Electromagnetic Pulse Propagation in Passive Media by the Lanczos Method

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Abstract

Maxwell’s equations are cast in the form of the Schrödinger equation. The Lanczos propagation method is used in combination with the fast Fourier pseudospectral method to solve the initial value problem. As a result, a time-domain, unconditionally stable, and highly efficient numerical algorithm is obtained for the propagation and scattering of broad-band electromagnetic pulses in dispersive and absorbing media. As compared to conventional finite-difference time-domain methods, an important advantage of the proposed algorithm is a dynamical control of accuracy: Variable time steps or variable computational costs per time step with error control are possible. The method is illustrated with numerical simulations of extraordinary transmission and reflection in metal and dielectric gratings with rectangular and cylindrical geometry.

Keywords: Lanczos algorithm; Maxwell’s equations; time-domain algorithms; pseudospectral methods; gratings

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I Introduction

Recent developments in photonics and nanostructure materials [1, 2] have increased interest in efficient and accurate algorithms for numerical simulations of the propagation and scattering of short (broad band) laser pulses in generic passive (dispersive and absorbing) media. Time-domain approaches for solving the Maxwell’s equations might be more suitable for this purpose than frequency domain methods because the sought-for information, e.g., the scattering matrix, can be obtained within a desired frequency range by a single propagation. Coupled with laser ellipsometry of broad band pulses, fast simulations of expected resonance patterns in the scattering amplitude appear to be an efficient tool to control quality of manufactured photonic devices. Unconditionally stable algorithms are especially advantageous for such tasks because of their applicability to practically all materials and geometries without any assessment of admissible values of the system parameters. Another attractive property of time domain methods is their universality. The very same algorithms can be used to calculate static properties of the system (e.g., a band structure of photonic crystals), to simulate the electromagnetic pulse propagation in non-linear materials as well as in media with time-dependent properties.

The advantages of time-domain methods have been for a long time recognized in quantum mechanics where they are extensively used in the fields of chemical reaction dynamics [3], laser-matter interactions [4], etc. Highly efficient and accurate tools have been developed for the wave packet propagation and analysis of the results [3, 5, 6, 7, 8, 9]. Since Maxwell’s equations can be cast in the form of the Schrödinger equation, it is then natural to extend time-domain methods of quantum mechanics to numerical electrody namics. Some realizations of this idea are rooted to the path integral representation of quantum theory (the Lie-Trotter product formula [10] or the split operator method [5, 11, 12]). The others exploit polynomial approximations of the fundamental solution of the Schrödinger equation. For instance, the Chebychev time-propagation technique has been recently used to simulate the electromagnetic pulse propagation in non-absorbing media [13, 14].

Here it is proposed to use the Lanczos algorithm [15] to obtain an unconditionally stable, time-domain solver of Maxwell’s equations for passive media. The method allows for a dynamical control of accuracy, meaning that computational costs are constantly optimized in due course of simulations with error control. In brief, the approach can be summarized as follows. Maxwell’s equations are written in the form of the Schrödinger equation which is then solved by the Lanczos propagation scheme [16, 5] (Section II). The difference with the well studied quantum mechanical case is that the wave function is a multi-dimensional vector field and the Hamiltonian is non-Hermitian for absorbing media. The split operator method [5, 11, 12] has been used to include attenuation into the Lanczos propagation scheme, while preserving its unconditional stability (Section III). The action of the Hamiltonian on the wave function is computed by means of the Fourier pseudospectral method introduced in [17].

The accuracy of the method is investigated in Section IV. In Section V the Lanczos propagation scheme is applied to various gratings. In particular, a resonant extraordinary
reflection of a periodic array of parallel dielectric cylinders is observed. This effect is similar to the Wood anomalies [18] and related to the existence of stationary (trapped) electromagnetic waves with wave vectors parallel to the discrete translation symmetry axis of the system. Simulations of the scattering of broad band pulses on metallic grating and grooves, whose dielectric properties are described by the Drude model, are performed to demonstrate that the Lanczos propagation scheme is able to reproduce the results known in the literature and obtained by different means (by finite differencing schemes or by the scattering matrix method).

