Electromagnetic pulse propagation in passive media by path integral methods

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Abstract

A novel time domain solver of Maxwell’s equations in passive (dispersive and absorbing) media is proposed. The method is based on the path integral formalism of quantum theory and entails the use of (i) the Hamiltonian formalism and (ii) pseudospectral methods (the fast Fourier transform, in particular) of solving differential equations. In contrast to finite differencing schemes, the path integral based algorithm has no artificial numerical dispersion (dispersive errors), operates at the Nyquist limit (two grid points per shortest wavelength in the wavepacket) and exhibits an exponential convergence as the grid size increases, which, in turn, should lead to a higher accuracy. The Gauss law holds exactly with no extra computational cost. Each time step requires $O(N \log_2 N)$ elementary operations where $N$ is the grid size. It can also be applied to simulations of electromagnetic waves in passive media whose properties are time dependent when conventional stationary (scattering matrix) methods are inapplicable. The stability and accuracy of the algorithm are investigated in detail.

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1 Introduction

In this study a time domain solver of Maxwell’s equation in passive (dispersive and absorbing) media is developed. The main motivation of this work is to bring methods of computational quantum physics into classical electromagnetic theory. One of the great advantages of time domain methods over stationary (scattering matrix) methods is that a single simulation of the scattering of a wide band wave packet can determine basic physical properties of the target (e.g., transmission and reflection coefficients) in the entire frequency band covered by the initial wave packet. Time domain methods also allow for a unique possibility to observe all immediate effects on fields caused by the target or by a surrounding passive medium, which greatly facilitates qualitative understanding of the interaction of an electromagnetic pulse with media and targets. Another important advantage is that the target geometry (or medium physical properties) may vary with time and this time dependence cannot be removed by going over to a moving reference frame. Stationary methods are simply inapplicable to these kind of problems.

From the computational point of view, the proposed approach is based on pseudospectral methods. The essential advantages of pseudospectral algorithms over conventional finite element or finite difference schemes in solving differential equations are [1]: (i) the exponential versus polynomial rate of convergence as the grid size (or the basis dimension) increases; (ii) the absence of dispersive errors and (iii) efficiency in numerical calculations. Time domain algorithms in combination with pseudospectral methods have become the state-of-the-art technique in numerical studies of quantum dynamics by solving the corresponding initial value problem for the Schrödinger equation (see, e.g., [2]). A typical algorithm entails an approximate computation of an object called the path integral (or functional integral) introduced by Feynman [3]. Here Maxwell’s theory in general dispersive media is reformulated in the Schrödinger (Hamiltonian) formalism. Then the path integral formalism is applied to the initial value problem in Maxwell’s theory in passive media to develop a numerical algorithm. The main objective of this work is to give a theoretical assessment of the path integral based solver of the initial value problem for Maxwell’s equations. Numerical tests and applications will be discussed elsewhere [4].

It is shown here that basic principles of the path integral formalism lead to a true time domain algorithm which indeed enjoys the advantages of pseudospectral methods. In particular, among the aforementioned features, (i) is provided by the use of the fast Fourier method [5] as a part of the algorithm, when applied to media whose parameters do not have discontinuities in space, (ii) is a consequence of Nelson’s construction [6] of the path integral which is embedded in our algorithm, (iii) is due to the fast Fourier method and some analytical results that speed up numerical computations. The algorithm has another great advantage over finite difference schemes: The Gauss law is implemented exactly with no extra computational cost (Theorem 8.2). For widely used multi-resonant Lorentz models of passive media, the algorithm is unitary, meaning that, the energy of a wave packet is preserved exactly in dispersive media with no attenuation (Theorem 6.1). It is also uncon-
ditionally stable (Theorems 7.1 and 7.3) versus conditionally stable finite element or finite difference algorithms [1] (see also [7]). A possible drawback of the algorithm (to be tested numerically) is that the use of the fast Fourier method in combination with Nelson’s construction of the path integral might require additional computational costs for boundary value problems with complicated boundary geometry. In our approach, conventional boundary conditions are not imposed on electromagnetic fields. Targets and medium interfaces are modeled by discontinuous medium parameters. The problem arises from well known features of the Fourier method [5]: Aliasing and low convergence rates for non-smooth functions. In this study we offer one possible way to deal with this problem while keeping the Fourier basis in the algorithm. Alternative pseudospectral approaches to circumvent the problem exist and are mentioned here, but not discussed in detail.

The basic idea of the path integral approach to solving linear, homogeneous, evolutionary differential equations (numerically or analytically) is based on the Hamiltonian formalism. In the framework of the Hamiltonian formalism, an original system of differential equations is transformed to an equivalent system of first-order (in time) differential equations by expanding the original configuration space, that is, by going over to a generalized phase space where all time derivatives, save for the one of highest order, become independent variables [8]. A generic linear homogeneous first-order system can be written in the form

\[ \partial_t \Psi_t = \mathcal{H} \Psi_t, \quad \Psi_{t=0} = \Psi_0, \]  

(1.1)

where \( \partial_t \) stands for the partial derivative with respect to time \( t \), a linear operator \( \mathcal{H} \) is called Hamiltonian, while \( \Psi_t \) is called a state vector (or wave function). It is an element of the generalized phase space of the system and viewed as a collection (column) of the original variables and their time derivatives. The generalized phase space is equipped with an inner product and becomes a Hilbert space. State vectors are typically vector-valued functions in \( \mathbb{R}^3 \), and the Hamiltonian is a differential operator. The choice of the inner product depends on the problem at hand. One usually requires that components of \( \Psi_t \) are elements of \( L_2(\mathbb{R}^3) \).

In general, upon going over to the Hamiltonian formalism, there might occur constraints [9, 10]

\[ C_a \Psi_t = 0, \]  

(1.2)

with \( C_a \) being a set of linear operators which do not contain time derivatives; \( a \) enumerates the constraint operators. The constraints must be preserved in the time evolution which is described by (1.1). In other words, the solution is sought in the subspace of the Hilbert space defined by (1.2). Depending on the type of constraints, there are different ways of developing the corresponding path integral formalism. In Maxwell’s theory, the constraint is the Gauss law, and it is of the “first class” in the Dirac terminology [10]. The characteristic feature of a first class constrained system is that

\[ \left[ \mathcal{H}, C_a \right] \sim C_a, \quad \left[ C_a, C_b \right] \sim C_c. \]  

(1.3)

A consequence of (1.3) is that if the initial configuration \( \Psi_0 \) satisfies the constraints, then so does the solution of (1.1). However, after the projection of the Hilbert space spanned by \( \Psi_t \),
onto a finite-dimensional subspace (e.g., a projection on a subspace associated with a finite spatial grid as is done in Section 3), which is required for numerical simulations, the involution condition (1.3) can be violated causing problems in simulations. For instance, the Gauss law is typically violated in any finite differencing approach to simulations of electromagnetic wave packet propagation. Special efforts have to be made to ensure the transversality of the radiation field in Maxwell’s theory, which, in turn, complicates simulation algorithms and increases computational costs (e.g., when enforcing the Gauss law in finite difference schemes on the grid via the Lagrange multiplier method). It is one of the advantages of the proposed path integral based algorithm that the Gauss law can be strictly enforced with no additional computational costs for generic passive media (Theorem 8.2).

The solution to Eq. (1.1) is

\[ \Psi_t = \exp(t\mathcal{H}) \Psi_0 \equiv U_t \Psi_0 , \quad t \geq 0 , \]  

(1.4)

assuming that the exponential of \( \mathcal{H} \) exists. If the Hamiltonian is time dependent then the following replacement has to be made in (1.4)

\[ \exp(t\mathcal{H}) \to T \exp \left( \int_0^t d\tau \mathcal{H}(\tau) \right) = U_t , \]

(1.5)

where \( T \exp \) stands for the time-ordered exponential. The operator \( U_t \) is defined as the fundamental solution of (1.1), \( \partial_t U_t = \mathcal{H} U_t \) with \( U_{t=0} \) being the identity operator. The fundamental solution has the semigroup property, \( U_{t_1 + t_2} = U_{t_1} U_{t_2} \). The action of the evolution operator \( U_t \) on the initial configuration can be written via its integral kernel,

\[ \Psi_t(r) = \int_{\mathbb{R}^3} dr' U_t(r, r') \Psi_0(r') . \]

(1.6)

Using the semigroup property of the evolution operator, the entire time evolution can be viewed as consecutive actions of the infinitesimal evolution operator \( U_{\Delta t} \), where \( \Delta t \) is a time step. If the kernel of the infinitesimal evolution operator is known, then the kernel of the evolution operator can be computed as the convolution

\[ U_t(r, r') = \int_{\mathbb{R}^3} dr_1 \cdots dr_n U_{\Delta t}(r, r_n) U_{\Delta t}(r_n, r_{n-1}) \cdots U_{\Delta t}(r_1, r') \]

(1.7)

with \( \Delta t(n+1) = t \). The integration variables can be regarded as points \( r_k = r(t_k) \), where \( t_k = k\Delta t, \quad k = 0, 1, ..., n+1 \), on a path \( r(\tau) \) connecting points \( r(\tau = t) = r \) and \( r(\tau = 0) = r' \). In the limit \( \Delta t \to 0 \) the convolution (1.7) can be viewed as a sum over all paths connecting the initial and final points. This is the gist of the Feynman path integral representation of the fundamental solution of (1.1). A nontrivial problem is to find the measure on the space of paths. For example, if \( \mathcal{H} = \Delta \) (the Laplace operator), it can be shown that the limit exists, and that the measure coincides with the Wiener measure which has support in the space of all continuous, but nowhere differentiable paths (trajectories of the Brownian motion) pinned at the end points. In quantum mechanics, the problem is more subtle, but
can still be solved [11]. The existence of the proper measure on the space of paths opens up an attractive possibility to use Monte-Carlo methods of computing the sum over paths which is the gold standard algorithm in quantum and statistical physics.

However, the present study does not intend to tackle the measure problem for the path integral representation of Maxwell’s theory, but rather offers a solution of a more modest problem. Namely, how the conventional way, outlined above, of deriving the path integral from the original differential equation can be used to obtain an algorithm for numerical simulations of the convolution (1.7) for a small, but finite $\Delta t$. Similar ideas have been applied to non-dispersive and/or random media as well as to scattering problems and waveguides [12]. Our approach applies to general passive media and goes beyond the eikonal approximation of geometric optics and/or the diffraction theory used in earlier works on path integrals in electromagnetic theory. The results obtained here are believed to be useful for further development of path integral methods in theoretical and numerical studies of propagation of electromagnetic wave packets in passive media.

The idea of numerical simulations follows from (1.7) rather straightforwardly, namely,

$$\Psi_{t+\Delta t} = U_{\Delta t}\Psi_t.$$  \hspace{1cm} (1.8)

Thus, finding a state of the system in a sequential moment of time amounts to computing the action of the exponential of a differential operator $H$ on the state at the preceding moment of time. Theoretically, it is sufficient to know $U_{\Delta t}$ up to $(\Delta t)^2$. The limit $\Delta t \to 0$ in (1.7) would not change if we replace the exact infinitesimal evolution operator kernel by such an approximation. In numerical simulations, the limit is never achieved. Therefore a higher accuracy is required to make errors small. Note that the errors are accumulated as more iterations (1.8) are taken. An expansion of $\exp(\Delta t H)$ into the power series up to some desired order is known to produce unstable algorithms. Yet another obvious drawback is the lack of unitarity of the time evolution, that is, if the Hamiltonian is skew-symmetric (anti-Hermitian, if a complex phase space is used), $H^* = -H$, then $U_{\Delta t}U_{\Delta t}^* = 1$. In the Maxwell theory, as we shall see, the squared norm of $\Psi_t$ with respect to the $L_2(\mathbb{R}^3)$ scalar product $(\Psi_1, \Psi_2) = \int d\mathbf{r} \Psi_1^* \Psi_2$ is proportional to the electromagnetic energy of the system. Consequently, for non-absorbing media the unitarity of the time evolution is required in simulations to provide the energy conservation.

We shall apply Nelson’s method of obtaining the path integral representation of the fundamental solution of Maxwell’s equations for passive media. It is based on the Kato-Trotter product formula for the exponential of a sum of two noncommuting operators and the use of the Fourier basis to compute exponentials of differential operators. Actually, in practical applications, a simpler version, known as the Lie-Trotter product formula, is used (see the textbooks [13] for details and references therein). In computational quantum mechanics this is also known as the split operator method. It allows one to keep the differential operators in the exponential, and thereby, ensures the correct dispersion relation of simulated electromagnetic waves. It will be shown that there exists a particular realization of this idea in which the Gauss law holds exactly in simulations. In general, the Gauss law can be enforced by the
projection operator formalism developed for the path integral representation of constrained dynamical systems (for a review see [14] and references therein, a numerical application to constrained wave packet propagation can be found in [15]). The idea is to replace the Hamiltonian by its projection on the subspace (1.3). If \( P \) is the projection operator, that is, \( C_a P \Psi = 0 \) for any \( \Psi \), \( P^2 = P \) and \( P^* = P \), then \( \mathcal{H} \) is replaced by \( P \mathcal{H} P \). In Maxwell’s theory the projection can be implemented in our algorithm with no extra computational costs. A significant difference from the quantum mechanical case is that the Hamiltonian \( \mathcal{H} \) (or its projection) is not normal, that is, it does not commute with its adjoint. This feature complicates the stability analysis because the von Neumann criteria is no longer sufficient for stability, while still being necessary [16]. Nevertheless, the stability, accuracy and convergence analysis of the algorithm can be carried out in rather general settings.

Since time domain simulations are performed on finite lattices, there is always a moment of time when the simulated signal first reaches the lattice boundary. One typically uses lattices with periodic boundary conditions. So, the pulse would appear on the other side of the lattice interfering with itself, thus leading to totally disastrous results for simulations. The problem is usually solved by introducing absorbing boundary conditions (see, e.g., [17] (for quantum mechanics) and [18] (for electrodynamics)). It is convenient to set a conducting layer at the grid boundary whose conductivity is chosen so that it neither transmits nor reflects within the designated accuracy in the frequency domain of the initial pulse. In Appendix we briefly describe how such a conducting layer can be obtained.

2 Maxwell theory in the Hamiltonian formalism

Dynamics of electromagnetic waves in continuous media is governed by Maxwell’s equations

\[
\begin{align*}
\partial_t D_t &= c \nabla \times H_t, \\
\partial_t B_t &= -c \nabla \times E_t,
\end{align*}
\]

(2.1)

(2.2)

where \( c \) is the speed of light, boldface letters denote three-vector fields in \( \mathbb{R}^3 \) whose spatial arguments are suppressed and the time dependence is indicated by a subscript. No external currents and charges (antennas) are included in this study. However, the formalism being developed is readily generalized to the case when external time dependent sources are present.

The electric and magnetic induction vectors, \( D_t \) and \( B_t \), respectively, are subject to the constraints (the Gauss law)

\[
\nabla \cdot D_t = \nabla \cdot B_t = 0.
\]

(2.3)

In linear response theory, assumed throughout the paper, the electric induction is related to the electric field as [19]

\[
D_t = E_t + \int_{-\infty}^{t} d\tau \chi_{t-\tau}^e E_\tau \equiv E_t + P_t,
\]

(2.4)
where $\chi_t^e$ is an electric response function of the medium and $P_t$ is the medium polarization vector. A similar relation can be written for the magnetic field and induction, $B_t = H_t + M_t$, where magnetization $M_t$ is determined by the applied magnetic field and the magnetic response function of the medium.

The relation between inductions and fields must be causal, meaning that the response of the medium, $P_t$ and $M_t$, can only depend on fields applied to the medium prior to the current time $t$, (e.g., $\chi_t^e = 0$ for $t < 0$) [19]. A natural way to ensure the causality is to require that the response function satisfies a differential equation. In other words, the response function is assumed to be the fundamental solution of some time evolution differential equation. This differential equation can be obtained from a particular physical model of the medium in question. A popular model is the multi-resonant Lorentz model. Let $\tilde{D}_\omega$ and $\tilde{E}_\omega$ be the Fourier transforms of the electric induction and field. Then from (2.4) it follows that $\tilde{D}_\omega = \varepsilon_\omega \tilde{E}_\omega$. The dielectric constant in the Lorentz model has the form

$$\varepsilon_\omega = 1 + \sum_{a=1}^{N} \frac{\omega_{pa}^2}{\omega_a^2 - \omega^2 - 2i\gamma_a\omega}, \quad (2.5)$$

and $M_t = 0$. The physical meaning of the model is transparent. The medium is assumed to be made of $N$ sorts of damped harmonic oscillators with resonant frequencies $\omega_a$ and damping coefficients $\gamma_a$. Parameters $\omega_{pa}$, called the plasma frequencies, are proportional to coupling constants of the oscillators to the external electric field (the electric dipole coupling) and also depend on the density of oscillators of the sort $a$. The density may vary in space. So $\omega_{pa}$ are assumed to be functions of spatial coordinates. In an empty space, $\omega_{pa} = 0$. If the resonant frequency is zero, the one-resonant Lorentz model is equivalent to the Drude model of metals [19]. In the Lorentz medium the magnetic response function is zero, while the electric response function can easily be found by taking the Fourier transform of (2.5). Its explicit form is omitted here because it will not be used. The medium polarization is determined by a set of second-order differential equations

$$\partial_t^2 P^a_t + 2\gamma_a \partial_t P^a_t + \omega_a^2 P^a_t = \omega_{pa}^2 E_t, \quad P_t = \sum_{a=1}^{N} P^a_t. \quad (2.6)$$

Together with Maxwell’s equations, Eq. (2.6) form a system of sought-for causal evolution equations which are to be transformed into a system of first order equations by means of the Hamiltonian formalism. In finite difference time domain numerical schemes, the Hamiltonian formalism for the Lorentz model has been used in [20] to study propagation of an electromagnetic pulse in homogeneous Lorentz media.

