Lanczos Pseudospectral Propagation Method for Initial-Value Problems in Electrodynamics of Passive Media

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Abstract

Maxwell’s equations for electrodynamics of dispersive and absorptive (passive) media are written in the form of the Schrödinger equation with a non-Hermitian Hamiltonian. The Lanczos time-propagation scheme is modified to include non-Hermitian Hamiltonians and used, in combination with the Fourier pseudospectral method, to solve the initial-value problem. The time-domain algorithm developed is shown to be unconditionally stable. Variable time steps and/or variable computational costs per time step with error control are possible. The algorithm is applied to study transmission and reflection properties of ionic crystal gratings with cylindric geometry in the infra-red range.

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1. **Introduction.** There is a demand for fast time-domain solvers of the Maxwell’s equations to model dynamics of broad band electromagnetic pulses in dispersive and absorptive media. This is driven by various applications that include photonic devices, communications, and radar technology, amongst many others. Efficiency, accuracy, and stability are the key criteria of choosing a concrete algorithm for specific applications. In the past decades, pseudospectral methods of solving the initial value problem for differential equations have been under intensive study [1]. Because of their high efficiency and accuracy, they have replaced finite differencing approaches in many traditional applications as well as scientific simulations, e.g., in quantum chemistry [2]. Unconditionally stable pseudospectral algorithms are particularly attractive for numerical simulations.

In the present paper we develop an unconditionally stable time-domain algorithm for solving the initial value problem for Maxwell’s equations in dispersive and absorptive (passive) media with sharp interfaces (discontinuities of medium parameters). It is a time-stepping algorithm that is based on the Hamiltonian formalism for electrodynamics of passive continuous media, the Lanczos propagation scheme [3, 4], and the Fourier pseudospectral method [5]. Apart from the unconditional stability, the algorithm has a dynamical control of accuracy, which allows one to automatically optimize computational costs with error control at each time step.

We apply the algorithm to the scattering of broad band electromagnetic pulses on gratings, the photonic devices that currently attract lots of attention because of their transmission and reflection properties [6]. As for the passive medium, we choose an ionic crystal material. From the numerical point of view, the model of the dielectric permeability of such a material is rather representative and used in the vast number of applications. From the physical point of view, the interest to gratings and photonic crystals made of this kind of material is due two types of effects in interaction with electromagnetic radiation: The structural and polaritonic ones [7, 8]. We show that in the infrared range the reflection and transmission properties of ionic crystal gratings change significantly in narrow frequency ranges due to structural and polaritonic resonances. Structural resonances are associated with the existence of trapped (quasistationary) electromagnetic modes supported by the grating geometry (guided wave resonances) [9]. Polaritonic resonances are associated with dispersive properties of the material. Such resonances appear when the incident radiation can cause polaritonic excitations in the medium. From the macroscopic point of view, this occurs in the anomalous dispersion region of the dielectric constant.

2. **Basic equations.** Maxwell’s equations in passive media can be written in the form of the Schrödinger equation in which the wave function is a multidimensional column, composed of electromagnetic field components and the medium polarization, and the Hamiltonian is, in general, non-Hermitian when attenuation is present. The initial-value problem (the time evolution of an electromagnetic pulse) is then solved by finding the fundamental solution (the evolution operator kernel) for the Schrödinger equation. Here this idea is applied to the ionic crystal material whose dielectric properties at the frequency ω are described by the dielectric constant

\[ \varepsilon(\omega) = \varepsilon_\infty + \frac{(\varepsilon_0 - \varepsilon_\infty)\omega_0^2}{\omega_0^2 - \omega^2 - i\eta\omega}, \]  

(1)
where \( \varepsilon_{\infty,0} \) are constants, \( \omega_T \) is the resonant frequency, and \( \eta \) is the attenuation. In particular, transmission and reflection properties of the periodic grating structure of circular parallel cylinders made of such a material are studied.

