), belong to $L^2(\Omega)^3$ and, secondly, $\mathbf{n} \times \mathbf{D}(t) = 0$ on $\partial\Omega$. Notice again that $\nabla \times \mathbf{D}(t) \in L^2(\Omega)^3$ ensures that $\mathbf{n} \times \mathbf{D}(t)$ makes sense in the trace sense, as pointed out in Remark 1. Below we shall strengthen the regularity assumptions on the data to ensure the well-posedness of the initial-boundary value problem for (13); see in particular Lemma 1 (iii) below.

As we are primarily interested in regular solutions, which are reasonably smooth in t , we shall assume enough regularity of the data to this end. Parts (i) and (ii) of the following basic lemma contain general and known results about the well-posedness of the Cauchy problem of this paper. The conditions on the data can be relaxed [5], [4]. In part (iii) stronger conditions are assumed to ensure a higher degree of regularity in time t , which will be of importance in the sequel.

Lemma 1. *Let Ω be a bounded, simply connected, open subset Ω of \mathbb{R}^3 with a Lipschitz boundary $\partial\Omega$ and with $\overline{\mathbb{C}\Omega}$ connected. Let Ω meet condition (5). Assume $\varepsilon, \mu \in C^3(\overline{\Omega})$ satisfy (6). Let \mathbf{J} belong to $C^1(\mathbb{R}; L^2(\Omega)^3)$ and $\mathbf{U}_0 \in \text{dom}(\mathcal{A})$. Moreover, assume that $\varrho \in C(\mathbb{R}; L^2(\Omega))$ and that (7) holds in $\mathcal{D}'(\mathbb{R} \times \Omega)$. Let also (8) be fulfilled. Then the following statements hold:*

- (i) *The problem (14), i.e., the initial-boundary problem for Maxwell's equations (1)–(4), has a unique classical solution $\mathbf{U} \in C^1(\mathbb{R}; L^2(\Omega)^6)$ with $\mathbf{U}(t) = (\mathbf{B}(t), \mathbf{D}(t)) \in \text{dom}(\mathcal{A})$ for all $t \in \mathbb{R}$. The solution is given by (15). Moreover, the classical solution $\mathbf{U} = (\mathbf{B}, \mathbf{D})$ satisfies (1)–(2) in the sense of $\mathcal{D}'(\mathbb{R} \times \Omega)$.*
- (ii) *We have $\nabla \cdot \mathbf{D} = \varrho$ in $\mathcal{D}'(\mathbb{R} \times \Omega)$ and $\mathbf{n} \times \mathbf{D}(t) = 0$ on the boundary for each $t \in \mathbb{R}$. Furthermore, if (9) is met, then $\nabla \cdot \mathbf{B}(t) = 0$ in Ω and $\mathbf{n} \cdot \mathbf{B}(t) = 0$ on $\partial\Omega$ for each $t \in \mathbb{R}$ and, moreover, $\mathbf{U} \in C(\mathbb{R}; H^1(\Omega)^6)$.*
- (iii) *Assuming condition (9) and the regularity $\mathbf{J} \in C^3(\mathbb{R}; L^2(\Omega)^3)$, $\varrho \in C^2(\mathbb{R}; L^2(\Omega))$, $\mathbf{F}(0) = (0, -\mathbf{J}(0)) \in \text{dom}(\mathcal{A}^2)$, and $\mathbf{U}_0 \in \text{dom}(\mathcal{A}^3)$, we have $\mathbf{U} \in C^3(\mathbb{R}; L^2(\Omega)^6) \cap C^2(\mathbb{R}; H^1(\Omega)^6)$*

Proof. A proof of part (i) can be found in [5] and [4, Chap. XVII]. Note, e.g., that $\mathbf{n} \times \mathbf{D}_0$ is well-defined on the boundary in the trace sense since by our

assumptions \mathbf{D}_0 and $\nabla \times \mathbf{D}_0$ are in $L^2(\Omega)^3$. Similarly, $\mathbf{n} \cdot \mathbf{B}_0|_{\partial\Omega}$ is defined in the trace sense for $\mathbf{B}_0 \in L^2(\Omega)^3$ when $\nabla \cdot \mathbf{B}_0 \in L^2(\Omega)$, in particular, when $\nabla \cdot \mathbf{B}_0 = 0$. See Remark 1 and Theorems 1 and 2 of [3, Chap. IX].

It was proved in [5, Thm. 5.1] that the classical solution is also a solution in the sense of distributions.

(ii) Taking the divergence of (2) and using (7) in the sense of distributions yields

$$\frac{\partial}{\partial t} \nabla \cdot \mathbf{D} = \frac{\partial \varrho}{\partial t}.$$

The equality $\nabla \cdot \mathbf{D}(t) = \varrho(t)$ ensues for any $t \in \mathbb{R}$, since it is assumed that $\nabla \cdot \mathbf{D}(0) = \varrho(0)$. Analogously, by taking the divergence of (1), it is proved that the divergence $\nabla \cdot \mathbf{B}(t) = 0$ for all times t provided $\nabla \cdot \mathbf{B}(0) = 0$. For proofs of the remaining parts of (ii) see Theorems 5.1–5.3 of [5] and [4, Chap. XVII].

We consider in detail the regularity assertions of (ii) and (iii).

The regularity proposition of (ii) can be proved as follows. Since $\mu \in C^3(\overline{\Omega})$ and $\nabla \times (\mu^{-1}\mathbf{B}) \in C(\mathbb{R}; L^2(\Omega)^3)$, we have $\nabla \times \mathbf{B} \in C(\mathbb{R}; L^2(\Omega)^3)$ and $\nabla \cdot \mathbf{B} = 0$, whence $\mathbf{B} \in C(\mathbb{R}; H^1(\Omega)^3)$. Similarly, it follows from $\nabla \times \mathbf{E} = -\mathbf{B}_t \in C(\mathbb{R}, L^2(\Omega)^3)$ and $\nabla \cdot \mathbf{D} = \varrho \in C(\mathbb{R}; L^2(\Omega))$ that $\mathbf{D}, \mathbf{E} \in C(\mathbb{R}; H^1(\Omega)^3)$. The assumptions on Ω , including (5), guarantee this degree of regularity of the fields, see Theorem 3 and Remark 2 of [3, Chap. IX].

(iii) By the extra assumptions, $\mathbf{F} = (0, -\mathbf{J})$ belongs to $C^3(\mathbb{R}; L^2(\Omega)^6)$. Writing $\mathbf{U}(t) = G(t)\mathbf{U}_0 + \mathbf{V}(t)$ where

$$\mathbf{V}(t) = \int_0^t G(t-\tau)\mathbf{F}(\tau) \, d\tau$$

and examining the terms separately, we first find that $d(G(t)\mathbf{U}_0)/dt = G(t)\mathcal{A}\mathbf{U}_0$. Proceeding to higher derivatives, using $\mathcal{A}\mathbf{U}_0 \in \text{dom}(\mathcal{A})$ and $\mathcal{A}^2\mathbf{U}_0 \in \text{dom}(\mathcal{A})$, we find that $d(G(t)\mathbf{U}_0)/dt = G(t)\mathcal{A}\mathbf{U}_0$ is again differentiable and $d^2(G(t)\mathbf{U}_0)/dt^2 = G(t)\mathcal{A}^2\mathbf{U}_0$ and $d^3(G(t)\mathbf{U}_0)/dt^3 = G(t)\mathcal{A}^3\mathbf{U}_0$ are continuous functions of t . As regards \mathbf{V} , writing $\mathbf{V}(t) = \int_0^t G(s)\mathbf{F}(t-s) \, ds$ and using the differentiability of $\mathbf{F}(t)$ we obtain that $\mathbf{V}(t)$ is differentiable with

$$(16) \quad \mathbf{V}'(t) = G(t)\mathbf{F}(0) + \int_0^t G(s)\mathbf{F}'(t-s) \, ds.$$

As $\mathbf{F} \in C^3(\mathbb{R}; L^2(\Omega)^6)$ and $\mathbf{F}(0) \in \text{dom}(\mathcal{A}^2)$, $\mathbf{V}''(t)$ as well as $\mathbf{V}'''(t)$ exist and constitute continuous functions of t . We have thus proved $\mathbf{U} \in C^3(\mathbb{R}; L^2(\Omega)^6)$.

In view of $\nabla \times (\mu^{-1}\mathbf{B}) = \mathbf{D}_t + \mathbf{J} \in C^2(\mathbb{R}; L^2(\Omega)^3)$ and the smoothness and positivity of μ , we have $\nabla \times \mathbf{B} \in C^2(\mathbb{R}; L^2(\Omega)^3)$ and $\nabla \cdot \mathbf{B} = 0$ and thus $\mathbf{B} \in$

$C^2(\mathbb{R}; H^1(\Omega)^3)$. Similarly, it follows from $\nabla \times \mathbf{E} = -\mathbf{B}_t \in C^2(\mathbb{R}, L^2(\Omega)^3)$ and $\nabla \cdot \mathbf{D} = \rho \in C^2(\mathbb{R}; L^2(\Omega))$ that $\mathbf{E} \in C^2(\mathbb{R}; H^1(\Omega)^3)$. We conclude that $\mathbf{U} \in C^2(\mathbb{R}; H^1(\Omega)^6)$. \square

3. POTENTIAL FORMALISM

We now introduce vector and scalar potentials representing the field. Let us first do this formally. Below precise statements are given.

Assuming that the divergence of $\mathbf{B}(t)$ vanishes for all $t \in \mathbb{R}$, $\mathbf{B} = \nabla \times \mathbf{A}$ for some vector field \mathbf{A} by Poincaré's theorem. Further, as $\mathbf{B}_t + \nabla \times \mathbf{E} = 0$ and $\mathbf{B} = \nabla \times \mathbf{A}$, we find that $\nabla \times (\mathbf{A}_t + \mathbf{E}) = 0$ and so, by another application of Poincaré's theorem, $\mathbf{A}_t + \mathbf{E} = -\nabla\varphi$ for some potential φ .

