Model Dispersive Media in Finite-Difference Time-Domain Method With Complex-Conjugate Pole-Residue Pairs

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***Abstract*—In this letter, we show that both Debye poles and Lorentz pole pairs are special cases of complex-conjugate pole-residue pairs, and the general form of such pairs is in fact far more efficient than the commonly used Debye poles and Lorentz pole pairs for modeling real dispersive media with the finite-difference time-domain method. We first derive an alternative formulation of the auxiliary differential equation method for arbitrary dispersive media based on general complex-conjugate pole-residue pairs. We then numerically demonstrate the efficiency of using these pairs in modeling dispersive media.**

***Index Terms*—Auxiliary differential equation method, dispersive medium, finite-difference time-domain (FDTD).**

I. Introduction

THE finite-difference time-domain (FDTD) method has been widely used to model dispersive media because it allows the treatment of broadband response in a single simulation run [1]–[18]. For this purpose, one needs to accurately and efficiently incorporate real material dispersions. At present, the common practice is to fit a given permittivity function as the sum of multiple Debye poles or Lorentz pole pairs. However, in many practical situations the number of poles required for such a fit can become quite large, which directly leads to a high computational cost.

Here, we propose to describe a permittivity function as the sum of multiple complex-conjugate pole-residue pairs. We show by numerical examples that this new fitting basis can lead to a substantial saving in both the memory space and CPU time consumption. We also derive a corresponding formulation of the auxiliary differential equation (ADE) method [7], [8], [12], in part because the ADE method is particularly attractive for modeling nonlinear dispersive effects [5], [15]. Also, the ADE method can be readily combined with other differential equations, e.g., the rate equation in laser simulations [9], [16], [17] to simulate complex device behaviors.

II. Formulation

We propose to model the permittivity of a given dispersive medium as the sum of complex-conjugate pole-residue pairs

permittivity inf freq

$$\varepsilon(\omega) = \varepsilon_0\varepsilon_\infty + \varepsilon_0 \sum_{p=1}^{P} c_p/(j\omega - a_p) + c_p^*/(j\omega - a_p^*), \quad (1)$$

cp,ap => units of freq

where the real part of a_p is negative such that $\varepsilon(\omega)$ is stable and causal. This model readily yields an ADE formulation. For each term in the summation in (1), we introduce two complex quantities $\vec{J_p}(\omega)$ and $\vec{J_p'}(\omega)$, defined as

$$\vec{J_p}(\omega) = \varepsilon_0 \frac{c_p}{j\omega - a_p} j\omega \vec{E}(\omega) \quad (2)$$

$$\vec{J_p'}(\omega) = \varepsilon_0 \frac{c_p^*}{j\omega - a_p^*} j\omega \vec{E}(\omega). \quad (3)$$

In the time domain, (2) and (3) become

$$\frac{d}{dt}\vec{J_p}(t) - a_p \vec{J_p}(t) = \varepsilon_0 c_p \frac{d}{dt}\vec{E}(t) \quad (4)$$

$$\frac{d}{dt}\vec{J_p'}(t) - a_p^* \vec{J_p'}(t) = \varepsilon_0 c_p^* \frac{d}{dt}\vec{E}(t). \quad (5)$$

Since $\vec{E}(t)$ is real in standard FDTD implementations, $\vec{J_p'}(t) = \vec{J_p^*}(t)$ always holds provided that they have the same initial values. Thus, we only need to store and update either $\vec{J_p}(t)$ or $\vec{J_p'}(t)$ instead of both. Combining the auxiliary differential equation (4) and the Maxwell curl equations, we arrive at the corresponding ADE-FDTD implementation

$$\vec{E}^{(n+1)\Delta t} = \left(\frac{2\varepsilon_0\varepsilon_\infty + \sum_{p=1}^{P} 2\mathrm{Re}(\beta_p) - \sigma\Delta t}{2\varepsilon_0\varepsilon_\infty + \sum_{p=1}^{P} 2\mathrm{Re}(\beta_p) + \sigma\Delta t}\right)\vec{E}^{n\Delta t} + \frac{2\Delta t \cdot \left[\nabla \times \vec{H}^{(n+1/2)\Delta t} - \mathrm{Re}\sum_{p=1}^{P}(1+k_p)\vec{J_p}^{n\Delta t}\right]}{2\varepsilon_0\varepsilon_\infty + \sum_{p=1}^{P} 2\mathrm{Re}(\beta_p) + \sigma\Delta t} \quad (6)$$

$$\vec{J_p}^{(n+1)\Delta t} = k_p \vec{J_p}^{n\Delta t} + \beta_p \left(\frac{\vec{E}^{(n+1)\Delta t} - \vec{E}^{n\Delta t}}{\Delta t}\right) \quad (7)$$

where

need to compute as complex number due to division
(Re(a/b) != Re(a)/Re(b)

$$k_p = \frac{1 + a_p\Delta t/2}{1 - a_p\Delta t/2}, \quad \beta_p = \frac{\varepsilon_0 c_p \Delta t}{1 - a_p\Delta t/2}$$