Let \( \mathbf{P} \) be a dispersive part of the total polarization vector of the medium. Then \( \mathbf{D} = \varepsilon_{\infty} \mathbf{E} + \mathbf{P} \), where \( \mathbf{D} \) and \( \mathbf{E} \) are the electric induction and field, respectively. By using the Fourier transform, it is straightforward to deduce that \( \mathbf{P} \) satisfies the second-order differential equation

\[
\dot{\mathbf{P}} + \eta \mathbf{P} + \omega_p^2 \mathbf{P} = \varepsilon_{\infty} \omega_p^2 \mathbf{E},
\]

where the overdot denotes the time derivative, \( \omega_p^2 = (\varepsilon_0 - \varepsilon_{\infty}) \omega_T^2 / \varepsilon_{\infty} \) if \( \varepsilon_0 - \varepsilon_{\infty} \) is positive, otherwise, \( \omega_p^2 \rightarrow -\omega_p^2 \) in (2). Equation (2) must be solved with the zero initial conditions, \( \mathbf{P} = \mathbf{0} \) at \( t = 0 \).

Define a set of auxiliary fields \( \mathbf{Q}_{1,2} \) by \( \mathbf{P} = \sqrt{\varepsilon_{\infty}} \omega_p \mathbf{Q}_1 / \omega_T \) and \( \dot{\mathbf{Q}}_1 = \omega_T \mathbf{Q}_2 \). For non-magnetic media (\( \mu = 1 \)), the Maxwell’s equations and (2) can be written as the Schrödinger equation, \( i \dot{\psi}(t) = \mathcal{H}\psi(t) \), in which the wave function and the Hamiltonian are defined by

\[
\psi = \begin{pmatrix} \varepsilon_{\infty}^{1/2} \mathbf{E} \\ \mathbf{B} \\ \mathbf{Q}_1 \\ \mathbf{Q}_2 \end{pmatrix}, \quad \mathcal{H} = \begin{pmatrix} 0 & ic\varepsilon_{\infty}^{-1/2} \nabla \times & 0 & -i\omega_p \\ -ic\nabla \times \varepsilon_{\infty}^{-1/2} & 0 & 0 & 0 \\ 0 & 0 & 0 & i\omega_T \\ i\omega_p & 0 & -i\omega_T & -i\eta \end{pmatrix},
\]

where \( c \) is the speed of light in the vacuum, and \( \mathbf{B} \) is the magnetic field. A solution to the initial-value problem is given by \( \psi(t) = \exp(-i\mathcal{H}t)\psi(0) \). Boundary conditions at medium interfaces are enforced dynamically, that is, parameters of the Hamiltonian \( \mathcal{H} \) are allowed to be discontinuous functions of position. In particular, \( \varepsilon_{\infty,0} \) are set to one in the vacuum, and to some specific values in the medium in question (see Section 4).

The norm of the wave function, \( \|\psi\|^2 = \int d\mathbf{r} \psi^\dagger \psi \), is proportional to the total electromagnetic energy of the wave packet [11, 12]. When the attenuation is not present, \( \eta = 0 \), the Hamiltonian is Hermitian, \( \mathcal{H}^\dagger = \mathcal{H} \), relative to the conventional scalar product in the space of square integrable functions, and the norm (energy) is conserved.

3. The algorithm. The Lanczos propagation scheme is based on a polynomial approximation of the short-time fundamental solution for the Schrödinger equation, \( \psi(t + \Delta t) = \exp(-i\Delta t \mathcal{H})\psi(t) \) [4, 10]. If the exponential is expanded into the Taylor series and the latter is truncated at the order \( O(\Delta t^n) \), then the approximation of \( \psi(t + \Delta t) \) belongs to the Krylov space \( \mathcal{K}_n = \text{Span} \{ \psi(t), \mathcal{H}\psi(t), ..., \mathcal{H}^{n-1}\psi(t) \} \). Let \( \mathcal{P}_n \) be a projection operator of the original Hilbert space onto the Krylov space, \( \mathcal{P}^2_n = \mathcal{P}_n \) and \( \mathcal{P}^\dagger_n = \mathcal{P}_n \). Let \( \mathcal{P}_n \psi = \psi_{(n)} \). The exact solution of the initial-value problem is approximated by a solution of the corresponding initial value problem in \( \mathcal{K}_n \), \( \psi_{(n)}(t + \Delta t) = \exp(-i\Delta t \mathcal{H}^{(n)})\psi_{(n)}(t) \), where \( \mathcal{H}^{(n)} = \mathcal{P}_n \mathcal{H} \mathcal{P}_n \). The accuracy of the approximation is of order \( O(\Delta t^n) \). Hence, for practical needs, it is sufficient to choose \( n \) not so large (typically, \( n \leq 9 \)). Then \( \mathcal{H}^{(n)} \) is a small matrix whose exponential is computed by direct diagonalization. If the Hamiltonian is Hermitian, then the corresponding matrix is symmetric tridiagonal in the Lanczos basis for \( \mathcal{K}_n \) [3, 4]. Therefore the propagation scheme is unitary, that is, the energy (norm) of the initial wave packet is preserved.
which also implies the unconditional stability of the algorithm. Another important feature of the Lanczos propagation scheme for Hermitian Hamiltonians is the dynamical control of accuracy [4, 10].