II The Lanczos method for Maxwell’s equations

Consider first the case of non-dispersive media. Let $D$ and $B$ be electric and magnetic inductions, respectively, and $E$ and $H$ the corresponding fields so that $D = \varepsilon E$ and $B = \mu H$ where $\varepsilon$ and $\mu$ are positive, symmetric, position dependent matrices for generic non-isotropic and non-homogeneous media. For isotropic media, $\varepsilon$ and $\mu$ are scalars. At interfaces of different media, the boundary conditions are enforced dynamically, that is, $\varepsilon$ and $\mu$ are allowed to have discontinuities. Maxwell’s equations are rewritten as:

$$i\dot{\psi} = \mathcal{H}\psi, \quad \psi = \begin{pmatrix} E \\ H \end{pmatrix}, \quad \mathcal{H} = \begin{pmatrix} 0 & ic\varepsilon^{-1}\nabla \times \\ -ic\mu^{-1}\nabla \times & 0 \end{pmatrix}. \quad (2.1)$$

The over-dot denotes the time derivative, and $c$ is the speed of light in the vacuum. One can also use the electromagnetic inductions as independent variables instead of the fields. The Hamiltonian $\mathcal{H}$ must then be modified accordingly. The initial value problem is solved by applying the evolution operator (or the fundamental solution) to the initial wave function

$$\psi(t) = e^{-it\mathcal{H}}\psi(0). \quad (2.2)$$

The Hamiltonian is a Hermitian operator, $\mathcal{H}^\dagger = \mathcal{H}$, with respect to the measure scalar product

$$(\psi_1, \psi_2) = \int (D_1 \cdot E_2 + B_1 \cdot H_2) \, dr \equiv \int \psi_1^\dagger \kappa \psi_2 \, dr. \quad (2.3)$$

The symmetric positive matrix $\kappa$ is block-diagonal, with the blocks being $\varepsilon$ and $\mu$. The norm of the wave function with respect to the scalar product (2.3) is proportional to the electromagnetic energy and is conserved because the evolution operator is unitary.

In numerical simulations, the Hilbert space is projected onto a finite dimensional Euclidean space so that $\psi$ becomes a vector whose components are values of the wave function at sites of a finite spatial grid. In the grid representation, $\mathcal{H}$ is a matrix. If the Hamiltonian is Hermitian, it is then convenient to have $\mathcal{H}$ as an explicitly Hermitian matrix. In the Maxwell theory, this can be achieved if, before projecting onto the grid, the wave function and the Hamiltonian are scaled

$$\psi \rightarrow \kappa^{-1/2}\psi, \quad \mathcal{H} \rightarrow \kappa^{-1/2}\mathcal{H}\kappa^{1/2}. \quad (2.4)$$
In the representation (2.1) we have

\[ E \rightarrow \varepsilon^{-1/2} E, \quad H \rightarrow \mu^{-1/2} H, \quad \mathcal{H} \rightarrow \begin{pmatrix} 0 & ic\varepsilon^{-1/2} \nabla \times \mu^{-1/2} \\ -ic\mu^{-1/2} \nabla \times \varepsilon^{-1/2} & 0 \end{pmatrix}. \]  

The scaled Hamiltonian is Hermitian with respect to the conventional scalar product in the space of square integrable functions, and, hence, it is a Hermitian matrix, when projected onto the grid. The action of spatial derivatives is calculated within the pseudospectral approach based on the Fourier grid representation of the wavefunction and the fast Fourier transform. In what follows, only consecutive actions of \( \mathcal{H} \) on wave functions are required.

A direct use of (2.2) implies a diagonalization of \( \mathcal{H} \), which is not feasible if the matrix size is too large. Various numerical approximations are based on the semigroup property of the evolution operator

\[ \psi(t + \Delta t) = e^{-i\Delta t \mathcal{H}} \psi(t). \]  

In a local propagation scheme the exponential can be approximated by a polynomial for a sufficiently small time step \( \Delta t \). The basic idea of the Lanczos propagation method is that the exact solution \( \psi(t + \Delta t) \) is projected onto the Krylov subspace associated with the initial state \( \psi(t) \) and the Hamiltonian, \( \psi(t + \Delta t) \rightarrow \psi^{(n)}(t + \Delta t) \equiv \mathcal{P}_n \psi(t + \Delta t) \in \mathcal{K}_n \), where \( \mathcal{P}_n^\dagger = \mathcal{P}_n \), \( \mathcal{P}_n^2 = \mathcal{P}_n \), and

\[ \mathcal{K}_n = \text{Span} \left( \psi(t), \mathcal{H} \psi(t), ..., \mathcal{H}^{n-1} \psi(t) \right). \]

The accuracy of such an approximation is \( O(\Delta t^n) \). The Hamiltonian is projected accordingly,

\[ \mathcal{H} \rightarrow \mathcal{H}^{(n)} \equiv \mathcal{P}_n \mathcal{H} \mathcal{P}_n. \]

Thus,

\[ \psi(t + \Delta t) \approx \psi^{(n)}(t + \Delta t) = e^{-i\Delta t \mathcal{H}^{(n)}} \psi^{(n)}(t). \]  