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we do E^(n+1/2) and H^(n+1)

and σ denotes the electric conductivity. During the simulation, each new time step starts with calculating $\vec{E}^{(n+1)\Delta t}$ using (6), then all the $\vec{J}_p^{(n+1)\Delta t}$ components are updated using (7), and finally $\vec{H}^{(n+3/2)\Delta t}$ are obtained from the standard Yee algorithm. In our derivation, we adopt the semi-implicit difference scheme [7] to achieve the full synchronism.

In particular, when $c_p = \Delta\varepsilon_p/(2\tau_p)$ and $a_p = -1/\tau_p$, the formulation described above is exactly the same as the known ADE formulation for a medium modeled by Debye poles [1]. On the other hand, when $c_p = j\Delta\varepsilon_p\omega_p^2/(2\sqrt{\omega_p^2 - \delta_p^2})$ and $a_p = -\delta_p - j\sqrt{\omega_p^2 - \delta_p^2}$, we get an alternative ADE formulation for a medium modeled by Lorentz pole pairs. Here, $\Delta\varepsilon_p, \tau_p, \omega_p$, and δ_p are the parameters for characterizing Debye poles and Lorentz pole pairs [1]. Therefore, in our ADE formulation Debye media and Lorentz media are treated in a unified manner. Compared to the current ADE formulations in which the two media are treated differently, our unified formulation reduces the implementation complexity.

As to the memory cost, to update each electrical field component, P auxiliary complex variables, i.e., $2P$ auxiliary real variables, are needed. That is the same as what are required by using P Lorentz pole pairs in the latest ADE formulation [12]. However, in contrast to a Lorentz pole pair in which c_p is purely imaginary, a complex-conjugate pole-residue pair can have a real part in its c_p. With these additional degrees of freedom, one should be able to fit a given permittivity function more accurately with the same number of poles than using Debye poles or Lorentz pole pairs. Below, we show that this is indeed the case. Thus, using complex-conjugate pole-residue pairs does increase the computational efficiency.

III. Numerical Result

We demonstrate the improved computational efficiency from the proposed fitting basis of complex-conjugate pole-residue pairs by modeling two material systems: metal Ag and GaAs/AlGaAs quantum wells.

The permittivity of a metal is usually approximated with the Drude–Lorentz model [19], in which the Drude part can be viewed as a special Lorentz pole pair with the resonance frequency ω_p set to zero. For Ag, however, the frequency range that the Drude–Lorentz model can cover is in fact quite limited [20]. We consider the optical constant data of Ag over a very broad frequency range (0.125–5.0 eV), which are taken from [21]. As shown in Fig. 1, with one Drude pole pairs and as many as five Lorentz pole pairs, the optimized fit of Ag's permittivity function [20] performs rather poorly at photon energies higher than 4.5 eV. Instead, if we do the fitting with six complex-conjugate pole-residue pairs, which have the same computational cost, a significant increase in both the accuracy and the covered frequency range can be achieved. The parameters for these pairs are listed in Table I. They are obtained through standard nonlinear least-square analysis.

Fig. 2 shows the FDTD simulation result of the transmittance of a 100 nm thick Ag slab in air. The spatial resolution in the simulation is chosen to be 1/40 of the shortest wavelength of interest. The transmittance spectrum calculated with the ADE formulation in Section II, using the six complex-conjugate pole-residue pairs in Table I, follows the analytic result closely. This further confirms the quality of the fit by using the complex-conjugate pole-residue pairs and verifies numerically the ADE formulation derived in Section II. In contrast, the transmittance spectrum calculated by using the one Drude and five Lorentz pole pairs [20] deviates significantly from the analytic result. For the same computational cost, there is clearly an advantage of using complex-conjugate pole-residue pairs for the FDTD broadband simulation of dispersive media.

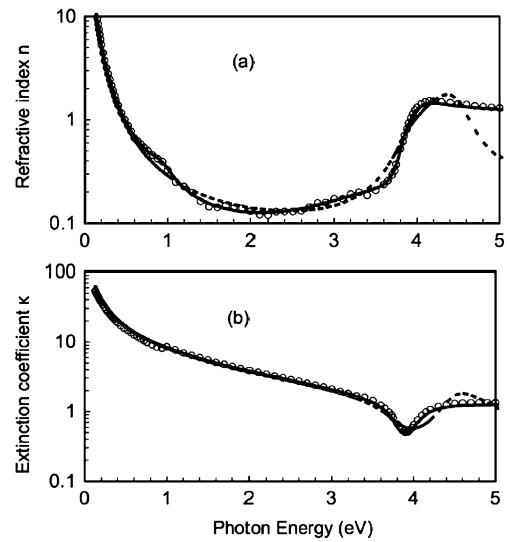

Fig. 1. (a) Real and (b) imaginary parts, i.e., n and κ, of Ag's complex refractive index $n - j\kappa$. The circles represent the experimental data taken from [21], the solid line represents the fitting result with the six pole-residue pairs listed in Table I, and the dashed line represents the fitting result with one Drude and five Lorentz pole pairs listed in [20].