Here \mathbf{A} and φ are the magnetic vector potential and the electric scalar potential, respectively. They are not defined in a unique manner because any specific choice $(\mathbf{A}^0, \varphi^0)$ can be replaced by

$$(17) \quad \mathbf{A} = \mathbf{A}^0 + \nabla\psi,$$

$$(18) \quad \varphi = \varphi^0 - \psi_t$$

for “any” scalar function ψ . A particular choice of (\mathbf{A}, φ) representing the electromagnetic field (\mathbf{E}, \mathbf{B}) is called a gauge; the transformation $(\mathbf{A}^0, \varphi^0) \mapsto (\mathbf{A}, \varphi)$ given by (17)–(18) is termed a gauge transformation; the electromagnetic field (\mathbf{E}, \mathbf{B}) is invariant under gauge transformations.

We recall that the Coulomb gauge (\mathbf{A}, φ) (denoted by $(\tilde{\mathbf{A}}, \tilde{\varphi})$ below) is characterized by $\nabla \cdot \mathbf{A} = 0$ and suitable boundary conditions. Starting from a vector potential \mathbf{A}^0 , it is obtained as (17) by setting the divergence of (17) to zero, i.e., by solving Poisson's equation $-\Delta\psi = \nabla \cdot \mathbf{A}^0$. However, the main role is played by the Lorenz gauge in this article. The Lorenz gauge is constructed from the Coulomb gauge in Section 3.2.

In the forthcoming sections we proceed to rigorous statements about the potentials. In doing so we rely on [3, Chap. IX] and [4, Chap. XVII]. In the sequel we assume the conditions of Lemma 1 (iii), under which each of the fields \mathbf{B} , \mathbf{E} , $\mathbf{D} = \varepsilon\mathbf{E}$ and $\mathbf{H} = \mu^{-1}\mathbf{B}$ belongs to the space

$$C^3(\mathbb{R}; L^2(\Omega)^3) \cap C^2(\mathbb{R}; H^1(\Omega)^3),$$

and

$$(19) \quad \nabla \cdot \mathbf{B}(t) = 0 \text{ in } \Omega \quad \text{and} \quad \mathbf{n} \cdot \mathbf{B}(t) = 0 \text{ on } \partial\Omega$$

for all $t \in \mathbb{R}$.

3.1. The Coulomb gauge

Let us first make the following specific choice of potentials according to the Coulomb gauge. Fix

$$(20) \quad \tilde{\mathbf{A}} \in C^3(\mathbb{R}; H^1(\Omega)^3)$$

with $\mathbf{B}(t) = \nabla \times \tilde{\mathbf{A}}(t)$ and $\nabla \cdot \tilde{\mathbf{A}}(t) = 0$ in Ω and $\mathbf{n} \times \tilde{\mathbf{A}}(t) = 0$ on $\partial\Omega$, at each time instant $t \in \mathbb{R}$. The existence and uniqueness of $\tilde{\mathbf{A}}$ follows from the results of [3, Chap. IX] (see also Remark 7, §4, Chap. XVII of [4]). Indeed, by Theorem 3, Remark 2, and Theorem 2 of [3, Chap. IX], $\mathbf{B}(t) \in H^1(\Omega)^3$ and (19) together ensure the existence and uniqueness of $\tilde{\mathbf{A}}(t) \in H^1(\Omega)^3$ with $\nabla \times \tilde{\mathbf{A}}(t) = \mathbf{B}(t)$ and $\nabla \cdot \tilde{\mathbf{A}}(t) = 0$ in Ω and $\mathbf{n} \times \tilde{\mathbf{A}}(t)|_{\partial\Omega} = 0$. In fact, the curl operator, $\text{curl}: X \rightarrow Y$, acts as an isomorphism of the space

$$X = \{\mathbf{v} \in H^1(\Omega)^3: \nabla \cdot \mathbf{v} = 0 \text{ in } \Omega \text{ and } \mathbf{n} \times \mathbf{v}|_{\partial\Omega} = 0\}, \text{ with the } H^1\text{-norm}$$

onto the subspace $Y = \text{curl } H^1(\Omega)^3$ of $L^2(\Omega)^3$. Indeed, by Corollary 6 and Remark 6 of [3, Chap. IX], using in particular the assumptions on Ω , for each $\mathbf{v}_0 \in H^1(\Omega)$ there exists a unique $\mathbf{v} \in H^1(\Omega)^3$ satisfying $\nabla \times \mathbf{v} = \nabla \times \mathbf{v}_0$ and $\nabla \cdot \mathbf{v} = 0$ in Ω as well as $\mathbf{n} \times \mathbf{v}|_{\partial\Omega} = 0$. Hence $\text{curl}: X \rightarrow Y$ is a continuous linear bijection. Furthermore, X and Y are closed subspaces of $H^1(\Omega)^3$ and $L^2(\Omega)^3$, respectively; see [3, Chap. IX, p. 223]. Therefore, the inverse operator, here simply denoted by $\mathcal{L}: Y \rightarrow X$, is continuous by Banach's open mapping theorem.

Returning to the relation $\mathbf{B}(t) = \nabla \times \tilde{\mathbf{A}}(t)$ where $\tilde{\mathbf{A}}(t) \in X$, we shall verify that $\tilde{\mathbf{A}}(t) = \mathcal{L}(\mathbf{B}(t))$ is a differentiable function of t . We have

$$h^{-1}(\tilde{\mathbf{A}}(t+h) - \tilde{\mathbf{A}}(t)) = \mathcal{L}(h^{-1}(\mathbf{B}(t+h) - \mathbf{B}(t))) \rightarrow \mathcal{L}(\mathbf{B}'(t)) \quad \text{as } h \rightarrow 0,$$

with convergence in $H^1(\Omega)^3$ thanks to $\mathbf{B} \in C^3(\mathbb{R}; L^2(\Omega)^3)$ and the recently discussed continuity of \mathcal{L} . Thus $\tilde{\mathbf{A}}'(t)$ exists and $\tilde{\mathbf{A}}'(t) = \mathcal{L}(\mathbf{B}'(t))$. This procedure can be repeated twice to yield $\tilde{\mathbf{A}} \in C^3(\mathbb{R}; H^1(\Omega)^3)$.

We proceed to the accompanying scalar potential. Since $\mathbf{B}_t + \nabla \times \mathbf{E} = 0$ and $\mathbf{B} = \nabla \times \tilde{\mathbf{A}}$, we find that $\nabla \times (\tilde{\mathbf{A}}_t + \mathbf{E}) = 0$ and so, by another application of Poincaré's theorem, $\tilde{\mathbf{A}}_t + \mathbf{E} = -\nabla\tilde{\varphi}$ for some $\tilde{\varphi}(t) \in H_0^1(\Omega)$ [3, Chap. IX]. Taking the divergence of $\tilde{\mathbf{A}}_t + \mathbf{E} = -\nabla\tilde{\varphi}$ and using $\nabla \cdot \tilde{\mathbf{A}} = 0$, the equation

$$(21) \quad -\Delta\tilde{\varphi} = \nabla \cdot \mathbf{E} \in C^3(\mathbb{R}; H^{-1}(\Omega)) \cap C^2(\mathbb{R}; L^2(\Omega))$$

ensues. Invoking the regularity theory for Poisson's equation we conclude that

$$(22) \quad \tilde{\varphi} \in C^3(\mathbb{R}; H_0^1(\Omega)) \cap C^2(\mathbb{R}; H^2(\Omega)),$$

since (5) is assumed.

In other words, $\tilde{\mathbf{A}}$ and $\tilde{\varphi}$ are the vector and scalar potentials of the Coulomb gauge satisfying $\nabla \cdot \tilde{\mathbf{A}}(t) = 0$ in Ω as well as the boundary conditions $\mathbf{n} \times \tilde{\mathbf{A}}(t) = 0$ and $\tilde{\varphi}(t) = 0$ on $\partial\Omega$ for every $t \in \mathbb{R}$.

3.2. The Lorenz gauge

We shall convert the Coulomb gauge into the Lorenz gauge. To this end, set

$$(23) \quad \mathbf{A} = \tilde{\mathbf{A}} + \nabla\psi, \quad \varphi = \tilde{\varphi} - \psi_t,$$

where ψ is the solution of the following wave equation with variable coefficients:

$$(24) \quad \begin{aligned} \varepsilon\mu\psi_{tt} - \Delta\psi &= \varepsilon\mu\tilde{\varphi}_t, & t \in \mathbb{R}, \\ \psi(0) &= 0, \\ \psi_t(0) &= \tilde{\varphi}(0), \\ \psi(t) &= 0 & \text{on } \partial\Omega \text{ for } t \in \mathbb{R}, \end{aligned}$$

$\tilde{\varphi}$ being known. The exact problem formulation is found below in Lemma 2.

Then the characteristic properties of the Lorenz gauge are fulfilled. To check the Lorenz condition (12) we calculate

$$(25) \quad \varepsilon\mu\varphi_t + \nabla \cdot \mathbf{A} = \varepsilon\mu(\tilde{\varphi}_t - \psi_{tt}) + \nabla \cdot \tilde{\mathbf{A}} + \Delta\psi = \varepsilon\mu(\tilde{\varphi}_t - \psi_{tt}) + \Delta\psi = 0$$

by (24). This construction requires the existence of a solution of the initial-boundary value problem (24), as is shown below. The imposed initial and boundary conditions on ψ give rise to a vector potential \mathbf{A} and scalar potential φ enjoying favorable properties.

Lemma 2. *Assume (22). Then the following three assertions are true:*

- (i) *The wave equation (24) has a unique variational solution ψ with $\psi \in C(\mathbb{R}; H_0^1(\Omega))$ and $\psi_t \in C(\mathbb{R}; L^2(\Omega))$ satisfying the initial conditions $\psi(0) = 0$ and $\psi_t(0) = \tilde{\varphi}(0)$. To be exact, ψ is uniquely determined by these regularity and initial conditions and the requirement that*

$$\frac{d}{dt} \int_{\Omega} \varepsilon(x)\mu(x)\psi_t(t,x)v(x) dx + \int_{\Omega} \nabla\psi(t,x) \cdot \nabla v(x) dx = \int_{\Omega} f(t,x)v(x) dx$$

holds in the sense of $\mathcal{D}'(\mathbb{R})$ for any $v \in H_0^1(\Omega)$, where $f = \varepsilon\mu\tilde{\varphi}_t$. The variational solution ψ is also a solution of (24) in the sense of $\mathcal{D}'(\mathbb{R} \times \Omega)$.

