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Optical conductivity of graphene and its Drude-like approximation for FDTD

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In this paper, the optical conductivity of a two-dimensional surface material of graphene is theoretically investigated. An effective method for interpolation of the surface conductivity of grapheme is proposed and worked out in the form of a polynomial expansion in Drude conductivities. The proposed expression will significantly facilitate further FDTD (Finite Difference Time Domain) numerical simulations of optical phenomena in the layered hyperbolic medium based on graphene-dielectric sandwich structure.

Key words: graphene, optical conductivity, resistivity, Formula Kubo in the linear response, Drude-like conductivity.
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1 Introduction

It was rather recently demonstrated both theoretically and experimentally that graphene is a two-dimensional crystal lattice of carbon atoms that exhibits a wide range of unique properties [1-3]. For example, the motion of free electrons inside of a two-dimensional structure of graphene can be described by the Dirac equation since charge carriers in graphene have linear dispersion law (dependence of the electron energy on their wave number) near the Dirac points. As a consequence, various transport effects, characteristic for Dirac fermions, can be observed in grapheme including the quantum Hall effect, the conductance quantization in strong magnetic fields and low temperatures, Shubnikov-de Haas oscillations of the conductivity of two-dimensional electron gas in a strong magnetic fields [4,5]. It was almost immediately shown that the charge carriers in graphene have high mobility, which makes it a promising material for use in a variety of applications, such as a future basis for nanoelectronics and possible substitution of silicon in integrated circuits [6].

In accordance with the aforesaid it is of great interest to study the electrodynamic properties of hyperbolic metamaterial media, which consist of periodically layered structures of graphene and dielectric. In order to adequately simulate the optical properties of graphene media with FDTD the general expression for its surface conductivity is impractical. On the other hand, the Drude-Lorentz model conductivity provides an easy-to-use expression that is routinely handled in FDTD simulations of optical phenomena in media of diverse physical nature. In this paper an idea is put forward to approximate the surface conductivity of graphene by its expansion in the Drude-Lorentz model conductivities with different internal parameters.

2 Conductivity of graphene

In order to consider multilayered hyperbolic metamaterial media based on graphene-dielectric sandwich structure, it is important to understand the behavior of electromagnetic waves at the interface between the graphene and the dielectric. Since the graphene is a two-dimensional conductive medium, its material equations in the Fourier space take the following form:

$$\begin{aligned} \tilde{\mathbf{D}} &= \varepsilon_0 \varepsilon_r \tilde{\mathbf{E}} - \varepsilon_0 \alpha \frac{\theta}{\pi} c_0 \tilde{\mathbf{B}}, \\ c_0 \tilde{\mathbf{H}} &= \frac{c_0 \tilde{\mathbf{B}}}{\mu_0 \mu_r} + \alpha \frac{\theta}{\pi} \frac{\tilde{\mathbf{E}}}{\mu_0 \mu_r}. \end{aligned} \tag{1}$$

Here α denotes the fine structure constant that takes an odd multiple number of π for nontrivial topological materials and zero otherwise.

The boundary conditions for the magnetic and electrical components of the electromagnetic field can be shown at the interface between the graphene and the dielectric as:

$$D_{2\perp} - D_{2\perp} = q_g, \qquad \mathbf{H}_{2\parallel} - \mathbf{H}_{1\parallel} = \mathbf{j}, \qquad (2)$$

where q_g, $\mathbf{j}$ stand for the surface charge and electric current, respectively.

Using the integral formula for Ohm's law, it can be shown that the following holds in the Fourier space:

$$\tilde{D}_{2\perp} - \tilde{D}_{2\perp} = q_g, \qquad \tilde{\mathbf{H}}_{2\parallel} - \tilde{\mathbf{H}}_{1\parallel} = \sigma_g(\omega)\tilde{\mathbf{E}}_{\parallel}, \quad (3)$$

where σ_g is simply the surface optical conductivity.

One of the main problems in the study of electrodynamic properties of graphene is the relative complexity of the representation of its surface conductivity. In most cases, the surface conductivity can be provided under the Kubo approach that takes into account both the electronic intraband and interband transitions. The intraband contribution is described by an expression similar to that of the Drude model, which is very convenient for handling in FDTD simulations. On the contrary the interband contribution is well presented by a rather complex integral. To overcome this difficulty, this work is aimed at interpolating the interband contribution by various methods.