In our approach no boundary conditions are imposed on electromagnetic fields at medium and/or target interfaces. The latter are modeled by spatially dependent couplings of media to electromagnetic fields which are included into the system Hamiltonian. At any interface, the couplings are allowed to have discontinuities, or, from a physical point of view, they remain smooth but change rapidly, $\lambda_w |\nabla\omega_p|/\omega_p >> 1$, at the interface, where $\lambda_w$ is a typical wave
length of the incoming wave packet. The conventional boundary conditions are automatically
generated by the dynamics \[19\]. Thus, the initial value problem is solved in \(L^2(\mathbb{R}^3)\) for every
matter and electromagnetic field component. This implies that the energy of the propagating
wave packet remains finite (in contrast to the scattering matrix approach based on plane
wave solutions).

Let us now formulate the initial value problem for a generic passive medium and then
apply the formalism to multi-resonant Lorentz models. Combine the fields, inductions and
medium responses into columns:

\[
\psi^F_t = \left( \begin{array}{c} E_t \\ H_t \end{array} \right), \quad \psi^I_t = \left( \begin{array}{c} D_t \\ B_t \end{array} \right), \quad \psi^R_t = \left( \begin{array}{c} P_t \\ M_t \end{array} \right).
\]

Assuming linear response theory, one can write for the Fourier transforms

\[
\tilde{\psi}_\omega = \tilde{\chi}_\omega \tilde{\psi}_\omega^F,
\]

where the Fourier transform of a general response function, \(\tilde{\chi}_\omega\), has to satisfy a dispersion
relation that ensures causality (like the Kramer-Kronig relations for the dielectric constant)
\[19\]. For anisotropic media, \(\tilde{\chi}_\omega\) is a symmetric matrix acting on components of electromagnetic
fields. With this type of generality all possible media are covered as long as linear
response theory is valid. The response function \(\tilde{\chi}_\omega\) can either be modeled or measured and
tabulated in some frequency range of interest (determined by the frequency bandwidth of
the initial wavepacket), say, \(\omega \in [\omega_1, \omega_2]\). Next, the components of \(\tilde{\chi}_\omega^{-1}\) are expanded in
a basis of suitable orthogonal polynomials. An optimal expansion is often achieved in the
Chebyshev polynomial basis. Chebyshev polynomials are defined in the interval \([-1, 1]\) so
a corresponding rescaling and translation of \([\omega_1, \omega_2]\) must be done. By taking the Fourier
transform of \(\tilde{\chi}_\omega^{-1} \tilde{\psi}_\omega^R = \tilde{\psi}_\omega^F\) we obtain the desired differential equation

\[
\sum_{n=0}^{N} \chi_n \partial_t^n \psi_t^R = \omega_p \psi_t^F,
\]

where \(\omega_p = \omega_p(r)\) plays the role of the coupling constant between matter and electromagnetic
fields. The order \(N\) is determined by the highest order of polynomials used to approximate
\(\tilde{\chi}_\omega^{-1}\). The expansion coefficients \(\chi_n\) and the coupling \(\omega_p\) are matrices for anisotropic media.

The basic idea of the Hamiltonian formalism is to convert the system (2.6) or (2.8) into
a system of first-order differential equations by introducing auxiliary (matter) fields. The
number of such fields is determined by the order of the original evolution equation for matter.
For instance, in the case of the multi-resonant Lorentz model, there are \(N\) fields \(P^a_t\) each of
which satisfies a second order differential equation. In the Hamiltonian formalism one would
have \(2N\) real vector fields, \(\xi_t^j, j = 1, 2, ..., 2N\). A simple possibility is to set

\[
P^a_t = \left( \frac{\omega_p}{\omega_a} \right) \xi_t^{2a-1},
\]

\[
\partial_t \xi_t^{2a-1} = \omega_a \xi_t^{2a},
\]

\[
\partial_t \xi_t^{2a} = -2\gamma_a \xi_t^{2a} - \omega_a \xi_t^{2a-1} + \omega_p E_t.
\]
The reason of inserting the factor $\omega_{pa}/\omega_a$ in the definition (2.9) of the auxiliary fields will be evident from what follows. Note that the medium polarization $\mathbf{P}_t$ must be zero in empty space where $\omega_{pa} = 0$. The factor $\omega_a^{-1}$ in (2.9) simplifies the energy conservation and stability analysis.

For the Lorentz model there is another convenient way to introduce the Hamiltonian formalism by using $N$ complex vector fields $\zeta^a_t$ which satisfy the first order differential equation

$$\partial_t \zeta^a_t = \lambda^a \zeta^a_t - i \omega_{pa} \mathbf{E}_t, \quad (2.12)$$

$$\mathbf{P}^a_t = \frac{\omega_{pa}}{2\nu_a} (\zeta^a_t + \bar{\zeta}^a_t), \quad (2.13)$$

where $\lambda^a = -\gamma^a + i\nu_a$ and $\nu_a = \sqrt{\omega_a^2 - \gamma_a^2}$. This representation is defined only if $\gamma_a < \omega_a$ (i.e., the attenuation is not high). From the numerical point of view, solving a decoupled system of $N$ first order differential equation and taking complex conjugation (denoted here by an over bar) is less expensive than solving an original system of differential equations to compute the medium polarization.

Returning to the general case, we introduce a set of auxiliary fields $\xi_t$ to convert (2.8) into a first-order system,

$$\partial_t \xi_t = \mathcal{H}_{FM}^F \xi_t + \mathcal{V}_{MF}^F \psi^F_t. \quad (2.14)$$

The operators $\mathcal{H}_{FM}^F$ and $\mathcal{V}_{MF}^F$ are determined by the details of going over to the Hamiltonian formalism. We shall call $\mathcal{H}_{FM}^F$ the matter Hamiltonian; it governs time evolution of the medium when no external fields are applied. The index $F$ indicates that the electromagnetic degrees of freedom are described by fields, not inductions. We shall see shortly that the matter Hamiltonian depends on whether $\psi^I_t$ or $\psi^F_t$ is used as independent electromagnetic variables. The matrix $\mathcal{V}_{MF}^F$ describes the coupling of matter to the electromagnetic fields, which is emphasized by the index $MF$ (matter-to-field coupling). We introduce a linear time independent operator $\mathcal{R}$ that acts in the space of auxiliary (matter) fields so that

$$\psi^R_t = \mathcal{R} \xi_t, \quad (2.15)$$

that is, the (response) operator $\mathcal{R}$ maps a given configuration of auxiliary fields onto the corresponding physical response field. It depends on the definition of the matter fields (cf. (2.9) and (2.13)). A passive medium is not excited, $\xi_t = 0$, if no external electromagnetic field is applied; that is, the initial condition for Eq. (2.14) is such that it has only the trivial solution whenever $\psi^F_t = 0$. Under this condition, the solution of (2.14) reads

$$\xi_t = \int_{-\infty}^t d\tau e^{(t-\tau)\mathcal{H}_{FM}^F} \mathcal{V}_{MF}^F \psi^F_{\tau}. \quad (2.16)$$

Hence, the linear response operator $\tilde{\chi}_\omega$ in (2.7) is the Fourier transform of the operator

$$\chi_t = \theta_t \mathcal{R} e^{i\mathcal{H}_{FM}^F} \mathcal{V}_{MF}^F, \quad (2.16)$$
where \( \theta_t \) is the Heaviside function. Or, vice versa, \( R, \mathcal{H}_M^F \) and \( \mathcal{V}_{MF} \) must be chosen so that the Fourier transform of \( \chi_t \) defined by (2.16) coincides with the known response function \( \tilde{\chi}_\omega \) of the medium in a designated frequency range.

Maxwell’s equations without external currents can be rewritten in the Hamiltonian form

$$
\partial_t \psi_t^F = \mathcal{H}_F \psi_t^F - \partial_t \psi_t^R = \mathcal{H}_F \psi_t^F + \mathcal{V}_{FM} \xi_t .
$$

(2.17)

The field-to-matter coupling \( \mathcal{V}_{FM} \) and the field Hamiltonian \( \mathcal{H}_F \) are deduced from (2.14) by acting on the latter by the operator \( R \), which yields

$$
\mathcal{V}_{FM} = -R \mathcal{H}_M^F ,
$$

(2.18)

$$
\mathcal{H}_F = \begin{pmatrix}
0 & c \nabla \\
-c \nabla & 0
\end{pmatrix} - R \mathcal{V}_{MF} \equiv \mathcal{H}_0 - R \mathcal{V}_{MF} .
$$

(2.19)

It is always possible to set up the Hamiltonian formalism so that \( R \mathcal{V}_{MF} \equiv 0 \) and, hence, \( \mathcal{H}_F = \mathcal{H}_0 \). It is not difficult to verify that this holds for the Lorentz model discussed above.

In the general case, the standard procedure of going over to the Hamiltonian formalism [8], where components of \( \xi_t \) are identified with time derivatives of the response field, \( \xi_t^k \sim \partial_t^k \psi_t^R \), leads to the same result that \( R \mathcal{V}_{MF} = 0 \). Thus, without loss of generality, the last term in the field Hamiltonian (2.19) can be omitted.

The auxiliary matter and electromagnetic fields (or inductions) are unified into a larger column

$$
\Psi_t^F = \begin{pmatrix}
\psi_t^F \\
\xi_t
\end{pmatrix}, \quad \Psi_t^I = \begin{pmatrix}
\psi_t^I \\
\xi_t
\end{pmatrix} .
$$

(2.20)

The wave function \( \Psi_t^F \) satisfies the Schrödinger equation

$$
\partial_t \Psi_t^F = \mathcal{H}_F \Psi_t^F , \quad \mathcal{H}_F = \begin{pmatrix}
\mathcal{H}_0 & \mathcal{V}_{FM} \\
\mathcal{V}_{MF} & \mathcal{H}_M^F
\end{pmatrix} .
$$

(2.21)

which has to be solved with the initial field configuration \( \psi_t^F = \psi_0 \), while the matter fields are assumed to be zero at the initial moment of time, \( \xi_{t=0} = 0 \), e.g., the initial wave packet is localized in an empty space region. Equations (2.14) and (2.17) are equivalent to (2.21). In a similar fashion, one can derive the Schrödinger equation for \( \Psi_t^I \). Note that

$$
\Psi_t^I = S \Psi_t^F , \quad S = \begin{pmatrix}
1 & R \\
0 & 1
\end{pmatrix} , \quad S^{-1} = \begin{pmatrix}
1 & -R \\
0 & 1
\end{pmatrix} .
$$

(2.22)

Hence,

$$
\partial_t \Psi_t^I = \mathcal{H}_I \Psi_t^I , \quad \mathcal{H}_I = S \mathcal{H}_F S^{-1} .
$$

(2.23)

The corresponding blocks of \( \mathcal{H}_I \) have the form

$$
\mathcal{H}_I = \mathcal{H}_0 , \quad \mathcal{V}_{MI} = \mathcal{V}_{MF} ,
$$

(2.24)

$$
\mathcal{V}_{IM} = \mathcal{V}_{FM} + R \mathcal{H}_M^F - \mathcal{H}_0 R = -\mathcal{H}_0 R ,
$$

(2.25)

$$
\mathcal{H}_M^I = \mathcal{H}_M^F - \mathcal{V}_{MF} R .
$$

(2.26)
To simplify $\mathcal{V}_{IM}$, Eq. (2.18) has been applied. Observe in (2.26) the aforementioned dependence of the matter Hamiltonian on the representation of electromagnetic degrees of freedom. The use of either (2.21) or (2.23) in numerical simulations has its own advantages and disadvantages which are discussed below.

As an example, we give an explicit form of the Hamiltonian for the Lorentz model when the auxiliary field are defined by (2.9)

$$
\mathcal{V}_{FM} = (\mathcal{V}_{FM1}, \mathcal{V}_{FM2}, \cdots, \mathcal{V}_{FMN}), \quad \mathcal{V}_{FMa} = \begin{pmatrix} 0 & -\omega pa \\ 0 & 0 \end{pmatrix}, \quad (2.27)
$$

$$
\mathcal{V}_{MF} = -\mathcal{V}_{FM}, \quad (2.28)
$$

$$
\mathcal{H}_{FM}^F = \text{diag} \left( \mathcal{H}_{M1}^F, \mathcal{H}_{M2}^F, \cdots, \mathcal{H}_{MN}^F \right), \quad \mathcal{H}_{Ma}^F = \begin{pmatrix} 0 & \omega_a \\ -\omega_a & -2\gamma_a \end{pmatrix}, \quad (2.29)
$$

where $\text{diag}$ indicates that the corresponding matrix is block-diagonal with blocks listed in the order from the upper left to lower right corners. Note that the matrices $\mathcal{V}_{FMa}$ and $\mathcal{H}_{FMa}$ act on a six-dimensional column $(\xi^{2a-1}_t, \xi^{2a}_t)^*$. Therefore they should be understood as composed of $3 \times 3$ blocks. Each block is obtained by multiplying the unit matrix by the number indicated in place of the block in (2.27) and (2.29).

Our final remark in this section concerns “canonical” transformations in the Hamiltonian formalism. As has been pointed out, the auxiliary fields are not uniquely defined. There is a freedom of making general complex nonsingular linear transformations such as

$$
\xi_t \to S_M \xi_t, \quad \det S_M \neq 0. \quad (2.30)
$$

If the infinitesimal evolution operator $U_{\Delta t}^{(F,I)} = \exp(\Delta t \mathcal{H}^{(F,I)})$ is computed with one choice of the auxiliary fields, a simple similarity transformation, like the one in (2.23), would allow us to compute it in any other basis of auxiliary fields. This is an important observation because the auxiliary field basis can be chosen in a way that facilitates computation of the evolution operator (e.g., to improve the convergence rate or speed up simulations). For instance, in the complex representation (2.13) of the auxiliary fields in the Lorentz model, the matter Hamiltonian is diagonal. The corresponding transformation of the auxiliary fields is given by

$$
\begin{pmatrix} \xi^{2a-1}_t \\ \xi^{2a}_t \end{pmatrix} = \frac{1}{2\nu_a} \begin{pmatrix} \omega_a & \omega_a \\ \lambda_a & \lambda_a \end{pmatrix} \begin{pmatrix} \xi^a_t \\ \xi^a_t \end{pmatrix} \equiv S_M \begin{pmatrix} \xi^a_t \\ \xi^a_t \end{pmatrix}. \quad (2.31)
$$

To transform the whole system into this representation, the Hamiltonian $\mathcal{H}^F$ is replaced by $S^{-1}\mathcal{H}^F S$ and the wave function $\Psi^F_t$ by $S\Psi^F_t$ where $S$ is block-diagonal with the unit matrix in the upper left (field) corner and with $S_M$ in the lower right (matter) corner.

### 3 The grid representation of Maxwell’s theory

Consider an equidistantly spaced finite grid with periodic boundary conditions. Let $\Delta r$ be the grid step and $n$ be a vector with integer valued components. Then the dynamical
variables are projected onto the grid by taking their values at grid points \( r = n \Delta r \),

\[
\Psi^Q_t(r) \rightarrow \Psi^Q_t(n \Delta r)
\]  

(3.1)

where \( Q \) denotes the representation, \( I \) or \( F \). For simplicity, a cubic grid is assumed here. It is straightforward to generalize the discussion to a generic rectangular grid. Consider a discrete Fourier transformation associated with the grid \([5, 21]\)

\[
\tilde{\Psi}^Q_t(nk_0) = \sum_{n'} F_{nn'} \Psi^Q_t(n' \Delta r)
\]  

(3.2)

where the dual lattice step is \( k_0 = 2\pi/\Delta r \). The grid spatial size \( L \) and step must be chosen so that the Fourier transform of the initial wavepacket has support within the region \( k \in [k_{\text{min}}, k_{\text{max}}] \) where \( k = |k| \), \( k_{\text{max}} = k_0 \) and \( k_{\text{min}} = 2\pi/L \). The Hamiltonian \( H^Q \) is split into a sum

\[
H^Q = H_0^Q + V^Q,
\]  

(3.3)

where all the spatial derivatives are included into \( H_0^Q \) and \( V^Q \) contains multiplications by position dependent functions. This is always possible for the Hamiltonian described in the preceding section. The operator \( V^Q \) is projected naturally

\[
V^Q(r)\Psi^Q_t(r) \rightarrow V^Q(n \Delta r)\Psi^Q_t(n \Delta r).
\]  

(3.4)

Consider \( H_0^Q \) in the Fourier basis, \( H_0^Q(\nabla) \rightarrow H_0^Q(jk) \). The projection is then done via the discrete Fourier transform

\[
H_0^Q(\nabla)\Psi^Q_t(r) \bigg|_{r=n\Delta r} \rightarrow \sum_{n'} (F^*)_{nn'} H_0^Q(in'k_0) \tilde{\Psi}^Q_t(n'k_0).
\]  

(3.5)

In what follows, the rules (3.4) and (3.5) define the action of the operators \( V^Q \) and \( H_0^Q \) and their functions on any state vector. The action of a product of \( V^Q \) and \( H_0^Q \) on any state vector is understood as consecutive actions of these operators according to the rules (3.4) and (3.5), in the order specified in the product.

The projection (3.5) as well as any action of \( H_0^Q \) on state vectors is performed by the fast Fourier method [5]. It requires \( N \log_2 N \) elementary operations (flops) with \( N \) being the grid size. In finite differencing schemes, the action of \( H_0^Q \) on a state vector would require \( mN_d \) operations where the integer \( m \) depends on a particular difference scheme used to approximate derivatives, and \( N_d \) is the grid size used in the differencing scheme. It should be noted that, as shown below, the use of the fast Fourier transform eliminates the phase error (because the correct electromagnetic dispersion relation is preserved) and operates at the Nyquist limit. These two features allows one to reduce substantially the grid size as compared with that in a finite differencing scheme, while providing the same accuracy in simulations. Recall that, in scattering problems, the phase of the return signal contains the most significant information about the target. So, in practice, grids in finite differencing schemes are significantly larger (more dense) than grids used in the fast Fourier method.
in order to reduce the phase errors in the former. Needless to say, the advantage of the fast Fourier method in reducing the phase error becomes even more significant in higher dimensions because \( N_d/N = (n_d/n)^D \) where \( n_d \) and \( n \) are the corresponding numbers of grid points per shortest wave length in the wave packet, and \( D \) is the grid dimension. The Nyquist limit is \( n = 2 \), while \( n_d \) is of order 10 or higher.

