Kramers-Kronig relations and causality conditions for graphene in the framework of the Dirac model

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We analyze the concept of causality for the conductivity of graphene described by the Dirac model. It is recalled that the condition of causality leads to the analyticity of conductivity in the upper half-plane of complex frequencies and to the standard symmetry properties for its real and imaginary parts. This results in the Kramers-Kronig relations, which explicit form depends on whether the conductivity has no pole at zero frequency (as in the case of zero temperature when the band gap of graphene is larger than twice the chemical potential) or it has a pole (as in all other cases, specifically, at nonzero temperature). Through the direct analytic calculation it is shown that the real and imaginary parts of graphene conductivity, found recently on the basis of first principles of thermal quantum field theory using the polarization tensor in (2 + 1)-dimensional space-time, satisfy the Kramers-Kronig relations precisely. In so doing, the values of two integrals in the commonly used tables, which are also important for a wider area of dispersion relations in quantum field theory and elementary particle physics, are corrected. The obtained results are not of only fundamental theoretical character, but can be used as a guideline in testing the validity of different phenomenological approaches and for the interpretation of experimental data.

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I. INTRODUCTION

Considerable recent attention has been focused on graphene, which is a two-dimensional sheet of carbon atoms packed in a hexagonal lattice [1,2]. This unique material is interesting not only for condensed matter physics due to its unusual electrical and mechanical properties, but for quantum field theory as well. The point is that the electronic excitations in graphene are either massless or very light. At energies below a few eV they possess the linear dispersion relation and obey (2+1)dimensional Dirac equation where the speed of light c is replaced with the Fermi velocity $v_F \approx c/300$ [1–3]. Thus, graphene makes possible testing many predicted effects of quantum field theory and quantum electrodynamics which are not experimentally feasible with much heavier ordinary electrons. Among other effects one could mention the Klein paradox [4], the creation of particle-antiparticle pairs from vacuum in a static [5,6] and time-dependent [7,8] electric field, and the relativistic quantum Hall effect in a strong magnetic field [9].

Graphene is also unique in that its response to external electromagnetic field and quantum fluctuations, described by the polarization tensor in (2 + 1)-dimensional space-time, can be found in an explicit form on the basis of first principles of thermal quantum field theory. Although some

special cases have been considered previously (see, e.g., Ref. [10] and literature therein), the complete expression for the polarization tensor of graphene in the one-loop approximation has been derived at zero temperature in Ref. [11] and at any nonzero temperature in Ref. [12], where the area of application was limited to the pure imaginary Matsubara frequencies. In doing so both cases of zero and nonzero width of the gap Δ between the energy bands (i.e., of gapless and gapped graphene) and chemical potential μ were considered. The results of Refs. [11,12] have been extensively used when investigating the Casimir and Casimir-Polder forces in graphene systems [13-23] (some other, more phenomenological, approaches used for this purpose are the density-density correlation functions, models of the response functions of graphene by Lorenztype oscillators, and the Kubo formalism [24–35]).

A more universal representation for the polarization tensor of graphene at nonzero temperature was derived in Ref. [36]. Unlike Ref. [12], the polarization tensor of Ref. [36] allows an analytic continuation to the entire plane of complex frequencies including the real frequency axis. At the pure imaginary Matsubara frequencies both representations take the same values. The novel representation was applied in investigations of the Casimir force [37–41] and, after a continuation to the real frequency axis, for

better understanding of the reflectances of graphene and graphene-coated plates [42–44]. In Ref. [45] the polarization tensor of Ref. [36] was generalized for the case of doped graphene with a nonzero chemical potential. This generalization was used [46] to investigate an impact of nonzero band gap and chemical potential on the thermal effect in the Casimir force.

One of the most important characteristics of graphene is its electrical conductivity. This quantity possesses many surprising properties connected with an existence of the socalled *universal* conductivity $\sigma_0 = e^2/(4\hbar)$ expressed via the fundamental constants, electron charge *e* and Planck constant \hbar . For a pure graphene, having the zero band gap and no doping, the conductivity is equal to σ_0 in the limit of zero temperature. This result might be considered as paradoxical if to take into account that with vanishing temperature the concentration of charge carriers in pure graphene goes to zero and there is no scattering and no dissipation processes.