The projection is done via an orthonormal basis for \( \mathcal{K}_n \) which is constructed by means of the Lanczos recursion algorithm [15]. In this basis, the matrix \( \mathcal{H}^{(n)} \) is Hermitian and tridiagonal. Typically, just a few orders are sufficient \( (n \leq 9) \) so that \( n \) is much smaller than the dimension of \( \mathcal{H} \) and the matrix \( \mathcal{H}^{(n)} \) can easily be diagonalized. The dimension \( n \) may be set differently at each time step, depending on the current vector \( \psi(t) \), and is determined by a pre-set required accuracy. In particular, it allows to avoid excessive actions of \( \mathcal{H} \) on the wave function. This feature leads to a dynamical optimization of computational costs with error control, which is one the greatest advantages of the Lanczos method.

A detailed discussion of the Lanczos recursion algorithm and its application to the wave packet propagation can be found elsewhere [16, 5]. Here only a brief summary is given with notations used later in the text. Let \( \psi_0 = \psi(t) \) where \( \psi(t) \) is assumed to be normalized so that \( \|\psi_0\| = 1 \). Due to the linearity of the Schrödinger equation one can always scale \( \psi_0 \) by a number and rescale it back after applying the infinitesimal evolution operator. Define

\[ \alpha_0 = (\psi_0, \mathcal{H} \psi_0), \quad \phi_1 = (\mathcal{H} - \alpha_0) \psi_0, \quad \psi_1 = \phi_1/\|\phi_1\|. \]
By construction, $\psi_1$ and $\psi_0$ are orthonormal. For $k = 2, 3, \ldots, n - 1$ the rest of the basis for $K_n$ is generated by the recursion relation

\begin{align*}
\alpha_{k-1} &= \langle \psi_{k-1}, \mathcal{H}\psi_{k-1} \rangle, \\
\beta_{k-2} &= \langle \psi_{k-2}, \mathcal{H}\psi_{k-1} \rangle, \\
\phi_k &= \langle \mathcal{H} - \alpha_k \rangle \psi_{k-1} - \beta_{k-2} \psi_{k-2}, \\
\psi_k &= \phi_k/\|\phi_k\|.
\end{align*}

By construction, the vector $\mathcal{H}\psi_j$ is a linear combination of $\psi_{j-1}$, $\psi_j$, and $\psi_{j+1}$. Hence, in the Lanczos basis the matrix $\mathcal{H}^{(n)}_{ij} = \langle \psi_i, \mathcal{H}\psi_j \rangle$ is tridiagonal. Elementary calculations show that the diagonal elements are $\mathcal{H}^{(n)}_{jj} = \alpha_j = \bar{\alpha}_j$, the upper and lower superdiagonals are $\mathcal{H}^{(n)}_{jj+1} = \mathcal{H}^{(n)}_{j-1j} = \beta_j = \bar{\beta}_j$.

Let $U$ be a unitary transformation such that $U^\dagger \mathcal{H}^{(n)} U$ is a diagonal matrix, and $E_j$ be eigenvalues of $\mathcal{H}^{(n)}$. The approximate solution (2.7) is obtained by expanding the wave function over the Lanczos basis and solving the Schrödinger equation for the expansion coefficients:

$$\psi^{(n)}(t + \Delta t) = \sum_{k,j=0}^{n-1} \bar{U}_{jk} e^{-i\Delta t E_j} U_{j0} \psi_k \equiv \sum_{k=0}^{n-1} c_k(\Delta t) \psi_k,$$

where the initial condition $c_k(0) = \delta_{k0}$ has been taken into account. Since $\mathcal{H}^{(n)}$ is Hermitian, the evolution preserves the norm

$$\|\psi^{(n)}(t + \Delta t)\|^2 = \|\psi^{(n)}(t)\|^2 = \|\psi_0\|^2 = 1.$$

Thus, the algorithm is unconditionally stable because the norm of the amplification matrix $\mathcal{G}^{(n)}(\Delta t)$, defined by $\psi^{(n)}(t + \Delta t) = \mathcal{G}^{(n)}(\Delta t) \psi(t)$, is uniformly bounded, $\|\mathcal{G}^{(n)}(t)\| \leq 1$, for all parameters of the Hamiltonian and $\Delta t \geq 0$.