4 The split operator method

Let \( |\Psi| \) denote the \( L_2(\mathbb{R}^3) \) norm of the wave function, or the Euclidean norm of the corresponding vector (3.1) in the grid representation. One possible way to compute numerically the path integral (1.7) is based on the Kato-Trotter product formula \([13]\)

\[
\lim_{n \to \infty} \left| e^{t(A+B)} \Psi - \left( e^{tA/2} e^{tB/n} e^{tA/2n} \right)^n \Psi \right| = 0 , \tag{4.1}
\]

for a general \( \Psi \) and under certain assumptions about the linear operators \( A \) and \( B \) in the Hilbert space spanned by \( \Psi \). For our purposes it is sufficient to note that for bounded operators, (4.1) always holds and is known as the Lie-Trotter product formula. In the grid representation, which would always be assumed, unless stated otherwise, operators \( A \) and \( B \) are finite matrices and, hence, bounded.

Let us apply (4.1) to the split (3.3), meaning that the operator \( \mathcal{H}_0^Q \) is used in place of \( A \) (or \( B \)) and, respectively, the operator \( \mathcal{V}^Q \) is used in place of \( B \) (or \( A \)). The infinitesimal evolution operator in (1.8) can be approximated by the first term in the following expansion

\[
\begin{align*}
\mathcal{U}^Q_{\Delta t} &= e^{t(A+B)} = \mathcal{G}^Q_{\Delta t} + \Delta t^3 \mathcal{W}_{\Delta t} \\
\mathcal{G}^Q_{\Delta t} &= e^{tA/2} e^{tB/n} e^{tA/2n} \tag{4.2} \\
\mathcal{W}_{\Delta t} &= -\frac{1}{24} ([A, [A, B]] - 2[B, [B, A]]) + O(\Delta t) \tag{4.3}.
\end{align*}
\]

By making \( n \) larger while keeping \( n\Delta t = t \) fixed, the strong convergence in (4.1) guarantees that the error can be made arbitrary small for any initial state,

\[
|(\mathcal{U}^Q_{\Delta t})^n \Psi_0 - (\mathcal{G}^Q_{\Delta t})^n \Psi_0| \to 0 \tag{4.5}
\]

as \( n \to \infty \) for any \( \Psi_0 \). The numerical iteration algorithm is then based on the replacement of the exact evolution (1.8) by the approximate one

\[
\Psi^Q_{t+\Delta t} = \mathcal{G}^Q_{\Delta t} \Psi^Q_t . \tag{4.6}
\]

The quantity \( t\Delta^2 |\mathcal{W}^Q_{\Delta t} \Psi_0|/|\Psi_0| \) can be used to roughly estimate the accuracy of the algorithm. A more detailed accuracy analysis is given in Section 8. By making use of the Campbell-Hausdorf formula for the exponential of the sum of operators it is possible to obtain the symmetric product formula in (4.2) to approximate \( \mathcal{U}_{\Delta t} \) up to any desired order.
in $\Delta t$, presumably achieving a higher accuracy [22]. This would come at the price of having more exponentials in the symmetric product $G_{\Delta t}^Q$. In numerical simulations, one should keep in mind that computational costs of decreasing $\Delta t$ in the third order split (4.2) (i.e., increasing the number of steps in the time evolution) might be less than those of computing a lesser number of actions of $G_{\Delta t}^Q$ in higher order splits. So, the higher order splits are not always optimal to achieve a better accuracy [2].

On the grid, the action of the amplification operator $G_{\Delta t}^Q$ is computed according to the rules (3.4) and (3.5) applied to, respectively, $\exp(\Delta t V^Q)$ and $\exp(\Delta t H^Q_0)$. Explicit formulas for the exponentials of the corresponding operators can be worked out in the field and induction representations. If the fields are used as independent variables, then a natural choice is

$$H^F = H^F_0 + V^F = \begin{pmatrix} H^F_0 & 0 \\ 0 & H^F_M \end{pmatrix} + \begin{pmatrix} 0 & V^F_{FM} \\ V^F_{MF} & 0 \end{pmatrix}.$$  (4.7)

The matter Hamiltonian $H^F_M$ can also be transferred into $V^F$ if so desired. This rearrangement affects the accuracy of the method, meaning that the operator (4.4) would change. In turn, a rearrangement of operators in the split can be used to improve the accuracy. We shall discussed this issue later. Using the Taylor series we infer that

$$\exp(tH^F_0) = \begin{pmatrix} \exp(tH^F_0) & 0 \\ 0 & \exp(tH^F_M) \end{pmatrix},$$

$$\exp(tH^F_0) = 1 + \left[ \cos(\sqrt{-\Delta}) - 1 \right] P^\perp + \frac{\sin(\sqrt{-\Delta})}{c\sqrt{-\Delta}} H^F,$$  (4.9)

where $\Delta = \nabla \cdot \nabla$ is the Laplace operator and $P^\perp = 1 - \nabla(\Delta^{-1}\nabla \cdot)$ is the projector on transverse fields, that is, $P^\perp E = E$ if $\nabla \cdot E = 0$ and $P^\perp E = 0$ if the vector field $E$ is conservative, $E = \nabla \phi$. The projector $P^\perp$ can be omitted in (4.9) if it is known (e.g. from a theoretical analysis of the system) that the fields remain transversal in due course. In this case, the two first terms in (4.9) are equal to $\cos(\sqrt{-\Delta})$. The action of $\exp(tH^F_0)$ is computed by the fast Fourier transform according to (3.5). In the Fourier basis, $-\Delta = k^2 = n^2k_0^2$. Note also that the Fourier transform of the fields $\psi^F_t$ is required, while the auxiliary fields remain in the grid basis all the time. The exponentials of $H^F_M$ and $V^F$ can either be computed analytically for simple models like the Lorentz model, as is shown Section 5, or, in general case, by direct diagonalization at each grid site.

Alternatively, the following approximation of the exponential of an operator can be used

$$e^{\Delta B} = \frac{1 + \Delta B/2 + \Delta^2 B^2/12}{1 - \Delta B/2 + \Delta^2 B^2/12} + O(\Delta^5) = 1 + \frac{\Delta B/2}{1 - \Delta B/2} + O(\Delta^3).$$  (4.10)

If the matrix $B$ is anti-hermitian, then the approximations (4.10) of the exponential of $B$ retain unitarity, which is important for stability of the split algorithm (see Theorems 7.1 and 7.3). On the other hand, costs of computing the inverse matrices in the right hand side of (4.10) can be less than those of computing the exponential.
If the inductions are used as independent variables, then a natural choice of the split would be
\[ \mathcal{H}^t = \mathcal{H}_0^t + \mathcal{V}^t = \begin{pmatrix} \mathcal{H}_0 & -\mathcal{H}_0 \mathcal{R} \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ \mathcal{V}_{MI} & \mathcal{H}_M^t \end{pmatrix}. \quad (4.11) \]

Making use of the Taylor expansion again we deduce that
\[ \exp(t\mathcal{H}_0^t) = \begin{pmatrix} \exp(t\mathcal{H}_0) & [1 - \exp(t\mathcal{H}_F)] \mathcal{R} \\ 0 & 1 \end{pmatrix}. \quad (4.12) \]

and, similarly,
\[ \exp(t\mathcal{V}^t) = \begin{pmatrix} 1 & 0 \\ (\mathcal{H}_M^t)^{-1}[\exp(t\mathcal{H}_M^t) - 1]\mathcal{V}_{MI} & \exp(t\mathcal{H}_M^t) \end{pmatrix}. \quad (4.13) \]

Now we can compare the two splits. The split (4.7) has an advantage over (4.11) because it requires less calls of the fast Fourier transform. Indeed, in the former the fast Fourier transform is called only for the fields \( \psi^F_t \). As it follows from (4.12), the operator \( \exp(t\mathcal{H}_0) \) acts on both the inductions \( \psi^I_t \) and the auxiliary fields. Hence the fast Fourier transform must be called for the entire column \( \Psi^I_t \). If the number of auxiliary fields is large, there might be a substantial difference in the computational speed of two algorithms. The latter, however, depends on the choice of the matter fields which, in turn, determines \( \mathcal{R} \) and therefore the number of calls of the fast Fourier transform. Note that the matter fields can always be chosen in such a way that only one of the components of \( \xi_t \) specifies the response field \( \psi^R_t \). Thus, the canonical transformation (2.30) can be used to reduce the number of calls of the fast Fourier transform. If \( \mathcal{R} \) is chosen so that it depends on position, multiplication of the matter fields by \( \mathcal{R} \) must be done before calling the fast Fourier transform. A significant advantage of the split in the induction representation is that the Gauss law can be exactly fulfilled without altering the algorithm (see Theorem 8.2).

In empty space either of the splits reproduces an exact solution of Maxwell’s equations for any period of time \( t \), provided the initial pulse is bandwidth limited. Indeed, on the grid, the initial wave packet is a superposition of a finite number of plane waves. Thanks to the linearity of the theory, each Fourier mode is evolved exactly, that is, without any phase error, by \( \exp(t\mathcal{H}_0) \) for any \( t > 0 \). As final remarks in this section, we note that the algorithm can operate at the Nyquist limit: Two grid points per shortest wavelength in the initial wave packet [5]. Yet, for the multiresonant Lorentz model, it is unconditionally stable (see Theorems 7.1 and 7.3). These features cannot be achieved in any finite difference scheme.

5 A multi-resonant Lorentz model

An analytical expression for the exponents of \( \mathcal{H}_M^Q \) and \( \mathcal{V}^Q \) helps to reduce computational costs. Here such analytical expressions are derived for multi-resonant Lorentz models. Let
us take first the field representation. Due to the block diagonal structure of $\mathcal{H}_M^F$, we get

\begin{equation}
\exp(t\mathcal{H}_M^F) = \text{diag} \left( \exp(t\mathcal{H}_{M1}^F), \exp(t\mathcal{H}_{M2}^F), \ldots, \exp(t\mathcal{H}_{MN}^F) \right),
\end{equation}

where $\tilde{\nu}_a = (\gamma_a^2 - \omega_a^2)^{1/2}$. The exponential (5.15) is easy to compute by expanding $\mathcal{H}_{Ma}^F$ in the Pauli matrix basis, which is also a basis for the Lie algebra $su(2)$, and then by using the well known formula for the exponential of a linear combination of Pauli matrices. For small attenuation, $\gamma_a < \omega_a$, we get $\tilde{\nu}_a = i\nu_a$. The hyperbolic functions in (5.15) become trigonometric ones and $\tilde{\nu}_a$ is replaced by $\nu_a$. The eigenvalues of the matter Hamiltonian are $\lambda_a = -\gamma_a \pm \nu_a$. Hence, $\text{Re} \lambda_a < 0$ and amplitudes of the matter fields are always exponentially attenuated as $t \to \infty$, unless $\gamma_a = 0$ leading to $\text{Re} \lambda_a = 0$.

Computation of $\exp(t\mathcal{V}^F)$ is a bit more subtle. We start with the observation that the characteristic polynomial of $\mathcal{V}^F$ has a simple form

\begin{equation}
\det (\mathcal{V}^F - \lambda) = \lambda^{2N} (\lambda^2 + \omega_p^2), \quad \omega_p^2 = \sum_{a=1}^{N} \omega_{pa}^2.
\end{equation}

This can be proved either by a direct computation or by mathematical induction. So, $\mathcal{V}^F$ has $2N$ zero eigenvalues and two non-zero ones, $\lambda = \pm i\omega_p$. Let $X$ be the eigenvector of $\mathcal{V}^F$ corresponding to the eigenvalue $i\omega_p$. Its components have the form

\begin{equation}
X_j = \omega_p^{-1} [\mathcal{V}^F_{j1} + i\omega_p \delta_{j1}], \quad j = 1, 2, \ldots, 2(N + 1),
\end{equation}

so that $\bar{X} \cdot X = 1$ and $\bar{X} \cdot \bar{X} = X \cdot X = 0$ where the dot denotes the Euclidean scalar product. The skew-symmetric matrix $\mathcal{V}^F$ has the following spectral decomposition

\begin{equation}
\mathcal{V}^F = i\omega_p \left( X \otimes \bar{X} - \bar{X} \otimes X \right).
\end{equation}

Taking the square of (5.17) we also infer that

\begin{equation}
X \otimes \bar{X} = -\omega_p^{-2} (\mathcal{V}^F)^2 - i\omega_p^{-1} \mathcal{V}^F.
\end{equation}

The exponential of (5.17) is obtained via the Taylor series and making use of (5.18). The final result reads

\begin{equation}
\exp(t\mathcal{V}^F) = 1 + \frac{\sin \omega_p t}{\omega_p} \mathcal{V}^F + 2 \left( \frac{\sin(\omega_p t/2)}{\omega_p} \right)^2 (\mathcal{V}^F)^2.
\end{equation}

In the induction representation, an explicit formula for $\exp(t\mathcal{H}_M^I)$ is not that simple. To avoid unnecessary technicalities, we limit the discussion to the simplest case of the one-resonant Lorentz model. We choose the matter fields so that $\xi_t^1 = \mathbf{P}_t$ and $\xi_t^2 = \partial_t \xi_t^1$. In this case, non-zero elements of the matter Hamiltonian are $\mathcal{H}_{M12}^I = 1$, $\mathcal{H}_{M21}^I = -\omega_0^2 - \omega_p^2$, and...
\( H_{M22} = -2\gamma \). The coupling matrix \( V_{MI} \) has only one non-zero element, \( V_{M121} = \omega_p^2 \). Here \( \omega_0 \) is the resonant frequency, \( \gamma \) is the attenuation constant and \( \omega_p \) is the plasma frequency. Using the Pauli matrix basis again, we find that the expression (5.15) holds for \( \exp(tH_M^I) \) if we replace in it \( \nu_a \) by \( \nu_p = \sqrt{\omega_0^2 + \omega_p^2 - \gamma^2} \), \( \gamma_a \) by \( \gamma \) and \( H_f^M \) by \( H_M^I \). The lower left corner of (4.13) has the form

\[
(H_M^I)^{-1} \left( \exp(tH_M^I) - 1 \right) V_{MI} = -\frac{\omega_p^2}{\omega_0^2 + \omega_p^2} (\exp(tH_M^I) - 1) \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}.
\]

(5.20)

A further simplification can be achieved by going over to the complex representation (2.12) of the auxiliary fields in which the matter Hamiltonian is diagonal. The transformation rule is explained in the paragraph after Eq. (2.31).

### 6 Energy and norm conservation

Consider the \( L_2(\mathbb{R}^3) \) norm of \( \Psi_t^Q \), \( |\Psi_t^Q|^2 = \int d\mathbf{r} \Psi_t^{Q*} \Psi_t^Q \equiv (\Psi_t^Q, \Psi_t^Q) \). In the grid representation, the norm coincides with the corresponding (complex) Euclidean norm, \( (\Psi_t^Q, \Psi_t^Q) = \sum_n \Psi_t^{Q*}(n\Delta r)\Psi_t^Q(n\Delta r) \) where the sum is taken over all grid sites. By taking the time derivative of \( |\Psi_t^Q|^2 \) and using the evolution equation (1.1), it is not hard to deduce that the norm is conserved, provided the Hamiltonian is anti-Hermitian

\[
H^* = -H^Q.
\]

(6.1)

For a generic passive media this is not the case. So the norm is generally not conserved in contrast to the quantum mechanical case. However, we shall see that in the case when the matter evolution is described by second order differential equations in time and no attenuation is present, the norm coincides with the system energy and is conserved. In numerical simulations, this important property can be used to help to control the accuracy.

Consider multi-resonant Lorentz models with no attenuation, \( \gamma_a = 0 \). We start with the observation that the field and matter evolution equations can be obtained from the variational principle for the action

\[
S = \int dt \int d\mathbf{r} \left[ \frac{1}{2} \left( E_t^2 - B_t^2 \right) + \frac{1}{2} \sum_a \left( (\partial_t \vartheta_t^a)^2 - \omega_a^2 \vartheta_t^{a2} \right) + \sum_a \omega_{pa} \vartheta_t^a \cdot \mathbf{E}_t \right],
\]

(6.2)

where the electromagnetic degrees of freedom are described by vector and scalar potentials, respectively, \( \mathbf{A}_t \) and \( \varphi_t \), so that \( \mathbf{E}_t = -\nabla \varphi_t - \partial_t \mathbf{A}_t \) and \( \mathbf{B}_t = \nabla \times \mathbf{A}_t \). The units are chosen in this Section so that \( c = 1 \). The polarization of the medium is expressed via the matter fields as \( \mathbf{P}_t = \sum_a \omega_{pa} \vartheta_t^a \). The least action principle for the scalar potential \( \varphi \) leads to the Gauss law, \( \nabla \cdot \mathbf{D}_t = 0 \), for the vector potential \( \mathbf{A}_t \) to the Maxwell’s equation, \( \partial_t \mathbf{D}_t = \nabla \times \mathbf{B}_t \), and for the matter field \( \vartheta_t^a \) to the medium polarization evolution equation of the Lorentz
model with no attenuation, $\gamma_a = 0$. The second Maxwell’s equation and the Gauss law for the magnetic field follow from the relation $B_t = \nabla \times A_t$ by taking its time derivative and divergence, respectively. The energy of the system coincides with the canonical Hamiltonian which is obtained by a Legendre transformation [8] of the Lagrangian $L$ for the velocities $\partial_t A_t$ and $\partial_t \theta^a_t$. Doing the Legendre transformation, we find the canonical Hamiltonian (energy) of the system

$$E_t = \frac{1}{2} \int dx \left[ E_t^2 + B_t^2 + \sum_a \left( \pi_t^a + \omega_a \theta^a_t \right)^2 \right] = \frac{1}{2} |\Psi^F_t|^2 ,$$

where $\pi_t^a = \delta L/\delta (\partial_t \theta^a)$ are canonical momenta of the matter fields. To get the last equality in (6.3), we have used the relations $\xi_t^{2a} = \pi_t^a$ and $\xi_t^{2a-1} = \omega_a \theta^a_t$ which follow from comparison of the canonical Hamiltonian equations of motion for the canonically conjugate variables $\theta^a_t$ and $\pi_t^a$ and Eqs. (2.10) and (2.11) with $\gamma_a = 0$. Note that the canonical momentum conjugate to the vector potential $A_t$ coincides with $-D_t = -E_t - P_t$, not $-E_t$ in this system. Therefore, the coupling between the electromagnetic and matter degrees of freedom is included into the term $E_t^2 = (D_t - P_t)^2$ of the canonical Hamiltonian. Equation (6.3) becomes the conventional expression for the electromagnetic energy in a passive medium [19] when $\pi_t^a$ and $\theta^a_t$ are replaced by the corresponding solutions of the equations of motion with initial conditions $\pi_0^a = \theta_0^a = 0$. The energy conservation can be deduced either from the Noether theorem (because $E_t$ is the Noether integral of motion corresponding to the time translational symmetry of the action) or directly from the norm conservation of $\Psi^F_t$ (because the evolution operator $\exp(t\mathcal{H}^F)$ is unitary when $\gamma_a = 0$).