The conductivity of graphene was extensively investigated by many authors using the current-current correlation functions, the Kubo formalism, the Boltzmann transport theory, and the two-dimensional Drude model (see the review papers [47–49] and references therein). Some of the results obtained employ simple intuitive models, phenomenological approaches of a limited application area and even do not agree with each other. To overcome these troubles, the conductivity of graphene at any temperature was investigated on the basis of first principles of quantum electrodynamics using the polarization tensor of Refs. [36,45] analytically continued to the real frequency axis. In Refs. [50,51] the cases of pure and gapped graphene were considered, respectively, and in Ref. [52] of both gapped and doped graphene characterized by nonzero band gap Δ and chemical potential μ . The real and imaginary parts of graphene conductivity have been found in an explicit form. It was shown that the major contribution to the conductivity of graphene calculated in the framework of Dirac model is local, whereas the nonlocal corrections are negligibly small.

In this paper, we consider the problem of causality in the response of graphene to electric field. The demand of causality leads to some constraints on the local conductivity of graphene. Specifically, it should be an analytic function in the upper half-plane of complex frequencies and satisfy certain symmetry conditions. These result in the Kramers-Kronig relations for the real and imaginary parts of the conductivity of graphene. Until the present time the Kramers-Kronig relations for graphene were discussed only using some approximate, phenomenological approaches leading to incomplete and even contradictory results (see, e.g., Refs. [53–56]). Thus, the form of Kramers-Kronig relations used in Refs. [53–55] does not take into account that the imaginary part of the conductivity of graphene has a pole at zero frequency. Furthermore, Ref. [53] arrives to the Kramers-Kronig relation expressing the real part of graphene conductivity via its imaginary part, but fails in obtaining a similar relation with interchanged real and imaginary parts. An existence of the universal conductivity of graphene σ_0 is not taken into account. Moreover, Ref. [56] admits that under some conditions the Kramers-Kronig relations for graphene do not hold. When it is considered that these relations are not only of fundamental theoretical character, but are used for interpretation of the measurement data (see, e.g., Ref. [55]), it is of prime importance to conclusively find out their specific form for graphene and directly prove their validity.

Below we establish an explicit form of the Kramers-Kronig relations for graphene and demonstrate that the real and imaginary parts of its conductivity, found independently on the basis of first principles of quantum electrodynamics, satisfy these relations precisely. Depending on temperature and a relationship between the band gap Δ and chemical potential μ , an additional pole term in the Kramers-Kronig relations may arise as it holds in a familiar case of metals [57]. The obtained relations take proper account for the universal conductivity of graphene σ_0 . In fact, there is no reason that the Kramers-Kronig relations were not satisfied for the conductivity determined from the first principles. The obtained results, however, are physically meaningful because they establish the specific form of the Kramers-Kronig relations for so unusual material as graphene and, by performing the direct verification of these relations, confirm the expressions for its conductivity found recently in Ref. [52] using the polarization tensor. In the course of our calculations, the values of two integrals, indicated incorrectly in the most comprehensive and widely used table of integrals [58], have been corrected. These integrals might be also useful in a wider context of dispersion relations for the scattering amplitudes in quantum field theory and physics of elementary particles.

The paper is organized as follows. In Sec. II, the brief summary for the polarization tensor, conductivity of graphene and causality conditions is presented. Section III contains the proof of the Kramers-Kronig relations for the conductivity of graphene at zero temperature. The validity of the Kramers-Kronig relations at nonzero temperature is demonstrated in Sec. IV. In Sec. V, the reader will find our conclusions and a discussion. Appendices A and B contain some details of several mathematical derivations.

II. POLARIZATION TENSOR, CONDUCTIVITY OF GRAPHENE AND CAUSALITY CONDITIONS

The polarization tensor of graphene in the one-loop approximation in the momentum representation is defined according to Refs. [59,60] with the following differences. We consider the (2 + 1)-dimensional space-time. In the free Dirac equation the speed of light *c* is replaced with the Fermi velocity $v_F \approx c/300$ although an interaction with the

electromagnetic field is governed, as usual, by the coupling constant e/c. In addition, one should take into account that we consider the polarization tensor at nonzero temperature *T*. Because of this, according to the Matsubara formalism, an integration over the zeroth component q_0 of the wave vector q^{μ} of a loop electronic excitation should be replaced with a summation over the pure imaginary fermionic Matsubara frequencies

