A closed-form approximate expression for the optical conductivity of graphene

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A closed-form approximate expression for the optical conductivity of graphene is developed, which generates results with less than 0.8% maximum absolute error for $\lambda > 250$ nm. The expression takes wavelength, temperature, chemical potential, and hopping parameter into account and provides a fast, easy, and reliable alternative to well-known methods that include singular integrals. Numerical results confirm that the effective complex electrical permittivity derived from the optical conductivity successfully represents this one atom thick material in three-dimensional electromagnetic simulations and analyses.

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Graphene, a one atom thick sheet of carbon atoms, has been receiving a great deal of interest since its invention [1] due to its exceptional electrical and optical properties. It has found different roles in a wide range of applications including optical modulators [2], transistors [3], p–n junctions [4], sensors [5], transformation optics [6], and many other subjects explained in [7].

One of the several properties of the graphene under careful examination, both theoretically and experimentally, is its two-dimensional (2D) complex optical conductivity ($\sigma_c = \sigma_r + i\sigma_i$) in different parts of the electromagnetic spectrum [8–17]. There are multiple factors determining σ_c: wavelength λ, temperature T, hopping parameter t, and chemical potential μ_c, which is a function of the carrier density and can be controlled by gate voltage, electric field, magnetic field, and/or chemical doping [13,15].

In the last decade, several methods have been developed to calculate the conductivity of graphene. In [8,9,13], Gusynin *et al.* developed a frequency dependent electrical conductivity tensor using the Kubo formulation. Peres *et al.* [10] studied the electronic properties of graphene in the presence of defects, and electron–electron interaction as a function of temperature, external frequency, gate voltage, and magnetic field. Wunsch *et al.* [11] and Hwang and Das Sarma [12] developed similar methods to calculate the conductivity of graphene from the polarization based on the Dirac cone approximation for finite chemical potential and arbitrary radian frequency, respectively. Stauber *et al.* also developed a method based on the Kubo formulation to calculate the optical conductivity of graphene by taking into account its full density of states and found that in the optical regime the corrections to the Dirac cone approximation are quite small [14]. Li *et al.* calculated the conductivity of a single graphene sheet for the infrared part of the spectrum [15].

In three-dimensional (3D) electromagnetic analyses, the graphene can be defined as an infinitely thin material with an optical conductivity of σ_c. However, such definition requires a special boundary condition treatment, which is not available in most of the commercial full-wave electromagnetic solvers. One might try to overcome this problem by treating the graphene as a 3D material with a finite thickness and refractive index (or electrical permittivity). For example, Bruna and Borini developed an extremely simple model to define the refractive index of graphene [17] but their model only depends on the frequency of the excitation. Therefore, it cannot be used in any study where the chemical potential or temperature changes.

This work is aimed to answer following two questions: (i) whether we can obtain a closed-form, integral-free expression for the optical conductivity of graphene, so that one could calculate it with a simple calculator not only in visible but also in infrared region of the electromagnetic spectrum, and (ii) whether we can safely convert the (2D) optical conductivity into (3D) electrical permittivity to represent graphene as a 3D material in 3D electromagnetic simulations.

In this direction, we first develop an approximate function in order to replace the momentum integral existing in the Kubo formulation and remove the singularity in the expression developed by Stauber *et al.* [14] for the imaginary component of the optical conductivity. Numerical results show that the approximate closed form expression generates results with a maximum absolute error of 0.8%. In the second part of this work, we convert the 2D optical conductivity into 3D effective electrical permittivity and evaluate the accuracy of the approach. Numerical results confirm that the effective electrical permittivity successfully represents this one atom thick material in 3D electromagnetic simulations and analyses.

According to [14], the real and imaginary parts of the conductivity can be calculated by using

$$\sigma_r = \sigma_0 \left[\frac{18 - (\hbar\omega/t)^2}{\pi 12\sqrt{(3)}} \right] \psi_r \kappa, \tag{1}$$

where

$$\psi_r = \tanh\left(\frac{\hbar\omega + 2\mu_c}{4k_B T}\right) + \tanh\left(\frac{\hbar\omega - 2\mu_c}{4k_B T}\right), \tag{2}$$

$$\kappa = \begin{cases} \frac{1}{\sqrt{F(\hbar\omega/2t)}}\mathbf{K}\left(\frac{2\hbar\omega/t}{F(\hbar\omega/2t)}\right), & \hbar\omega < 2t \\ \frac{1}{\sqrt{2\hbar\omega/t}}\mathbf{K}\left(\frac{F(\hbar\omega/2t)}{2\hbar\omega/t}\right), & \hbar\omega \geq 2t \end{cases}, \tag{3}$$