In numerical simulations, an exact unitary evolution operator $U_{\Delta t}^Q$ is replaced by its approximation $\mathcal{G}_{\Delta t}^Q$. However, the energy remains conservative:

**Theorem 6.1.** The split algorithm is unitary for multiresonant Lorentz models with no attenuation, that is, the split algorithm preserves the energy $E_{t+\Delta t} = E_t$.

**Proof.** In the field representation, $\mathcal{H}^F = -\mathcal{H}^0_F$ and $\mathcal{V}^F = -\mathcal{V}^F$ and, therefore, $\mathcal{G}_{\Delta t}^F$ is unitary. As a result, the algorithm preserves the initial wave packet energy and the norm,

$$|\mathcal{G}_{\Delta t}^F \Psi^F_t| = |\Psi^F_{t+\Delta t}| = |\Psi^F_t| .$$

In the induction representation, the energy coincides with the norm of $\Psi^I_t$ in the measure space. The measure is determined by the transformation law $\Psi^I_t = S\Psi^F_t$,

$$E_t = \frac{1}{2} (\Psi^F_t, \Psi^F_t) = \frac{1}{2} (\Psi^I_t, \mu \Psi^I_t) \equiv \frac{1}{2} |\Psi^I_t|_\mu ^2 , \quad \mu = S^{-1} S^{-1} .$$

Since $\mathcal{H}^I$ is similar to $\mathcal{H}^F$, the Hamiltonian $\mathcal{H}^I$ is anti-Hermitian relative to the $\mu$ scalar product,

$$\mathcal{H}^I^* \mu = -\mu \mathcal{H}^I .$$

The norm conservation (unitarity) in the split algorithm requires in addition that the amplification matrix $\mathcal{G}_{\Delta t}^I$ satisfies the unitarity condition

$$\mathcal{G}_{\Delta t}^I \mathcal{G}_{\Delta t}^I = \mu .$$
This is indeed the case. To prove (6.7), we show that $H^I_0$ and $V^I$ satisfy the condition (6.6) and, hence, the product of their exponentials is a unitary operator relative to the $\mu$ scalar product. Consider $H^I = SH^FS^{-1} = H^I_0 + V^I$ so that $H^F = S^{-1}H^I_0S + S^{-1}V^I S$. For the Lorentz model,

$$S^{-1}H^I_0S = \begin{pmatrix} H^I_0 & 0 \\ 0 & 0 \end{pmatrix} = -(S^{-1}H^I_0S)^* . \quad (6.8)$$

Therefore $H^I_0$ satisfies (6.6). From the anti-Hermiticity of $H^F$ and (6.8) it follows that

$$(S^{-1}V^I S)^* = -S^{-1}V^I . \quad (6.9)$$

Hence, $\Psi^I$ also satisfies (6.6). Thus,

$$|G^I_{\Delta t} \Psi^I_t|_\mu = |\Psi^I_{t+\Delta t}|_\mu = |\Psi^I_t|_\mu , \quad (6.10)$$

which completes the proof.

The norm (energy) conservation can be used to control numerical convergence, especially when the aliasing problem in the fast Fourier transform is present, i.e., when parameters of the medium are discontinuous functions in space. In a properly designed algorithm the loss of energy (norm) due to attenuation should be controlled by the symmetric part of the Hamiltonian operator

$$\partial_t E_t = -\sum_a \gamma_a |\xi^2_a t|^2 \equiv \frac{1}{2} (\Psi^Q_t, \Psi^Q_t \Psi^Q_t) \leq 0 , \quad (6.11)$$

where $V^Q = V^Q = (H^Q + H^Q)/2 \leq 0$ (a negative semidefinite operator) which is, in this case, a diagonal matrix with nonpositive elements.

### 7 Stability of the algorithm

The norm of an operator $H$ is defined as

$$\|H\| = \sup_{|\Psi|=1} |H\Psi| . \quad (7.1)$$

If the operator is normal, that is, it commutes with its adjoint, then its norm coincides with its spectral radius $\rho(H)$, the supremum absolute value of its eigenvalues. In general, $\rho(H) \leq \|H\|$. A family of amplification operators (matrices) $G_{\Delta t}(\alpha)$ is called conditionally stable if there exists a constant $C(\tau, T)$ such that [16]

$$\|G^\alpha_{\Delta t}(\alpha)\| \leq C(\tau, T) , \quad (7.2)$$

for all $\Delta t \in (0, \tau)$, all $0 \leq n\Delta t \leq T$ for some positive $\tau$ and $T$, and all parameters $\alpha$. The unconditional stability of $G^\alpha_{\Delta t}(\alpha)$ means that (7.2) holds uniformly in $n \geq 0$ for any
\( \Delta t > 0 \) and for all \( \alpha \), that is, \( C \) is independent of \( T \) and \( \tau \). Parameters \( \alpha \) can be all wave vectors \( \vec{k} \) supported by the grid or simply grid values of the position vector \( \vec{x} \). They can also include parameters of the medium. Note that if \( G_{\Delta t} \) is not normal, then \( \rho(G_{\Delta t}) \leq \|G_{\Delta t}\| \)
and, therefore, the von Neumann condition \( \rho(G_{\Delta t}) \leq 1 \) is no longer sufficient for stability, while still being necessary.

**Theorem 7.1.** For multiresonant Lorentz models, the split algorithm in the field representation is unconditionally stable.

**Proof.** We shall prove that
\[
\|G_{\Delta t}^F\| \leq 1, \tag{7.3}
\]
which leads to the theorem statement
\[
\|(G_{\Delta t}^F)^n\| \leq \|G_{\Delta t}^F\|^n \leq 1. \tag{7.4}
\]
By definition and making use of the inequality, \( \|A B\| \leq \|A\| \|B\| \), we get
\[
\|G_{\Delta t}^F\| = \| e^{\Delta t H_{0}^F/2} e^{\Delta t \nu F} e^{\Delta t H_{0}^F/2} \| \\
\leq \| e^{\Delta t H_{0}^F/2} \|^2 \tag{7.5}
\]
because \( e^{\Delta t \nu F} \) is a unitary operator, so its norm equals 1. The operator \( e^{t H_{0}^F} \) is block-diagonal (see (4.8) and (5.14)). The norm of a block-diagonal operator is the maximal norm of its blocks. The upper left corner block is given by the unitary operator \( e^{t H_{0}^F} \) whose norm equals 1. We have then
\[
\|e^{t H_{0}^F}\| = \max_a \left\{ 1, \|e^{t H_{0}^F_{Ma}}\| \right\}. \tag{7.6}
\]
The norm of the exponential of \( H_{Ma}^F \) can be found by direct calculation using the fact that \( \|A\|^2 = \|A^* A\| = \nu(\lambda^* A) \) and the explicit form of \( e^{t H_{Ma}^F} \) given in (5.15). For small attenuation, \( \omega_a^2 - \gamma_a^2 = \nu_a^2 \geq 0 \), we define \( z_a = (\gamma_a/\nu_a) \sin(\nu_a t) \) so that the largest eigenvalue has the form
\[
\|e^{t H_{Ma}^F}\|^2 = \|(e^{t H_{Ma}^F})^* e^{t H_{Ma}^F}\| \\
= e^{-2\gamma_a t} \left( 1 + 2z_a^2 + 2z_a \sqrt{1 + z_a^2} \right). \tag{7.7}
\]
Since \( z_a \leq \gamma_a t \equiv y \) for \( t \geq 0 \), the function (7.7) is bounded from above by \( f(y) = e^{-2y} (1 + 2y^2 + 2y \sqrt{1 + y^2}) \). It is not hard to verify that the derivative \( f'(y) \) is negative for all \( y > 0 \), and that \( f(0) = 1 \). Hence, replacing \( t \) by \( \Delta t/2 \), we conclude that
\[
\|e^{\Delta t H_{Ma}^F/2}\| \leq 1, \tag{7.8}
\]
from which (7.3) follows. For large attenuation (like in Drude metals), \( \omega_a^2 - \gamma_a^2 = -\nu_a^2 \leq 0 \), in (7.7) we get \( z_a = (\gamma_a/\nu_a) \sinh(\nu_a t) \equiv z_a(t) \). For \( t \geq 0 \) the latter relation defines the inverse function \( t = t(z_a) \). Once again, the derivative of (7.7) with respect to \( z_a \) can be shown to be negative for all positive \( z_a \) while at \( z_a = 0 \) the function equals 1. So inequalities (7.8) and (7.3) hold in this case too. This completes the proof.
The proof of Theorem 7.1 given above is not the most economical. However, the idea of estimating the norm of the exponential of the matter Hamiltonian in order to investigate stability of the algorithm can be applied numerically to systems more general than the Lorentz model because $H_M^F$ is local on the grid, that is, it does not contain derivatives. So the exponentials of $H_M^F$ and its adjoint are not expensive to calculate numerically for some trial values of $\Delta t$ to see if (7.8) holds.

We give an alternative proof of the unconditional stability in the case of the induction representation of the multi-resonant Lorentz model where an analytical expression of the exponent of the matter Hamiltonian is too hard to find, not to mention its norm. We shall make use of the following obvious lemma.

**Lemma 7.2.** Let a vector $\psi_t, t \geq 0$, be a solution of the linear equation $\partial_t \psi_t = (H + V)\psi_t$ where the linear operators $H$ and $V$ satisfy the conditions $H^* = -H$ and $V^* = V \leq 0$ (negative semidefinite). Then $|\psi_t| \leq |\psi_0|$ for all $t \geq 0$.

The proof follows from an obvious relation

$$\partial_t |\psi_t|^2 = 2(\psi_t, V\psi_t) \leq 0 \tag{7.9}$$

As a consequence we also get

$$\|e^{t(H+V)}\| \leq 1 \tag{7.10}$$

for all $t \geq 0$.

**Theorem 7.3.** For multiresonant Lorentz models, the split algorithm in the induction representation is unconditionally stable.

**Proof.** If the attenuation is absent, the amplification matrix $G_{\Delta t}$ is unitary with respect to the energy scalar product ($\mu$-scalar product) as is shown in (6.10). Hence, $\|(G_{\Delta t})^n\|_\mu = 1$. When the attenuation is switched on, the unitarity of the amplification matrix can get violated only through $\exp(\Delta t V^I)$ because the operator $\exp(\Delta t H_0^I)$ remains unitary with respect to the $\mu$-scalar product. The idea is to prove the unconditional stability with respect to the $\mu$-norm. The theorem statement would follow from the equivalence of the Euclidean and $\mu$- norms. Recall that two norms $|\Psi|$ and $|\Psi'|$ are equivalent if there exist two positive constants $C_1, C_2$ such that

$$C_1 |\Psi| \leq |\Psi'| \leq C_2 |\Psi| \tag{7.11}$$

for all $\Psi$. All topological properties of the space spanned by $\Psi$ are the same in one norm as in the other; in particular convergence of a sequence, boundedness of a set, boundedness of a linear operator, and uniform boundedness of a family of operators are all invariant concepts under a change of one norm to the other. If $|\Psi'| = |\Psi|_\mu$, then $\|A\|_\mu = \|S^{-1}AS\|$ and

$$|\Psi|_\mu = |S^{-1}\Psi| \leq \|S^{-1}\| |\Psi|, \quad |\Psi| = |S\Psi|_\mu \leq \|S\| |\Psi|_\mu = \|S\| |\Psi|_\mu,$$
so that the two norms are indeed equivalent

\[ \|S\|^{-1}|\Psi| \leq |\Psi|_\mu \leq \|S^{-1}\| |\Psi| . \]  \hspace{1cm} (7.12)

Since \( \|AU\| = \|A\| \) for any bounded operator \( A \) and a unitary operator \( U \), we infer that

\[ \|(G^I_{\Delta t})^n\|_\mu \leq \|G^I_{\Delta t}\|_\mu = \|e^{\Delta t\nu^I}\|_\mu = \|e^{\Delta tS^{-1}\nu^I S}\|^n . \]  \hspace{1cm} (7.13)

When \( \gamma_a = 0 \) (no attenuation), the operator \( S^{-1}\nu^I S \) is skew-symmetric (cf. (6.9)). When \( \gamma_a \neq 0 \), the operator \( S^{-1}\nu^I S \) acquires an addition which is a diagonal operator with nonpositive elements as follows from (2.26) and (2.29). Therefore the inequality (7.10) must hold for it as a consequence of Lemma 7.2,

\[ \|e^{\Delta tS^{-1}\nu^I S}\| \leq 1 , \]

from which the uniform boundedness of the family \( (G^I_{\Delta t})^n \) with respect to the \( \mu \)-norm immediately follows. By the equivalence of the two norms (7.12), the family \( (G^I_{\Delta t})^n \) is also uniformly bounded in the Euclidean norm,

\[ \|(G^I_{\Delta t})^n\| \leq \|S\| \|S^{-1}\| \]  \hspace{1cm} (7.14)

which completes the proof.

**Comment.** The same idea of making use of the norm equivalence, which actually goes in line with the Kreiss matrix theorem (its last part) [23, 16], can be applied to analyze the stability of the split algorithm for generic passive media. It is not hard to find a quadratic Lagrangian local in time such that the corresponding Euler equations describe propagation of an electromagnetic pulse in generic non-absorbing media. Due to time translation symmetry, the system should have a conserved quantity according to the Noether theorem [8]. This integral of motion coincides with the canonical Hamiltonian which is a quadratic form of \( \Psi^Q_t \) if the linear response approximation is valid. By analogy with the \( \mu \)-norm, one could try to identify the canonical Hamiltonian with the new norm of \( \Psi^Q_t \) which is conserved by construction and, hence, in an attenuation-free medium the corresponding evolution operator is unitary. Thus, it would always be possible to arrange the split so that the amplification operator is unitary too. From the physical point of view, it is then naturally expected that, when absorption is added to the system, the attenuation operator \( \nu^Q \) would generally satisfy the condition (6.11) because Fourier amplitudes of fields are exponentially attenuated in passive media. The latter would make it possible to apply Lemma 7.2 to prove the unconditional stability of the amplification operator with respect to the norm defined by the canonical Hamiltonian along the lines similar to the proof of Theorem 7.3. An obstacle for this rather natural idea to generalize Theorem 7.3 to generic passive media is that the canonical Hamiltonian is not, in general, positive definite. It becomes positive only on solutions of the equations of motion for matter fields, which is a rather common feature of Lagrangian systems with higher order time derivatives. Thus, the canonical Hamiltonian does not always define a positive definite quadratic form in the Hilbert space for a generic...
passive media, and, hence, cannot serve as a new (conservative) norm. The study of conditions on attenuation-free media under which a positive definite and conserved quadratic form does exist goes beyond the scope of this paper since it would require the canonical formalism and the Noether theorem for theories with higher-order time derivatives, which is rather involved for generic passive media. The question can be addressed more easily for each particular medium model of interest. However, the unconditional stability might be excessive as far as practical needs are concerned. It is more important to make the split algorithm convergent for a generic passive medium. Then one should use the equivalence of (conditional) stability and convergence according to the fundamental convergence theorem due to Kantorovich [24, 16].

Our findings in this latter approach are summarized in the following theorem.

**Theorem 7.4.** Suppose that the medium response function satisfies the causality conditions (that is, its Fourier transform has poles only in the lower half of the frequency plane, Im $\omega \leq 0$). Let $U_t$ be an exact evolution matrix in the grid representation (as defined in Section 3), and $G_{\Delta t}$ be an amplification matrix in some third order split algorithm. Then for band-width limited wave packets the split algorithm is (conditionally) stable and for all $0 \leq n \leq N$, $T = N \Delta t$, and $0 < \Delta t < \tau$, there exist a constant $C_m$, which depends only on the medium parameters, and a constant $W_m$, which depends also on $\tau$, such that

$$\|G_{\Delta t}^n\| \leq C_m + \delta(\Delta t, T),$$

$$\delta(\Delta t, T) = C_m \left(e^{W_m T \Delta t^2} - 1\right) = O(\Delta t^2),$$

$$\|U_{n \Delta t} - G_{\Delta t}^n\| \leq \delta(\Delta t, T).$$

**Remark.** Before proving the theorem, let us discuss its significance for practical applications. Inequality (7.15) implies conditional stability, while (7.17) establishes a relation between the accuracy (and convergence) of the split approximation and the uniform bound in the stability condition (7.15). By making the time step $\Delta t$ smaller, any desired accuracy can be achieved during the total (fixed) simulation time $T$. The latter implies, of course, that the grid is assumed to be chosen fine enough (in accord with the Shannon sampling theorem) to accurately reproduce the initial pulse configuration via the fast Fourier method. Indeed, let $\Psi_{n \Delta t}^{app} = G_{\Delta t}^n \Psi_0$ be a simulated solution, and $\Psi_t = U_t \Psi_0$ be an exact solution, then from (7.17) it follows that

$$|\Psi_t - \Psi_t^{app}| \leq \delta(\Delta t, T) |\Psi_0| = O(\Delta t^2),$$

for all $0 \leq t \leq T$ and any fixed total simulation time $T$ which is roughly $2L/c$ where $L$ is the simulation box size and $c$ the speed of light. Now we turn to the proof.

