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Time Domain Modeling of Tunable Response of Graphene

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Abstract: We present a causal numerical model for time domain simulations of the optical response of graphene. The dielectric function is approximated with a conductivity term, a Drude term and a number of the critical points terms.
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1. Introduction

Graphene has lately received a lot of interest for plasmonics due to its tunable optical response that can be controlled by an applied voltage and temperature, see e.g. [1]. Recently we have demonstrated a graphene-antenna hybrid device for controlling the damping of a plasmonic resonance with an applied voltage [2] and studied the tunability of Fano resonances in a dolmen structure with graphene [4]. For the dielectric function of graphene we use the local random-phase approximation [3], where the intraband and interband conductivities are represented as integrals of a Fermi-Dirac distribution. The interband integral does not have an antiderivative in elementary functions (except for asymptotes in a limited range of parameters) and was previously evaluated by numerical integration in our frequency-domain simulations [2, 4].

However, the time domain simulation of electrically controlled graphene devices involving non-linear regimes and ultrafast optical processes would require the evaluation of a broadband, multi-parameter dielectric function for graphene in the time domain, which is complicated with the interband integral. In [5], this integral was fitted with a single Pade approximant and then used in the FDTD simulation. However, the obtained approximation (1) has limited accuracy, (2) is valid in the NIR only, and (3) works solely for a given chemical potential and a given temperature. In this work, we have developed an approach to approximate the dielectric function of graphene with a causal time domain model involving a finite conductivity, a Drude term and a number of critical points terms [6, 7]. This approximation works through a range of chemical potentials, temperatures and scattering rates, providing full control over the parameters in time domain simulations. The model has been tested for one-dimensional graphene structures with a FDTD Maxwell's Equations solver; it shows accurate results and demonstrates the stability of the solver coupled with the proposed model.

2. Numerical Approach and validation

In the frequency domain, the dielectric function of graphene can be derived within the local random-phase approximation [3] as a sum of intraband and interband contribution (left to right)

$$\varepsilon_r(\omega) = \frac{4\sigma_0}{\pi(\omega/\hbar)t_g}\left(\frac{1}{\omega+\iota\Gamma}\int_{\mathbb{R}}|\alpha|f'(\alpha)d\alpha + (\omega+\iota\Gamma)\int_{\mathbb{R}}\frac{\mathrm{sgn}(\alpha)f(\alpha)}{(\omega+\iota\Gamma)^2-4\alpha^2}d\alpha\right),$$

where $f(\alpha) = (1+\exp[T^{-1}(\alpha-\mu)])^{-1}$ is the Fermi-Dirac distribution, t_g is the effective thickness of the graphene sheet [m], ω is the frequency of light [eV], ε_0 is the permittivity of vacuum [F/m], Γ is the carrier scattering rate [eV], T is the temperature normalized by the Boltzmann constant [eV], μ is the chemical potential [eV], $\hbar$ is the reduced Planck constant [eV·s], and $\sigma_0 = e^2/4\hbar$ is conductivity of the undoped graphene [S].

For time domain simulations, this model can be represented as a combination of conductivity, the Drude term, and an integral of critical points terms

$$\varepsilon_r(\omega) = -\frac{\sigma}{\iota\varepsilon_0(\omega/\hbar)} - \frac{\omega_p^2}{\iota\omega\Gamma+\omega^2} + \int_0^\infty \frac{1}{2}\Delta\varepsilon_\alpha\Omega_\alpha\left(\frac{\mathrm{e}^{-\iota\varphi_\alpha}}{\omega+\iota\Gamma+\Omega_\alpha} - \frac{\mathrm{e}^{\iota\varphi_\alpha}}{\omega+\iota\Gamma-\Omega_\alpha}\right)d\alpha\,,$$