In particular, the optical conductivity of the graphene is written under Kubo approximation in the following form:

$$\sigma_g(\omega,\mu_c,\Gamma,\mathrm{T}) = -\frac{ie^2(\omega+i2\Gamma)}{\pi\hbar^2}\left[\frac{1}{(\omega+i2\Gamma)^2}\int_0^\infty \varepsilon\left(\frac{\partial f_d(\varepsilon)}{\partial\varepsilon} - \frac{\partial f_d(-\varepsilon)}{\partial\varepsilon}\right)d\varepsilon - \int_0^\infty\left(\frac{f_d(-\varepsilon)-f_d(\varepsilon)}{(\omega+i2\Gamma)^2 - 4(\varepsilon/\hbar)^2}\right)d\varepsilon\right], \quad (4)$$

where ε is the energy, $\hbar$ denotes the Planck's constant, e designates the elementary charge, k_B stands for the Boltzmann constant, μ_c is a chemical potential, Γ denotes the scattering parameter, T is the system temperature, $f_d(\varepsilon) = (1+\exp((\varepsilon-\mu_c)/k_BT))^{-1}$ represents the Fermi-Dirac distribution.

3 Drude-like approximation

As a rule expression (4) is not directly applied in the numerical evaluations, various approximations are used instead to calculate the integral over the energy, thus, imposing some restrictions on the range of physical parameters involved. In order to consider the time evolution of the system using, for example, FDTD method together with boundary conditions (2) and material equations (1), it is necessary to interpolate and bring the expression for the surface conductivity to a more convenient form.

In particular, it is convenient to carry out the interpolation of $\rho = 1/\sigma_g$, i.e. of the optical resistance. The main point of this is to write the interpolation expression for the optical conductivity of graphene and topological insulator, in the form of the Drude model-like expansion:

$$\rho_g(\omega) \approx \rho_\infty + \sum_{j=1}^{j=N}\rho_j(\omega), \qquad (5)$$

where

$$\rho_j(\omega) = \begin{cases} \dfrac{r_j}{i\omega - p_k}, & \text{for real part of } r_j \text{ and } p_k \\ \dfrac{r_j}{i\omega - p_k} + \dfrac{r_j^*}{i\omega - p_k^*}, & \text{for imaginary part of } r_j \text{ and } p_k \end{cases}.$$

In most cases, it is enough to take four terms in (5):

$$\rho_l(\omega) = \frac{\left(A_0 - A_2\omega^2 + A_4\omega^4 - A_6\omega^6\right) + i\omega\left(A_1 - A_3\omega^2 + A_5\omega^4 - A_7\omega^6\right)}{\left(1 - B_2\omega^2 + B_4\omega^4 - B_6\omega^6\right) + i\omega\left(B_1 - B_3\omega^2 + B_5\omega^4 - B_7\omega^6\right)} = \frac{N(\omega)}{D(\omega)}, \qquad (6)$$

where A_j, B_j are the real coefficients of interpolation sought.

Introducing the difference between the directly calculated function ρ_g and the interpolating function ρ_l as

$$\varepsilon = \rho_g - \rho_l = \rho_g - \frac{N(\omega)}{D(\omega)}, \qquad (7)$$

it is possible to rewrite it in the form $D(\omega)\varepsilon = D(\omega)\rho_g - N(\omega) = a(\omega) + ib(\omega)$.

The final goal is to minimize the function $E = \sum_{k=1}^{N}(a^2(\omega_k) + b^2(\omega_k))$, which yields the following set of equations for the interpolation coefficients:

$$\frac{\partial E}{\partial A_j} = 0, \qquad \frac{\partial E}{\partial B_j} = 0, \qquad (8)$$

Thus the function ρ_l is obtained from the solution of the set of the linear algebraic equations