**Proof.** In the grid Fourier basis, $U_t \Psi_0^Q = \sum_k \Psi_t^Q(k) e^{ikx}$, where $k$ spans the dual lattice. By construction of the Hamiltonian, each Fourier mode $\Psi_t^Q(k)$ evolves exactly as in the continuum case. Since the medium response function satisfies the causality conditions, Fourier
amplitudes of the electromagnetic and response fields as well as their time derivatives are bounded functions of time. The amplitudes cannot grow infinitely large because of dissipation [19]. The number of Fourier modes is finite on the grid (only bandwidth limited initial wave packets are considered) and, hence, $|\Psi_t^Q| \leq C_Q$ for all $t \geq 0$ because components of the auxiliary field $\xi_t$ are linear combinations of the response field and its time derivatives. The latter inequality is equivalent to the evolution matrix being uniformly bounded for all $t \geq 0$,

$$\|U_t\| \leq C_m. \quad (7.19)$$

Let $U_{\Delta t} - G_{\Delta t} = \Delta t^3 W_{\Delta t}$ and $W_{\Delta t} = W_0 + O(\Delta t)$ for small $\Delta t$ according to a third order split (cf. (4.2) - (4.4)). Let $W_m = C_m \sup_{\Delta t} \|W_{\Delta t}\|$ for $0 < \Delta t < \tau$ and some positive finite $\tau$. Using the semigroup property $U_{\Delta t}^k = U_{k\Delta t}$ and (7.19) we infer that

$$\|G_{\Delta t}^n\| = \|U_{\Delta t}^n - (U_{\Delta t}^n - G_{\Delta t}^n)\|$$

$$\leq \|U_{\Delta t}^n\| + \|U_{\Delta t}^n - G_{\Delta t}^n\| \quad (7.20)$$

$$\leq C_m + \|U_{\Delta t}^n - (U_{\Delta t} - \Delta t^3 W_{\Delta t})^n\| \quad (7.21)$$

$$= C_m + \| - \Delta t^3 \left( \sum_{k=0}^{n-1} U_{\Delta t(n-k-1)} W_{\Delta t} U_{k\Delta t} \right) + \cdots \| \quad (7.22)$$

$$\leq C_m + C_m \left[ (1 + \Delta t^3 W_m)^n - 1 \right] \quad (7.23)$$

$$\leq C_m + \delta(\Delta t, T). \quad (7.24)$$

Inequality (7.17) readily follows from comparing the right hand side of (7.20) with those of (7.21)-(7.24). This completes the proof.

8 Convergence and accuracy analysis

To estimate the accuracy of the algorithm at a fixed finite grid size $N$, consider the following quantity

$$\beta_n(N, \Delta t) = \left| \left( (U_{\Delta t}^Q)^n - (G_{\Delta t}^Q)^n \right) \Psi_0^Q \right| / |\Psi_0| \leq \left\| (U_{\Delta t}^Q)^n - (G_{\Delta t}^Q)^n \right\| \quad (8.1)$$

which specifies a deviation of the approximate solution from the exact one relative to a given norm. Here $U_{\Delta t}^Q$ is an exact evolution operator. The accuracy estimate $\beta_n(N, \Delta t)$ is a norm dependent quantity. The choice of norm is usually determined by practical needs. We use the norm related to the electromagnetic energy of the system and investigate, first, the behavior of $\beta_n(N, \Delta t)$ as $\Delta t$ goes to zero, while $\Delta t n = t$ remains fixed and does not exceed some positive constant, $t \leq T$.

**Theorem 8.1.** For multi-resonant Lorentz models, there exists a positive constant $W_Q$ such that

$$\left\| (U_{\Delta t}^Q)^n - (G_{\Delta t}^Q)^n \right\| \leq \Delta t^2 W_Q c_Q^2, \quad (8.2)$$

where $c_F = 1$ and $c_I = ||S|| ||S^{-1}||$, for all $\Delta t \in (0, \tau)$ and $n\Delta t \leq T$. 


Proof. In the field representation $Q = F$, $\|(U^F_{\Delta t})^n\| \leq 1$ and $\|(G^F_{\Delta t})^n\| \leq 1$ for any integer $n$, as a consequence of Lemma 7.2 for the multi-resonant Lorentz model. The same inequalities hold in the induction representation if the norm is replaced by the $\mu$-norm. According to the split algorithm (4.2)-(4.4), $U^Q_{\Delta t} - G^Q_{\Delta t} = \Delta t^3 W^Q_{\Delta t}$. Let $W^Q = \sup_{\Delta t} \|W^Q_{\Delta t}\|$ for $\Delta t \in (0, \tau)$ for some positive $\tau$ (a maximal time step used in simulations). We then have the following chain of inequalities that lead to the theorem statement

$$\|(U^F_{\Delta t})^n - (G^F_{\Delta t})^n\| = \left\| \sum_{k=1}^{n-1} (U^F_{\Delta t})^k (U^F_{\Delta t} - G^F_{\Delta t}) (G^F_{\Delta t})^{n-k} \right\| \leq (n - 1) \Delta t^3 \|W^F_{\Delta t}\| \leq \Delta t^2 TW^F.$$  

In the case of the induction representation, inequality (8.4) holds relative to the $\mu$-norm. The theorem statement (8.2) follows from the norm equivalence (7.12), $c_I^{-1} \|A\| \leq \|A\|_{\mu} \leq c_I \|A\|$ for any operator $A$. The proof is complete.

Remark. In simulations, the continuum limit $N \to \infty$ is never achieved. Hence the operators in the split algorithm (4.1) remain bounded versus the unbounded case of (4.1). It is known that the convergence rate of $\beta_n(\infty, \Delta t)$ as $\Delta t \to 0$ estimated by the operator norm as in the right hand side of (8.1) is no longer of order $O(\Delta t^2)$ but rather of $O(\sqrt{\Delta t})$ (see, e.g., [25] and references therein). For unbounded operators, the estimate (8.5) is not valid. This suggests that the convergence rate $\beta_n(N, \Delta t)$ may depend, even significantly, on the initial vector $\Psi_0$ as $N$ increases.

In a general case, the quantity $\delta(\Delta t, T)$ in Theorem 7.4 determines the accuracy of the split algorithm with respect to the norm (7.1) on a finite grid. To make simulation errors small, it is sufficient to require that

$$\|U_{\Delta t} - G^Q_{\Delta t}\| = \Delta t^3 \|W^Q_{\Delta t}\| \ll 1.$$  

Making use of (4.4) and the fact that the norm of a matrix does not exceed the maximal norm of its blocks, we infer for a multi-resonant Lorentz model that, in order for (8.6) to hold, the following inequalities are sufficient:

$$\omega_{pa}\Delta t \ll 1, \quad \omega_{max}\Delta t \ll 1, \quad \omega_a\Delta t \ll 1, \quad \gamma_a\Delta t \ll 1,$$  

and, yet another one,

$$|\nabla \omega_{pa}| c\Delta t \ll 1.$$  

Here $\omega_{max}$ is the maximal frequency of the initial wave packet. The right hand side of (8.6) is a sum of two types of terms. There are terms of the cubic order in numbers (8.7) as well as a term linear in (8.8) with the coefficient being quadratic in (8.7). The ratio in (8.8) can roughly be estimated from $|\nabla \omega_{pa}| \leq \omega_{pa}/\Delta r$ with $\Delta r$ being the grid step. The condition (8.8) implies then that the distance traveled by the wave packet during one time step should be much smaller than the grid step.
To complete the discussion, one should also analyze the accuracy of the Gauss law (2.3). Note that the constraints are automatically fulfilled in the continuum theory due to the Dirac involution relations (1.3). By projecting the continuum theory onto a finite grid and replacing the exact evolution operator by its approximation in the split algorithm, the involution relations might be violated, thus leading to errors and potential instabilities of the algorithm. A good example of this kind is numerical general relativity (although the nonlinearity of the equations of motion plays the central role in generating instabilities due to the violation of the Dirac involution relations).

It is not hard to be convinced that the Gauss law (2.3) is equivalent to the following constraint on state vectors

\[ \mathcal{C}^I \Psi^I_t = 0, \quad \mathcal{C}^I = \begin{pmatrix} C & 0 \\ 0 & 0 \end{pmatrix}, \quad \mathcal{C} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \mathcal{P}_\parallel, \quad \mathcal{P}_\parallel = 1 - \mathcal{P}_\perp. \] (8.9)

The operator \( \mathcal{P}_\parallel \) projects a vector field onto its longitudinal component. In other words, it acts as the identity operator if the vector field is conservative, and it annihilates any rotational vector field (which is the curl of another vector field). In the field representation we get \( \mathcal{C}^F = S^{-1} \mathcal{C}^I S \) with \( S \) defined in (2.22). On the grid, the action of the operator \( \mathcal{C}^Q \) is defined by the rule (3.5), that is, by (8.9) we understand \( \mathcal{F} \mathcal{C}^Q \mathcal{F}^* \mathcal{F} \Psi^Q_t = 0 \). Thus, the Gauss law requires that the Fourier transform of the inductions should not acquire components parallel to wave vectors of the dual grid. This is obviously guaranteed if the exact evolution operator, \( U^Q_t = \exp(t \mathcal{H}^Q) \), is used to generate the time evolution because

\[ \mathcal{C}^Q \mathcal{H}^Q = 0, \] (8.10)

and, hence, \( \mathcal{C}^Q U^Q_t \Psi^Q_0 = \mathcal{C}^Q \Psi^Q_0 = 0 \). A problem may arise when the approximate evolution operator, \( (\mathcal{G}^Q_{\Delta t})^n \), is used to evolve the initial wave packet \( \Psi^Q_0 \). From linearity of the system, it is natural to expect that the Gauss law violation should be of the same order as the accuracy of a numerical solution of dynamical Maxwell’s equations. However, we shall take a closer look at the problem and find a pleasant result important in practice, which is stated in the following theorem.

**Theorem 8.2.** Assuming linear response theory for any passive medium, the Gauss law holds exactly in the split algorithm in the induction representation.

**Proof.** In the induction representation, identity (8.10) is equivalent to two identities for the blocks of \( \mathcal{C}^Q \mathcal{H}^Q \), namely, \( \mathcal{C}^Q_0 = 0 \) and \( \mathcal{C}^Q_{IM} = 0 \). The first one is obvious. The second one follows from (2.25) established for any passive medium. The key observation is that the identity

\[ \mathcal{C}^I \mathcal{H}^I_0 = 0 \] (8.11)

holds thanks to the two above identities and (4.11). Indeed, in the Fourier basis (8.11) is equivalent to the vanishing of the triple vector product \( \mathbf{k} \cdot (\mathbf{k} \times \mathbf{A}) \) for some \( \mathbf{A} \) regular at \( \mathbf{k} = 0 \). Then from (8.9) and (8.11) it follows that

\[ \mathcal{C}^I \mathcal{V}^I = \mathcal{C}^I (\mathcal{H}^I - \mathcal{H}^I_0) = 0. \] (8.12)
As a consequence of (8.11) and (8.12), we infer that
\[
C^I (G^I_{\Delta t})^n \Psi^I_0 = C^I e^{\Delta t H^I_{\Delta t}/2} e^{\Delta t V^I} e^{\Delta t H^I_{\Delta t}/2} (G^I_{\Delta t})^{n-1} \Psi^I_0 = C^I (G^I_{\Delta t})^{n-1} \Psi^I_0 = C^I \Psi_0 = 0 , \tag{8.13}
\]
which is the statement of the theorem.

In the field representation the Gauss law can be enforced by means of the projection formalism discussed in Section 1. The projection operator is, obviously, \( P = 1 - C^F \). Its action is computed in the grid representation by the fast Fourier method according to the rule (3.5). Without the use of the projection formalism, the accuracy of the Gauss law is stated in the following technical proposition.

**Proposition 8.3.** Let \( W = ||W_{\Delta t}^F|| \) and \( W_C = ||[C^F, W_{\Delta t}^F]|| C_m (1 + \delta(\Delta t, T)) \) where \( C_m \) and \( \delta(\Delta t, T) \) are defined in Theorem 7.4, then
\[
|C^F (G^I_{\Delta t})^n \Psi^F_0|/|\Psi^F_0| \leq TW_C \Delta t^2 + \Delta t^4 W_C e^{TW_{\Delta t}} (\Delta t^2 + T^2/2) = O(\Delta t^2) , \tag{8.14}
\]
for all \( 0 \leq n \leq N, T = N\Delta t \) and any positive \( \Delta t \).

**Proof.** Since \( C^F U^F_t = C^F \), assuming that the initial state \( \Psi^F_0 \) satisfies the Gauss law we get
\[
C^F (G^I_{\Delta t})^n \Psi^F_0 = -C^F \left\{ (U^F_{\Delta t})^n - (G^I_{\Delta t})^n \right\} \Psi^F_0 \\
= -C^F \sum_{k=1}^{n-1} (U^F_{\Delta t})^k (U^F_{\Delta t} - G^I_{\Delta t}) (G^I_{\Delta t})^{n-k} \Psi^F_0 \\
= -\Delta t^3 [C^F, W_{\Delta t}^F] \sum_{k=1}^{n-1} (G^I_{\Delta t})^{n-k} \Psi^F_0 + \Delta t^3 W_{\Delta t}^F \sum_{k=1}^{n-1} C^F (G^I_{\Delta t})^{n-k} \Psi^F_0 . \tag{8.15}
\]
Denoting the left hand side of (8.14) by \( \alpha_n \), we infer from (8.15), by taking the norm of both sides, that
\[
\alpha_n \leq \Delta t^3 \|[C^F, W_{\Delta t}^F]|| \sum_{k=1}^{n-1} ||(G^I_{\Delta t})^{n-k}|| + \Delta t^3 \|[W_{\Delta t}^F]|| \sum_{k=1}^{n-1} \alpha_{n-k} ,
\]
for \( n > 1 \) and \( \alpha_1 \leq W_C \Delta t^3 \). By Theorem 7.4, powers of the amplification matrix \( G^I_{\Delta t} \) are bounded. Hence the following recursion inequality holds
\[
\alpha_n \leq (n - 1)\Delta t^3 W_C + \Delta t^3 W (\alpha_{n-1} + \alpha_{n-2} + \cdots + \alpha_1) . \tag{8.16}
\]
Iterating (8.16) \( n - 1 \) times, we deduce that
\[
\alpha_n \leq (n - 1)\Delta t^3 W_C + \Delta t^3 W \left\{ (n - 2)\Delta t^3 W_C + (1 + \Delta t^3 W)(\alpha_{n-2} + \alpha_{n-3} + \cdots + \alpha_1) \right\} \\
\leq (n - 1)\Delta t^3 W_C + \Delta t^6 W W_C \left\{ \sum_{k=0}^{n-2} (n - 2 - k)(1 + \Delta t^3 W)^k + (1 + \Delta t^3 W)^{n-2} \right\} .
\]
One can find an explicit form for the sum in the latter equation. However, it is a cumbersome expression. For practical purposes, we give a simpler estimate which is stated in (8.14). First, factor out \((1 + \Delta t^3 W)^{n-2}\) in the brackets, and then use obvious inequalities \((1 + \Delta t^3 W)^{-k} \leq 1\) and \((1 + \Delta t^3 W)^{n-2} \leq \exp(TW \Delta t^2)\), which leads to (8.14).

In the case of the Lorentz model, \(W_C = \| [C^F, W_{\Delta t}] \|\) because all powers of the amplification matrix are uniformly bounded by 1. For small \(\Delta t\), a good estimate can be obtained by computing \(W_C\) for \(\Delta t = 0\) using (4.4).

The convergence rate as the number of grid points \(N\) increases is determined by the convergence rate of the fast Fourier transform which is exponential versus polynomial in finite difference schemes, provided parameters of the medium are smooth functions of position [1, 5]. As is well known from Fourier analysis, the convergence rate can be affected for functions which have discontinuities [5]. The latter is, unfortunately, the case in electromagnetic scattering problems. Suppose there is an interface between two media. It can be deduced from the Maxwell’s equations that the components of the electric and magnetic fields, \(E_t\) and \(H_t\), tangential to the interface must be continuous, provided there is no surface electric current on the interface. From the Gauss law it follows that the components of the inductions, \(D_t\) and \(B_t\), normal to the interface must be continuous, provided there is no surface charge on the interface. In contrast, the normal components of the fields and the tangential components of the inductions can be discontinuous. Their discontinuities are proportional to discontinuities of medium parameters (e.g., discontinuities in plasma frequencies in Lorentz models). Therefore, in either the induction or field representation, there are components which suffer discontinuities at the interface. Consequently, the convergence rate of the split algorithm for Maxwell’s theory might be slower than that in quantum mechanics with a discontinuous potential because in the latter case the wave function remains continuous.

Another source of errors that affects the convergence rate as \(N\) increases is the aliasing problem in the fast Fourier transform on the grid. Note that, even though the initial wave packet is band-width limited and the grid is chosen fine enough to eliminate errors in doing its fast Fourier transform back and forth, the wave packet loses this property after the operator \(\exp(\Delta t \mathcal{V}^Q)\) is applied to it. As a result, the aliasing problem arises in spatial domains where \(\mathcal{V}^Q\) varies (typically at interfaces between different types of media).