For non-Hermitian Hamiltonians, one possibility is to use the split method in combination with the Lanczos propagation scheme for the Hermitian part of the Hamiltonian [13]. While the unconditional stability is maintained, the accuracy is limited by the accuracy of the split approximation of the infinitesimal fundamental solution, typically, by $O(\Delta t^2)$. An alternative, mathematically sound, and more accurate procedure is based on the use of the dually orthonormal Lanczos basis in which $H^{(n)}$ retains the tridiagonal complex symmetric structure [3]. In the particular case of a complex symmetric $H$, the use of the dual Krylov space can be avoided. There is an orthogonal Lanczos basis for $K_n$ in which $H^{(n)}$ is also complex symmetric tridiagonal, but the orthogonality is now understood with respect to a new scalar product (without complex conjugation of vectors) [14]. However, in both the cases, the projector $P_n$ is no longer Hermitian. This has an unpleasant consequence. One can show that, while the accuracy remains of the order $O(\Delta t^n)$, the unconditional stability is typically lost. The algorithm is only conditionally stable. A more detailed study of such schemes will be given elsewhere. Here we focus on developing an unconditionally stable algorithm. For this purpose we construct an orthonormal basis for $K_n$ itself, ignoring the dual Krylov space and making $P_n$ Hermitian. In this basis $H^{(n)}$ has a Hessenberg form, that is, it is upper-triangular with one extra non-zero lower superdiagonal [14]. A direct diagonalization of such a matrix is still not expensive for small $n$. The dynamical control of accuracy is also preserved.

Let $\psi_j$, $j = 0, 1, ..., n - 1$, form an orthonormal basis for $K_n$ that is constructed as follows. Set $\phi_0 = \psi(t)$ and $\psi_0 = \phi_0 / \| \phi_0 \|$. Compute $h_{00}^{(n)} = (\psi_0, H\psi_0)$ where $(\cdot, \cdot)$ denotes the conventional scalar product in the Hilbert space of square integrable functions. For $j = 1, 2, ..., n - 1$, compute

$$
\phi_j = H\psi_{j-1} - \sum_{k=0}^{j-1} h_{kj-1}^{(n)} \psi_k, \quad \psi_{j} = \frac{\phi_j}{\| \phi_j \|}, \quad h_{jj-1}^{(n)} = (\psi_{j}, H\psi_{j-1}),$$

and, for $k = 0, 1, ..., j$, compute

$$
h_{kj}^{(n)} = (\psi_k, H\psi_j). \quad (6)
$$

By construction, $(\psi_j, \psi_k) = \delta_{jk}$. Let $\psi_{(n)}(t + \Delta t) = P_n\psi(t + \Delta t) = \sum_{k=0}^{n-1} c_k(\Delta t)\psi_k$ where $c_k(\Delta t) = (\psi_k, \psi(t + \Delta t))$. Note that the basis functions $\psi_j$ depend on $t$ and so do $c_j$. For brevity of notations, the dependence on $t$ of all quantities involving $\psi_j$ is not explicitly shown in what follows. The expansion coefficients $c_k$ are united into a complex column $c$ with $n$ entries. It is straightforward to infer that $c(\Delta t)$ satisfies the Schrödinger equation $i\dot{c} = h^{(n)}c$ with the initial condition $c_k(0) = \delta_{k0}$. The matrix $h^{(n)}$ has a Hessenberg form and is the projected Hamiltonian $H^{(n)}$ in the basis constructed. Thus $c(\Delta t) = \exp(-i\Delta th^{(n)})c(0)$. The exponential of the Hessenberg matrix $h^{(n)}$ is computed by direct diagonalization.