TABLE I
Values of the Complex-Conjugate Pole-Residue Pairs for Modeling the Permittivity of Ag

Parameters	*Values (unit:eV)*
(c_1, a_1)	$(5.987\times10^{-1}+j4.195\times10^{3},\ -2.502\times10^{-2}-j8.626\times10^{-3})$
(c_2, a_2)	$(-2.211\times10^{-1}+j2.680\times10^{-1},\ -2.021\times10^{-1}-j9.407\times10^{-1})$
(c_3, a_3)	$(-4.240+j7.324\times10^{2},\ -1.467\times10^{1}-j1.338)$
(c_4, a_4)	$(6.391\times10^{-1}-j7.186\times10^{-2},\ -2.997\times10^{-1}-j4.034)$
(c_5, a_5)	$(1.806+j4.563,\ -1.896-j4.808)$
(c_6, a_6)	$(1.443-j8.219\times10^{1},\ -9.396-j6.477)$

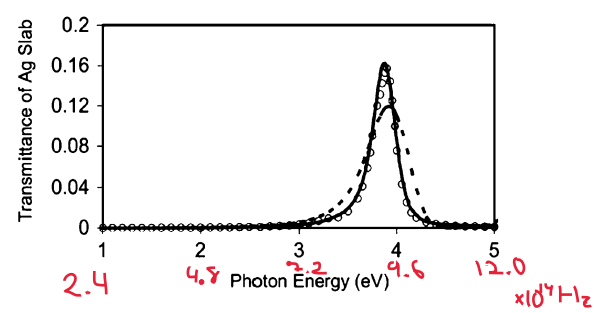

Fig. 2. Transmittance of a 100-nm-thick Ag slab. The circles represent the analytic results, the solid line represents the FDTD simulation result by using the six complex-conjugate pole-residue pairs in Table I, and the dashed line represents the FDTD simulation result by using the one Drude and five Lorentz poles pairs in [20].

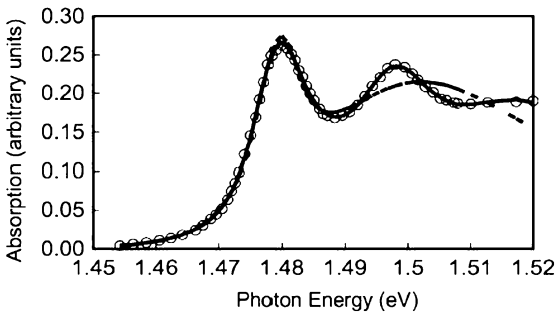

Fig. 3. Electroabsorption spectrum of GaAs/$Al_{0.4}Ga_{0.6}As$ quantum wells at room temperature. The reverse-biased voltage is zero, the well thickness is 95 Å, and the barrier thickness is 65 Å. The circles represent the measured data taken from [23], the solid line represents the fitting result with three complex-conjugate pairs, and the dashed line represents the fitting result with three Lorentz pole pairs.

As a second example, we consider the electroabsorption coefficient of semiconductor quantum wells. The use of quantum wells as a voltage-controllable absorber is important for active micro-resonator devices [22]. For these applications, the frequency range of interest is much narrower than that in the first example. Nevertheless, due to the strong dispersion, it still requires a large number of Lorentz pole pairs to fit the permittivity function well. As Fig. 3 shows, for the electroabsorption spectrum of a GaAs/$Al_{0.4}Ga_{0.6}As$ quantum well given in [23], using three Lorentz pole pairs cannot accurately reproduce the whole spectrum of interest. On the contrary, three complex-conjugate pole-residue pairs are sufficient for this purpose. To obtain a comparable accuracy with Lorentz pole pairs, as many as five pairs have to be used.

Finally, we note that although in this letter we focus on the ADE method, the proposed complex-conjugate pole-residue pairs can be implemented in the piecewise-linear recursive convolution (PLRC) method as well. A similar extension of the PLRC method was in fact discussed in [10], yet no example was given beyond the well-known Debye and Lorentz media types. In conclusion, the use of complex-conjugate pole-residue pairs, which can be implemented with minor modifications of standard FDTD algorithms, results in substantial improvement in the modeling of realistic dispersive media.

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