The accuracy of the algorithm can be estimated from the following observation [16]. The norm of a projection of the exact solution onto the orthogonal complement of $K_n$ can be used as a measure of accuracy of the Lanczos algorithm. By expanding the exponential in the right hand side of (2.6) into the Taylor series, it is clear that the contribution of the term $(\Delta t \mathcal{H})^{n+1} \psi(t)$, which has no projection onto $K_n$, can only be captured by the approximate solution if the larger Krylov space $K_{n+2}$ is used in the Lanczos algorithm, which, in turn, implies that the vector $c_j(\Delta t)$ acquires two additional components. Thus, the accuracy of the Lanczos algorithm can be controlled, for example, by demanding that the absolute value of $c_{n-1}(\Delta t)$ is less than a specified small number $\epsilon$. Note that $|c_{n-1}(\Delta t)| \sim O(\Delta t^{n-2})$ as one can deduce from (2.15) and the tridiagonal structure of $\mathcal{H}^{(n)}$ in the Lanczos basis. To ensure that the norm of the projection of $\psi(t + \Delta t)$ onto the orthogonal complement of $K_n$ is small, we demand that

$$|c_{n-3}(\Delta t)|^2 + |c_{n-2}(\Delta t)|^2 + |c_{n-1}(\Delta t)|^2 \leq \epsilon$$

(2.17) where $\epsilon \sim 10^{-14}$ in our calculations. To satisfy (2.17), the time step $\Delta t$, or the dimension of the Krylov subspace $n$, or both can be varied to minimize computational costs. This is the aforementioned dynamical control of accuracy in the Lanczos propagation method. In our simulations, $\Delta t$ has been kept fixed, while (2.17) has been used to determine a minimal $n$ for each time step.
III Including attenuation by the split method

The response function of a passive medium in an applied electromagnetic field must satisfy the causality condition. A common way to model the causal response function is to assume that the medium polarization and magnetization satisfy a linear differential equation in time in which a non-homogeneous term is proportional to the applied field (for linear media). The Maxwell’s equations in passive media appear then to be a system of (high-order) differential equations to which numerical algorithms are applied [19, 20]. Any system of high-order differential equations can be converted into a system of first-order differential equations by introducing auxiliary dynamical variables. This idea is used to convert Maxwell’s equations for passive media into the Schrödinger equation (2.1) in which the wave function contains additional components that describe dynamics of the medium polarization and magnetization. Due to absorption the time evolution is no longer unitary.

It must be noted that absorption of the wave packet is required in numerical simulations of scattering problems in which the pulse shape is to be computed in the asymptotic region. Indeed, when the front edge of the pulse reaches the grid boundary, it will be reflected or re-appear on the other side of the grid, depending on the boundary conditions. To avoid an artificial interference of the scattered pulse with itself, a layer of an absorbing medium is necessary at the grid boundary [21].

Here a simple way is proposed to include the attenuation of the wave packet amplitude into the Lanczos method, while maintaining the unconditional stability of the algorithm. The procedure is illustrated with the Drude model of metals.

Let \( \mathcal{H} = \mathcal{H}_0 - i \mathcal{V} \) where \( \mathcal{H}_0^\dagger = \mathcal{H}_0 \) and \( \mathcal{V}^\dagger = \mathcal{V} \). The system is absorbing and, therefore, \( \mathcal{V} \) must be a positive semidefinite operator, that is, for any \( \psi \), \( (\psi, \mathcal{V} \psi) \geq 0 \). This readily follows from the condition that the norm of a solution of (2.1) cannot increase with time. The exact time evolution (2.6) is approximated by means of the Lie-Trotter formula

\[
\psi(t + \Delta t) = e^{-\Delta t \mathcal{V}/2} e^{-i \Delta t \mathcal{H}_0/2} e^{-\Delta t \mathcal{V}/2} \psi(t) + O(\Delta t^3). \tag{3.1}
\]

The action of the exponential of \( \mathcal{H}_0 \) is computed by the Lanczos method as before. The attenuation potential \( \mathcal{V} \) typically does not involve spatial derivatives and, hence, the action of its exponential on a wave function is far less expensive than that for \( \mathcal{H}_0 \). The norm of any power of the amplification matrix still remains uniformly bounded by one because \( \|e^{-\Delta t \mathcal{V}/2}\| \leq 1 \) for \( \Delta t \geq 0 \). Hence the unconditional stability is preserved.