To compute the basis functions, multiple actions of the Hamiltonian $H$ on the current
wave function $\psi(t)$ are required. This is done by the Fourier pseudospectral method on a finite grid [5]. To suppress reflections of the wave packet from grid boundaries, absorbing boundary conditions are enforced by a conducting layer placed at the grid edges (see, e.g., [15]). The position dependence of the conductivity $\sigma$ is adjusted to suppress reflections with desired accuracy in the frequency range of interest. The Hamiltonian $H$ is modified accordingly. In the upper left corner of $H$ in (3), the function $-4\pi i\sigma$ is inserted instead of zero.

Let us discuss the stability of the algorithm. In a time-stepping algorithm, an amplification matrix $G(\Delta t)$ is defined by $\psi(t + \Delta t) = G(\Delta t)\psi(t)$. The algorithm is unconditionally stable if $\|G^N(\Delta t)\| \leq \text{const}$ uniformly for all integers $N > 0$, $\Delta t \geq 0$ and all other parameters characterizing the system [16]. The norm of an operator is defined by $\|G\| = \sup \|G\psi\|/\|\psi\|$. For any $H$ the following decomposition holds: $H = H_0 + iV$ where $H_0$ and $V$ are Hermitian. Clearly, $V$ is responsible for attenuation in any physically reasonable model of a passive medium. The norm of the initial-value problem solution decreases with time if $V$ is negative semidefinite, that is, for any $\psi$, $(\psi, V\psi) \leq 0$. Now we prove that the Lanczos algorithm with the Hessenberg projected Hamiltonian (6) is unconditionally stable, provided $V$ of the total Hamiltonian is negative semidefinite.

Observe that $\|\exp(-i\Delta t H)\| \leq 1$ for $\Delta t > 0$ and all parameters of $H$ for which $V$ remains negative semidefinite. The amplification matrix has the form $G(\Delta t) = \exp(-i\Delta t H^{(n)})$. Thanks to the Hermiticity of $P_n$, it is sufficient to show that $V^{(n)} = P_n V P_n$ is negative semidefinite because the latter implies that $\|G^N(\Delta t)\| \leq \|G(\Delta t)\|^N \leq 1$ uniformly for all integers $N > 0$, $\Delta t > 0$, and all parameters of $H$. For any $\psi$, the following chain of equalities holds, $(\psi, V^{(n)}\psi) = (\psi, P_n V P_n \psi) = (\psi^{(n)}, V\psi^{(n)}) \leq 0$. In the first equality, the definition of $V^{(n)}$ has been used, in the second one, the Hermiticity of the projection operator has been invoked, and the final inequality is valid since $V$ is negative semidefinite. The proof is completed.