The above two problems that also reduce the accuracy of the algorithm are well known and studied in the theory of the fast Fourier transform [5]. The only way to cope with them is to make the grid finer in the areas where medium parameters have discontinuities. However, the fast Fourier algorithm requires a uniform equispaced lattice, which might lead to wasting computer resources if the increased resolution is necessary only in relatively small areas of the computational volume of the problem (e.g., only near an interface between two media). There are several ways to modify the algorithm when the above problems are too expensive to overcome by making a uniform grid finer.

First, the grid can be made fine enough so that the action of powers of the Hamiltonian
$H^Q$ on the state vector $\Psi^Q_0$ is sufficiently accurate in the Fourier basis as specified by the rules (3.4) and (3.5). The operator $H^Q$ is projected onto the Krylov space spanned by vectors $(H^Q)^k\Psi^Q_0, k = 0, 1, \ldots, n$. Its exponent (the evolution operator) is then computed by diagonalizing $H^Q$ instead of using the Lie-Trotter formula. Usually, it is sufficient to take a low dimensional Krylov space. This method is known as the Lanczos method [26]. A detailed study of the Krylov-Lanczos method as well as other similar pseudospectral methods in Maxwell theory will be given elsewhere.

Second, one can give up a uniform grid, while preserving basic advantages of pseudospectral methods such as, e.g., exponential convergence. A possible way to emulate a non-uniform grid in a multiscale problem is to use wavelet bases. The problem here is to compute the action of $\exp(\Delta t H^Q_0)$ in the split algorithm because the derivative operator $\nabla$ is not diagonal in this basis (in contrast to the Fourier basis). However, $H^Q_0$ is expected to be sparse in a wavelet basis so that its direct diagonalization might not be expensive, and a significant reduction of computational costs can be achieved in the split algorithm, by using the fast wavelet transform, as compared to that in the Fourier basis. Otherwise, the use of (4.10) might be helpful in place of the direct diagonalization method. This approach has proved to be successful in solving multiscale initial value problems for the Schrödinger equation [27].

In the framework of Maxwell’s theory for passive media, additional studies of several issues in time domain wavelet based algorithms, like, e.g., stability, would still be needed.

Third, the fast Fourier transform algorithm remains in place but is applied to an auxiliary uniform grid that is related to a non-uniform grid in physical coordinates by a change of variables. Consider a change of variables $y = y(x)$. A uniform grid in the new variables $y$ would generate a non-uniform grid in the original Euclidean (physical) coordinates $x$. A desired local density of grid points in the physical space, to enhance the sampling efficiency in designated regions, can be achieved by an appropriate choice of the functions $y(x)$ [28]. By necessity, the auxiliary grid spans a rectangular box (with periodic boundary conditions). Its pre-image in the physical space would not be a box in general, save for the case when the map $y(x)$ splits into three individual one-dimensional maps $y_j = y_j(x_j), j = 1, 2, 3$. Since, the derivatives are transformed as $\nabla_x = A(y) \nabla_y$, where the $3 \times 3$ matrix $A$ is position dependent, the operator $H^Q_0$ cannot be kept in the exponential. The action of its exponential on the state vector can be approximated by the leapfrog method in which only the action of $H^Q_0$ on $\Psi^Q$ is required. The latter can be done by the fast Fourier method according to the rules (3.5) and (3.4) applied to an operator being a product of position and derivative dependent operators. In contrast to the well studied quantum mechanical case, the algorithm appears to be unstable for media with absorption. In Section 9 a modification of the leapfrog scheme is proposed to achieve conditional stability.
9 The temporal leapfrog scheme

Here we discuss a temporal finite difference scheme applied to the Maxwell theory for passive media in the Hamiltonian formalism. As has been pointed out, such a scheme might be helpful for reducing computational costs by using non-uniform grids in combination with some pseudospectral methods (e.g., wavelet bases or the fast Fourier method with a change of variables). A temporal finite difference scheme can be obtained by the following procedure. Let us integrate (1.1) over the interval \((t, t + n\Delta t)\). We have

\[
\Psi_{t+n\Delta t} = \Psi_t + \mathcal{H} \int_t^{t+n\Delta t} d\tau \Psi_\tau = \Psi_t + \Delta t \mathcal{H} \left( \sum_{k=0}^{n-1} C_k^{(n)} \Psi_{t+k\Delta t} \right) + O(\Delta t^{n+1}) ,
\]

(9.1)

where the coefficients \(C_k^{(n)}\) used to approximate the integral are well known for any \(n\) as well as the accuracy of the approximation. For example, one can use the 3/8 Simpson rule for \(n = 3\) or Bode’s rule for \(n = 4\). The iterating scheme allows one to compute the wave function at the sequential moment of time if it is known for \(n\) preceding moments of time. Only the simplest case \(n = 2\), for which the mid-point approximation for the integral is taken, leading to \(C_0^{(2)} = 0\) and \(C_1^{(2)} = 2\), will be considered in detail. It is also known as the leapfrog scheme:

\[
\Psi_{t+\Delta t} = \Psi_{t-\Delta t} + 2\Delta t \mathcal{H} \Psi_t .
\]

(9.2)

The action of the Hamiltonian is computed in a suitable basis (as has been noted above). Apart from violation of the dispersion relation of electromagnetic waves, temporal finite difference schemes would generally be unstable in media with absorption, in contrast to the quantum mechanical case. The reason is that the Hamiltonian in (9.2) is not anti-Hermitian. Consequently, convergence to the continuum solution would also be violated.

A general solution to (9.2) can be written in the form

\[
\Psi_{n\Delta t} = \left( G_{\Delta t}^{(+)} \right)^n \Psi_+ + \left( G_{\Delta t}^{(-)} \right)^n \Psi_-, \quad G_{\Delta t}^{(\pm)} = \mathcal{H} \Delta t \pm \sqrt{1 + \mathcal{H}^2 \Delta t^2} ,
\]

(9.3)

(9.4)

for some initial state vectors \(\Psi_0\) and \(\Psi_{\Delta t}\) (the vectors \(\Psi_{\pm}\) are determined by them). Stability requires that there exists a positive constant \(C\) such that

\[
|\Psi_{n\Delta t}| \leq C (|\Psi_+| + |\Psi_-|) ,
\]

(9.5)

for all \(0 \leq n \leq N\), \(T = N\Delta t\) and \(0 < \Delta t < \tau\). Note that in general a solution of (1.1) may have a legitimate exponential growth if the hermitian part of the Hamiltonian, \(\mathcal{H} + \mathcal{H}^*\), is not negative semidefinite (see Lemma 7.2). For this reason, a typical stability criterion would be equivalent to the condition [16] that there exists some positive constant \(K_1\) such that \(\|G_{\Delta t}^{(\pm)}\| \leq 1 + K_1 \Delta t\) uniformly for all parameters of \(G_{\Delta t}^{(\pm)}\) and for \(0 < \Delta t < \tau\), which is clearly the case for (9.4) if \(\mathcal{H}\) is bounded. The latter leads to

\[
\left\| \left( G_{\Delta t}^{(\pm)} \right)^n \right\| \leq e^{K_1 T}
\]

(9.6)

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so that a legitimate exponential growth of the solution is allowed, i.e., $C \sim e^{K_1 t}$ in (9.5). For passive media, the Hamiltonian satisfies the conditions of Lemma 7.2 and, hence, no legitimate exponential growth should be present in a numerical solution in order to achieve convergence. However, as we shall see shortly, the scheme (9.2) always generates an exponentially growing solution for media with attenuation.

Let complex numbers $z = Re^{i\varphi}$ be eigenvalues of $H\Delta t$. Since the spectral radius of $G^{(\pm)}_{\Delta t}$ does not exceed its norm, the necessary (von Neumann) condition to suppress an exponential growth of the solution (9.3) reads

$$\rho(G^{(\pm)}_{\Delta t}) = \max_{z \in D} \left| z \pm \sqrt{1 + z^2} \right| \leq 1 .$$  \hspace{1cm} (9.7)

The aim is to analyze the domain $D$ of the complex plane for which (9.7) holds. Let $\eta = \sqrt{1 + z^2}$ and $|\eta| = r$. The two inequalities in (9.7) require that for $z \in D$, $R^2 + r^2 \pm \xi \leq 1$, where $\xi = \bar{z} \eta + z \bar{\eta}$. By combining the latter inequalities, one gets $R^2 + r^2 \leq 1$ or $r^4 \leq (1 - R^2)^2$. On the other hand, $r^4 = 1 + R^4 + 2R^2 \cos(2\varphi)$. Hence, $\cos(2\varphi) \leq -1$ which is only possible if $\varphi = \pm \pi/2$ or $z = \pm iR$. The necessary condition (9.7) is satisfied if

$$\varphi = \pm \pi/2 , \quad R^2 \leq 1 .$$  \hspace{1cm} (9.8)

This does not yet guarantee that there is no norm growth. A norm growth, which is polynomial in time, can still occur.

Let us investigate general properties of the solution of (1.1) when the Hamiltonian satisfies the von Neumann condition (9.8). For any matrix $H$ there exists a similarity transformation so that $S^{-1}HS$ has the Jordan normal form. Let $h_z$ be a block of the Jordan normal form corresponding to an eigenvalue $z$ of $H$. Any block $h_k$ is a $q_k \times q_k$ bi-diagonal matrix, $q_k \geq 1$, with all the elements of the diagonal being equal to $z$ and all the elements on the upper superdiagonal being equal to one. For $q_k = 1$, $h_z = z$ is just a complex number. The norm of any solution of (1.1) cannot grow faster than $\| \exp(tH) \|$. Let a $q_z$-dimensional vector $\phi_t$ satisfy the equation $\partial_t \phi_t = h_z \phi_t$. For a generic initial condition, the solution norm grows polynomially, $|\phi_t| = O(t^{q_z-1})$ as $t \rightarrow \infty$. Using the similarity transformation $S$, we define the corresponding $\mu$-norm of state vectors and the corresponding matrix norm (cf. (6.5)) by setting $\mu = S^{-1} S^{-1}$. From the equivalence of the norms $\| \cdot \|$ and $\| \cdot \|_\mu$ (see the proof of Theorem 7.3), the norm growth cannot be faster than

$$\| e^{tH} \| = \| e^{tS^{-1}HS} \| = \max_z \| e^{th_z} \| = O(t^{q_z-1}) , \quad q = \max_z q_z , \quad t \rightarrow \infty ,$$  \hspace{1cm} (9.9)

provided $z = \pm iR$. However, a state vector norm growing polynomially with time is unacceptable from the physical point of view because in any passive medium there is no physical mechanism for such amplification of the field amplitudes in the large time limit. Consequently, we demand that any model Hamiltonian for a passive medium should be similar to a diagonal matrix (i.e., $H$ is diagonalizable). In this latter case, the blocks $h_z$ of the Jordan normal form of $H$ are just complex numbers $z$. Hence $\| \exp(th_z) \| = | \exp(\pm itR) | = 1$ so that the $\mu$-norm of any solution of (1.1) is conserved according to (9.9).
Two important conclusions about the leapfrog scheme (9.2) follow from our analysis. First, the von Neumann condition (9.8) is also sufficient for stability. Indeed, if (9.8) holds then \[ \|G_{\Delta t}^{(\pm)}\|_\mu = \|S G_{\Delta t}^{(\pm)} S^{-1}\| = \rho(G_{\Delta t}^{(\pm)}) = 1 \] and, hence, \[ \|G_{\Delta t}^{(\pm)}\|^n \|_\mu \leq 1 \text{ uniformly in } n \geq 0. \] By the norm equivalence, \[ \|G_{\Delta t}^{(\pm)}\|^n \] is also bounded uniformly in \( n \geq 0 \). Second, reversing the argument, we conclude from the norm conservation of the stable leapfrog solution that no attenuation can be added to the Hamiltonian without destroying the stability and, consequently, the convergence to the continuum solution. Whenever the attenuation is added, the leapfrog solution would always contain an exponentially growing component, while this would not be so for a continuum solution (see Lemma 7.2).

Since \( G_{\Delta t}^{(\pm)} G_{\Delta t}^{(-)} = 1 \), only one of the two independent solutions in (9.3) would grow exponentially whenever the attenuation is added. Theoretically, for \( \mathcal{H} + \mathcal{H}^* \leq 0 \) the exponentially growing solution can be eliminated by choosing the initial condition so that \( \Psi_- = 0 \) which is equivalent to the initial condition \( \Psi_{\Delta t} = G_{\Delta t}^{(+)\Psi_0}. \) Practically, this is never possible due to rounding errors and/or numerical errors in computing \( G_{\Delta t}^{(+)\Psi_0}. \) Even for a small \(|\Psi_-|\) in (9.3) the growing part would eventually become comparable with the exponentially attenuating solution generated by \( \Psi_+\). A reduction of the time step would not be helpful since the constant \( K_1 \) in (9.6) is independent of \( \Delta t \) while the simulation time \( T \) is fixed by the dimension of the simulation volume and the speed of light. One needs at least to modify the scheme so that there exists a constant \( K_p \) such that

\[ \|G_{\Delta t}^{(\pm)}\| \leq 1 + K_p \Delta t^p, \quad p > 1, \quad (9.10) \]

for \( 0 < \Delta t < \tau \). Indeed, it follows from (9.10) that \[ \|(G_{\Delta t}^{(\pm)})^n\| \leq \exp(K_p T \Delta t^{p-1}) = 1 + O(\Delta t^{p-1}) \] for all \( 0 \leq n \leq N \) where \( N \Delta t = T \). The norm growth could be reduced as much as desired by making the time step smaller. Next we show how to modify the leapfrog scheme to make (9.10) valid for at least \( p = 3 \) and, if the Hamiltonian is normal, an even stronger result holds, namely, \( K_p = 0 \).

Let \( \mathcal{H} = \mathcal{H}_0 + \mathcal{V} \) where \( \mathcal{V}^* + \mathcal{V} \leq 0 \) (negative semidefinite) and \( \mathcal{H}_0^* = -\mathcal{H}_0 \). In (1.1) we make a substitution \( \Psi_t = \exp(t \mathcal{V}) \Phi_t \). The new state vector \( \Phi_t \) satisfies an equation with a time dependent Hamiltonian,

\[ \partial_t \Phi_t = e^{-t \mathcal{V}} \mathcal{H}_0 e^{t \mathcal{V}} \Phi_t \equiv \mathcal{H}_t \Phi_t, \quad (9.11) \]

and with the same initial condition \( \Phi_0 = \Psi_0 \). Applying the leapfrog method to (9.11) we get \( \Phi_{t+\Delta t} = \Phi_{t-\Delta t} + 2\Delta t \mathcal{H}_t \Phi_t \) valid up to \( O(\Delta t^3) \). Returning to the initial variables, we arrive at the following recurrence relation

\[ \Psi_{t+\Delta t} = \mathcal{L}_{\Delta t} \Psi_{t-\Delta t} + 2\Delta t \mathcal{L}_{\Delta t} \mathcal{H}_0 \Psi_t, \quad (9.12) \]

where \( \mathcal{L}_{\Delta t} = \exp(\Delta t \mathcal{V}) \). All the derivative operators are included into the anti-Hermitian part \( \mathcal{H}_0 \) of the Hamiltonian \( \mathcal{H} \), while the attenuation operator \( \mathcal{V} \) might even be independent of position and, hence, \( \mathcal{L}_{\Delta t} \) has to be computed only once for given medium parameters and
time step. It can often be done analytically as, for example, in multiresonant Lorentz models (see Section 10). On the other hand, by Lemma 7.2, \( \|L_\Delta t\| \leq 1 \) for any \( \Delta t > 0 \), and one might hope to stabilize the leapfrog scheme by satisfying the stability condition (9.8) for \( \mathcal{H}_0 \) only, that is, \( 1 + \mathcal{H}_0^2 \Delta t^2 \) is positive semidefinite. This is indeed the case. The amplification matrix, \( \Psi_{t+\Delta t} = \mathcal{G}_{\Delta t} \Psi_t \), for the recurrence (9.12), satisfies the equation

\[
\mathcal{G}_{\Delta t} = L_{2\Delta t} \mathcal{G}_{\Delta t}^{-1} + 2\Delta t L_{\Delta t} \mathcal{H}_0 .
\]

(9.13)

According to our analysis of the von Neumann stability condition (9.8), the anti-Hermiticity condition of \( \mathcal{H}_0 \) in (9.12) and (9.13) can be weakened by demanding that \( \mathcal{H}_0 \) is related to an anti-Hermitian matrix by a similarity transformation. Some important properties of the amplification matrix obtained from (9.13) are stated in the following theorem.

**Theorem 9.1.** Suppose there exists a similarity transformation such that \( \mathcal{S}^{-1} \mathcal{H} \mathcal{S} = \mathcal{H}_S + \mathcal{V}_S \) where \( \mathcal{H}_S^* = -\mathcal{H}_S \), the Hermitian part of \( \mathcal{V}_S \) is negative semidefinite, \( \mathcal{V}_S^* + \mathcal{V}_S \leq 0 \), and \( \mathcal{H}_S \) also satisfies the von Neumann stability condition for the leapfrog scheme, \( 1 + \mathcal{H}_S^2 \Delta t^2 \geq 0 \) (positive semidefinite). Consider the amplification matrix \( \mathcal{G}_{\Delta t} \) of the modified leapfrog scheme (9.13) with \( \mathcal{H}_0 = \mathcal{S} \mathcal{H}_S \mathcal{S}^{-1} \) and \( \mathcal{V} = \mathcal{S} \mathcal{V}_S \mathcal{S}^{-1} \). Then there exists a norm \( \| \cdot \|_\mu \) equivalent to \( \| \cdot \| \) such that \( \mathcal{G}_{\Delta t} \) has the following properties:

(A) if \( [\mathcal{H}_0, \mathcal{V}] = 0 \),

\[
\| \mathcal{G}_{\Delta t}\|_\mu \leq 1
\]

uniformly in \( n \geq 0 \);

(B) if \( [\mathcal{H}_0, \mathcal{V}] \neq 0 \), there exists a non-negative constant \( K_3 \) such that

\[
\| \mathcal{G}_{\Delta t}\|_\mu \leq 1 + K_3 \Delta t^3 ,
\]

for \( 0 < \Delta t < \tau \) and some positive \( \tau \).