$$F(x) = (1+x)^2 - 0.25(x^2-1)^2, \tag{4}$$

$$\mathbf{K}(m) = \int_0^1 ((1-x^2)(1-mx^2))^{-1/2}\mathrm{d}x \tag{5}$$

and

$$\sigma_i = \frac{\sigma_0}{\pi}\left\{\frac{4\mu_c}{\hbar\omega}\left[1 - 2\left(\frac{\mu_c}{3t}\right)^2\right] - \left[1 - \left(\frac{\hbar\omega}{6t}\right)^2\right]\Upsilon\right\}, \tag{6}$$

where

$$\Upsilon = \log\frac{|\hbar\omega + 2\mu_c|}{|\hbar\omega - 2\mu_c|} \tag{7}$$

and $\sigma_0 = e^2/4\hbar$, t is the hopping parameter of graphene, $\hbar$ is the reduced Planck constant, and k_B is the Boltzmann constant. Note that the above formulation assumes a positive chemical potential. For a negative chemical potential, one can use $\sigma_c(\mu_c) = \sigma_c(-\mu_c)$.

In [14], Stauber *et al.* provide an approximate expression for the real part of the conductivity for the visible range of the electromagnetic spectrum. If the frequency is not in that range, then one needs to evaluate the singular integral given in Eq. (5). Moreover, the approximate expression developed by Stauber *et al.* for the imaginary part of the conductivity is singular at $\hbar\omega = 2\mu_c$. Apart from a mathematical singularity, the logarithmic function in Eq. (7) suggests a dramatic dip at $\hbar\omega = 2\mu_c$; however, when we examine the experimental results provided in [15], we do not observe such a huge drop in the imaginary part of the conductivity near $\hbar\omega = 2\mu_c$.

In the light of these mathematical and physical observations, we propose to replace the κ and Υ functions with the following ones:

$$\kappa' = \begin{cases} 4.6936 - 2.897\tanh(|\hbar\omega - 2t|^{0.546}), & \hbar\omega < 2t \\ 4.6936\exp(-0.7714|\hbar\omega - 2t|^{0.4727}), & \hbar\omega \geq 2t \end{cases}, \tag{8}$$

$$\Upsilon' = \log\left(\frac{|\hbar\omega + 2\mu_c| - \psi_i}{|\hbar\omega - 2\mu_c| + \psi_i}\right), \tag{9}$$

where

$$\psi_i = 2k_BT\left\{\tanh\left(\frac{|\hbar\omega + 2\mu_c|}{4k_BT}\right) - \tanh\left(\frac{|\hbar\omega - 2\mu_c|}{4k_BT}\right)\right\}. \tag{10}$$

The numbers in Eq. (8) are obtained with the help of a MATLAB search algorithm yielding a minimum root mean squared error. The new ψ_i term in Eq. (9) removes the singularity without damaging the general behavior of σ_i near $\hbar\omega = 2\mu_c$, similar to the singularity treatment implemented in [18]. Moreover, ψ_i makes σ_i a temperature-dependent variable [19].

In Figs. 1(a) and 1(b), we plot the real and imaginary parts of the complex conductivity of graphene at $T = 45$ K as a function of frequency for three chemical potential values, assuming 2.7 eV of hopping parameter. The results plotted with solid lines are obtained with Eqs. (1)–(7) and admitted as "exact results," while the results shown by markers are generated with the approximate expressions. These results indicate that Eqs. (8)–(10) can successfully approximate σ_r and removes the singularity in σ_i without changing its general behavior. Figures 1(c) and 1(d) show real and imaginary parts, respectively, in the visible region as a function of chemical potential for 0 eV $< \mu_c <$ 4 eV. Compared to exact solution, the maximum relative error is less than 0.8% except for the $\hbar\omega \approx 2\mu_c$ region due to logarithmic singularity in Eq. (7).

In Fig. 2, we plot the imaginary part of the conductivity only for $\omega = 3$ eV and $1 < \mu_c < 2$ eV to show the effect of smoothing factor ψ_i. While Eq. (7) suggests an infinite conductivity at $\hbar\omega = 2\mu_c$, the ψ_i term removes the singularity in Eq. (7) without changing the main character of σ_i.

In order to verify the accuracy of the approximate formulation, we reproduce two sets of numerical results plotted in Figs. 2 and 6 of [14], which are not provided here for the sake of brevity. In short, we first calculate graphene's conductivity at two different temperatures ($T = 10$ K and $T = 300$ K) for two chemical potential values ($\mu_c = 0$ eV and $\mu_c = 0.2$ eV), then we calculate the transmittivity and reflectivity for normal incidence for a two-layer medium which are separated by an infinitely thin graphene layer. Both sets of approximate results are in a perfect agreement with the exact results provided in [14].