- (ii) *The variational solution ψ enjoys the following regularity: $\psi \in C^2(\mathbb{R}; H_0^1(\Omega)) \cap C^1(\mathbb{R}; H^2(\Omega))$, $\psi_{ttt} \in C(\mathbb{R}; L^2(\Omega))$. Moreover, $\Delta\psi \in C(\mathbb{R}; H_0^1(\Omega))$.*

(iii) The solution ψ satisfies $\psi(0) = 0$, $\psi_t(0) = \tilde{\varphi}(0)$, $\psi_{tt}(0) = \tilde{\varphi}_t(0)$ and $\psi_{ttt}(0) = \tilde{\varphi}_{tt}(0) - (\varepsilon\mu)^{-1}\nabla \cdot \mathbf{E}(0)$.

Notice that it implicitly follows from $\psi(t) \in H_0^1(\Omega)$ that $\psi(t)$ vanishes in the trace sense on the boundary $\partial\Omega$.

Proof. First, by (22),

$$f = \varepsilon\mu\tilde{\varphi}_t \in C^2(\mathbb{R}; H_0^1(\Omega)) \cap C^1(\mathbb{R}; H^2(\Omega)).$$

In particular, $f \in L_{\text{loc}}^2(\mathbb{R}; L^2(\Omega))$.

(i) This assertion follows as a special case of ‘‘Mathematical Example 3’’ in Chapter XVIII of [4]; see also [13, Chap. V] or [6, Chap. 7]. These results guarantee the existence and uniqueness of a variational solution $u \in C(\mathbb{R}; H_0^1(\Omega))$ with $u_t \in C(\mathbb{R}; L^2(\Omega))$ of the wave equation $\varepsilon\mu u_{tt} - \Delta u = g$ with initial conditions $u(0) = u_0$ and $u_t(0) = v_0$ provided $g \in L_{\text{loc}}^2(\mathbb{R}; L^2(\Omega))$, $u_0 \in H_0^1(\Omega)$ and $v_0 \in L^2(\Omega)$. This more general proposition is invoked not only here but below in the proof of part (ii).

(ii) Differentiating (24) with respect to t we see that $y = \psi_t$ formally solves

$$(26) \quad \begin{aligned} \varepsilon\mu y_{tt} - \Delta y &= \varepsilon\mu\tilde{\varphi}_{tt}, \\ y(0) &= \tilde{\varphi}(0), \\ y_t(0) &= \tilde{\varphi}_t(0), \\ y(t) &= 0 \quad \text{on } \partial\Omega \text{ for } t \in \mathbb{R}. \end{aligned}$$

The third equality follows from $y_t(0) = \psi_{tt}(0) = \tilde{\varphi}_t(0) + (\varepsilon\mu)^{-1}\Delta\psi(0) = \tilde{\varphi}_t(0)$. Since the initial data $\tilde{\varphi}(0)$ and $\tilde{\varphi}_t(0)$ both belong to $H_0^1(\Omega)$ and the right-hand side $\varepsilon\mu\tilde{\varphi}_{tt}$ belongs to $L_{\text{loc}}^2(\mathbb{R}; L^2(\Omega))$, the initial-value problem (26) is well-posed; it has a unique variational solution $y \in C(\mathbb{R}; H_0^1(\Omega))$ with $y_t \in C(\mathbb{R}; L^2(\Omega))$. Again this follows from ‘‘Mathematical Example 3’’ in Chapter XVIII of [4]; see also the proof of (i). Just as in the proof of Theorems 30.1–30.2 of [13] one then shows that the formal equation $\psi_t = y$ is in fact rigorous. This is done by demonstrating that $\int_0^t y(s) ds$ is a variational solution of (24) and hence is equal to $\psi(t)$.

Equation (26) permits one more time differentiation. Setting formally $z = y_t$, we have

$$(27) \quad \begin{aligned} \varepsilon\mu z_{tt} - \Delta z &= \varepsilon\mu\tilde{\varphi}_{ttt}, \\ z(0) &= \tilde{\varphi}_t(0) \in H_0^1(\Omega), \\ z_t(0) &= \tilde{\varphi}_{tt}(0) + (\varepsilon\mu)^{-1}\Delta\tilde{\varphi}(0) \in L^2(\Omega), \\ z(t) &= 0 \quad \text{on } \partial\Omega \text{ for } t \in \mathbb{R}. \end{aligned}$$

We have here made use of (22). As for (26), the initial-value problem (27) has a unique variational solution $z \in C(\mathbb{R}; H_0^1(\Omega))$ with $z_t \in C(\mathbb{R}; L^2(\Omega))$. Again and for the same reasons the formal identity is rigorous: $z = y_t = \psi_{tt}$ are true identities.

So far we have proved that

$$(28) \quad \begin{aligned} \psi &\in C^2(\mathbb{R}; H_0^1(\Omega)), \quad \psi_{ttt} \in C(\mathbb{R}; L^2(\Omega)); \quad \psi(0) = 0, \quad \psi_t(0) = \tilde{\varphi}(0), \\ \psi_{tt}(0) &= \tilde{\varphi}_t(0), \quad \psi_{ttt}(0) = \tilde{\varphi}_{tt}(0) + (\varepsilon\mu)^{-1}\Delta\tilde{\varphi}(0). \end{aligned}$$

To investigate the regularity with respect to the space variables, we observe that

$$-\Delta\psi = \varepsilon\mu(\tilde{\varphi}_t - \psi_{tt}) \in C(\mathbb{R}; H_0^1(\Omega)),$$

which implies $\psi \in C(\mathbb{R}; H^2(\Omega))$ thanks to the hypotheses on the domain. Similarly, since $y = \psi_t$ is the solution of (26) we have $-\Delta\psi_t \in C(\mathbb{R}; L^2(\Omega))$, which ensures $\psi_t \in C(\mathbb{R}; H^2(\Omega))$.

(iii) Use (28) in combination with $-\Delta\tilde{\varphi}(0) = \nabla \cdot \mathbf{E}(0)$, which holds by (21). \square

We summarize what we have achieved so far.

Theorem 1. *Let Ω be a bounded, simply connected, open subset Ω of \mathbb{R}^3 with a Lipschitz boundary $\partial\Omega$. Let $\mathbb{C}\overline{\Omega}$ be connected and assume Ω meets condition (5). Assume $\varepsilon, \mu \in C^3(\overline{\Omega})$ are positive on $\overline{\Omega}$. Let $\mathbf{J} \in C^3(\mathbb{R}; L^2(\Omega)^3)$, $\varrho \in C^2(\mathbb{R}; L^2(\Omega))$, $\mathbf{F}(0) = (0, -\mathbf{J}(0)) \in \text{dom}(\mathcal{A}^2)$ and $\mathbf{U}_0 = (\mathbf{B}_0, \mathbf{D}_0) \in \text{dom}(\mathcal{A}^3)$. Moreover, assume conditions (7)–(9). Let $\mathbf{U} = (\mathbf{B}, \mathbf{D})$ be the classical solution of (1)–(4) furnished by Lemma 1.*

Then each of the fields \mathbf{B} , \mathbf{D} , \mathbf{E} , \mathbf{H} belongs to $C^3(\mathbb{R}; L^2(\Omega)^3) \cap C^2(\mathbb{R}; H^1(\Omega)^3)$. Moreover, there exist a vector potential \mathbf{A} and a scalar potential φ , the Lorenz gauge, representing the electromagnetic field as (10), (11), (12). These potentials can be chosen so as to have the following properties:

- (i) *Regularity: $\varphi \in C(\mathbb{R}; H^2(\Omega)) \cap C^1(\mathbb{R}; H_0^1(\Omega))$ and $\varphi_{tt} \in C(\mathbb{R}; L^2(\Omega))$ while $\mathbf{A} \in C^1(\mathbb{R}; H^1(\Omega)^3)$ and $\mathbf{A}_{tt} \in C(\mathbb{R}; L^2(\Omega)^3)$. The Lorenz condition is fulfilled in $C(\mathbb{R}; H_0^1(\Omega))$, i.e., φ_t and $\nabla \cdot \mathbf{A}$ belong to $C(\mathbb{R}; H_0^1(\Omega))$ and (12) is met. Moreover, $\nabla \times \mathbf{A} \in C^3(\mathbb{R}; L^2(\Omega)^3) \cap C^2(\mathbb{R}; H^1(\Omega)^3)$.*
- (ii) *\mathbf{A} satisfies the initial conditions $\nabla \cdot \mathbf{A}(0) = 0$, $\mathbf{A}_t(0) = -\mathbf{E}(0) = -\varepsilon^{-1}\mathbf{D}_0$ and $\mathbf{A}_{tt}(0) = -\mathbf{E}_t(0) = \varepsilon^{-1}(\mathbf{J}(0) - \nabla \times (\mu^{-1}\mathbf{B}_0))$ as well as the boundary conditions $\mathbf{n} \times \mathbf{A}(t) = 0$ and $\nabla \cdot \mathbf{A}(t) = 0$ on $\partial\Omega$ for every t ; in fact, $\nabla \cdot \mathbf{A} \in C(\mathbb{R}; H_0^1(\Omega))$. The scalar potential satisfies the initial conditions $\varphi(0) = 0$, $\varphi_t(0) = 0$, $\varphi_{tt}(0) = (\varepsilon\mu)^{-1}\nabla \cdot \mathbf{E}(0)$ as well as the homogeneous boundary condition encoded in $\varphi \in C^1(\mathbb{R}; H_0^1(\Omega))$.*

Proof. First, by Lemma 1 (iii), the fields \mathbf{B} and \mathbf{E} belong to the space $C^3(\mathbb{R}; L^2(\Omega)^3) \cap C^2(\mathbb{R}; H^1(\Omega)^3)$. As we have seen, this degree of regularity guarantees that the potentials of the Coulomb gauge satisfy, in particular, (20) and (22). The assertions of the theorem on the Lorenz gauge follow from relation (23) between the Coulomb and Lorenz gauges, where ψ has the properties discovered in Lemma 2. For instance,

$$\mathbf{n} \times \mathbf{A}(t) = \mathbf{n} \times \tilde{\mathbf{A}}(t) + \mathbf{n} \times \nabla \psi(t) = 0 + 0,$$

the term $\mathbf{n} \times \nabla \psi(t)$ being the vanishing tangential derivative (since $\psi(t) = 0$ on $\partial\Omega$). The calculation (25) verifying the Lorenz condition is justified in the sense of distributions. \square

Remark 2. It follows from Theorems 2–4 below that \mathbf{A} and φ are uniquely determined by the stated conditions.