$$cq_{0n} = 2\pi i \left(n + \frac{1}{2} \right) \frac{k_B T}{\hbar},\tag{1}$$

where k_B is the Boltzmann constant and $n = 0, \pm 1, \pm 2, ...$ Finally it is necessary to replace the zeroth component k_0 of the wave vector k^{μ} of an external photon in the argument of the polarization tensor with the pure imaginary bosonic Matsubara frequencies

$$i\xi_l = ck_{0l} = 2\pi i l \frac{k_B T}{\hbar},\tag{2}$$

where $l = 0, \pm 1, \pm 2,$

As a result, the polarization tensor takes the form [11,12,36,59,60]

$$\Pi^{\mu\nu}(i\xi_{l},\boldsymbol{k}) = -8\pi\alpha k_{B}T\sum_{n=-\infty}^{\infty}\left(n+\frac{1}{2}\right)$$

$$\times \int \frac{d\boldsymbol{q}}{(2\pi)^{2}}\operatorname{tr}\frac{1}{i\tilde{\gamma}^{\mu}q_{\mu}-\Delta/(2\hbar)}\tilde{\gamma}^{\mu}$$

$$\times \frac{1}{i\tilde{\gamma}^{\mu}q_{\mu}-i\tilde{\gamma}^{\mu}k_{\mu}-\Delta/(2\hbar)}.$$
(3)

Here, $\alpha = e^2/(\hbar c) \approx 1/137$ is the fine structure constant, $q^{\mu} = (q_{0n}, q^1, q^2), k^{\mu} = (k_{0l}, k^1, k^2), \mu = 0, 1, 2, \mathbf{k} = (k^1, k^2),$ $\tilde{\gamma}^{\mu} = \eta^{\mu}_{\nu} \gamma^{\nu}$ where $\eta^{\mu}_{\nu} = \text{diag}(c, v_F, v_F)$ and γ^{ν} are the Dirac matrices. Note also that the numerical factor on the righthand side of Eq. (9) takes into account four fermion species for graphene [1–3].

The polarization tensor (3) was calculated over the entire axis of imaginary frequencies in Ref. [36], analytically continued to the real frequency axis and used for different purposes in Refs. [36,42–44,50,51]. In Ref. [45] this tensor was generalized for the case of graphene with nonzero chemical potential μ [this is reached by the replacement $q_{0n} \rightarrow q_{0n} + \mu/(\hbar c)$] and analytically continued to the real frequency axis in Ref. [52]. The longitudinal (in-plane of graphene) and transverse (out-of-plane) electrical conductivities are expressed via the polarization tensor as [22,50–52]

$$\sigma_{\parallel}(\omega, k, T) = -i \frac{\omega}{4\pi\hbar k^2} \Pi_{00}(\omega, k, T),$$

$$\sigma_{\perp}(\omega, k, T) = i \frac{c^2}{4\pi\hbar\omega k^2} \Pi(\omega, k, T), \qquad (4)$$

where

$$\Pi(\omega, k, T) = k^2 \operatorname{tr} \Pi_{\mu\nu}(\omega, k, T) + \left(\frac{\omega^2}{c^2} - k^2\right) \Pi_{00}(\omega, k, T)$$
(5)

and $k = |\mathbf{k}|$. The conductivities of graphene are the complex quantities as well as the polarization tensor along the real frequency axis.

Calculations show that the major contributions to both the real and imaginary parts of $\sigma_{\parallel(\perp)}$ are given in the local limit k = 0, whereas the nonlocal corrections are of the order of $(v_F/c)^2 \sim 10^{-5}$. In the local limit one has

$$\sigma(\omega, T) \equiv \sigma_{\parallel}(\omega, 0, T) = \sigma_{\perp}(\omega, 0, T).$$
(6)

Note that the quantities Π_{00} and Π in Eq. (4) go to zero as k^2 when k goes to zero, whereas $tr\Pi_{\mu\nu}$ goes to a nonzero constant. Expanding all these quantities up to the first power in the parameter $(v_F k/\omega)^2 < (v_F/c)^2$ and using Eqs. (28), (40), and (43) in Ref. [52], one obtains that in this perturbation order

$$\Pi(\omega, k, T) = -\frac{\omega^2}{c^2} \Pi_{00}(\omega, k, T).$$
(7)

Taking into account Eq. (4), it is seen that Eq. (7) is in agreement with Eq. (6).

