Graphene: A Two Dimensional Material in Three Dimensional Structures

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***Abstract*—This work addresses the need for a closed form expression to calculate the two dimensional (2D) conductivity of graphene that allows researchers to include graphene either as a 2D or a 3D material in their theoretical and numerical electromagnetic analysis. The closed form expression is developed based on the Kubo formula and experimental results found in the literature. Numerical studies reveal that the maximum absolute error is less than 1 per cent for $\lambda > 250$ nm.**

I. Introduction

There has been a growing interest on graphene since its invention [1] due to its exceptional electrical and optical properties. Its high optical transmittance and conductivity make graphene an "almost transparent" conductive electrode [1], [5]–[12]. In comparison to traditional transparent conductive electrodes such as indium tin oxide, graphene films are more flexible, chemically stable and mechanically stronger .

From the electronic point of view, graphene is an excellent material due to its linear dispersion and more interestingly the broad optical absorption in graphene can be controlled through electrical gating: by shifting the electronic Fermi level, one can controllably change graphenes optical transitions. This property makes graphene a promising material to be implemented in new ultrafast opto-electronic devices such as modulators [2], transistors [3] and non-linear frequency generators [4]. This is why the conductivity of graphene has been one of its most examined properties both from experimentalists and theoreticians. In this direction, several models have been developed based on Kubo formulation and Dirac-cone approximation [5]–[12].

In this work, we first studied the previously developed theoretical models and evaluated their accuracy under different bias voltages at different temperatures in different parts of the electromagnetic spectrum. Then, based on the performance of these methods, we developed a new closed form expression for the conductivity of graphene that is valid for a wide range of wavelengths. In the last part, we convert two dimensional (2D) conductivity to effective complex electrical permittivity and refractive index to be used in three dimensional electromagnetic simulations. Numerical results show that graphene, a 2D structure, can be successfully modeled as a 3D structure using these effective complex electrical permittivity and refractive index.

II. 2D Conductivity of Graphene Based on the Kubo Formula

The 2D complex conductivity of graphene, which depends on the angular frequency (ω), temperature (T), and chemical potential (μ_c), can be written as $\sigma_c = \sigma_r + i\sigma_i$. According to [9], 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

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

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

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

$$\mathbf{K}(m) = \int_0^1 \left((1-x^2)(1-mx^2)\right)^{-1/2} dx, \tag{5}$$

and

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

where

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

and $\sigma_0 = \pi e^{/} 2h$, t is hopping parameter of graphene, h and $\hbar$ are regular and reduced Planck constants, respectively, and k_B is Boltzmann constant. Note that (6) is an approximation. The approach based on the Dirac Hamiltonian can be found in [8].

The results obtained with these two different approaches, Kubo formula and Dirac Hamiltonian, become distinguishable in the visible range of the electromagnetic spectrum. While the former estimates that σ_r is very close to σ_0, the latter claims $\sigma_r \approx 0.9\sigma_0$. Moreover, the former suggests a finite σ_i as we continue to increase μ_c, the latter estimates a linear increase. The difference between the results obtained with these approaches decreases as the wavelength is increased to

20 μm. However, the approximation derived from the Kubo formula estimates a peak for the real part at $\hbar\omega = 2t$ and a dip for the imaginary part at $\hbar\omega = 2\mu_c$ [9]. In fact, the approximation formula provided in [9] is singular at $\hbar\omega = 2\mu_c$. When we compare these predictions with the experimental results provided in [10], we do not observe such a dip. This singularity comes from the logarithmic function in (7). In this work, we first handle this singularity by adding an appropriate analytical expression to both the numerator and denominator of (7). Furthermore, we develop an approximate formula to replace κ function, which allows us to calculate σ_c without a numerical integration. The accuracy of the developed closed form expression is verified by comparing the approximate results with the Kubo formula results (without any approximation) and numerical results reveal that the maximum absolute error is 0.8 per cent. As an example, in Fig. 1 we plot the real and imaginary parts of the conductivity of graphene at $T = 45$ K for 7 values of chemical potential chosen at $0.15 \text{ eV} \leq \mu_c \leq 0.3 \text{ eV}$. These numerical results have a very good agreement with the experimental results provided in [10].

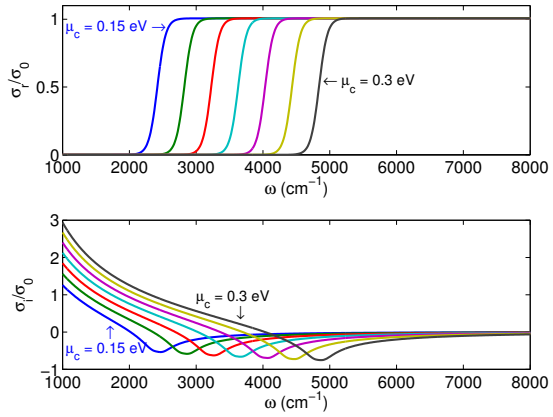

Fig. 1. The real (σ_r) and imaginary (σ_i) parts of the conductivity of graphene normalized by σ_0 as a function of frequency at $T = 45$ K. The chemical potential is increased from 0.15 eV (blue) to 0.3 eV (black), linearly, in 7 steps.

The 2D conductivity of graphene can be converted to a complex effective electrical permittivity by using

$$\epsilon_{eff} = 1 - \frac{\sigma_c}{i\omega\epsilon_0 d} \tag{8}$$

where d is the thickness of the graphene layer, which is equal to 0.335 nm. Fig. 2 shows the real and imaginary parts of the effective complex permittivity of graphene as a function of chemical potential at room temperature in the visible range of the electromagnetic spectrum. We notice that the real part of the graphene permittivity can attain negative and positive values in different ranges of frequencies depending on the level of chemical potential [8].

In the last part of our study, we analyze the accuracy of the effective permittivity approach. In this direction, we

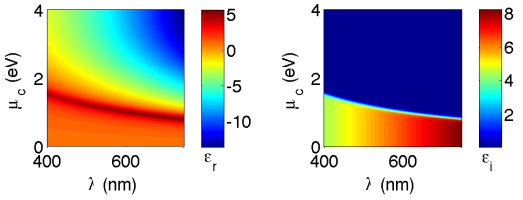

Fig. 2. The real (ϵ_r) and imaginary (ϵ_i) parts of the relative permittivity of graphene as a function of chemical potential at room temperature ($T = 300$ K) in the visible range of the electromagnetic spectrum.

first calculate the reflection/transmission from/through the two dimensional graphene by assuming it is an infinitely thin layer with a 2D conductivity σ_c. Then, we calculate the reflection/transmission from/through a graphene layer with a thickness of d and relative permittivity of ϵ_{eff}. These two completely different methods generate almost the same results that are in a perfect agreement with the experimental results provided in [12].

III. Conclusion

An accurate closed form expression is developed for the two dimensional complex conductivity of graphene, which can be converted to effective complex electrical permittivity allowing researchers to include graphene as a 3D material in electromagnetic simulations and analysis.

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