3.3. The wave equation

Substituting (10) and (11) into Ampere's law, (\mathbf{A}, φ) (still in the Lorenz gauge) satisfies in $C(\mathbb{R}; L^2(\Omega)^3)$ the equation

$$(29) \quad \varepsilon(\nabla \varphi_t + \mathbf{A}_{tt}) + \nabla \times (\mu^{-1} \nabla \times \mathbf{A}) = \mathbf{J}.$$

It follows from (12) that $-\nabla \varphi_t = \nabla((\varepsilon\mu)^{-1} \nabla \cdot \mathbf{A})$. Using this relation to eliminate φ in (29) one finds that \mathbf{A} is a solution of the wave equation (13), i.e.,

$$\varepsilon(\mathbf{A}_{tt} - \nabla((\varepsilon\mu)^{-1} \nabla \cdot \mathbf{A})) + \nabla \times (\mu^{-1} \nabla \times \mathbf{A}) = \mathbf{J}.$$

We have hence derived the following theorem.

Theorem 2. *Under the conditions of Theorem 1, the vector potential \mathbf{A} of the Lorenz gauge satisfies in $C(\mathbb{R}; L^2(\Omega)^3)$ the wave equation (13).*

We proceed to the uniqueness problem for (13).

Theorem 3. *Let Ω be a bounded, simply connected, open subset Ω of \mathbb{R}^3 with a Lipschitz boundary $\partial\Omega$. Let $\overline{\Omega}$ be connected and assume Ω meets condition (5). Assume $\varepsilon, \mu \in C^3(\overline{\Omega})$. Let $\mathbf{A} \in C^1(\mathbb{R}; H^1(\Omega)^3)$ fulfil $\mathbf{A}_{tt} \in C(\mathbb{R}; L^2(\Omega)^3)$, $\nabla \cdot \mathbf{A} \in C(\mathbb{R}; H_0^1(\Omega))$ and $\nabla \times \mathbf{A} \in C(\mathbb{R}; H^1(\Omega)^3)$, and the boundary condition $\mathbf{n} \times \mathbf{A}(t) = 0$ on $\partial\Omega$ for all $t \in \mathbb{R}$, as well as the initial conditions $\mathbf{A}(0) = 0$ and $\mathbf{A}_t(0) = 0$. Assume \mathbf{A} satisfies in $C(\mathbb{R}; L^2(\Omega)^3)$ the homogeneous wave equation*

$$(30) \quad \varepsilon(\nabla((\varepsilon\mu)^{-1} \nabla \cdot \mathbf{A}) - \mathbf{A}_{tt}) - \nabla \times (\mu^{-1} \nabla \times \mathbf{A}) = 0.$$

Then \mathbf{A} vanishes identically.

Proof. We define φ by

$$\varphi(t) = -\frac{1}{\varepsilon\mu} \int_0^t \nabla \cdot \mathbf{A}(\tau) \, d\tau, \quad t \in \mathbb{R}.$$

Then $\varphi \in C^1(\mathbb{R}; H_0^1(\Omega))$ and, by (30), in the sense of $C(\mathbb{R}; L^2(\Omega)^3)$,

$$(31) \quad \varepsilon(-\nabla\varphi - \mathbf{A}_t)_t - \nabla \times (\mu^{-1}\nabla \times \mathbf{A}) = 0.$$

Next we set

$$\mathbf{E} = -\nabla\varphi - \mathbf{A}_t \quad \text{and} \quad \mathbf{B} = \nabla \times \mathbf{A},$$

which have by our assumptions the following regularity: $\mathbf{E} \in C(\mathbb{R}; L^2(\Omega)^3)$ and $\mathbf{B} \in C(\mathbb{R}; H^1(\Omega)^3)$. In view of (31), Ampere's law is fulfilled, i.e.,

$$\varepsilon\mathbf{E}_t - \nabla \times (\mu^{-1}\mathbf{B}) = 0 \quad \text{in } C(\mathbb{R}; L^2(\Omega)^3).$$

In particular, $\mathbf{E}_t \in C(\mathbb{R}; L^2(\Omega)^3)$ and so $\mathbf{E} \in C^1(\mathbb{R}; L^2(\Omega)^3)$. Also $\mathbf{B} \in C^1(\mathbb{R}; L^2(\Omega)^3)$ since $\mathbf{B}_t = \nabla \times \mathbf{A}_t \in C(\mathbb{R}; L^2(\Omega)^3)$.

Clearly, Faraday's law is fulfilled, i.e.,

$$\mathbf{B}_t + \nabla \times \mathbf{E} = 0.$$

In particular, $\nabla \times \mathbf{E} \in C(\mathbb{R}; L^2(\Omega)^3)$ and by hypothesis $\mathbf{B} \in C(\mathbb{R}; H^1(\Omega)^3)$, and so $(\mathbf{B}(t), \mathbf{D}(t)) = (\mathbf{B}(t), \varepsilon\mathbf{E}(t)) \in \text{dom}(\mathcal{A})$. The constructed fields satisfy homogeneous initial conditions: $\mathbf{E}(0) = -\nabla\varphi(0) - \mathbf{A}_t(0) = 0$ and $\mathbf{B}(0) = \nabla \times \mathbf{A}(0) = 0$. We check that $\mathbf{n} \times \mathbf{E}(t) = 0$ on the boundary for all t . Since $\varphi(t) \in H_0^1(\Omega)$ and $\mathbf{n} \times \mathbf{A}(t)|_{\partial\Omega} = 0$ in the trace sense, we have $\mathbf{n} \times \mathbf{E}(t) = -\mathbf{n} \times \nabla\varphi(t) - \mathbf{n} \times \mathbf{A}'(t) = 0 + 0$ on $\partial\Omega$. To justify that $\mathbf{n} \times \mathbf{A}'(t) = 0$ on the boundary, we recall the trace theorem for $H(\text{curl}, \Omega)$, see Remark 1. First, the hypothesis $\mathbf{A} \in C^1(\mathbb{R}; H^1(\Omega)^3)$ ensures that $\gamma_\tau(\mathbf{A}(t))$ and $\gamma_\tau(\mathbf{A}'(t))$ make sense in $H^{-1/2}(\Omega)$ for each $t \in \mathbb{R}$. By assumption, the trace $\gamma_\tau(\mathbf{A}(t)) = 0$. Therefore, $\gamma_\tau(h^{-1}(\mathbf{A}(t+h) - \mathbf{A}(t))) = 0$ and since, as $h \rightarrow 0$, $h^{-1}(\mathbf{A}(t+h) - \mathbf{A}(t)) \rightarrow \mathbf{A}'(t)$ in $H^1(\Omega)$, hence in $H(\text{curl}, \Omega)$, it follows that $\gamma_\tau(\mathbf{A}'(t)) = 0$, as was to be verified.

Hence $\mathbf{B}(t) = 0$ and $\mathbf{E}(t) = 0$ for all $t \in \mathbb{R}$ owing to the uniqueness of classical solutions [5], [3]. Finally, since \mathbf{B} and \mathbf{E} vanish, \mathbf{A} vanishes as well. Indeed, we have shown that

$$(32) \quad \nabla \times \mathbf{A} = 0,$$

$$(33) \quad -\nabla\varphi - \mathbf{A}_t = 0,$$

$$(34) \quad \varepsilon\mu\varphi_t + \nabla \cdot \mathbf{A} = 0.$$

Eliminating \mathbf{A} from (33)–(34), we *formally* find the wave equation $\varepsilon\mu\varphi_{tt} - \Delta\varphi = 0$ with the homogeneous initial conditions $\varphi(0) = 0$ and $\varphi_t(0) = 0$ and with homogeneous boundary conditions. By uniqueness, $\varphi = 0$ everywhere and so (33) reduces to $\mathbf{A}_t = 0$. Since $\mathbf{A}(0) = 0$ by assumption we must have $\mathbf{A}(t) = 0$ for all $t \in \mathbb{R}$, which was to be proved.

However, to rigorously complete the proof we need to justify that φ is the unique solution of the wave equation in a proper sense. According to the uniqueness proof of Lemma 2 (i), because $\varphi \in C^1(\mathbb{R}; H_0^1(\Omega))$, it suffices to demonstrate that it follows from (32)–(34) that φ (satisfying the homogeneous initial and boundary conditions) is the variational solution of $\varepsilon\mu\varphi_{tt} - \Delta\varphi = 0$, i.e., that

$$(35) \quad \frac{d}{dt} \int_{\Omega} \varepsilon(x)\mu(x)\varphi_t(t, x)v(x) dx + \int_{\Omega} \nabla\varphi(t, x) \cdot \nabla v(x) dx = 0$$

is fulfilled in the sense of $\mathcal{D}'(\mathbb{R})$ for any $v \in H_0^1(\Omega)$.

Making use of (33) and (34), it is evident that (35) boils down to

$$(36) \quad -\frac{d}{dt} \int_{\Omega} (\nabla \cdot \mathbf{A})v dx - \int_{\Omega} \mathbf{A}_t \cdot \nabla v dx = 0.$$

Since $\nabla \cdot \mathbf{A} \in C(\mathbb{R}; H_0^1(\Omega))$, (36) is proved in two steps:

$$-\frac{d}{dt} \int_{\Omega} (\nabla \cdot \mathbf{A})v dx = \frac{d}{dt} \int_{\Omega} \mathbf{A} \cdot \nabla v dx = \int_{\Omega} \mathbf{A}_t \cdot \nabla v dx.$$

The first equality holds by the definition of the divergence in the sense of distributions and the density of $\mathcal{D}(\Omega)$ in $H_0^1(\Omega)$. For the second equality we have used $\mathbf{A} \in C^1(\mathbb{R}; H^1(\Omega)^3)$ and $\nabla v \in L^2(\Omega)^3$ which ensure that $F(\mathbf{A}(t)) = \int_{\Omega} \mathbf{A} \cdot \nabla v dx$ is a C^1 real function of t whose derivative is $F(\mathbf{A}'(t)) = \int_{\Omega} \mathbf{A}_t \cdot \nabla v dx$. Indeed, the functional

$$F(\mathbf{u}) = \int_{\Omega} \mathbf{u} \cdot \nabla v dx, \quad \mathbf{u} \in L^2(\Omega)^3,$$

is linear and continuous on $L^2(\Omega)^3$. Therefore, because $\mathbf{A} \in C^1(\mathbb{R}; H^1(\Omega)^3)$, we have

$$h^{-1}(F(\mathbf{A}(t+h)) - F(\mathbf{A}(t))) = F(h^{-1}(\mathbf{A}(t+h) - \mathbf{A}(t))) \rightarrow F(\mathbf{A}'(t)), \quad h \rightarrow 0,$$

and $F(\mathbf{A}'(t))$ is a continuous function of t .