The explicit expressions for the quantity $\sigma(\omega, T)$ in the most general case of graphene with nonzero Δ and μ have been derived from Eq. (4) in Ref. [52]. It is convenient to present the local conductivity of graphene (6) as the sum of two contributions

$$\sigma(\omega, T) = \sigma^{(0)}(\omega) + \sigma^{(1)}(\omega, T).$$
(8)

The quantity $\sigma^{(0)}$ on the right-hand side of this equation is the contribution to the conductivity which does not depend on *T* and μ . It is given by [52]

$$\operatorname{Re}\sigma^{(0)}(\omega) = \sigma_0 \theta(\hbar\omega - \Delta) \frac{(\hbar\omega)^2 + \Delta^2}{(\hbar\omega)^2},$$
$$\operatorname{Im}\sigma^{(0)}(\omega) = \frac{\sigma_0}{\pi} \left[\frac{2\Delta}{\hbar\omega} - \frac{(\hbar\omega)^2 + \Delta^2}{(\hbar\omega)^2} \ln \left| \frac{\hbar\omega + \Delta}{\hbar\omega - \Delta} \right| \right], \quad (9)$$

where Δ is the width of the gap in Dirac's spectrum and $\theta(x)$ is the step function equal to unity for $x \ge 0$ and zero for x < 0. Note that under the condition $\Delta > 2\mu$ the quantity $\sigma^{(0)}(\omega)$ defined in Eq. (9) has the physical meaning of the total conductivity of graphene at zero temperature $\sigma(\omega, 0)$. This means that under the condition $\Delta > 2\mu$ it holds [52]

$$\sigma^{(1)}(\omega, 0) = \lim_{T \to 0} \sigma^{(1)}(\omega, T) = 0.$$
(10)

Thus, if $\Delta > 2\mu$ the conductivity $\sigma(\omega, 0)$ does not depend on μ (even if μ is not equal to zero but is smaller than $\Delta/2$) and $\text{Re}\sigma^{(0)}$ vanishes if $\hbar\omega < \Delta$. The conductivity of graphene at T = 0 and $\Delta < 2\mu$ is considered in Sec. III.

The quantity $\sigma^{(1)}$ on the right-hand side of Eq. (8) depends on *T*, Δ and μ . It can be represented in the form [52]

$$\operatorname{Re}\sigma^{(1)}(\omega,T) = -\sigma_0 \theta(\hbar\omega - \Delta) \frac{(\hbar\omega)^2 + \Delta^2}{(\hbar\omega)^2} F(\omega,T),$$

$$\operatorname{Im}\sigma^{(1)}(\omega,T) = \frac{2\sigma_0}{\pi} \int_{\frac{\Delta}{\hbar\omega}}^{\infty} dt \left[1 + \frac{(\hbar\omega)^2 + \Delta^2}{(\hbar\omega)^2} \frac{1}{t^2 - 1} \right]$$

$$\times F(\omega t,T), \qquad (11)$$

where the function F(x, T) is defined as

$$F(x,T) = \sum_{\kappa=\pm 1} \left[\exp\left(\frac{\hbar x + 2\kappa\mu}{2k_BT}\right) + 1 \right]^{-1}.$$
 (12)

It is convenient to introduce the new integration variable $v = \hbar \omega t / \Delta$ in the second line of Eq. (11) which takes the form

$$\operatorname{Im}\sigma^{(1)}(\omega, T) = \frac{2\sigma_0}{\pi} \frac{\Delta}{\hbar\omega} \int_1^\infty dv \left[1 + \frac{\Delta^2 + (\hbar\omega)^2}{(v\Delta)^2 - (\hbar\omega)^2} \right] \times F\left(\frac{v\Delta}{\hbar}, T\right).$$
(13)

This expression has the pole term $C(T)/\omega$ at $\omega = 0$, where

$$C(T) = \frac{2\sigma_0}{\pi} \frac{\Delta}{\hbar} \int_1^\infty dv \frac{v^2 + 1}{v^2} F\left(\frac{v\Delta}{\hbar}, T\right).$$
(14)