The most expensive operation of the algorithm is the action of the Hamiltonian on the wave function. Bearing also in mind the accumulation of round-off errors, when computing powers of $H$ with broad spectrum (cf. [3]), this implies that the dimension of the Krylov space has to be as small as possible at each time step while controlling the approximation error. In the case of Hermitian Hamiltonians, the $n$ needed at a specified time step can be deduced from the condition [4] that $|c_{n-1}(\Delta t)|^2 \leq \epsilon$ where $\epsilon$ is a small number. This condition is based on the fact that $c_{n-1}(\Delta t) \sim O(\Delta t^{n-1})$. Note that $c_{n-1}$ determines the weight of $H^{n-1}\psi(t)$ in the Taylor expansion of $\psi(t + \Delta t)$. In our algorithm for a non-Hermitian $H$, the time evolution of the vector $c$ is generated by a Hessenberg matrix $h^{(n)}$. By examining the Taylor expansion of the exponential in $\exp(-i\Delta th^{(n)}c(0))$ it is easy to convince oneself that $c_{n-1}(\Delta t) \sim O(\Delta t^{n-1})$ remains valid thanks to $c_j(0) = \delta_{j0}$. Thus, the same dynamical accuracy control can be used. In particular, in our simulations the dimension of the Krylov space at each time step is determined by $|c_{n-3}|^2 + |c_{n-2}|^2 + |c_{n-1}|^2 \leq \epsilon$ at a fixed $\Delta t$ to control weights of three highest Krylov vectors in the approximate solution, and $\epsilon \sim 10^{-14}$ with $\Delta t$ being fixed. Note, however, that both the propagation parameters $n$ and $\Delta t$ can be varied at each time step to minimize computational costs at the given accuracy level.
4. Ionic crystal gratings. The algorithm has been applied to simulate the scattering of broad band electromagnetic (laser) pulses on a grating structure consisting of circular parallel ionic crystal cylinders periodically arranged in vacuum. Our primary interest is to study the effect of trapped modes (guided wave resonances) and polaritonic excitations on transmission and reflection properties of the grating in the infrared range. The dielectric function of the ionic crystal material is approximated by the single oscillator model (1). Following the work [7], we choose the parameters representative for the beryllium oxide: 
\[ \epsilon_\infty = 2.99, \quad \epsilon_0 = 6.6, \quad \omega_T = 87.0 \text{ meV}, \quad \text{and} \quad \eta = 11.51 \text{ meV}. \]
The packing density \( R/D_g = 0.1 \), where \( R \) is the radius of cylinders and \( D_g \) is the grating period, has been kept fixed in simulations. The cylinders are set parallel to the \( y \) axis. The structure is periodic along the \( x \) axis, and the \( z \) direction is transverse to the grating. A Gaussian wave packet propagating along the \( z \) axis is used as an initial configuration. It is linearly polarized with the electric field oriented along the \( y \) axis, i.e., parallel to the cylinders (the so called TM polarization). 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 periodic structure [17]. The zero diffraction mode is studied here for wavelengths \( \lambda \geq D_g \) so that reflected and transmitted beams propagate along the \( z \)-axis. Similar to our previous works [11, 13] we use a change of variables in both \( x (x = f_1(\xi)) \) and \( z (z = f_2(\zeta)) \) coordinates to enhance the sampling efficiency in the vicinity of medium interfaces. A typical size of the mesh corresponds to \( -17D_g \leq z \leq 15D_g \), and \( -0.5D_g \leq x \leq 0.5D_g \) with, respectively, 384 and 64 knots. Note that, because of the variable change, a uniform mesh in the auxiliary coordinates \( (\xi, \zeta) \) corresponds to a non-uniform mesh in the physical \( (x, z) \) space.

Two types of resonances are expected for the gratings studied here. Structure resonances are associated with the existence of guided wave modes [9, 13]. They are characteristic for periodic dielectric gratings and, in the absence of losses, lead to the 100% reflection within a narrow frequency interval(s) for wavelengths \( \lambda \sim D_g \). The second type of resonances arise because of polariton excitations for wavelengths \( \lambda \sim D_T = 2\pi c/\omega_T \). Calculations have been done for different values of \( D_g \) so that the polaritonic excitation can be tuned throughout the wavelength range of interest \( (\lambda/D_g \geq 1) \) by changing the ratio \( D_T/D_g \).

In Fig. 1 we show the results obtained for the transmission (blue curves) and reflection (red curves) coefficients for the beryllium oxide gratings characterized by the period \( D_g \) such that \( D_T/D_g = 0.5, 2.5, \) and \( 4 \) as indicated in the figure. The results are presented as a function of the radiation wavelength measured in units of the grating period. Note that the logarithmic scale is used for the horizontal axis in order to improve the resolution at small wavelengths. Consider first the following two limiting cases. According to (1), for short wavelengths \( \lambda \ll D_T \) \( (D_g \ll D_T) \), the medium behaves as a dielectric with \( \epsilon \approx \epsilon_\infty \). In the long wavelength limit \( \lambda \gg D_T \) \( (D_g \gg D_T) \), the medium responds as a dielectric material characterized by \( \epsilon \approx \epsilon_0 \). In Fig. 1 the dashed and solid black curves represent the reflection coefficient of the grating made of a lossless, non-dispersive dielectric with \( \epsilon = \epsilon_\infty \) and \( \epsilon = \epsilon_0 \), respectively. In agreement with the previously published results [13], the reflection coefficient in these two cases reaches 1 within a narrow frequency range for \( \lambda \sim D_g \). This 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 [9, 11]. The width of the resonances is determined by the lifetime of the corresponding quasi-stationary trapped mode which is a standing wave along the $x$ axis and is excited by the incoming wave. The width increases with $\varepsilon$ while the resonant wavelength gets redshifted, which explains the difference between the dashed and solid black curves ($\varepsilon_0 > \varepsilon_\infty$).