Let us turn to the Drude model which is used in numerical simulations presented below. Another popular model, a multi-resonance Lorenz model, can be treated similarly. Let \( \mathbf{D} = \mathbf{E} + \mathbf{P} \) and \( \mathbf{B} = \mathbf{H} \). In the Drude model, the medium polarization is described by the second order differential equation

\[
\ddot{\mathbf{P}} + \eta \dot{\mathbf{P}} = \omega_p^2 \mathbf{E} , \tag{3.2}
\]

where \( \eta > 0 \) is the attenuation constant and \( \omega_p \) is the plasma frequency. Equation (3.2) must be solved with zero initial conditions, \( \mathbf{P}(0) = \dot{\mathbf{P}}(0) = 0 \). Define an auxiliary field \( \mathbf{Q} \)
by $\dot{\mathbf{P}} = \omega_p \mathbf{Q}$. Rewriting the Maxwell’s equations and (3.2) in terms $\mathbf{E}$, $\mathbf{B}$, and $\mathbf{Q}$ and their first-order time derivatives, the Schrödinger equation is obtained in which

$$
\psi = \begin{pmatrix} \mathbf{E} \\ \mathbf{B} \\ \mathbf{Q} \end{pmatrix}, \quad \mathcal{H} = \begin{pmatrix} 0 & ic \nabla \times & -i \omega_p \\ -ic \nabla \times & 0 & 0 \\ i \omega_p & 0 & -i \eta \end{pmatrix} .
$$

(3.3)

The Hamiltonian is Hermitian when $\eta = 0$ (no attenuation). The attenuation potential $\mathcal{V}$ is a diagonal matrix, $\text{diag}(0, 0, \eta)$, that is positively semidefinite since $\eta > 0$.

For an absorber at the grid boundaries, a layer of a conducting medium has been used with a position dependent conductivity $\sigma$. As the induced current in a conducting medium has the form $\mathbf{J} = \sigma \mathbf{E}$, the matrix $\mathcal{V}$ is changed to $\text{diag}(-4\pi \sigma, 0, \eta)$. The function $\sigma$ is constructed according to the frequency band of the initial pulse.

### IV Free space propagation. Phase and amplitude errors

To illustrate the efficiency of the Lanczos time-propagation method, we compare it with a widely adopted Second Order Finite Differencing (SOD, or leapfrog) propagation method [5, 20, 22], using the simplest example of the electromagnetic pulse propagation in vacuum. The action of the Hamiltonian on wave functions in the Lanczos and leapfrog methods are done in the same way, that is, by the fast Fourier pseudospectral method on the same grid.

Consider a Gaussian wave packet linearly polarized along the $y$ axis and propagating along the $z$ axis. The amplitude of the fields at the initial time $t = 0$ is given by

$$
E_y(z) = e^{-z^2/D^2} e^{ik_0 z}, \quad H_x(z) = -E_y(z) ,
$$

(4.1)

where $k_0 = 5.5/D$, and $D$ determines the width of the wave packet. The carrier wave length $\lambda = 2\pi/k_0$ so that $D = 0.875\lambda$. We take $D = 1.75 \mu m$, or $\lambda = 2 \mu m$. The step of the grid is $\Delta z = 0.1D$. An exact solution directly follows from (4.1) $E_y(z, t) = E_y(z - ct)$. The wave packet propagates in the direction of positive $z$. With our settings the pulse duration is about $25 fs$.

Numerical solutions are obtained by the Lanczos and leapfrog algorithms for the Schrödinger equation (2.1) in which $\varepsilon = \mu = 1$. Recall that the leapfrog propagation scheme is based on the third-order finite difference approximation of the time derivative

$$
\psi(t + \Delta t) = \psi(t - \Delta t) - 2i\Delta t \mathcal{H} \psi(t) .
$$

(4.2)

The scheme is conditionally stable, and the time step must be chosen accordingly. The simulated electric field is recorded by a detector placed at $z = z_{\text{det}} = 18D$. Its phase and amplitude are compared with those of the exact solution. For a signal $E(t) = E_0(t) e^{i\varphi(t)}$, 

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where \( E_0(t) = |E(t)| \), the phase and amplitude errors are defined, respectively, by

\[
\delta^P = \left| \frac{\phi^{\text{exact}} - \phi^{\text{approx}}}{\phi^{\text{exact}}} \right|, \quad \delta^A = \left| \frac{E_0^{\text{exact}} - E_0^{\text{approx}}}{E_0^{\text{exact}}} \right|
\]  \tag{4.3}

The errors \( \delta^P, \delta^A \) are plotted respectively in Figs 1 and 2 as functions of \( S = (z_{\text{det}} - ct) / D \), the position of the pulse center relative to the detector measured in units of \( D \). The results are shown for \( |S| \leq 2.5 \) where the signal on the detector is sufficient. Dashed and solid lines correspond to the leapfrog and Lanczos methods, respectively, for various settings of the time step.