Now we separate the pole term in the imaginary part of conductivity by adding and subtracting the quantity $C(T)/\omega$ on the right-hand side of Eq. (13). Leaving the first expression in Eq. (11) unchanged, both $\text{Re}\sigma^{(1)}$ and $\text{Im}\sigma^{(1)}$ can be rewritten as

$$\operatorname{Re}\sigma^{(1)}(\omega, T) = -\sigma_0 \theta(\hbar\omega - \Delta) \frac{(\hbar\omega)^2 + \Delta^2}{(\hbar\omega)^2} F(\omega, T),$$

$$\operatorname{Im}\sigma^{(1)}(\omega, T) = \frac{C(T)}{\omega} + \frac{2\sigma_0}{\pi} \hbar\omega \Delta \int_1^\infty dv \frac{v^2 + 1}{v^2[(v\Delta)^2 - (\hbar\omega)^2]} \times F\left(\frac{v\Delta}{\hbar}, T\right).$$
(15)

Now we discuss the requirements of causality imposed on the conductivity $\sigma(\omega, T)$ and its constituents $\sigma^{(0)}(\omega)$ and $\sigma^{(1)}(\omega, T)$. According to the principle of causality, the electric current density j(t) must not depend on the values of electric field E(t) at times greater than t, i.e.,

$$\mathbf{j}(t,T) = \int_0^\infty \sigma(\tau,T) \mathbf{E}(t-\tau) d\tau.$$
(16)

Multiplying both sides of this equation by $e^{i\omega t}$ and integrating with respect to t from $-\infty$ to ∞ , we obtain an equation for the Fourier images of the field and current density

$$\boldsymbol{j}(\boldsymbol{\omega},T) = \boldsymbol{\sigma}(\boldsymbol{\omega},T)\boldsymbol{E}(\boldsymbol{\omega}), \qquad (17)$$

where

$$\sigma(\omega, T) = \int_0^\infty \sigma(\tau, T) e^{i\omega\tau} d\tau.$$
(18)

Repeating the well-known reasoning contained in Ref. [57] for the case of frequency-dependent dielectric permittivity, it is easy to find the analytic properties of $\sigma(\omega, T)$ in the plane of complex frequencies and the symmetry properties of its real and imaginary parts. Specifically, from Eq. (18) it follows that in the upper half-plane (Im $\omega > 0$) $\sigma(\omega, T)$ is an analytic function with no singularities. The real and imaginary parts of $\sigma(\omega, T)$ are the even and odd functions of real frequency, respectively. From Eq. (18) it is seen also that for the complex ω it holds $\sigma(-\omega^*, T) = \sigma^*(\omega, T)$. Then at the pure imaginary frequencies $\sigma(\omega, T)$ takes the real values. Equation (16) is also valid for the contributions $\sigma^{(0)}(\tau)$ and $\sigma^{(1)}(\tau, T)$ to the conductivity $\sigma(\tau, T)$ [with the corresponding contributions to the total current $j^{(0)}(t)$ and $j^{(1)}(t, T)$ on the left-hand side]. From this it follows that all the above properties of $\sigma(\omega, T)$ are inherent also in $\sigma^{(0)}(\omega)$ and $\sigma^{(1)}(\omega, T)$.

Note that the explicit expressions (9) and (15) may appear in disagreement with the formulated above general properties of conductivity following from the causality condition (16). The point is that it may exist several equivalent representations for some quantity along the positive frequency axis, but only one of them allows immediate analytic continuation to the entire plane of complex frequencies. Equations (9) and (15) are written in the form which is most convenient for applications only at the real, positive frequencies and can be easily compared with the results obtained using various approximate and phenomenological approaches (see below). These equations, however, can be identically rewritten in the form where the analytic continuation from the real, positive frequency axis to the entire complex frequency plane is achieved by simply putting frequency ω complex. For example, Eq. (9) can be rewritten in the form

$$\sigma^{(0)}(\omega) = i \frac{2\sigma_0}{\pi} \left[\frac{\Delta}{\hbar\omega} - \frac{(\hbar\omega)^2 + \Delta^2}{(\hbar\omega)^2} \operatorname{arctanh} \frac{\hbar\omega}{\Delta} \right], \quad (19)$$

where all the above properties are evidently satisfied. An equivalence of Eqs. (9) and (19) along the real, positive frequency axis follows from the identities [61]

$$\operatorname{arctanh} x = \frac{1}{2} \ln \frac{1+x}{1-x}, \qquad 0 \le x^2 < 1,$$
$$\operatorname{arctanh} x = \operatorname{arctanh} \frac{1}{x} + i\frac{\pi}{2}, \qquad (20)$$

where the last identity is used for x > 1 at the upper bank of the cut which passes from unity to ∞ .