All these numerical analyses confirm that the developed approximate formulation provides a very robust and efficient method to calculate the optical conductivity

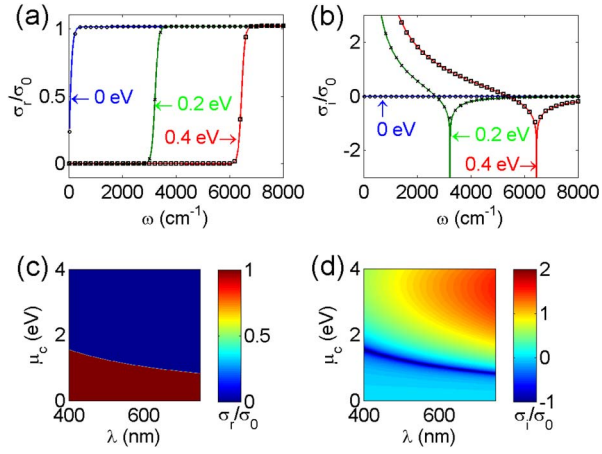

Fig. 1. (a) σ_r and (b) σ_i for $\mu_c = 0$ eV (blue), $\mu_c = 0.2$ eV (green), and $\mu_c = 0.4$ eV (red) as a function of wavelength at $T = 45$ K. Solid lines are generated using Eqs. (1)–(7) and approximate results shown by markers are obtained using Eqs. (8)–(10). (c) and (d) show real and imaginary parts, respectively, in the visible region as a function of chemical potential.

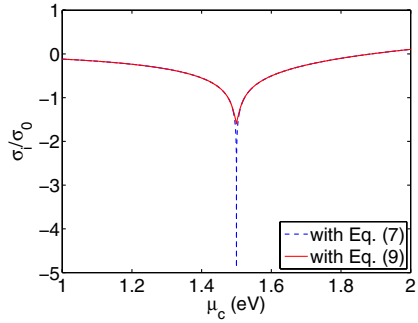

Fig. 2. σ_i calculated with Eq. (7) (blue dashed line), which has a singularity at $\hbar\omega = 2\mu_c$, and with Eq. (9) (red solid line). ω is taken as 3 eV.

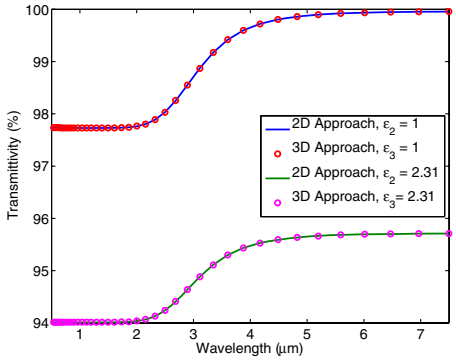

Fig. 3. Transmissivity for normal incident as a function of λ for $T = 300$ K and $\mu_c = 0.2$ eV where the top medium is vacuum and the bottom medium is either vacuum or glass. Solid lines and circles represent 2D and 3D approach results, respectively.

of graphene at any temperature or chemical potential for a wide range of wavelengths ($\lambda > 250$ nm).

In the second part of this work, we examine the accuracy of the effective electrical permittivity approach in which graphene is modeled as a 3D material with a finite thickness and a complex electrical permittivity. In this direction, we first convert the optical conductivity of graphene to a complex effective electrical permittivity by using $\epsilon_{\text{eff}} = 1 + i\sigma_c/\omega\epsilon_0 d$, where d is the thickness of the graphene layer, which is equal to 0.335 nm. Then we calculate the transmittivity with two different methods. First, we follow the 2D approach where graphene is represented with a 2D conductivity only (without any thickness) for $T = 300$ K, $\mu_c = 0.2$ eV, $\epsilon_1 = 1$, $\epsilon_2 = 1$ 1 or 2.31 (glass), where ϵ_1 and ϵ_2 represent the first and second layer's electrical permittivity. Then, we calculate the transmission through a three-layer medium, assuming the graphene layer has a finite thickness ($d = 0.335$ nm) and a complex effective permittivity; and $\epsilon_1 = 1$, $\epsilon_3 = 1$ 1 or 2.31 (glass), where ϵ_1 and ϵ_3 represent the first and third layer's electrical permittivity. Figure 3 compares the results for a wide range of wavelengths 500 nm $< \lambda <$ 7.5 μm. Clearly, these two completely different approaches yield almost the same results, which means that graphene can be successfully represented by a finite thickness and effective complex permittivity in 3D electromagnetic simulations and analyses.

In conclusion, a closed-form approximate expression is developed for the optical conductivity of graphene. The new formulation takes several factors into account including wavelength, temperature, chemical potential, and hopping parameter. Numerical results confirm the accuracy of the formulation. Since effective complex electrical permittivity derived from the optical conductivity successfully represents the graphene as a 3D material, developed closed-form expression can help all researchers working in different areas of nanotechnology who need graphene's optical conductivity, complex refractive index, or electrical permittivity.

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