The time step for the black dashed line is a reference time step, \( \Delta t_0 \approx 0.01 \) fs. If \( N_H \) is the number of elementary operations required to compute the action of the Hamiltonian on a wave function, then the total number of operations reads \( N = sN_HN_t \), where \( s \) is the number of actions of the Hamiltonian per a time step, \( N_t = t / \Delta t \) is the total number of time steps. For the leapfrog method, \( s = 1 \) for all time steps. In the Lanczos method, \( s = n - 1 \), with \( n \) being the dimension of the Krylov space. Despite that the dynamic control of accuracy has been activated, \emph{de facto} \( n \) does not vary in due course of simulations in vacuum.

Let \( N = N_0 \) for the black dashed curve. The red dashed curve is obtained by reducing the time step, \( \Delta t = \Delta t_0 / 2 \), and, hence, the total number of operations increases accordingly, \( N = 2N_0 \). In the Lanczos method, the black solid curve corresponds to \( \Delta t = 10\Delta t_0 \) and \( s = 7 \), the blue solid curve to \( \Delta t = 5\Delta t_0 \) and \( s = 7 \), and the red one to \( \Delta t = 2.5\Delta t_0 \) and \( s = 6 \). The total number of operations is, respectively, \( N = 0.7N_0 \), \( N = 1.4N_0 \), and \( N = 2.4N_0 \). It is readily seen that at roughly the same number of operations, the Lanczos algorithm has phase and amplitude errors that are less than those in the leapfrog method by several orders of magnitude.

A few remarks are in order. There are, of course, algorithms that would be more efficient than the Lanczos propagation method in free space. For instance, the split propagation method [12] essentially reproduces an exact solution and is also unconditionally stable. However, the split method would not be applicable when the Hamiltonian involves products of operators that depend on spatial derivatives and positions. The accuracy of the leapfrog scheme can be improved by, for example, taking into account the next term of the Taylor expansion of \( \psi(t \pm \Delta t) \) in powers of \( \Delta t \) in (4.2) [23],

\[
-2i\Delta t H\psi \rightarrow -2i\Delta t H(1 - \Delta t^2 H^2 / 3)\psi .
\]

In this case, \( s = 3 \). The method is still conditionally stable where the stability condition of the SOD, \( \Delta t \| H \| \leq 1 \), changes accordingly to \( \Delta t \| H (1 - \Delta t^2 H^2 / 3) \| \leq 1 \). Even though \( s \) has tripled, the new stability condition allows one to increase the time step by the factor of 2.1. Therefore the total number of operations increases only slightly. The accuracy of the scheme will be of \( O(\Delta t^5) \) which is still not as high as in the Lanczos method, \( O(\Delta t^n) \) with \( n = 8,7 \) in the above examples.

Some care should be taken regarding a known drawback of the Lanczos algorithm – a possible loss of orthogonality of basis functions due to round-off errors [15, 24]. This is why
the time step has to be adjusted so that only low dimensional Krylov spaces, \( n \leq 9 \), are invoked in contrast to the conventional use of the Lanczos method for solving linear systems.

V Applications to gratings

In this section the Lanczos propagation scheme is applied to the scattering of a broad band wave packet on nanostructure periodic materials such as gratings and grooves. We are particularly interested in transmission (reflection) properties currently being a subject of intense research [2, 26, 27, 28]. The results obtained here are compared with those available in the literature. The time-dependent approach allows us to underline the role played by trapped modes or resonances in the existence of extraordinary transmittance and reflectance of periodic structures. The longer lives a trapped mode, the more narrow resonance occurs in the reflection and/or transmission coefficient.

All systems considered here have a translation symmetry along one of the Euclidean axes, chosen to be the \( y \) axis. The structures are periodic along the \( x \) axis with the period \( D_g \), and the \( z \) direction is transverse to the structure. The initial wave packet is Gaussian and propagates along the \( z \) axis. Its spectrum is broad enough to cover the frequency range of interest. The zero diffraction mode is studied for wavelengths \( \lambda \geq D_g \) so that reflected and transmitted beams propagate along the \( z \)-axis. As in our previous work [25] we use a change of variables to enhance the sampling efficiency in the vicinity of medium interfaces so that the boundary conditions at sharp interfaces are accurately reproduced by the Fourier-grid pseudospectral method. A typical size of the mesh corresponds to \(-15D_g \leq z \leq 15D_g \), and \(-0.5D_g \leq x \leq 0.5D_g \) with, respectively, 512 and 128 knots. The frequency resolved transmission and reflection coefficients are obtained via the time-to-frequency Fourier transform of the signal on “virtual detectors” placed at some distance in front and behind the slab with a periodic structure [29].