where $\omega_p = \sqrt{8\hbar\pi^{-1}t_g^{-1}\varepsilon_0^{-1}\sigma_0 T\ln\left[2\cosh(\mu/2T)\right]}$, $\sigma = \frac{4\sigma_0\Gamma}{\pi t_g}\int_0^\infty \frac{g(\alpha,\mu,T)}{4\alpha^2+\Gamma^2}d\alpha$, $\Delta\varepsilon_\alpha = \frac{2\sigma_0\hbar}{\pi\varepsilon_0 t_g}\frac{g(\alpha,\mu,T)}{\alpha\sqrt{4\alpha^2+\Gamma^2}}$, $\Omega_\alpha = 2\alpha, \varphi_\alpha = \tan^{-1}\Gamma/2\alpha$, $g(\alpha,\mu,T) = \sinh(\alpha/T)\left[\cosh(\mu/T)+\cosh(\alpha/T)\right]^{-1}$. In this representation, all the terms are casual and physically comprehensive. Each critical points term (integrand) corresponds to a decaying oscillator with resonance frequency Ω_α, decay Γ, and phase shift φ_α with an amplitude $\Delta\varepsilon_\alpha$ controlled by the Fermi-Dirac distribution depending on the chemical potential μ and temperature T.

For the numerical implementation, the improper integral is transformed to an integral with finite limits. Then we use the Gauss-Kronrod (GK) integration scheme with adaptive bisection splitting to obtain a quadrature with a given accuracy. The subintervals are combined for a given range of frequencies, temperatures, potentials, and scattering rates to provide the accurate approximation through the needed range of parameters.

Though conventional integration methods with lower accuracy can lead to an overwhelming number of subintervals, with the adaptive GK scheme and 1 percent error tolerance, we obtain only about 80 critical points terms for the wavelength range between 400 nm and 4 μm, for 0 to 0.6 eV chemical potentials, for 4 to 300 K temperatures and for 0.011 eV scattering rates. This 80-term model has been implemented on a one-dimensional FDTD Maxwell's Equations solver with second-order ADE (Auxiliary Differential Equations) and RC (Recursive Convolution) schemes and tested with representative graphene structures. The validation shows stable calculations and accurate results compared to frequency-domain analytical reflection and transmission calculations.

3. Conclusion and future work

Graphene is an exciting new material that is gaining attention as an elementary material for constructing flexible, electrically driven, novel devices. However, the time domain simulations of graphene are complicated with by the restriction of having an accurate, multi-parameter, broadband, casual dielectric function for graphene. In this work we've proposed such a dispersion model derived from the frequency-domain, local random-phase approximation, which is well-suited for broadband, time domain simulations with varying parameters. The validation of our model with a FDTD Maxwell's equations solver shows stable calculations and accurate results. With this model, we plan to extend our simulations to the time domain to support studies of tunable devices with graphene [2, 4].

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4. References

[1] A. Grigorenko, M. Polini, and K. Novoselov, "Graphene plasmonics," Nature Photonics 6, 749-758 (2012).
[2] N. K. Emani, T.-F. Chung, X. Ni, A. V. Kildishev, Y. P. Chen, and A. Boltasseva, "Electrically Tunable Damping of Plasmonic Resonances with Graphene," Nano Letters 12, 5202-5206 (2012).
[3] F. H. L. Koppens, D. E. Chang, and F. J. García de Abajo, "Graphene Plasmonics: A Platform for Strong Light–Matter Interactions," Nano Letters 11, 3370-3377 (2011).
[4] N. K. Emani, T.-F. Chung, L. Prokopeva, A. Kildishev, Y. P. Chen, and A. Boltasseva, "Tuning Fano Resonances with Graphene", CLEO Proceedings, 2013 (submitted)
[5] A. Mock, "Pade approximant spectral fit for FDTD simulation of graphene in the near infrared", Opt. Material Express 2, 771-781 (2012).
[6] P. G. Etchegoin, E. C. Le Ru, and M. Meyer, "An Analytic Model for the Optical Properties of Gold", J. Chem. Phys. **125**, 164705 (2006).
[7] L. Prokopeva, J. Borneman, and A. Kildishev, "Optical dispersion models for time-domain modeling of metal-dielectric nanostructures", IEEE Trans. on Magn. 47, 1150-1153 (2011).