The analytic properties of the functions $\sigma(\omega, T)$, $\sigma^{(0)}(\omega)$ and $\sigma^{(1)}(\omega, T)$ result in the validity of the Kramers-Kronig relations which can be proven in exactly the same manner as it is done in Ref. [57] for the case of dielectric permittivity. The form of the Kramers-Kronig relations depends on the behavior of σ at zero frequency. As is seen in Eq. (9), both the real and imaginary parts of $\sigma^{(0)}$ are regular at $\omega = 0$ (the first order pole in the first term of Im $\sigma^{(0)}$ is canceled by a similar pole with an opposite sign in the second term). At $\omega \to \infty$ the quantity $\text{Re}\sigma^{(0)}$ goes to σ_0 . Because of this, the Kramers-Kronig relation is valid for the function $\text{Re}\sigma^{(0)} - \sigma_0$. The result is similar to that presented in Ref. [57] for the dielectric permittivity

$$\operatorname{Re}\sigma^{(0)}(\omega) = \sigma_0 + \frac{2}{\pi} \int_0^\infty \frac{\xi \operatorname{Im}\sigma^{(0)}(\xi)}{\xi^2 - \omega^2} d\xi,$$

$$\operatorname{Im}\sigma^{(0)}(\omega) = -\frac{2\omega}{\pi} \int_0^\infty \frac{\operatorname{Re}\sigma^{(0)}(\xi)}{\xi^2 - \omega^2} d\xi,$$
(21)

where the crossed sign of integration means that the principal value of the integral is taken. We note also that

$$\int_{0}^{\infty} \frac{d\xi}{\xi^2 - \omega^2} = 0.$$
 (22)

Because of this it is not necessary to subtract σ_0 in the nominator of the second equality in Eq. (21).

Now we consider the second contribution to the conductivity of graphene, i.e., $\sigma^{(1)}$. As is seen in Eq. (15), the imaginary part of $\sigma^{(1)}$ has the first-order pole. Because of this, the Kramers-Kronig relations are similar to those obtained in Ref. [57] for the dielectric permittivity of conductors

$$\operatorname{Re}\sigma^{(1)}(\omega,T) = \frac{2}{\pi} \int_{0}^{\infty} \frac{\xi \operatorname{Im}\sigma^{(1)}(\xi,T) - C(T)}{\xi^{2} - \omega^{2}} d\xi,$$
$$\operatorname{Im}\sigma^{(1)}(\omega,T) = -\frac{2\omega}{\pi} \int_{0}^{\infty} \frac{\operatorname{Re}\sigma^{(1)}(\xi,T)}{\xi^{2} - \omega^{2}} d\xi + \frac{C(T)}{\omega}, \quad (23)$$

where C(T) is defined in Eq. (14). We note that both the real and imaginary parts of $\sigma^{(1)}$ defined in Eq. (15) go to zero when $\omega \to \infty$. Because of this, it is not needed to subtract any constant from $\text{Re}\sigma^{(1)}$ like it was done in Eq. (21). At the same time, it is necessary to subtract C(T)in the nominator of the first dispersion relation in Eq. (23). This subtraction does not change the value of the integral at all $\omega \neq 0$ due to Eq. (22), but makes the Kramers-Kronig relation correct at $\omega = 0$ (see the relevant discussions in Ref. [57] for the dielectric permittivity of metals and in Sec. III).

By combining Eqs. (21) and (23), one arrives to the Kramers-Kronig relations for the total conductivity of graphene at any temperature

$$\operatorname{Re}\sigma(\omega,T) = \sigma_0 + \frac{2}{\pi} \int_0^\infty \frac{\xi \operatorname{Im}\sigma(\xi,T) - C(T)}{\xi^2 - \omega^2} d\xi,$$

$$\operatorname{Im}\sigma(\omega,T) = -\frac{2\omega}{\pi} \int_0^\infty \frac{\operatorname{Re}\sigma(\xi,T)}{\xi^2 - \omega^2} d\xi + \frac{C(T)}{\omega}.$$
(24)

The Kramers-Kronig relations (21), (23), and (24) follow from the discussed above general analytic properties of the local conductivity of graphene. None of the expressions for the graphene conductivity obtained in the previous literature using various approximate and phenomenological methods satisfy these relations precisely. Below we demonstrate, however, that the conductivity (8), (9), (15), derived independently on the basis of first principles of quantum electrodynamics at nonzero temperature using the polarization tensor, is in full agreement with the Kramers-Kronig relations and, thus, with the demands of causality.