V.1 Array of dielectric cylinders

The significance of trapped modes is first illustrated with a periodic array of non-dispersive dielectric cylinders, the system which has not received as much attention as metal or dielectric gratings. Consider an array of parallel, periodically positioned, dielectric cylinders in vacuum oriented along the \( y \) axis. The radius \( R \) of cylinders is small as compared to the array period \( D_g = 1.75 \mu \text{m} \). In simulations, the ratio \( R/D_g \) is taken to be 0.0857. The incident wave packet is linearly polarized. The electric field is oriented along the \( y \) axis, i.e., parallel to the cylinders (the so-called TM polarization). The Hamiltonian for the Lanczos scheme has the form (2.1) where \( \mu = 1 \).

In Fig. 3 the reflection coefficient \( R \) is shown as a function of the wave length expressed in units of \( D_g \). In the Schrödinger formulation of Maxwell’s theory the norm of the wave function is proportional to the total electromagnetic energy. Hence, for a lossless medium the
transmission $T$ can simply be obtained from the energy conservation: $T + R = 1$. Recall that the Lanczos propagation method preserves the norm. The solid-blue and dashed-red curves correspond, respectively, to $\varepsilon = 2$ and $\varepsilon = 4$. As one can see the array becomes a perfect reflector within a fairly narrow wavelength range centered at the resonant wavelength that is slightly larger than the period $D_g$. Similar results have been obtained for dielectric grating structures. The resonant pattern is associated with the so-called Wood anomalies [18], and can be explained by the existence of trapped modes or guided wave resonances [25, 30]. The widths of the resonances in the reflection (transmission) coefficient are determined by the lifetime of a corresponding quasi-stationary trapped mode which is a standing wave along the $x$ axis and is excited by the incoming wave.

The existence of trapped modes can easily be inferred from the temporal evolution of the electromagnetic field. Figure 4 shows the transmitted electric field as a function of time measured by a detector placed behind the layer of dielectric cylinders. The main transmitted pulse is clearly visible. It has a significant amplitude and duration about $25 \text{ fs}$. After the main pulse passes the array, it leaves behind an excited quasi-stationary mode which looses its energy by radiating almost monochromatic waves with the same amplitude, but an opposite phase, in the transmission and reflection directions. The lasing effect of the trapped mode appears as exponentially dumped oscillations coming after the main signal. The exponential decay due to a finite lifetime of the quasi-stationary state is clearly seen. By the symmetry, the same lasing effect is registered by a detector placed in front of the layer (not shown here). A 100% reflection at the resonant frequency can be understood from the fact that the field emitted by the trapped mode in the transmission direction and the corresponding frequency component of the initially transmitted pulse have an opposite phase, thus compensating each other. The solid-blue and dashed-red curves correspond, respectively, to $\varepsilon = 2$ and $\varepsilon = 4$. The radiation coming from the narrow resonance (the blue curve) has a lower amplitude and a much longer duration. The lifetime of the trapped mode in this case is in the picosecond range, i.e., thousand times longer than the initial pulse duration. Note that the more narrow resonance is the less energy gets trapped from the initial pulse. This explains the amplitude difference of the blue and red curves. Finally, the concept of trapped modes localized on successive layers and interacting with each other provides a theoretical framework for the light propagation in layered structures such as photonic crystal slabs [31].

V.2 Metal gratings and grooves

Metal gratings and grooves have been extensively studied in micro-wave and optical domains [26, 27]. The purpose of this section is to show that the Lanczos propagation method can successfully be applied to metals described by the Drude model. The Hamiltonian has the form (3.3). The attenuation and the plasma frequency are taken to be representative for silver: $\omega_p = 9eV$, and $\eta = 0.1eV$ [26]. The grating geometry is sketched in the inset of Fig. 5. The grating period is $D_g = 1.75 \text{ \mu m}$, the thickness (along the $z$ axis) is $h = 0.8 \text{ \mu m}$, and the grating width $a = 0.3 \text{ \mu m}$. The corresponding grooves are obtained by attaching a solid metal plate on one side of the gratings so that no transmission is possible. The polarization of the incident wave packet is such that the electric field vector is oriented along the $x$ axis,
i.e., perpendicular to the gratings (the so called TE polarization). The difference with the non-dispersive case discussed above is the presence of attenuation. The trapped mode loses its energy due to (non-perfect) conductivity of the metal. This leads to broadening of the resonance.