Now we turn to the discussion of the effects due to dispersive properties of the ionic crystal material. For $D_T/D_g = 0.5$, the resonant excitation of polaritons is impossible within the range of wavelengths of interest, and the dielectric constant is close to $\varepsilon_0$. The result for the reflection coefficient in this case is similar to the data shown by the black solid curve. However, there is an essential difference as compared to the case of a lossless, non-dispersive dielectric grating. Indeed, for a lossless medium the sum of the reflection and transmission coefficients must be one, which is not the case for the beryllium oxide model because of the damping (the dashed-dotted green curve). The maximal loss of energy corresponds to the resonant wavelength. It is easily understood because the trapped mode remains in contact with the material much longer than the main pulse, and, therefore, can dissipate more energy.

For $D_T/D_g = 2.5$, two resonances emerge leading to the enhanced reflection within the corresponding frequency ranges. The one at $\lambda/D_g \sim 2.5$, i.e., $\lambda \sim D_T$, is associated with polaritonic excitations of the ionic crystal. The resonance at $\lambda \sim D_g$ is a structure resonance. As follows from (1), the dielectric constant in this case approaches $\varepsilon_\infty$ for small wavelengths $\lambda \sim D_g$. Then the width and position of the structure resonance are close to the data given by the dashed black curve. The imaginary part of the dielectric function is large enough through out the entire wavelength range to produce a substantial energy loss at both the resonances.

Finally, for $D_T/D_g = 4$ the polariton excitation appears at $\lambda \sim 4D_g$ and the two resonances are well separated. The structure resonance at $\lambda \sim D_g$ closely matches the result for a lossless, non-dispersive dielectric grating characterized by $\varepsilon = \varepsilon_\infty$. Observe that the reflection coefficient is close to 1 in this case and the energy loss is small because the imaginary part of $\varepsilon(\omega)$ is small far from $\omega = \omega_T$.

Figs 2 and 3 show the reflection and transmission coefficients of the grating as functions of the incident radiation wavelength and the grating period $D_g$. The polariton resonance wavelength $D_T = 2\pi c/\omega_T$ and the packing density $R/D_g$ are kept fixed. The results for the two limiting cases in which $\varepsilon = \varepsilon_0$ and $\varepsilon = \varepsilon_\infty$ are represented by the left most and right most colored columns, respectively. The resonance pattern of the system is clearly visible, in particular, the transformation of the structure resonance at $\varepsilon = \varepsilon_0$ into the polaritonic one. Thus, by increasing the ratio $D_T/D_g$, the “broad” structure resonance associated with $\varepsilon = \varepsilon_0$ is turned into the polaritonic resonance and follows the diagonal of the plot ($\lambda/D_g = D_T/D_g$). At the same time, starting approximately with $D_T/D_g = 2$, the “narrow” structure resonance associated with $\varepsilon = \varepsilon_\infty$ emerges and fully develops for $D_T/D_g = 4$.

Finally we would like to show the sensitivity of the results to the attenuation in the present system. In Fig. 4, the transmission and reflection coefficients are presented for two different choices of the attenuation $\eta$ in (1). The geometry of the grating structure is set
by $D_T/D_g = 2.5$. The upper panel of the figure corresponds to $\eta = 11.51$ meV as used throughout this paper. The lower panel of the figure corresponds to the damping reduced by the factor of 20: $\eta \to \eta/20$. Overall features are qualitatively the same in both the cases. Thus, both the structure resonance at $\lambda \sim D_g$ and polaritonic resonance at $\lambda \sim 2.5D_g$ are present, accompanied by the reduced transmission and enhanced reflection. As the wavelength increases from the structure resonance, the reflectivity of the grating drops to zero. Its subsequent onset for $\lambda > 1.683D_g$ is linked with the metal-type behavior of the ionic crystal ($\varepsilon$ becomes negative). The characteristic frequency for the “metallization” can be deduced from the Lyddane-Sachs-Teller relation $\omega_L = \omega_T \sqrt{\varepsilon_0 / \varepsilon_\infty}$, leading to $\lambda_L = 1.683D_g$ for $\lambda_T = 2.5D_g$. Despite these common features, the reduction of the attenuation leads to essential changes. In contrast to the upper panel of the figure, for $\eta \to \eta/20$ the transmission coefficient reaches nearly 0 at both the resonances, and the reflection coefficient is close to 1. Moreover, new structures appear in the polaritonic resonance for $\lambda = D_T$, i.e., as $\varepsilon$ changes from large negative to large positive values. These structures are completely washed out for the medium with large damping. This result indicates the importance of accurate modeling of losses in polaritonic media in order to make reliable predictions of transmission and reflection properties of grating structures and photonic crystals.