$$\begin{pmatrix}
\lambda_0 & 0 & -\lambda_2 & 0 & \lambda_4 & 0 & -\lambda_6 & 0 & T_1 & S_2 & -T_3 & -S_4 & T_5 & S_6 & -T_7 \\
0 & \lambda_2 & 0 & -\lambda_4 & 0 & \lambda_6 & 0 & -\lambda_8 & -S_2 & T_3 & S_4 & -T_5 & -S_6 & T_7 & S_8 \\
\lambda_2 & 0 & -\lambda_4 & 0 & \lambda_6 & 0 & -\lambda_8 & 0 & T_3 & S_4 & -T_5 & -S_6 & T_7 & S_8 & -T_9 \\
0 & \lambda_4 & 0 & -\lambda_6 & 0 & \lambda_8 & 0 & -\lambda_{10} & -S_4 & T_5 & S_6 & -T_7 & -S_8 & T_9 & S_{10} \\
\lambda_4 & 0 & -\lambda_6 & 0 & \lambda_8 & 0 & -\lambda_{10} & 0 & T_5 & S_6 & -T_7 & -S_8 & T_9 & S_{10} & -T_{11} \\
0 & \lambda_6 & 0 & -\lambda_8 & 0 & \lambda_{10} & 0 & -\lambda_{12} & -S_6 & T_7 & S_8 & -T_9 & -S_{10} & T_{11} & S_{12} \\
\lambda_6 & 0 & -\lambda_8 & 0 & \lambda_{10} & 0 & -\lambda_{12} & 0 & T_7 & S_8 & -T_9 & -S_{10} & T_{11} & S_{12} & -T_{13} \\
0 & \lambda_8 & 0 & -\lambda_{10} & 0 & \lambda_{12} & 0 & -\lambda_{14} & -S_8 & T_9 & S_{10} & -T_{11} & -S_{12} & T_{13} & S_{14} \\
T_1 & -S_2 & -T_3 & S_4 & T_5 & -S_6 & -T_7 & S_8 & U_2 & 0 & -U_4 & 0 & U_6 & 0 & -U_8 \\
S_2 & T_3 & -S_4 & -T_5 & S_6 & T_7 & -S_8 & -T_9 & 0 & U_4 & 0 & -U_6 & 0 & U_8 & 0 \\
T_3 & -S_4 & -T_5 & S_6 & T_7 & -S_8 & -T_9 & S_{10} & U_4 & 0 & -U_6 & 0 & U_8 & 0 & -U_{10} \\
S_4 & T_5 & -S_6 & -T_7 & S_8 & T_9 & -S_{10} & -T_{11} & 0 & U_6 & 0 & -U_8 & 0 & U_{10} & 0 \\
T_5 & -S_6 & -T_7 & S_8 & T_9 & -S_{10} & -T_{11} & S_{12} & U_6 & 0 & -U_8 & 0 & U_{10} & 0 & -U_{12} \\
S_6 & T_7 & -S_8 & -T_9 & S_{10} & T_{11} & -S_{12} & -T_{13} & 0 & U_8 & 0 & -U_{10} & 0 & U_{12} & 0 \\
T_7 & -S_8 & -T_9 & S_{10} & T_{11} & -S_{12} & -T_{13} & S_{14} & U_8 & 0 & -U_{10} & 0 & U_{12} & 0 & -U_{14}
\end{pmatrix} \times \begin{pmatrix} A_0 \\ A_1 \\ A_2 \\ A_3 \\ A_4 \\ A_5 \\ A_6 \\ A_7 \\ B_1 \\ B_2 \\ B_3 \\ B_4 \\ B_5 \\ B_6 \\ B_7 \end{pmatrix} = \begin{pmatrix} S_0 \\ T_1 \\ S_2 \\ T_3 \\ S_4 \\ T_5 \\ S_6 \\ T_7 \\ 0 \\ U_2 \\ 0 \\ U_4 \\ 0 \\ U_6 \\ 0 \end{pmatrix}$$

Here

$$\lambda_h = \sum_{k=1}^{k=N} \omega^h; \qquad S_h = \sum_{k=1}^{k=N} \omega^h \Re(\rho_g(\omega_k));$$
$$T_h = \sum_{k=1}^{k=N} \omega^h \Im(\rho_g(\omega_k)); \qquad U_h = \sum_{k=1}^{k=N} \omega^h \,|\, \rho_g(\omega_k) \,| \qquad (9)$$

Figures 1 and 2 display the comparison of the direct numerical integration of the surface conductivity with the interpolation formula to find a very good agreement in a wide range of frequencies. In Fig. 3 the relative error of the absolute value is presented for two fixed values of the chemical potential.

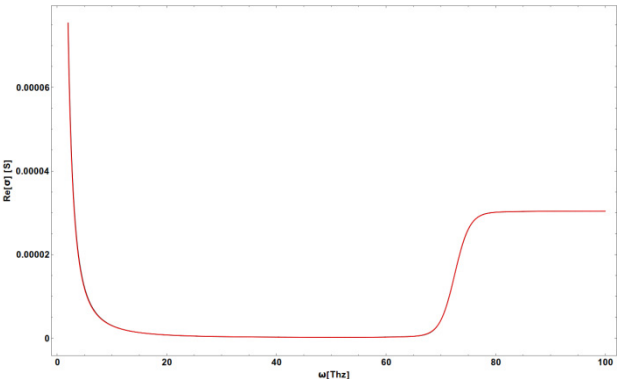

Figure 1 – The real part of the surface conductivity of the exact formula (4) (red curve) and the result of interpolation (blue).

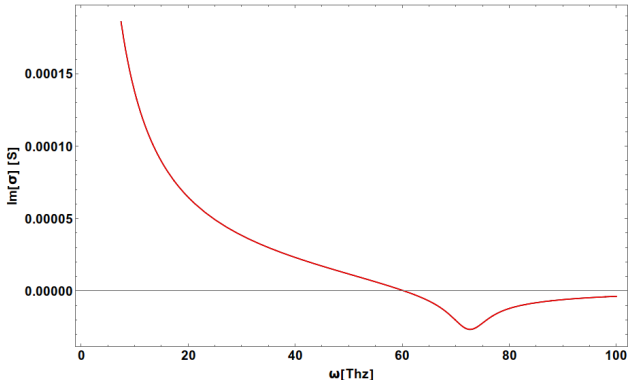

Figure 2 – The imaginary part of the surface conductivity of the exact formula (4) (red curve) and the result of interpolation (blue).