**Proof.** Part (A). If \( \mathcal{H}_0 \) and \( \mathcal{V} \) commute, the amplification matrix \( \mathcal{G}_{\Delta t} = L_{\Delta t} \mathcal{G}_0_{\Delta t} \) satisfies (9.13), provided \( \mathcal{G}_0_{\Delta t} \) satisfies the same equation for \( \mathcal{V} = 0 \) (or \( L_{\Delta t} = 1 \)), which one can easily check by substituting the solution into (9.13). Consider the norm associated with the similarity transformation \( \mathcal{S} \) of the Hamiltonian, \( \| \mathcal{A} \|_\mu = \| \mathcal{S}^{-1} \mathcal{A} \mathcal{S} \| \). The norms \( \| \cdot \|_\mu \) and \( \| \cdot \| \) are equivalent (see the proof of Theorem 7.3). Since \( \mathcal{H}_0 \) satisfies the von Neumann stability condition and is anti-Hermitian relative to the \( \mu \) scalar product, \( \| \mathcal{G}_0_{\Delta t}\|_\mu = \rho(\mathcal{G}_0_{\Delta t}) = 1 \) (according to the analysis after (9.7)). By Lemma 7.2, \( \| L_{\Delta t}\|_\mu \leq 1 \), and we infer that \( \| \mathcal{G}_{\Delta t}\|_\mu = \| (L_{\Delta t} \mathcal{G}_0_{\Delta t})^n \|_\mu \leq \| L_{\Delta t}\|_\mu^n \leq 1 \) uniformly for \( n \geq 0 \).

Part (B). Solving (9.13) by the perturbation theory in \( \Delta t \), it is not hard to find that

\[
\mathcal{G}_{\Delta t} - \mathcal{G}_{\Delta t}^V = \Delta t^3 \mathcal{K}_{\Delta t} , \quad \mathcal{G}_{\Delta t}^V = L_{\Delta t/2} \mathcal{G}_0_{\Delta t} L_{\Delta t/2} ,
\]

(9.16)

where \( \mathcal{K}_{\Delta t} \) is regular in the vicinity of \( \Delta t = 0 \) and vanishes whenever \( \mathcal{H}_0 \) and \( \mathcal{V} \) commute. On the grid, \( \mathcal{H}_0 \) and \( \mathcal{V} \) are bounded operators. Hence we can find a constant \( K_3 = \sup_{\Delta t} \| \mathcal{K}_{\Delta t}\|_\mu \)
for some open interval $0 < \Delta t < \tau$. Making use of the inequality $\|G_{\Delta t}^V\|_\mu \leq \|L_{\Delta t/2}\|_\mu^2 \leq 1$, we find

$$\|G_{\Delta t}\|_\mu = \|G_{\Delta t}^V + \Delta t^3 K_{\Delta t}\|_\mu \leq 1 + \Delta t^3 K_3,$$

which completes the proof.

The norm deviation of the solution generated by the modified leapfrog scheme (9.12) from the stable solution generated by $G_{\Delta t}^V$ is of order $O(\Delta t^2)$ for the entire simulation time $T$ and, hence, by reducing $\Delta t$ a possible norm growth can be suppressed as much as desired. Indeed,

$$\|G_{\Delta t}^V - (G_{\Delta t}^V)^n\|_\mu \leq \Delta t^3 K \sum_{k=1}^{n-1} \|G_{\Delta t}^{n-k}\|_\mu \leq K_3 \Delta t^3 e^{K_3 T \Delta t^2} = O(\Delta t^2).$$

Since in the continuum limit $\Delta t \to 0$, both the amplification matrices $G_{\Delta t}^V$ and $G_{\Delta t}$ generate the same solution and all the powers of the former are uniformly bounded by construction, a natural question to ask is whether one can find a recurrence relation for the function $\Psi_{n\Delta t} = (G_{\Delta t}^V)^n \Psi_0$ which could be used in place of (9.12). It is not difficult to derive an equation for $G_{\Delta t}^V$ similar to (9.13), but, unfortunately, this equation cannot be converted into a simple recurrence relation for the wave function itself, like (9.12), suitable for numerical applications.

It should be noted that if the operator $L_{\Delta t}$ in the modified leapfrog scheme (9.12) is replaced by another $L_{\Delta t}^s$ such that $L_{\Delta t} - L_{\Delta t}^s = O(\Delta t^3)$ and $\|L_{\Delta t}^s\|_\mu \leq 1$, then the convergence is not violated because Part B of Theorem 9.1 still holds. This observation is useful for analytic computation of $L_{\Delta t}$. For example, in the conditions of Theorem 9.1, put $S = 1$. Let $V = V_1 + V_2$ so that both $V_{1,2}$ have their hermitian parts negative semidefinite. By using the split (4.2) we get

$$L_{\Delta t} = e^{\Delta t V} = e^{\Delta t V_{1,2}} e^{\Delta t V_{1,2}} + O(\Delta t^3) = L_{\Delta t}^s + O(\Delta t^3).$$

By Lemma 7.2, $\|L_{\Delta t}^s\|_\mu \leq 1$ for $\Delta t \geq 0$. The operators $V_{1,2}$ can be chosen so that their exponentials can be computed analytically.

### 10 Examples of the temporal leapfrog algorithm

There are many possibilities to split the original Hamiltonian $H$ into two parts that satisfy the conditions of Theorem 9.1 and thereby to make the leapfrog scheme stable and convergent. Basic guidelines for doing that are as follows. The Hamiltonian $H_0$ should contain all the derivative operators in $H$ and, yet, the von Neumann condition is easy to establish for
\( \mathcal{H}_0 \). It would also be helpful to have an analytic expression for \( \mathcal{L}_{\Delta t} \) at least up to order \( O(\Delta t^3) \). As an illustration, we discuss multiresonant Lorentz models and geometric optics. To distinguish between the splits of the Hamiltonian in the split and leapfrog algorithms, we shall use an index \( l \) ("leapfrog") in the latter.

## I Lorentz models

In the field representation of the Hamiltonian for multiresonant Lorentz models, we make the following decomposition

\[
\mathcal{H}^F = \begin{pmatrix} \mathcal{H}_0 & \mathcal{V}_{FM} \\ \mathcal{V}_{MF} & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & \mathcal{H}_M^F \end{pmatrix} \equiv \mathcal{H}_0^F + \mathcal{V}_l^F
\]  

(10.1)

Thanks to (2.28) and \( \mathcal{H}_0^F = -\mathcal{H}_0 \), the operator \( \mathcal{H}_0^F \) is anti-Hermitian. From (2.29) it follows that the Hermitian part of \( \mathcal{V}_l^F \) is negative semidefinite (\( \gamma_a \geq 0 \)). The exponential of \( \mathcal{V}_l^F \) is easily computed according to (5.14) and (5.15). Let \( \xi_t^a \) denote a six-component column whose three upper components coincide with \( \xi_{t-1}^a \) and three lower components equal \( \xi_{t+1}^a \) (see (2.9)–(2.11)). As a result we arrive at the following scheme

\[
\psi_{t+\Delta t}^F = \psi_{t-\Delta t}^F + 2\Delta t \mathcal{H}_0^F \psi_{t-\Delta t}^F + 2\Delta t \sum_a \mathcal{V}_{FMa} \xi_t^a,
\]  

(10.2)

\[
\xi_{t+\Delta t}^a = e^{2\Delta t \mathcal{H}_M^F} \xi_{t-\Delta t}^a + 2\Delta t e^{\Delta t \mathcal{H}_M^F} \mathcal{V}_{MFa} \psi_{t-\Delta t}^F.
\]  

(10.3)

Stability is ensured if \( \mathcal{H}_0^F \) satisfies the von Neumann condition (9.8). Eigenvalues of \( \mathcal{H}_0^F \) satisfy the equation

\[
\det(z - \mathcal{H}_0^F) = z^q \det(z^2 - z\mathcal{H}_0 - \mathcal{V}_{FM} \mathcal{V}_{MF}) = 0
\]  

(10.4)

where the non-negative integer \( q \) depends on the number of resonances in the Lorentz model. Non-zero eigenvalues satisfy the so-called pencil equation whose theory is well developed and might be useful for more general models [29]. Here we shall find a simpler (practical) criterion sufficient for (9.8) to hold. Since the plasma frequencies may depend on position, we apply the following general idea [30]. Suppose we have a finite difference scheme with variable coefficients in space. Consider a corresponding finite difference scheme with frozen coefficients. It is obtained from the original scheme by fixing the coefficients to particular values everywhere in space. A finite difference scheme with variable coefficients is stable if all the corresponding finite difference schemes with frozen coefficients are stable [30, 16]. So let us fix the plasma frequencies to particular values. The spatial dependence of the eigenfunctions for the pencil problem in (10.4) is given by a harmonic factor \( \exp(ik \cdot x) \) and the corresponding eigenvalues are \( z = \pm i \sqrt{c^2k^2 + \omega^2_p} \), where \( \omega^2_p \) is defined in (5.16). Let \( k_{max} \) be the maximal norm of all wave vectors of the initial wave packet and \( \omega^p_{max} \) be the maximal value of \( \omega_p \) as a function of position, then a sufficient criterion for stability reads

\[
\Delta t \sqrt{c^2k_{max}^2 + (\omega^p_{max})^2} \leq 1.
\]  

(10.5)
The scheme (9.12) becomes especially simple in the case of small attenuation, $\gamma_a < \omega_a$. In the complex representation of the auxiliary fields (2.31) (cf. (2.12)) the matter Hamiltonians $H_{Ma}$ are diagonal and the action of its exponential is reduced to multiplication by a complex number $e^{i\nu_0 \Delta t}$ (see Section 5).

The stability condition (10.5) can be improved if one uses the induction representation arranging the split according to (4.11), that is, $H_{01}^I = H_0^I$ and $V_{1}^I = V^I$. In this case the conditions of Theorem 9.1 are met if instead of (10.5) we demand a weaker condition

$$\Delta t c k_{\text{max}} \leq 1. \quad (10.6)$$

To prove this, we note first that by the similarity transformation defined in (2.23) we get

$$S^{-1} H^I S = \begin{pmatrix} H_0 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & V_{FM} \\ V_{MF} & H_M^F \end{pmatrix} = H_S^I + V_S^I. \quad (10.7)$$

Then (10.6) is obviously the von Neumann stability condition for $H_S^I$, while the Hermitian part of $V_S^I$ is negative semidefinite if $\gamma_a \geq 0$. The scheme is obtained from (9.12) by replacing $\Psi_t \rightarrow \Psi_t^I$, $H \rightarrow H_0^I$ and $V \rightarrow V^I$ as defined in (4.11). Since the left hand side of (10.7) coincides with $H_F^I$, it can also be viewed as the leapfrog scheme in the field representation but with the split different from (10.1). This illustrates the point that the stability condition of the scheme (9.12) depends strongly on the choice of $H_{01}$. The price for a simpler stability condition in the induction representation is the lack of an explicit form of $L_{\Delta t}$. However, this problem can be circumvented by making use of (9.18). Indeed, $V_S^I = V_F^I + V_{I1}^F$ where $V_F^I$ is defined in (4.7). The exponentials of these operators are computed in Section 5. We also have $\| \exp(\Delta t V_F^I) \| = 1$ because $V_F^* = -V_F^I$ and $\| \exp(\Delta t V_{I1}^F) \| \leq 1$ by Lemma 7.2 for a non-negative $\Delta t$. We set

$$L_{\Delta t}^I = S e^{\Delta t V_I^F / 2} e^{\Delta t V_{I}\gamma^F / 2} S^{-1} \quad (10.8)$$

so that $\| L_{\Delta t}^I \|_{\mu} = \| S^{-1} L_{\Delta t}^I S \| \leq 1$. The operator (10.8) differs from $L_{\Delta t} = \exp(\Delta t V_I)$ by terms of order $O(\Delta t^3)$ and, hence, according to (9.18), can be used in place of $L_{\Delta t}$ in the leapfrog scheme without destroying its convergence and stability.

II Geometric optics

Another simple example is the case of geometric optics. For sake of simplicity we assume the medium to have no magnetic properties. A generalization is straightforward. Let $\varepsilon = \varepsilon(x)$ be the dielectric constant of the medium. If the medium is not isotropic, then $\varepsilon$ is symmetric positive definite $3 \times 3$ matrix everywhere in space. We rewrite Maxwell’s equations in the form

$$\partial_t \psi_t^I = H_G \psi_t^I, \quad H_G = \begin{pmatrix} 0 & c \nabla \times (\varepsilon^{-1}) \\ -c \nabla \times (\varepsilon^{-1}) & 0 \end{pmatrix}, \quad (10.9)$$
where the parentheses in \((\varepsilon^{-1})\) mean that the induction is first multiplied by \(\varepsilon^{-1}\) and then the curl of the resulting vector field is computed. Consider the scalar product

\[
\langle \psi_1^I, \psi_2^I \rangle = \int d \mathbf{r} \, \psi_1^{I*} \mu \psi_2^I, \quad \mu = \begin{pmatrix} \varepsilon^{-1} & 0 \\ 0 & 1 \end{pmatrix}.
\]  

(10.10)

In the grid representation of Section 3, the integral is replaced by the sum over grid points and \(\mathcal{H}_G\) becomes a finite matrix. The Hamiltonian is anti-Hermitian with respect to this scalar product, \(\mathcal{H}_G^* \mu = -\mu \mathcal{H}_G\). Therefore the corresponding \(\mu\) norm is preserved in the time evolution generated by \(\exp(t\mathcal{H}_G)\), that is, \(\langle \psi_t^I, \psi_t^I \rangle = \langle \psi_0^I, \psi_0^I \rangle\). The electromagnetic energy of the wave packet is conserved because it is proportional to the \(\mu\) norm of the initial state vector. Consequently, we expect that for a sufficiently small \(\Delta t\) the original leapfrog scheme (9.2),

\[
\psi_{t+\Delta t}^I = \psi_{t-\Delta t}^I + 2\Delta t \mathcal{H}_G \psi_t^I,
\]  

(10.11)

becomes stable. To find a sufficient condition for stability, the same idea of finite difference schemes with frozen coefficients can be used. It obviously leads to a condition similar to (10.6),

\[
\Delta t \epsilon k_{\text{max}}^e \leq 1,
\]

where \(k_{\text{max}}^e\) is the maximal norm of all wave vectors in the medium which can be estimated by \(\sqrt{\rho(\varepsilon)k_{\text{max}}}\) with \(k_{\text{max}}\) being the maximal wave vector of the initial pulse in vacuum. The spectral radius \(\rho(\varepsilon)\) is understood as the maximal spectral radius of \(\varepsilon(\mathbf{x})\) over \(\mathbf{x}\). If the Fourier basis is used to compute the derivatives, the algorithm does not violate the Gauss law. However, the algorithm would not conserve the \(\mu\) norm (or energy), rather a quantity which, in many cases, approximates the energy. Multiplying (10.11) by \(\psi_t^I\) using the scalar product (10.10), we infer that

\[
\langle \psi_{t+\Delta t}^I, \psi_t^I \rangle = \langle \psi_t^I, \psi_{t-\Delta t}^I \rangle = \cdots = \langle \psi_{\Delta t}^I, \psi_0^I \rangle.
\]  

(10.12)

By expanding the exponential in \(\psi_{t+\Delta t}^I = \exp(\Delta t \mathcal{H}_G) \psi_t^I\) into a Taylor series in both sides of (10.12) and making use of the anti-Hermiticity of \(\mathcal{H}_G\), we find that the energy conservation violation is of order \(O(\Delta t^2)\). Thus, it can be made as small as desired by reducing the time step.

**11 Conclusions**

The initial value problem in Maxwell theory for passive media has been reformulated in the Hamiltonian formalism. The path integral representation of the fundamental solution of the Hamiltonian evolution equation has been used to develop a time domain numerical algorithm for solving the initial value problem. The algorithm exhibits the main advantages of pseudospectral methods for solving differential equations such as an exponential convergence (and, hence, a greater accuracy), the absence of dispersive errors and numerical efficiency.
addition, the algorithm is unitary, meaning that the energy of the initial pulse is conserved whenever the medium attenuation vanishes (Theorem 6.1). For widely used multiresonant Lorentz models, the algorithm is unconditionally stable (Theorems 7.1 and 7.3), and, for a generic passive medium, conditional stability can always be achieved (Theorem 7.4). As the time step $\Delta t$ goes to zero, the algorithm accuracy is of order $O(\Delta t^2)$ (Theorem 8.1). It is possible to increase the convergence rate (accuracy) up to any desired order $O(\Delta t^n)$, $n \geq 2$. However, computational costs for increasing the accuracy in such a way are not necessarily lower than those for decreasing the time step in the original algorithm. An important advantage of the algorithm is that the Gauss law holds exactly in the process of numerical simulations with no extra computational cost (Theorem 8.2).

A drawback of the algorithm is related to well known problems of the fast Fourier method. Namely, a slower rate of convergence for non-smooth functions and aliasing. This might, perhaps, limit the advantages of the algorithm in some type of scattering problems with complex target geometries. Numerical tests are needed for a quantitative conclusion. There are several pseudospectral methods for approximating the fundamental solution of the Hamiltonian evolution equation that can help to circumvent this problem. We have analyzed one of them and formulated its stability criteria in the case of general passive media (Theorem 9.1). Numerical tests of the modified leapfrog scheme are presented in [4]. The results are compared with known theoretical and experimental studies of the system investigated (extraordinary transmission gratings [31]). Other methods will be discussed elsewhere as well as the case when radiation sources (antennas) are included.

It is believed that the proposed algorithm would be useful in numerical studies of electromagnetic pulse propagation in passive media (e.g., foliage, soil, etc), photonic crystals and devices, nonostructured materials, and also in applications to scattering problems with targets made of dispersive materials.