In Fig. 5 the dashed red and solid blue curves represent the transmission and reflection coefficients, respectively, as functions of the wavelength expressed in units of the grating period, $D_g$. The resonance is again associated with the existence of a trapped stationary wave in the grating. The transmittance does not reach 100% due to dissipative loss of energy in the Drude metal. While for a lossless medium the sum of the reflection and transmission coefficients must be one, this is not the case for the Drude metal (the dashed-dotted green curve in Fig. 5). The maximal loss of energy corresponds to the resonant wavelength. It is easily understood because the trapped mode remains in contact with the metal much longer than the main pulse, and, therefore, can dissipate more energy through exciting surface electrical currents in metal. The black curve in Fig. 5 shows the reflectance of the grooves. Since the light cannot be transmitted through the grooves, a resonance structure in the reflection coefficient is directly related to the enhanced energy loss at the wavelength of the trapped mode. Note that as compared to the metal gratings, the resonance is broadened and shifted to the lower frequencies (larger wavelength). The results obtained here are in a full agreement with previous theoretical and numerical analysis [26, 27].

VI Conclusions

It has been demonstrated that the Lanczos algorithm can be used to develop a highly efficient, accurate, and unconditionally stable propagation scheme to simulate scattering of broad band electromagnetic pulses in passive media. The accuracy and efficiency of the algorithm have been illustrated with an example of the electromagnetic wave propagation in vacuum. At the same computational costs, a significant reduction of phase and amplitude errors has been observed in the Lanczos propagation method as compared to the second-order finite-difference (leapfrog) scheme.

As an example of possible applications, the Lanczos propagation method has been applied to study resonant transmission and reflection of various periodic nano-structures: An array of periodically placed parallel cylinders made of a non-dispersive dielectric material, metallic gratings and grooves. The time-domain study clearly demonstrates the role played by quasi-stationary (trapped) electromagnetic waves supported by the corresponding periodic structure in the extraordinary transmission (reflection) properties of the grating. The results for metallic gratings and grooves coincide with those obtained earlier by means of other numerical algorithms and are also in agreement with theoretical studies. The unconditional stability of the Lanczos propagation scheme for media with attenuation has been achieved via the split method, which reduces the accuracy. It is possible to restore the accuracy up to the level gained for non-absorbing media. However, stability conditions require a further study that will be reported elsewhere.
In summary, the Lanczos algorithm has been shown to lead to a highly accurate, efficient, and unconditionally stable time-propagation numerical solver for the Maxwell’s equations. Variable time steps and/or variable computational costs with accuracy control are possible. The method is applicable to various electromagnetic systems (no restrictions on the Hamiltonian). All these virtues are hardly available in other unconditionally stable algorithms in numerical electrodynamics of passive media.

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Figure captions

Fig. 1. The phase errors for the propagation of an electromagnetic gaussian pulse in vacuum. Results are presented as a function of the position of the pulse center relative to the detector, $S$, measured in units of the pulse width $D$. Dashed and solid curves correspond, respectively, to the leapfrog and Lanczos propagation methods. Different colors represent computational costs of simulations measured as the total number of actions of the Hamiltonian on the wave function for fixed propagation time. Further details are given in the text.

Fig. 2. The amplitude errors for the propagation of an electromagnetic gaussian pulse in vacuum. Results are presented as a function of the position of the pulse center relative to the detector, $S$, measured in units of the pulse width $D$. Dashed and solid curves correspond, respectively, to the leapfrog and Lanczos propagation methods. Different colors represent computational costs of simulations measured as the total number of actions of the Hamiltonian on the wave function for fixed propagation time. Further details are given in the text.

Fig. 3 Calculated zero-order reflection coefficient for a periodic array of dielectric cylinders in vacuum described in the text. Results are presented as a function of the wavelength of the incident radiation measured in units of the period $D_g$. The solid blue and dashed red curves correspond, respectively, to the array of cylinders with dielectric constants $\varepsilon = 2$ and $\varepsilon = 4$.

Fig. 4 The electric field measured by a detector placed behind the periodic layer of dielectric cylinders. Only the field corresponding to the zero-order transmitted wave propagating along the $z$-axis is represented. It is obtained by the Fourier analysis of the $x$-coordinate dependence of the field at the detector position. The signal is shown as a function of time measured in femtoseconds. The solid blue and dashed red curves correspond, respectively, to the array of cylinders with dielectric constants $\varepsilon = 2$ and $\varepsilon = 4$.

Fig. 5. Calculated zero-order reflection and transmission coefficients for metallic gratings and grooves described in the text. Results are presented as a function of the wavelength of the incident radiation measured in units of the period $D_g$. The inset of the figure gives a schematic view on the grating geometry. The black line shows the reflection coefficient for metallic grooves. Blue and (dashed red) line shows the reflection (transmission) coefficient for metallic gratings. The sum of the reflection and transmission coefficients for metallic gratings is shown as the dashed-dotted green curve. Its deviation from 1 represents the loss of electromagnetic energy because of the absorption in metal.
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