Thus the key equation (36) is satisfied, and so φ as well as \mathbf{A} must vanish. \square

4. THE MAIN THEOREM FOR THE VECTOR POTENTIAL

We have obtained in Theorem 1 the existence of the potentials \mathbf{A} and φ of the Lorenz gauge, with respect to which (10)–(12) hold. It follows from Theorems 2 and 3 that \mathbf{A} is the unique solution of a wave problem. We are now in a position to state and prove the theorem that constitutes the analytical backbone of this paper.

Theorem 4. *Let Ω be a bounded, simply connected, open subset Ω of \mathbb{R}^3 with a Lipschitz boundary $\partial\Omega$. Let $\overline{\Omega}$ be connected and assume Ω meets condition (5). Assume $\varepsilon, \mu \in C^3(\overline{\Omega})$ are positive. Let $\mathbf{J} \in C^3(\mathbb{R}; L^2(\Omega)^3)$, $\varrho \in C^2(\mathbb{R}; L^2(\Omega))$, $\mathbf{F}(0) = (0, -\mathbf{J}(0)) \in \text{dom}(\mathcal{A}^2)$ and $\mathbf{U}_0 = (\mathbf{B}_0, \mathbf{D}_0) \in \text{dom}(\mathcal{A}^3)$. Then there exists exactly one $\mathbf{A}_0 \in H^1(\Omega)^3$ such that $\mathbf{B}_0 = \nabla \times \mathbf{A}_0$ and $\nabla \cdot \mathbf{A}_0 = 0$ in Ω and $\mathbf{n} \times \mathbf{A}_0 = 0$ on $\partial\Omega$. Furthermore, the vector potential \mathbf{A} of the Lorenz gauge is uniquely determined as the solution of the following initial-boundary value problem: find the solution \mathbf{A} of the wave equation (13) in the sense of $C(\mathbb{R}; L^2(\Omega)^3)$ fulfilling the initial conditions $\mathbf{A}(0) = \mathbf{A}_0$ and $\mathbf{A}_t(0) = -\mathbf{E}(0) = -\varepsilon^{-1}\mathbf{D}_0$ as well as the regularity and boundary conditions*

$$\begin{aligned} \mathbf{A} &\in C^1(\mathbb{R}; H^1(\Omega)^3), \quad \mathbf{A}_{tt} \in C(\mathbb{R}; L^2(\Omega)^3), \\ \nabla \times \mathbf{A} &\in C(\mathbb{R}; H^1(\Omega)^3), \quad \nabla \cdot \mathbf{A} \in C(\mathbb{R}; H_0^1(\Omega)), \quad \mathbf{n} \times \mathbf{A} = 0 \quad \text{on } \mathbb{R} \times \partial\Omega. \end{aligned}$$

Proof. We have seen, in Subsection 3.1 above, that there is a unique \mathbf{A}_0 possessing the stated properties. As regards the wave equation, according to Theorem 1 and Theorem 2 there exists a solution \mathbf{A} possessing the claimed regularity. By Theorem 3, this solution is unique. Indeed, if \mathbf{A}_1 and \mathbf{A}_2 are solutions, set $\hat{\mathbf{A}} = \mathbf{A}_1 - \mathbf{A}_2$. Then $\hat{\mathbf{A}}$ is a solution of the homogeneous wave equation considered in Theorem 3; hence $\hat{\mathbf{A}} = 0$, and the proof is complete. \square

Let us summarize how we compute the vector potential \mathbf{A} as a solution of a wave equation and how we construct the field (\mathbf{E}, \mathbf{B}) from this potential. First, notice that the wave equation (13) can be written as

$$(37) \quad \mathbf{A}_{tt} + L(\mathbf{A}) = \varepsilon^{-1}\mathbf{J} \quad \text{in } \mathbb{R} \times \Omega,$$

with

$$L(\mathbf{A}) = -\frac{1}{\varepsilon\mu} \left[\Delta\mathbf{A} + \frac{\nabla\mu}{\mu} \times (\nabla \times \mathbf{A}) - \frac{\nabla(\varepsilon\mu)}{\varepsilon\mu} (\nabla \cdot \mathbf{A}) \right]$$

and the boundary conditions

$$(38) \quad \nabla \cdot \mathbf{A} = 0, \quad \mathbf{n} \times \mathbf{A} = 0 \quad \text{on } \mathbb{R} \times \partial\Omega.$$

The boundary and initial conditions, supplemented with which the wave equation (37) is well-posed, are specified in Theorem 4. Having the solution \mathbf{A} , we determine φ_t by the Lorenz condition (12). Since $\varphi(0) = 0$, the time integral of φ_t from 0 to t then gives $\varphi(t)$ as

$$\varphi(t) = -\frac{1}{\varepsilon\mu} \int_0^t \nabla \cdot \mathbf{A}(\tau) \, d\tau, \quad t \in \mathbb{R}.$$

Finally, given the field (\mathbf{A}, φ) , the field (\mathbf{E}, \mathbf{B}) can be computed as well by (10) and (11).

5. NUMERICAL METHOD

Numerically, this description of the field through \mathbf{A} laid down in the first part of the paper has its pros and cons.

- (a) The operator L does not have zero for an eigenvalue, i.e., the system of equations

$$\begin{aligned} L(\mathbf{A}) &= \omega^2 \mathbf{A} \quad \text{in } \Omega, \\ \nabla \cdot \mathbf{A} &= 0, \quad \mathbf{n} \times \mathbf{A} = 0 \quad \text{on } \partial\Omega \end{aligned}$$

has no nontrivial (time-independent) solution \mathbf{A} if $\omega^2 = 0$. This fact can be seen from the Gauss divergence theorem. Hence no spurious modes, corresponding to $\omega = 0$, can contaminate the numerical solution to the time-domain problem (37), (38). When starting from the equations for the primitive field (\mathbf{E}, \mathbf{B}) , or the electric field \mathbf{E} , or the magnetic induction field \mathbf{B} , and neglecting the divergence equations for \mathbf{B} or \mathbf{E} , one may meet with erroneous results. Spurious modes may appear unless they are precautioned [8], [10], [2], [1].

- (b) The electric Gauss law $\nabla \cdot \mathbf{D} = \rho$ is not required for the calculation of \mathbf{A} , φ or (\mathbf{E}, \mathbf{B}) . (It is, however, enforced at $t = 0$ by condition (8).) Instead, in our method, the computed values of $\nabla \cdot \mathbf{D} - \rho$ provide a measure of accuracy.
- (c) Numerical differentiations are needed to reach (\mathbf{E}, \mathbf{B}) from the computed \mathbf{A} . This fact is the main disadvantage of the description through \mathbf{A} .

The initial-boundary value problem for (37) as specified in Theorem 4 can be handled by standard numerical methods. We employ the trapezoidal rule for time-integration and a Chebychev collocation method for approximations of partial derivatives. This spectral method is suitable since the material properties vary continuously, and smooth solutions \mathbf{A} to (37) and (38) are anticipated. The computed field \mathbf{A} then becomes continuous, as well as the computed fields \mathbf{E} and \mathbf{B} , while the electric Gauss law turns out to be satisfied asymptotically.

The numerical method and the geometry are presented in this section. Medium and antenna models are laid down in Section 6, and the outcomes of the method are compared with the ones for a standard finite element method. In addition, convergence properties are studied, and time histories of the field \mathbf{A} are given.

5.1. Time discretization

The initial conditions for \mathbf{A} and \mathbf{J} , as specified by Theorem 4, are fulfilled if the field and its source vanish identically at the outset. The numerical implementation of this assumption reads

$$(39) \quad \mathbf{A} = \mathbf{A}_t = 0, \quad \text{and} \quad \mathbf{J} = 0 \quad \text{on} \quad \bar{\Omega} \quad \text{at} \quad t = 0.$$

It can be seen that these initial conditions are consistent with wave equation (37) and boundary conditions (38).

Equation (37) is time-discretized by the trapezoidal rule, which is implemented in a way described in a textbook by Hughes [7, Chap. 9]. Below the implementation for the vector potential \mathbf{A} is given.

Let the time-step be Δt , and let $t^k = k\Delta t$, where k is a nonnegative integer. The approximations of the vector potential \mathbf{A} and its time derivative \mathbf{A}_t at time t^k are denoted by \mathbf{A}^k and \mathbf{A}_t^k , respectively. Similarly, $\mathbf{J}^k = \mathbf{J}(t^k)$. According to the trapezoidal rule

$$(40) \quad \mathbf{A}^{k+1} - \mathbf{A}^k = \frac{\Delta t}{2}(\mathbf{A}_t^{k+1} + \mathbf{A}_t^k)$$

and

$$(41) \quad \mathbf{A}_t^{k+1} - \mathbf{A}_t^k = \frac{\Delta t}{2}(\mathbf{A}_{tt}^{k+1} + \mathbf{A}_{tt}^k),$$

where terms quadratic in Δt have been neglected. Combining these equations one finds

$$(42) \quad \mathbf{A}_{tt}^{k+1} = \frac{4}{\Delta t^2}(\mathbf{A}^{k+1} - \mathbf{A}^k) - \frac{4}{\Delta t}\mathbf{A}_t^k - \mathbf{A}_{tt}^k.$$

Inserting (42) in (37) gives

$$(43) \quad \mathbf{A}^{k+1} + \frac{\Delta t^2}{4}L(\mathbf{A}^{k+1}) = \frac{\Delta t^2}{4\varepsilon}\mathbf{J}^{k+1} + \mathbf{A}^k + \Delta t\mathbf{A}_t^k + \frac{\Delta t^2}{4}\mathbf{A}_{tt}^k.$$

This equation applies to Ω . No time derivatives are involved on $\partial\Omega$.