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I Initial pulse configurations

In principle, any field configuration can serve as the initial configuration. However it is often desired to have an initial pulse with some specific properties (bandwidth, polarization, direction of propagation, etc). Yet, the initial wave packet should be built of radiation (propagating) electromagnetic fields. A simple method based on the fast Fourier transform algorithm is given below to obtain initial configurations made of radiation fields with designated properties.

A general solution of the Maxwell equations in vacuum can be written in the form

\[ E_t(r) = \int dk \left( C_0^{(+)}(k) e^{i k \cdot r - i \omega t} + C_0^{(-)}(k) e^{i k \cdot r + i \omega t} \right) \equiv C_t^{(+)}(r) + C_t^{(-)}(r) \]  

(12.1)

\[ B_t(r) = i \frac{\sqrt{-\Delta}}{\nabla} \times \left( C_t^{(+)}(r) - C_t^{(-)}(r) \right) . \]  

(12.2)

The representation (12.2) for the magnetic induction follows from the Maxwell equations and that the complex amplitudes \( C_0^{(\pm)}(k) \) satisfy the transversality and reality conditions which are, respectively,

\[ k \cdot C_0^{(\pm)}(k) = 0 , \quad \overline{C_0^{(\pm)}(k)} = C_0^{(\mp)}(-k) . \]

The representation (12.1) and (12.2) holds for any moment of time. Hence, we can set \( t = 0 \) to generate suitable initial conditions for an electromagnetic pulse propagating in empty space by choosing specific functions \( C_0^{(\pm)}(r) \).

Consider a few examples. Let there be translational invariance along the \( y \) axis. In this case the fields depend only on \( x \) and \( z \), i.e., \( r = (x, 0, z) \). Accordingly, the wave vector has the form \( k = (k_x, 0, k_z) \) and \( dk = dk_x dk_z \). Let \( \hat{e}_2 = (0, 1, 0) \) be the unit vector along the \( y \) axis. Introduce

\[ C_0^{(\pm)}(r) = \frac{1}{2} \hat{e}_2 A_0 e^{-\kappa^2 r^2/2} e^{i k_0 \cdot r} \equiv \hat{e}_2 C_0^{(\pm)}(r) , \]  

(12.3)

where \( A_0 \) and \( \kappa \) are real constants, and \( k_0 \) is a fixed wave vector. Note that the field \( C_0^{(\pm)}(r) \) is automatically transversal. The corresponding fields determine suitable initial conditions to generate a pulse propagating in the direction of \( k_0 \) whose frequency band is centered at \( \omega_0 = c k_0 \) and its width is proportional to \( c \kappa \). The pulse is linearly polarized along the \( y \) axis:

\[ E_0 = \hat{e}_2 E_0 , \quad E_0 = C_0^{(+)} + C_0^{(-)} , \]  

(12.4)

\[ B_0 = \frac{i}{\sqrt{-\Delta}} \nabla \times \hat{e}_2 \left( C_0^{(+)} - C_0^{(-)} \right) . \]  

(12.5)

The action of the differential operator is defined via the fast Fourier transform (see Section 3) on the grid fine enough to support the bandwidth limited function (12.3). In the Fourier basis, \( i \nabla / \sqrt{-\Delta} \rightarrow -k/k \).
To obtain suitable initial conditions for a pulse propagating in the direction $\mathbf{k}_0$ and whose polarization lies in the $xz$-plane, we make use of the electromagnetic duality of Maxwell theory which states that the dynamics remains unchanged when electric and magnetic charges switch places and simultaneously $\mathbf{E}_t \rightarrow -\mathbf{B}_t$ and $\mathbf{B}_t \rightarrow \mathbf{E}_t$. According to the duality theorem, we can take

$$
\mathbf{E}_0 = \frac{i}{\sqrt{-\Delta}} \nabla \times \hat{\mathbf{e}}_2 \left( C_0^{(+)} - C_0^{(-)} \right) \quad (12.6)
$$

$$
\mathbf{B}_0 = -\hat{\mathbf{e}}_2 \left( C_0^{(+)} + C_0^{(-)} \right) . \quad (12.7)
$$

Finally, suitable initial conditions for a pulse propagating in the direction $\mathbf{k}_0$ with a generic elliptic polarization are obtained by taking a linear combination of the above two initial conditions for two independent linear polarizations of the pulse. The amplitudes $C_0^{(\pm)}(r)$ can also be set numerically from actual measurements of a particular pulse of interest.

II Conductivity and absorbing boundary conditions

In numerical simulations, the grid in coordinate space is of necessity finite. In scattering problems we are interested in the pulse shape and polarization which we wish to compute in the asymptotically large coordinate region. This requires that not only the leading edge of the reflected pulse should have reached the asymptotic region, but also the trailing edge should have done so as well. This is essential if the reflected pulse propagates in a highly dispersive medium, or the target has a complex shape, or both. A complication arises from the very nature of the fast Fourier transform method. The method is designed to describe periodic functions and, consequently, if the pulse has a finite amplitude at the edge of the grid, this finite value would appear back at the other edge, with totally disastrous results for the computation. In quantum computational physics this problem is often solved by using an optical potential that absorbs the signal as it reaches the grid boundary. A similar method can be developed for our treatment of Maxwell’s theory. Before we do so let us point out that an absorbing boundary condition is not the only way to solve the problem. For instance, in the case of a complex target, an ancillary grid may be defined in one of the coordinates which extends to large distances. The pulse may be transferred in a gradual manner from the small grid (near the target) to this larger grid to prevent the pulse from ever reaching the edge of the small grid. This technique can also be applied to generate a pulse by an antenna of a complex construction. The dynamics of the portion of the pulse on the larger grid may be treated analytically (if dispersion properties of the medium are not too complex).

In quantum mechanics absorbing boundary conditions are made by adding an imaginary potential to the Hamiltonian with support near the grid edges. In the Maxwell theory, the same can be achieved by adding conductivity which gradually increases as the grid edges are
approached. An interaction of conducting media with electromagnetic radiation is described by Ohm’s law,

\[ J_t = \sigma E_t , \]  

combined with Maxwell’s equation (2.1), where the displacement current is amended as \( \partial_t D_t \rightarrow \partial_t D_t + (4\pi \sigma/c) E_t \) with \( \sigma = \sigma(r) \) being the conductivity of the medium. Consider a linearly polarized plane wave moving along the \( z \) axis. Let \( \tilde{E}_\omega \) be the Fourier transform of the only component of the electric field \( E_t \). Disregarding for a moment any possible anomalous dispersion of the medium, we find that \( \tilde{E}_\omega \) satisfies the equation

\[ \partial_z^2 \tilde{E}_\omega(z) + \left[ \frac{\omega^2}{c^2} - \frac{4\pi i \omega}{c} \sigma(z) \right] \tilde{E}_\omega(z) = 0 . \]  

Equation (12.9) is identical to the stationary Schroedinger equation with an optical (absorbing) potential being proportional to \( \sigma(z) \). In simulations of quantum wave packets it has been found that one of the optimal potentials has the form \[17\]

\[ \sigma(z) = (n + 1)^{-1} \sigma_n (z/L)^n , \quad n \geq 2 , \]  

in the interval \( z \in [0, L] \) and \( \sigma(z) = 0 \) otherwise. So, our next task is to find an optimal constant \( \sigma_n \) such that the conducting layer would not reflect or transmit electromagnetic energy in some designated frequency band. Maxwell’s equations in a conducting medium are form-invariant under the scaling transformations

\[ \omega \rightarrow \beta \omega , \quad \sigma(r) \rightarrow \beta \sigma(\beta r) , \quad \tilde{\psi}^F(\omega) \rightarrow \alpha \tilde{\psi}^F(\beta \omega) , \]  

where \( \alpha \) and \( \beta \) are positive constants. If the conductivity \( \sigma(r) \) was found optimal for a frequency \( \omega \) and over a length \( L \), then the optimal conductivity for a frequency \( \beta \omega \) would be \( \beta \sigma(\beta r) \) and the new length over which it is taken to act would be \( L/\beta \).

Let us first study the reflectivity of the absorbing layer. Suppose, \( \sigma(z) = \sigma_0 \theta(z) \) where \( \theta(z) \) is the Heaviside function. If a monochromatic linearly polarized wave coming from the negative \( z \) region has an amplitude one, then the reflected wave has the amplitude \[19\]

\[ \eta_\omega = \frac{1 - \nu_\omega}{1 + \nu_\omega} , \quad \nu_\omega = 1 + \frac{4\pi i \sigma_0}{\omega} \equiv 1 + iq_\omega \]  

The energy of the reflected wave is

\[ R_\omega = |\eta_\omega|^2 = q_\omega^2/4 + O(q_\omega^4) . \]  

\( R_\omega \) increases as the ratio \( q_\omega \) gets higher and is small if \( q_\omega^2/4 \ll 1 \). Consider now \( \sigma(z) \) which monotonically increases from \( z = 0 \) in the positive \( z \) direction. Let \( k_\omega = k_\omega(z) \) be a local wave vector of the wave in the conducting medium,

\[ k_\omega(z) = c^{-1} \omega \sqrt{1 + iq_\omega(z)} . \]  

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We shall argue that the reflection is negligibly small if the local wave vector does not significantly change over a distance of order $k^{-1}$, that is,

$$\left| \frac{k_\omega(z + \delta z) - k_\omega(z)}{k_\omega(z)} \right| \ll 1, \quad \delta z \sim k^{-1}. \quad (12.15)$$

Making a linear approximation in (12.15), we infer that

$$|\partial_z q_\omega(z)| \ll (2c)^{-1} \omega \left(1 + q_\omega^2(z)\right)^{3/4}, \quad (12.16)$$

which must be valid for all values of $q_\omega(z)$ including small ones when the reflection is small. Inequality (12.16) allows us to reverse the argument, that is, the reflection is small if $|\partial_z q_\omega(z)| \ll (2c)^{-1} \omega$. Let $\sigma_L$ be an average conductivity over a layer of width $L$, $\sigma_L = \frac{1}{L} \int_0^L dz \sigma(z)$. In particular, for (12.10), $\sigma_L = \sigma_n$. For a monotonically increasing function, the derivative can be approximated as $|\partial_z q_\omega(z)| \approx \sigma_L/L$. This leads to a necessary condition on conductivity to suppress the reflection, namely,

$$\sigma_L < \frac{\omega^2 L}{8\pi c}. \quad (12.17)$$

Our analysis is valid if the higher derivatives of $\sigma(z)$ are not large. This condition requires that the exponent $n$ in (12.10) should not be less than two to insure a smooth behavior at $z = 0$.

The transmission can be estimated as follows. Suppose the pulse occupies a compact region $\Omega$. Let $E_\Omega^t$ be the pulse energy. The pulse looses its energy as it propagates through a conducting medium according to Ohm’s law, so that

$$e^{-1} \partial_t E_\Omega^t = -(2c)^{-1} \int_\Omega d\mathbf{r} \, \sigma \, \mathbf{E}_\Omega^2 \leq -8\pi \sigma_\Omega E_\Omega^t, \quad (12.18)$$

where $\sigma_\Omega = \max_\Omega \sigma$. Therefore the pulse energy decay can be bounded from above by

$$E_\Omega^t \leq e^{-8\pi \sigma_\Omega} E_\Omega^0. \quad (12.19)$$

In the one dimensional case (12.10), $\sigma_\Omega = \sigma_L/(n + 1)$. For the time $t = L/c$ needed for a pulse to get through the layer of width $L$, the attenuation should be large, that is, $8\pi L \sigma_L/c(n + 1) \gg 1$. Thus, the necessary conditions to suppress both transmission and reflection (that is, to ensure an almost total absorption) of the pulse are

$$\frac{(n + 1)c}{8\pi L} < \sigma_L < \frac{\omega^2 L}{8\pi c}. \quad (12.20)$$

By changing the Hamiltonian $H^Q$, the conducting layer can be included into the split or leapfrog algorithm. Since the conducting layer produces attenuation, the conductivity $\sigma$ must be included into the operator $L_{\Delta t}$ in the modified leapfrog scheme. It is also possible to create an absorbing and non-reflecting layer by using a passive medium (e.g. a Lorentz model). The analysis of the medium properties would be similar to that for a conducting layer. In fact, using a layer of a passive medium would offer more flexibility in solving the grid boundary problem.
References

[1] B. Fornberg, *A practical guide to pseudospectral methods*, Cambridge University Press, Cambridge, 1996;
J.P. Boyd, *Chebyshev and Fourier spectral methods*, Springer-Verlag, New York, 1989.

[2] C. Leforestier *et al*, J. Comput. Phys. 94 (1991) 59.

[3] R.P. Feynman, Rev. Mod. Phys. 20 (1948) 367;
R.P. Feynman and A.R. Hibbs, *Quantum mechanics and path integrals*, McGraw-hill, New York, 1965.

[4] A.G. Borisov and S.V. Shabanov, *Applications of the wave packet method to resonant transmission and reflection gratings*, LANL electronic archive, physics/0312xxx, 2003 (submitted to J. Comput. Phys.)

[5] M. Pickering, *An introduction to fast Fourier transform methods for partial differential equations*, Research Study Press, John Wiley & Sons Inc., New York, 1986;
E.O. Brigham, *The fast Fourier transform and applications*, Prentice-Hall, Inc., Eglewood Cliffs, New Jersey, 1988.

[6] E. Nelson, J. Math. Phys. 5 (1964) 332.

[7] P.G. Petropoulos, IEEE Trans. Antennas Propagat., 42 (1994) 62;
S. A. Cummer. IEEE Trans. Antennas Propagat., 45 (1997) 392;
J.L. Yong, *et al*, IEEE Trans. Microwave Theory and Technique, 43 (1995) 1902.

[8] V.I. Arnold, *Mathematical methods of classical mechanics*, Springer-Verlag, Berlin, 1989.

[9] V.I. Arnold, V.V. Koslov and A.I. Neishtadt, *Mathematical aspects of classical mechanics* in: *Encyclopaedia of Mathematical Science, Vol. III, Dynamical Systems*, Springer-Verlag, Berlin, 1988.

[10] P.A.M. Dirac, *Lectures on Quantum Mechanics*, Yeshiva University, New York, 1964.

[11] I. Daubechies and J.R. Klauder, J. Math. Phys. 26 (1985) 2239.

[12] V.S. Buslaev, in: *Topics in Mathematical Physics* (Ed. M. Birman), Consultants Bureau, New York, 1968;
V.I. Klyatskin and V.I. Tatarskii, Sov. Phys. JETP, 30 (1970) 335;
R. Dashen, J. Math. Phys. 20 (1979) 894;
M. Eve, Proc. Roy. Soc. London, 347A (1976) 405;
I.M. Besieris, J. Opt. Soc. Amer. 2 (1985) 2095;
R.H. Hardin and F.D. Tappet, SIAM Rev. 15 (1973) 423;
R.D. Nevels, J.A. Miller and R.E. Miller, IEEE Trans. Antennas Propagat., 48 (2000) 565.
[13] G. Roepstorff, *Path integral approach to quantum physics: an introduction*, Springer-Verlag, Berlin, 1994;
L.S. Schulman, *Techniques and Applications of Path Integration*, Wiley, New York, 1981.

[14] S.V. Shabanov, Phys. Rept. 326 (2000) 1.

[15] A.G. Borisov, J.P. Gauyacq and S.V. Shabanov, Surf. Sci. 487 (2001) 243.

[16] R. Richtmyer and K. Morton, *Difference Methods for Initial-Value Problems*, Wiley, New York, 1967.

[17] D. Neuhauser and M. Baer, J. Chem. Phys. 90 (1989) 4351;
G.G. Balint-Kurti and Á. Vábók, in: *Numerical Grid Methods and Their Applications to Schrödinger’s Equation*, (ed. C. Cerjan), Kluwer Academic Publisher, Netherlands, 1993, p.195.

[18] J.P. Bérenger, J. Comput. Phys. 114 (1994) 185; 127 (1996) 363;
P.G. Petropoulos, L. Zhao and Cangellaris, J. Comput. Phys. 139 (1998);
J.-L. Vay, J. Comput. Phys. 165 (2000) 511.

[19] L.D. Landau and E.M. Lifshitz, *Electrodynamics of continuous media, Theoretical Physics, Vol. VIII*, Oxford, Pergamon, New York, 1984.

[20] R.M. Joseph, S.C. Hagness, and A. Taflove, Opt. Lett. 16 (1991) 1412;
L.Gilles, S.C. Hagness, and L. Vázquez, J. Comput. Phys. 161 (2000) 379;
A. Taflove, *Advances in Computational Electrodynamics: The Finite-Difference Time-Domain Method*, Artech House, Norwood, MA, 1998.

[21] M.D. Feit, J.A. Fleck Jr. and A. Steiger, J. Comput. Phys. 47 (1982) 418.

[22] H. De Raedt, Comput. Phys. Rep. 7 (1987) 1.

[23] H.O. Kriess, Nordisk Tidskr. Informations-Behandlung, 2 (1962) 153.

[24] L.W. Kantorovich, Uspekhi Math. Nauk, USSR, 3 (1948) 89.

[25] T. Ichinose and H. Tamura, Proc. Indian Acad. Sci. (Math. Sci.) 112 (2002) 99.

[26] C. Lanczos, J. Res. Nat. Bur. Stand. 45 (1950) 255;
T.J. Park and J.C. Light, J. Chem. Phys. 85 (1986) 5870.

[27] A.G. Borisov and S.V. Shabanov, Chem. Phys. Lett. 361 (2002) 15.

[28] E. Fattal, R. Baer and R. Kosloff, Phys. Rev. E 53 (1996) 1217;
D. Lemoine, Chem. Phys. Lett. 320 (2000) 492.

[29] D. Inman, *Vibration and Control, Measurement and Stability*, Prentice Hall, 1989.

[30] H. Shintani and K. Tomoeda, Hiroshima Math. J., 7 (1977) 309.

[31] T.W. Ebbesen et al, Nature, 391 (1998) 667.