5. Conclusions. We have developed an unconditionally stable (time-domain) algorithm for initial value problems in electrodynamics of inhomogeneous, dispersive, and absorptive media. The method is based on the three essential ingredients: (i) the Hamiltonian formalism in electrodynamics of passive media, (ii) the Lanczos propagation scheme, modified to account for attenuation, and (iii) the Fourier pseudospectral method on non-uniform grids induced by change of variables to enhance the sampling efficiency in the vicinity of sharp inhomogeneities of the medium. Apart from the unconditional stability, the algorithm allows for a dynamical accuracy control, meaning that the two propagation parameters, the dimension of the Krylov space and the time step, may automatically be adjusted to minimize computational costs in due course of simulations, while controlling error.

The algorithm has been tested by simulating the scattering of infrared electromagnetic pulses on periodic gratings composed of parallel cylinders that are made of the ionic crystal material. The Lorentz model describing dielectric properties of such a material is rather representative and used to model a vast variety of dielectric materials. Our results demonstrate the role of structure (or guided wave) resonances and polaritonic excitations for the transmission and reflection properties of grating structures. The results are also shown to be sensitive to the attenuation of polaritonic media.

Acknowledgments. S.V.S. thanks the LCAM of the Universeity of Paris-Sud and, in particular, Dr. V. Sidis for support and warm hospitality extended to him during his stay in Orsay. S.V.S. is also grateful to Dr. R. Albanese (US Air Force Brooks Research Center, TX), Profs. J.R. Klauder and T. Olson (University of Florida) for the continued support of this project. The authors thank Dr. D. Wack (KLA-Tencor, San Jose, CA) for stimulating and supporting the work on this project.
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Figure captions

Fig. 1. Calculated zero-order reflection (red curves) and transmission (blue curves) coefficients for the ionic crystal grating described in the text. The results are presented as a function of the incident radiation wavelength measured in units of the grating period $D_g$. Different panels of the figure correspond to different values of the grating period as compared to the resonance wavelength for the polaritonic excitation of the material, $D_T = 2\pi c/\omega_T$. The dashed and solid black curves represent the reflection coefficient calculated for the grating made of a lossless, non-dispersive dielectric characterized by $\varepsilon = \varepsilon_\infty$ and $\varepsilon = \varepsilon_0$, respectively. The sum of the reflection and transmission coefficients is shown as the dashed-dotted green curve. Its deviation from 1 represents the electromagnetic energy loss because of the attenuation.

Fig. 2. The zero-order transmission coefficient for the ionic crystal grating described in the text as a function of the incident radiation wavelength and the grating period. The horizontal axis represents the ratio $D_T/D_g$ of the resonance wavelength for the polaritonic excitation of the material $D_T = 2\pi c/\omega_T$ and the grating period $D_g$. The vertical axis represents the incident radiation wavelength $\lambda$ measured in units of $D_g$. Color codes used for the plot are shown in the inset.

Fig. 3. The zero-order reflection coefficient for the ionic crystal grating described in the text as a function of the incident radiation wavelength and the grating period. The horizontal axis represents the ratio $D_T/D_g$ of the resonance wavelength for the polaritonic excitation of the material $D_T = 2\pi c/\omega_T$ and the grating period $D_g$. The vertical axis represents the incident radiation wavelength $\lambda$ measured in units of $D_g$. Color codes used for the plot are shown in the inset.

Fig. 4. Calculated zero-order reflection (red curves) and transmission (dashed blue curves) coefficients for the ionic crystal grating. The sum of the reflection and transmission coefficients is shown as the dashed-dotted green curve. The geometry of the grating structure is set by $D_T/D_g = 2.5$. The upper panel of the figure corresponds to the attenuation $\eta = 11.51$ meV as used throughout the paper. The lower panel of the figure corresponds to the damping reduced by the factor of 20: $\eta \rightarrow \eta/20$. The vertical black line defines the resonant wavelength $\lambda = D_T = 2\pi c/\omega_T$. 
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