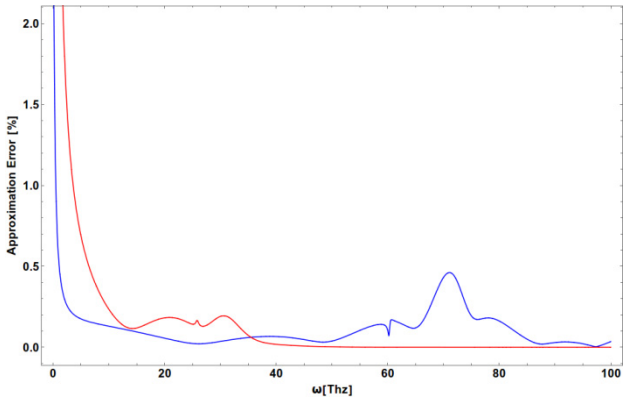

Figure 3. The relative interpolation error ($|1-\sigma_{int}/\sigma_g|\times 100\%$): blue curve: $\mu_c = 150$ [meV]; red curve: $\mu_c = 65$ [meV].

If it is needed for numerical calculations to dynamically change the parameters of the grapheme, the corresponding interpolation must be executed for the range of temperature and/or chemical potential. In this case to perform an interpolation over the frequency and one of the parameters it is necessary to interpolate the coefficients A_j, B_j.

When the chemical potential in the function $\rho_g(\omega, T)$ is treated fixed, the coefficients A_j, B_j are sought in the form of the polynomial relation:

$$A_j = \frac{r_0 + r_1 T + r_2 T^2 + r_3 T^3 + r_4 T^4 + r_5 T^5}{r_6 + r_7 T + r_8 T^2 + r_9 T^3 + r_{10} T^4 + r_{11} T^5}. \quad (10)$$

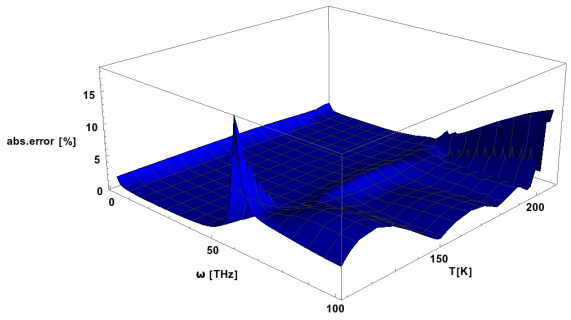

Figure 4 – The relative error of the interpolation for the function $\rho_g(\omega, T)$ at the fixed value of the chemical potential $\mu_c = 150$ [meV].

Figure 4 shows the relative error of the interpolation for the function $\rho_g(\omega, T)$ at the fixed value of the chemical potential $\mu_c = 150$ [meV].

In the case of interpolation with a fixed temperature in the function $\rho_g(\omega, \mu_c)$, the coefficients A_j, B_j are interpolated as a sum of the exponential functions as:

$$A_j = r_0 \exp[r_1 \mu_c] + r_2 \exp[r_3 \mu_c].$$

Figure 5 shows the relative error of interpolation for the function $\rho_g(\omega, \mu_c)$ at a fixed value of the temperature $T = 150$ [meV].

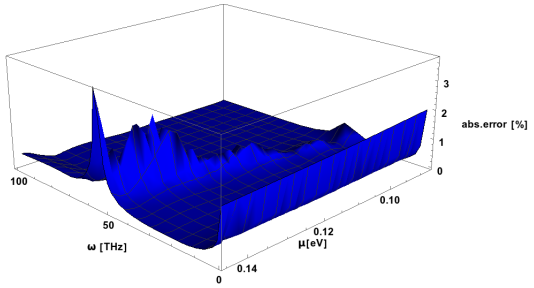

Figure 5 – The relative error of the interpolation for the function $\rho_g(\omega, \mu_c)$ at the fixed value of the temperature $T = 150$ [meV].

4 Conclusion

Thus, in this paper the analysis has been made of the electrodynamic properties of the grapheme. In particular, the surface conductivity has been

studied as a function of the frequency, the chemical potential μ and the temperature T. The effective method has been developed for the interpolation of the surface conductivity of the graphene as a polynomial expansion to find a good agreement for the entire range of values of the chemical potential and the temperature. This ensures effective integration of Maxwell's equations by FDTD simulations with further applications for studying optical phenomena in composite materials based on graphene and topological insulators [7].

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