To proceed from step k to step $k+1$, equations (43) and (38) are solved for \mathbf{A}^{k+1} . The derivatives \mathbf{A}_t^{k+1} and \mathbf{A}_{tt}^{k+1} are then calculated by (40) and (41). The initial

values \mathbf{A}^0 , \mathbf{A}_t^0 are given by (39), and the current \mathbf{J}^k is known (cf. Section 6.1). Therefore, $\mathbf{A}^0 = 0$, $\mathbf{A}_t^0 = 0$, and it is consistent to add $\mathbf{A}_{tt}^0 = 0$.

5.2. Space discretization

We study a cubic cavity $\Omega = (-1, 1)^3$. The faces of the cube are orthogonal to the coordinate axes; the unit outward normal vector is $\mathbf{n} = (0, 0, 1)$ on the side where $x_3 = 1$. The edges and the corners are looked upon as rounded in a symmetric way. Therefore, e.g., on the edge where $x_1 = x_2 = 1$ and $-1 < x_3 < 1$, $\mathbf{n} = \sqrt{2}^{-1}(0, 1, 1)$ and at the corner $(1, 1, 1)$, $\mathbf{n} = \sqrt{3}^{-1}(1, 1, 1)$.

The cube is discretized using the Gauss-Lobatto-Chebyshev collocation points (x_{1i}, x_{2j}, x_{3k}) where $x_{1i} = \cos(\pi i/m_1)$, $i = 0, \dots, m_1$, $x_{2j} = \cos(\pi j/m_2)$, $j = 0, \dots, m_2$, and $x_{3k} = \cos(\pi k/m_3)$, $k = 0, \dots, m_3$. Thus, there are altogether $(m_1 + 1) \times (m_2 + 1)(m_3 + 1)$ collocation points. These are classified as interior (b), side (s), edge (e), or corner points (c); b stands for bulk. They are ordered b, s, e, c and the points of each class in the partition $\{b, s, e, c\}$ are numbered by one index. Below is the pseudocode for the class b , where each collocation point $xb = (x_{1i}, x_{2j}, x_{3k})$ in b is assigned an index mb :

for $k = 1$ to $m_3 - 1$; for $j = 1$ to $m_2 - 1$; for $i = 1$ to $m_1 - 1$;

$$mb = i + (j - 1)(m_1 - 1) + (k - 1)(m_1 - 1)(m_2 - 1),$$

$$xb_{mb} = (x_{1i}, x_{2j}, x_{3k}).$$

Obviously, $mb = 1, \dots, (m_1 - 1)(m_2 - 1)(m_3 - 1)$. Similar pseudocodes describe the numbering of the points of the classes s, e and c .

Above, bold face vectors have three components, e.g., $\mathbf{A} = (A_1, A_2, A_3)$. For convenience, let the column vector a represent the values of \mathbf{A} at all collocation points, and let us distinguish between the interior (b), side (s), edge (e), and corner (c) values of a . Thus, $a^T = (ab^T, as^T, ae^T, ac^T)$, where $ab^T = (ab1^T, ab2^T, ab3^T)$ with the column vectors $ab1$, $ab2$ and $ab3$ each ordered in the same way as the interior collocation points xb , and abq , $q = 1, 2, 3$, representing A_q in class q .

Similarly, for $\gamma = s, e$ or c , $a\gamma^T = (a\gamma1^T, a\gamma2^T, a\gamma3^T)$ with the column vectors $a\gamma1$, $a\gamma2$ and $a\gamma3$ each ordered in the same way as the collocation points $x\gamma$ in class γ , and $a\gamma q$, $q = 1, 2, 3$, representing A_q in class γ .

5.3. Differentiating matrices

A standard Chebyshev method is adopted, where a scalar function f , defined on the cube $\bar{\Omega}$, is represented by the sum

$$\sum_{i=0}^{m_1} \sum_{j=0}^{m_2} \sum_{k=0}^{m_3} \hat{f}(i, j, k) T_i(x_1) T_j(x_2) T_k(x_3).$$

Here $\hat{f}(i, j, k)$ are the expansion coefficients and $T_i(x_q) = \cos(i \arccos x_q)$. The values of f at all collocation points yield the values of all expansion coefficients, and the sum approximates f on the cube and equals f at all collocation points. Below, simplified notation is used for the collocation points. We introduce $(i, j, k) = (x_{1i}, x_{2j}, x_{3k})$ whence $f(i, j, k) = f(x_{1i}, x_{2j}, x_{3k})$.

The basic differentiating matrix with respect to the space variables is der . It gives the partial derivatives of f at a collocation point in terms of the values of f at this and other collocation points. The Chebyshev collocation partial derivative with respect to x_1 is

$$f_{x_1}(l, j, k) = \sum_{i=0}^{m_1} der(l, i) f(i, j, k),$$

where the expression for the matrix der is well-known [9]. The Chebyshev collocation partial derivatives f_{x_2} and f_{x_3} are defined analogously using the matrix der . This matrix derivative procedure is translated to apply to the partitioning of the collocation points. We now let the domain of f be all collocation points. Using the enumeration that has been decided upon, the three-dimensional matrix $f(i, j, k)$ is represented by $(fb^T, fs^T, fe^T, fc^T)^T$, where fb , fs , fe and fc are column vectors. The vector f_{x_q} , $q = 1, 2, 3$, giving the x_q -derivative at the collocation points, can then be calculated by the matrix product

$$\begin{bmatrix} fb_{x_q} \\ fs_{x_q} \\ fe_{x_q} \\ fc_{x_q} \end{bmatrix} = \begin{bmatrix} dbbdxq & dbsdxq & dbedxq & dbcdxq \\ dsbdxq & dssdxq & dsedxq & dscdxq \\ debdxq & desdxq & deedxq & decdxq \\ dcbdxq & dcsdxq & dcedxq & dccdxq \end{bmatrix} \begin{bmatrix} fb \\ fs \\ fe \\ fc \end{bmatrix}.$$

The d -matrices, $dbbdx1, \dots, dccdx3$, are renumbered and expanded versions of parts of der . Some of these matrices are blocks of zeros. For instance, $dbedx1$ and $dbcdx1$ are zero matrices, since a line in the x_1 -direction passing through an interior point never ends at an edge point or a corner point.

Also the operators ∇ , $\nabla \cdot$ and $\nabla \times$ are approximated by matrices built by the matrices $dbbdx1, \dots, dccdx3$. Second-order derivatives are built by first-order differentiating matrices.

A study of the domain and range of the d -matrices yields, in generic terms, that if the discretized version of the equation $\mathbf{W} = \nabla \times \mathbf{V}$ is defined on both b and s then the discretized version of $\nabla \cdot \mathbf{W}$ vanishes in b . However, if $\mathbf{W} = \nabla \times \mathbf{V}$ is defined only in b , then $\nabla \cdot \mathbf{W} = 0$ is not enforced in b . These facts are significant for the fulfilment of the electric Gauss law. See Section 6.3, equation (47), where the substitution $\mathbf{V} = \mu^{-1}(\nabla \times \mathbf{A})$ gives an equation for $\mathbf{W} = \nabla \times \mathbf{V}$ in b alone.

5.4. Governing matrix equation

Approximating the space derivatives by matrices, equation (43) with boundary conditions yields a matrix equation of the form

$$(44) \quad mat * a = r,$$

where the asterisk $*$ denotes matrix product. Here the unknown vector a and the input vector r are arranged as explained in Section 5.2. The square matrix mat is of size $[3(m_1 + 1)(m_2 + 1)(m_3 + 1)]^2$, and is partitioned as follows:

$$mat = \begin{bmatrix} mbb11 & mbb12 & mbb13 & mbs11 & mbs12 & mbs13 & 0 & 0 \\ mbb21 & mbb22 & mbb23 & mbs21 & mbs22 & mbs23 & 0 & 0 \\ mbb31 & mbb32 & mbb33 & mbs31 & mbs32 & mbs33 & 0 & 0 \\ msb11 & msb12 & msb13 & mss11 & mss12 & mss13 & mse1 & 0 \\ msb21 & msb22 & msb23 & mss21 & mss22 & mss23 & mse2 & 0 \\ msb31 & msb32 & msb33 & mss31 & mss32 & mss33 & mse3 & 0 \\ 0 & 0 & 0 & mes1 & mes2 & mes3 & mee & mec \\ 0 & 0 & 0 & 0 & 0 & 0 & mce & mcc \end{bmatrix}.$$

The vectors a and r have the structure

$$(45) \quad a = [ab1^T, ab2^T, ab3^T, as1^T, as2^T, as3^T, ae^T, ac^T]^T$$

and

$$(46) \quad r = [rb1^T, rb2^T, rb3^T, 0, 0, 0, 0, 0]^T.$$

The matrix mat is built by block matrices, which are formed by the derivative matrices $dbbdx1, \dots, dccdx3$. Some of the blocks are zero matrices. In addition, $rs1, rs2, rs3, re, rc$ are all zero vectors, since the boundary conditions are homogeneous. All diagonal block matrices, $mbb11, \dots, mcc$, are well-conditioned, and it is possible to reduce the matrix equation (44) to a matrix equation for only the corner values, ac , by repeated block Gauss elimination. In the first step $ab1$ is eliminated. The first block row and first block column of mat become superfluous and some matrices are changed to account for the influence of $ab1$. Then $ab2$ is eliminated. The procedure is repeated, and after seven steps one obtains a matrix equation which gives ac :

$$m7cc * ac = r7c.$$

Here we use the Gauss transform (Schur complement)

$$m7cc = mcc - mce * (m6ee)^{-1} * me$$

and $r7c = rc - mce * (m6ee)^{-1} * r6e$, where $m6ee$ is known from the previous step. Back-substitution then gives the other parts of a .