III. KRAMERS-KRONIG RELATIONS FOR THE CONDUCTIVITY AT ZERO TEMPERATURE

We begin with the case $\Delta \ge 2\mu$ when the total conductivity of graphene at T = 0 is given by Eq. (9), i.e., $\sigma(\omega, 0) = \sigma^{(0)}(\omega)$. It is straightforward to substitute the first line of Eq. (9) in the right-hand side of the second Kramers-Kronig relation in Eq. (21) and obtain

$$-\frac{2\omega}{\pi} \int_{0}^{\infty} \frac{\operatorname{Re}\sigma^{(0)}(\xi)}{\xi^{2} - \omega^{2}} d\xi$$
$$= -\frac{2\sigma_{0}}{\pi} \hbar \omega \left[\int_{\Delta}^{\infty} \frac{d\zeta}{\zeta^{2} - \hbar^{2} \omega^{2}} + \Delta^{2} \int_{\Delta}^{\infty} \frac{d\zeta}{\zeta^{2} (\zeta^{2} - \hbar^{2} \omega^{2})} \right], \quad (25)$$

where the integration variable $\zeta = \hbar \xi$ is introduced. Integrating on the right-hand side of Eq. (25) we find

$$-\frac{2\omega}{\pi} \int_{0}^{\infty} \frac{\operatorname{Re}\sigma^{(0)}(\xi)d\xi}{\xi^{2} - \omega^{2}} = \frac{\sigma_{0}}{\pi} \left[\frac{2\Delta}{\hbar\omega} -\frac{(\hbar\omega)^{2} + \Delta^{2}}{(\hbar\omega)^{2}} \ln \left| \frac{\hbar\omega + \Delta}{\hbar\omega - \Delta} \right| \right] = \operatorname{Im}\sigma^{(0)}(\omega) \quad (26)$$

if to take into account Eq. (9). Thus, the second Kramers-Kronig relation in Eq. (21) is really satisfied.

Now we substitute the second line of Eq. (9) in the righthand side of the first Kramers-Kronig relation in Eq. (21) and obtain

$$\sigma_0 + \frac{2}{\pi} \int_0^\infty \frac{\xi \mathrm{Im}\sigma^{(0)}(\xi)}{\xi^2 - \omega^2} d\xi = \sigma_0 - \frac{2\sigma_0}{\pi^2} \int_0^\infty \frac{\xi}{\xi^2 - \omega^2} \left[\ln \left| \frac{\hbar\xi + \Delta}{\hbar\xi - \Delta} \right| + \frac{\Delta^2}{(\hbar\xi)^2} \ln \left| \frac{\hbar\xi + \Delta}{\hbar\xi - \Delta} \right| \right] d\xi, \tag{27}$$

where we have taken into account Eq. (22).

In Appendix A, we calculate the following important integral:

$$I(b) \equiv \int_{0}^{\infty} \frac{y}{y^{2} - b^{2}} \ln \left| \frac{y + 1}{y - 1} \right| dy = \begin{cases} \frac{\pi^{2}}{2}, & |b| < 1, \\ 0, & |b| > 1 \end{cases}$$
(28)

and indicate relevant incorrect results contained in Ref. [58].