The matrix $mbb11$ on the diagonal of mat and the diagonal Gauss transforms $m1bb22$, $m2bb33$, $m3ss11$, $m4ss22$, $m5ss33$, $m6ee$ and $m7cc$ are calculated in a preparatory step and then stored. They are well-conditioned. Totally, at each time level, 27 matrices are stored for the calculation of the reduced vectors $r7c$, $r6e$, $r5s3$, $r4s2$, $r3s1$, $r2b3$, $r1b2$, $rb1$ and the solution vector a .

6. NUMERICAL RESULTS

6.1. Material and antenna models

The permittivity ε and permeability μ are prescribed on the cube $[-1, 1]^3$. In our numerical experiments,

$$\varepsilon(x) = C \prod_{i=1}^3 \left(2 + \sin\left(\alpha_i \frac{\pi}{2} x_i + \beta_i\right) \right)$$

where α_i are specified below and $\beta_i = 0.1$, $i = 1, 2, 3$. The constant factor C is chosen such that the minimum value of ε equals 1. We let $\mu = 1$, i.e., dielectrics will be considered in the sequel.

Three different dielectrics will be used for numerical computations:

- (i) $\varepsilon = 1$, $\alpha_i = 0$ for $i = 1, 2, 3$, i.e., vacuum;
- (ii) $\varepsilon = \varepsilon(x_1, x_2)$ is independent of x_3 , $(\alpha_1, \alpha_2, \alpha_3) = (0.2, 0.2, 0.0)$;
- (iii) $\varepsilon = \varepsilon(x_1, x_3)$ is independent of x_2 , $(\alpha_1, \alpha_2, \alpha_3) = (0.2, 0.0, 0.2)$.

In (ii) and (iii), ε varies between 1 and 1.8 in the cube. Of course, the dielectric in (ii) is the same as that in (iii), but the current \mathbf{J} is chosen such that $\mathbf{J} \cdot \nabla \varepsilon = 0$ in (ii) whereas $\mathbf{J} \cdot \nabla \varepsilon$ does not vanish in (iii).

The prescribed current \mathbf{J} is similar to that of a linear antenna placed in the middle of the cavity. We let \mathbf{J} be directed along the x_3 -axis, vanish on $\partial\Omega$, and be given in Ω as a product of four regular functions of x_1 , x_2 , x_3 and t , respectively. These are chosen such that \mathbf{J} vanishes initially and that the time integral of \mathbf{J} from 0 to T_p is zero. The time-dependent factor of \mathbf{J} , J^t , is plotted in Fig. 1.

6.2. Comparison with FEM software results

All programs are run on the same platform, a sunu sparc SUNW, Sun-Fire-V210 with real memory 2048M, half of which is available for one user. The spectral code is implemented in the programming language MATLAB[®] 7 [15].

To check the spectral results, the governing equations are also implemented in a finite element software FEMLAB 2.2, using Lagrange-quadratic elements. (FEMLAB 2.2 is an old version of COMSOL[®] 3.2 [14].) The wave equation is written as

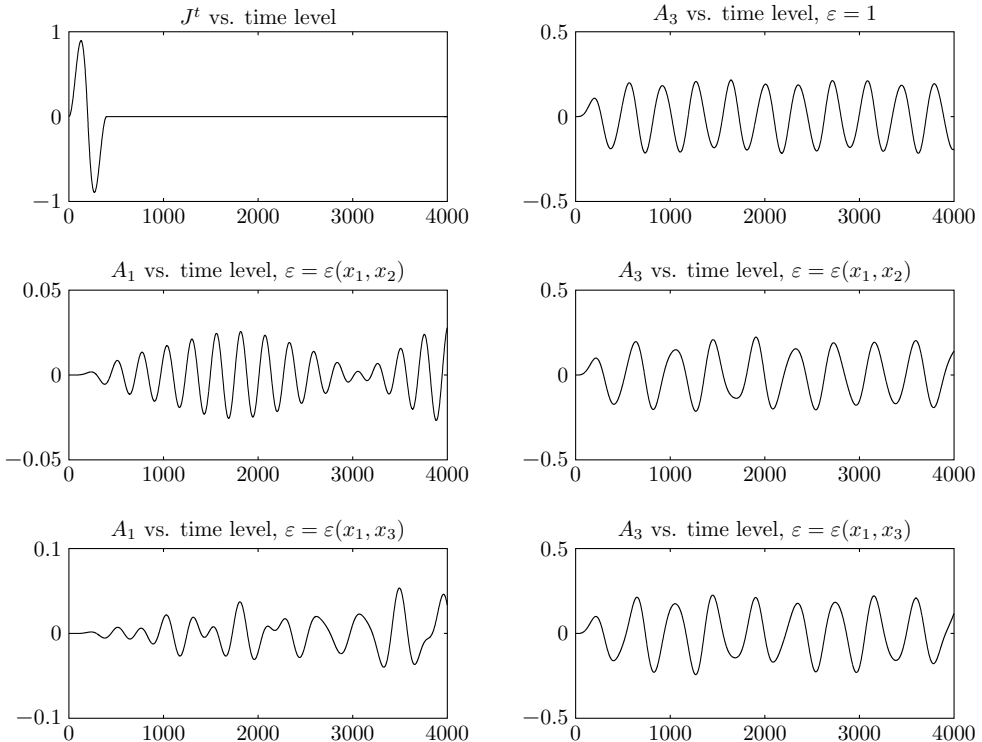


Figure 1. Time-dependent factor of imposed current \mathbf{J} and field components A_1 , A_3 at a point with Euclidian coordinates $(-0.71, 0.38, 0.38)$, at time levels 1–4000. Discretization: $(m_1, m_2, m_3) = (8, 8, 16)$, $\Delta t = \pi/400$. Top left: J^t . Top right: A_3 for $\varepsilon = 1$, vacuum, case (i). Middle: left, A_1 , and right, A_3 , for $\varepsilon = \varepsilon(x_1, x_2)$, case (ii). Bottom: left, A_1 , and right, A_3 , for $\varepsilon = \varepsilon(x_1, x_3)$, case (iii).

a system containing first order time-derivatives of $(\mathbf{A}, \mathbf{A}_t)$. To get a tractable problem, we use for time integration a backward Euler method of second order, and solve the linear system by an iterative method GMRES with incomplete LU-factorization with drop tolerance 0.01. The relative tolerance is set to 0.01 and the absolute tolerance is 0.001. Using these adjustments, we compute $(\mathbf{A}, \mathbf{A}_t)$ at time $t = 0.01\pi$ and $t = 0.02\pi$ for the dielectrics (i) $\varepsilon = 1$, (ii) $\varepsilon = \varepsilon(x_1, x_2)$ and (iii) $\varepsilon = \varepsilon(x_1, x_3)$; see Section 6.1. The results are presented in Tab. 1, where S stands for size and T_c for computation time. By definition, S is the maximal amount of memory needed during the computation. The corresponding results by the spectral code are given in Tab. 2. In Tabs. 1 and 2, $\max(\mathbf{A}) = \max(\max(A_1), \max(A_2), \max(A_3))$ and the other extreme values are defined analogously. (Below we use the shorthand notation $1.686 - 7$ for 1.686×10^{-7} .)

The finite element code has about 150 000 degrees of freedom, which is the minimal number of degrees of freedom to meet comparable precision with the collocation

medium	t	$\max(\mathbf{A})$	$\min(\mathbf{A})$	$\max(\mathbf{A}_t)$	$\min(\mathbf{A}_t)$	S and T_c
$\varepsilon = 1$	$.01\pi$	$1.686 - 7$	$-.007 - 7$	$2.081 - 5$	$-.008 - 5$	962 Mb
	$.02\pi$	$2.581 - 6$	$-.008 - 6$	$1.644 - 4$	$-.004 - 4$	9.9 h
$\varepsilon = \varepsilon(x_1, x_2)$	$.01\pi$	$1.227 - 7$	$-.007 - 7$	$1.516 - 5$	$-.008 - 5$	964 MB
	$.02\pi$	$1.879 - 6$	$-.008 - 6$	$1.197 - 4$	$-.004 - 4$	13.9 h
$\varepsilon = \varepsilon(x_1, x_3)$	$.01\pi$	$1.229 - 7$	$-.006 - 7$	$1.518 - 5$	$-.007 - 5$	964 Mb
	$.02\pi$	$1.882 - 6$	$-.007 - 6$	$1.199 - 4$	$-.004 - 4$	12.3 h

Table 1. Maximum and minimum of \mathbf{A} and \mathbf{A}_t , finite element method.

medium	t	$\max(\mathbf{A})$	$\min(\mathbf{A})$	$\max(\mathbf{A}_t)$	$\min(\mathbf{A}_t)$	S and T_c
$\varepsilon = 1$	$.01\pi$	$1.655 - 7$	$-.000 - 7$	$2.076 - 5$	$-.000 - 5$	222 Mb
	$.02\pi$	$2.605 - 6$	$-.000 - 6$	$1.651 - 4$	$-.000 - 4$	13.4 s
$\varepsilon = \varepsilon(x_1, x_2)$	$.01\pi$	$1.200 - 7$	$-.001 - 7$	$1.504 - 5$	$-.000 - 5$	225 Mb
	$.02\pi$	$1.888 - 6$	$-.000 - 6$	$1.197 - 4$	$-.000 - 4$	16.3 s
$\varepsilon = \varepsilon(x_1, x_3)$	$.01\pi$	$1.199 - 7$	$-.001 - 7$	$1.504 - 5$	$-.000 - 5$	234 Mb
	$.02\pi$	$1.888 - 6$	$-.000 - 6$	$1.197 - 4$	$-.000 - 4$	14.2 s

Table 2. Maximum and minimum of \mathbf{A} and \mathbf{A}_t , spectral method, $(m_1, m_2, m_3) = (4, 4, 12)$, $\Delta t = \pi/1000$.

solver. The spectral code uses polynomials of order 4, 4 and 12 in x_1 -, x_2 -, and x_3 -direction, respectively. Maximum and minimum values of \mathbf{A} and \mathbf{A}_t in Tab. 2 do not change if these orders are increased.

The time integration procedure influences the outcome. As for the finite element code, we use a backward Euler method of order three for $\varepsilon = \varepsilon(x_1, x_3)$, and $(\max(\mathbf{A}), \max(\mathbf{A}_t))$ takes the values $(1.175 - 7, 1.505 - 5)$ and $(1.883 - 6, 1.202 - 4)$ at $t = 0.01\pi$ and $t = 0.02\pi$, respectively. As for the spectral code, the time step is $\Delta t = \pi/1000$ in Tab. 2. The trapezoidal rule suffers from relative period errors [7, Chap. 11], and underestimates values that increase with time. If we use $\Delta t = \pi/8000$ instead, then $(\max(\mathbf{A}), \max(\mathbf{A}_t))$ assumes the values $(1.176 - 7, 1.497 - 5)$ and $(1.879 - 6, 1.195 - 4)$ at $t = 0.01\pi$ and $t = 0.02\pi$, respectively, for $\varepsilon = \varepsilon(x_1, x_3)$. Further decrease of the time step does not change these figures. In conclusion, the results of the two different implementations seem to be consistent.

Tabs. 1 and 2 indicate that the FEM solver is slow as compared with the spectral solver. We will comment on this fact.

- (i) The governing system of the FEM solver comprises six dependent scalar variables, while the governing system of the spectral solver comprises three dependent scalar variables.
- (ii) At every time step the FEM solver performs substantial numerical integration, but reassembles only the time-dependent quantities. The spectral solver is based

upon a partitioning and storing method constructed so that the computational cost per time step is low.

- (iii) The solution field is smooth. Hence, the spectral solver computes the field with sufficient accuracy when using polynomials limited to low order.

To sum up, the FEM solver is slow because of its generality, and the spectral solver is fast since it takes advantage of the cubic geometry and the smooth solution field.

6.3. Fulfilment of Maxwell's equations

Faraday's law and the magnetic Gauss law are satisfied automatically by the field represented by (\mathbf{A}, φ) , since analytically

$$\begin{aligned}\mathbf{B}_t + \nabla \times \mathbf{E} &= (\nabla \times \mathbf{A})_t - \nabla \times \mathbf{A}_t - \nabla \times \nabla \varphi = 0, \\ \nabla \cdot \mathbf{B} &= \nabla \cdot (\nabla \times \mathbf{A}) = 0.\end{aligned}$$

These relations are valid also for the discretized field as mentioned in Section 5.3.

Ampere's law and the electric Gauss law remain to be considered. Ampere's law is enforced in Ω , at the collocation points of b , through equation (37), so it is fulfilled there, while Ampere's law is not enforced at the collocation in $\partial\Omega$ (on s , e or c), where boundary conditions (38) apply. Analytically, the electric Gauss law is an implication of Ampere's law and the continuity equation. Numerically, if Ampere's law is enforced in Ω , at the collocation points b and s , the electric Gauss law is valid on b , but the former law is only enforced on b . It is therefore of interest to study the latter law further.

Introduce two quantities which measure how well Ampere's law and the electric Gauss law are fulfilled:

$$(47) \quad amp = \nabla \times (\mu^{-1}(\nabla \times \mathbf{A})) + \varepsilon(\nabla \varphi_t + \mathbf{A}_{tt})$$

with $\varphi_t = -(\varepsilon\mu)^{-1}\nabla \cdot \mathbf{A}$, and

$$(48) \quad rho = -\nabla \cdot (\varepsilon(\nabla \varphi + \mathbf{A}_t)),$$

where φ is obtained by time integration of φ_t and $\varphi(0) = 0$.

After the pulse ($t \geq T_p$) the source vanishes and amp and rho each equals zero if Ampere's law and the electric Gauss law hold exactly. We have computed amp and rho on b and s for $t \in [T_p, 10T_p]$. The corresponding relative errors on b are defined by

$$amp_{rb} = \|amp\|_b / \|\mathbf{B}\|_b, \quad rho_{rb} = \|rho\|_b / \|\mathbf{D}\|_b,$$

where $\|\mathbf{B}\|_b = \max(\max|B_1|, \max|B_2|, \max|B_3|)$ is the maximum value of the numerically computed vector \mathbf{B} on b . The relative errors on s are amp_{rs} and rho_{rs} .

The errors decrease as the space discretization increases and they depend slightly on the time discretization. The errors also depend on permittivity ε and current \mathbf{J} . The current \mathbf{J} varies faster in the x_3 -direction than in the x_1 - or x_2 -direction. Hence, in order to get small errors, it is suitable to let m_3 be larger than m_1 and m_2 .

medium	m_3	$amprb$	$amprs$	$rhorb$	$rhors$
$\varepsilon = 1$, case (i)	8	.18 -10	.17 -1	.29 -1	.12 -0
	16	.25 -10	.98 -3	.35 -1	.14 -0
	24	.26 -10	.10 -3	.33 -2	.13 -1
$\varepsilon = \varepsilon(x_1, x_2)$, case (ii)	8	.61 -4	.46 -1	.30 -1	.10 -0
	16	.67 -4	.87 -2	.30 -1	.99 -1
	24	.67 -4	.69 -2	.42 -2	.14 -1
$\varepsilon = \varepsilon(x_1, x_3)$, case (iii)	8	.21 -3	.31 -1	.25 -0	.76 -0
	16	.81 -4	.68 -2	.25 -1	.83 -1
	24	.81 -4	.68 -2	.24 -2	.78 -2

Table 3. Relative errors at $t = T_p$ vs. space discretization (m_1, m_2, m_3) and permittivity ε . $\Delta t = \pi/400$, $m_1 = m_2 = 8$.

It can be seen from Tab. 3 that the error $ampb$ comes from round-off if $\varepsilon = 1$. If ε varies in space there appear discretization errors of $ampb$ in spite of the fact that Ampere's law is enforced on b . The explanation is as follows: We implement (37) employing the exact expressions for μ , $\varepsilon\mu$, $\nabla\varepsilon$ and $\nabla(\varepsilon\mu)$, while we compute amp by inserting ε and μ^{-1} into (47). Then we replace the gradient, divergence and curl operators by our matrix operators and compute $ampb/\varepsilon$. In conclusion, the left-hand side of (37) differs numerically from $ampb/\varepsilon$ given by (47).

The data in Tab. 3 refer to a time t just after the current pulse, $t = T_p$. During the following nine time periods ($t \in [T_p, 10T_p]$) the errors vary strongly with no trend of increase or decrease. The minimum, mean and maximum values of $amprb$, $amprs$, $rhorb$ and $rhors$ are (.87 -5, .93 -4, .39 -3), (.44 -2, .15 -1, .55 -1), (.13 -2, .15 -1, .20 -0) and (.41 -2, .53 -1, .68 -0), respectively, provided $\varepsilon = \varepsilon(x_1, x_3)$ and $\Delta t = \pi/400$ and $(m_1, m_2, m_3) = (8, 8, 16)$.

The values of Tab. 3 have been obtained by repeated operations on the vector potential. The quantity amp is calculated by two space derivatives and two time derivatives of \mathbf{A} , while rho is calculated by three space derivatives, one time derivative and one time integration of \mathbf{A} . These facts explain the fluctuating values of amp and rho , and why the convergence of amp and rho towards zero is not straightforward.

6.4. Time histories

First, we will describe three representative runs which yield Fig. 1. All three simulations are run 4000 steps with a time increment $\Delta t = \pi/400$ and a space

discretization given by $(m_1, m_2, m_3) = (8, 8, 16)$. The source \mathbf{J} is non-zero during time levels 2 through 399, i.e. for $t \in (0, T_p)$ with $T_p = \pi$.

- (i) $\varepsilon = 1$, vacuum. $\mathbf{A} = (0, 0, A_3^T)^T$, $\mathbf{B} = (B_1^T, B_2^T, 0)^T$, $\mathbf{E} = (E_1^T, E_2^T, E_3^T)^T$, where the amplitudes of E_1 and E_2 are much smaller than that of E_3 . E_1 and E_2 come from the scalar potential φ and the main contribution to E_3 is the inductive part A_{3t} .
- (ii) $\varepsilon = \varepsilon(x_1, x_2)$. $\mathbf{A} = (A_1^T, A_2^T, A_3^T)^T$, where A_1 essentially coincides with A_2 because of the choice of parameters that define case (ii). See Section 6.1.
- (iii) $\varepsilon = \varepsilon(x_1, x_3)$. $\mathbf{A} = (A_1^T, 0, A_3^T)^T$. The field pattern (\mathbf{E}, \mathbf{B}) is complicated. All components of \mathbf{E} and \mathbf{B} are of approximately the same size.

We make fft-analyses of time histories of the components of \mathbf{A} in Fig. 1 and find spectra with peaks. For further information, simulations are run 48 000 time steps with $\Delta t = \pi/400$ and $(m_1, m_2, m_3) = (8, 8, 8)$. Then clear beats appear in cases (ii) and (iii). Analyses of the time histories of A_1 and A_3 at time levels 401–48 000 yield spectra with sharp peaks. The peak at the lowest frequency is identified with the fundamental frequency ω_f , and any other peak is denoted by ω_p . In cases (i), (ii), (iii) one has $\omega_f = 2.218, 1.882$ and 1.882 , respectively. Recall that the theoretical value of the fundamental frequency is $\pi/\sqrt{2} \approx 2.221$ for a $2 \times 2 \times 2$ vacuum cube [11, Chap. 13]. In Tab. 4 values of peak quotients ω_p/ω_f are shown. As can be realized from [11, Chap. 13], for a vacuum cube the exact value of ω_p/ω_f is $\sigma/\sqrt{2}$ provided σ^2 takes any of the values $1 + 1, 1 + 1 + 1, 1 + 2^2, 1 + 1 + 2^2, 2^2 + 2^2, 1 + 2^2 + 2^2, \dots$ (see row 2). The computed values are given in rows 3–5.

σ^2	2	3	5	6	8	9
$\sigma/\sqrt{2}$	1	1.225	1.581	1.732	2.000	2.121
(i) ω_p/ω_f	1	–	–	1.735	–	–
(ii) ω_p/ω_f	1	–	1.575	1.732	2.018	2.116
(iii) ω_p/ω_f	1	1.244	1.577	1.744 1.774	–	2.143

Table 4. Peak frequencies of A_3 compared with the fundamental peak frequency. (i) $\varepsilon = 1$, (ii) $\varepsilon = \varepsilon(x_1, x_2)$, (iii) $\varepsilon = \varepsilon(x_1, x_3)$.

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