Introducing the variable $y = \hbar \xi / \Delta$ in the first integral on the right-hand side of Eq. (27) and using Eq. (28), one obtains

$$\begin{aligned} \int_{0}^{\infty} \frac{\xi}{\xi^{2} - \omega^{2}} \ln \left| \frac{\hbar \xi + \Delta}{\hbar \xi - \Delta} \right| d\xi &= \int_{0}^{\infty} \frac{y}{y^{2} - b^{2}} \ln \left| \frac{y + 1}{y - 1} \right| dy \\ &= \begin{cases} \frac{\pi^{2}}{2}, & \hbar \omega < \Delta, \\ 0, & \hbar \omega > \Delta, b \equiv \frac{\hbar \omega}{\Delta}. \end{cases} \end{aligned}$$

$$(29)$$

The second integral on the right-hand side of Eq. (27) can be evaluated similarly

$$\frac{\Delta^2}{\hbar^2} \int_0^\infty \frac{1}{\xi(\xi^2 - \omega^2)} \ln \left| \frac{\hbar\xi + \Delta}{\hbar\xi - \Delta} \right| d\xi = \int_0^\infty \frac{1}{y(y^2 - b^2)} \ln \left| \frac{y + 1}{y - 1} \right| dy$$

$$= \frac{1}{b^2} \left[\int_0^\infty \frac{y}{y^2 - b^2} \ln \left| \frac{y + 1}{y - 1} \right| dy - \int_0^\infty \frac{dy}{y} \ln \left| \frac{y + 1}{y - 1} \right| \right]$$

$$= \begin{cases} 0, & \hbar\omega < \Delta, \\ -\frac{1}{2} (\frac{\pi\Delta}{\hbar\omega})^2, & \hbar\omega > \Delta. \end{cases}$$
(30)

In obtaining this result we have used Eq. (28) for two times, namely with $b \neq 0$ and b = 0.

Substituting Eqs. (29) and (30) in the right-hand side of Eq. (27) and using the first line of Eq. (9), one arrives at

$$\sigma_{0} + \frac{2}{\pi} \int_{0}^{\infty} \frac{\xi \mathrm{Im}\sigma^{(0)}(\xi)}{\xi^{2} - \omega^{2}} d\xi = \begin{cases} 0, & \hbar\omega < \Delta, \\ \sigma_{0} \frac{(\hbar\omega)^{2} + \Delta^{2}}{(\hbar\omega)^{2}}, & \hbar\omega > \Delta \end{cases}$$
$$= \mathrm{Re}\sigma^{(0)}(\omega). \tag{31}$$

Thus, the conductivity $\sigma^{(0)}$ in Eq. (9) satisfies the first Kramers-Kronig relation in Eq. (21).

Now we continue to consider the case of zero temperature, but assume that $\Delta < 2\mu$. In this case it holds

$$\sigma^{(1)}(\omega,0) = \lim_{T \to 0} \sigma^{(1)}(\omega,T) \neq 0$$
(32)

and

$$\sigma(\omega, 0) = \sigma^{(0)}(\omega) + \sigma^{(1)}(\omega, 0). \tag{33}$$

Calculations show that under the condition $\Delta < 2\mu$ we have [52]

$$\operatorname{Re}\sigma(\omega,0) = \sigma_0 \theta(\hbar\omega - 2\mu) \frac{(\hbar\omega)^2 + \Delta^2}{(\hbar\omega)^2},$$

$$\operatorname{Im}\sigma(\omega,0) = \frac{\sigma_0}{\pi} \left[\frac{4\mu}{\hbar\omega} - \frac{(\hbar\omega)^2 + \Delta^2}{(\hbar\omega)^2} \ln \left| \frac{\hbar\omega + 2\mu}{\hbar\omega - 2\mu} \right| \right]. \quad (34)$$

Similar to Eq. (9), this result is valid at the real, positive frequency axis. It is easily seen that in the limiting case $\omega \rightarrow 0$ one has

$$\operatorname{Im}\sigma(\omega,0) = \frac{C(0)}{\omega} + O\left(\frac{\hbar\omega}{2\mu}\right),\tag{35}$$

where

$$C(0) = \frac{\sigma_0}{\pi} \frac{(2\mu)^2 - \Delta^2}{\hbar\mu}.$$
 (36)

The last equation is also obtainable as a particular case of Eq. (14) if one puts there T = 0. In so doing it is necessary to take into account that at $T \rightarrow 0$ only the interval of v from unity to $2\mu/\Delta$ contributes to the integral.

Taking into account that $\text{Im}\sigma(\omega, 0)$ has a pole at zero frequency, the Kramers-Kronig relations are given in this case by Eq. (24) where one should replace $\sigma(\omega, T)$ with $\sigma(\omega, 0)$ and C(T) with C(0). It is easily seen that both of them are satisfied. Really, substituting the first line of Eq. (34) in the right-hand side of the second Kramers-Kronig relation in Eq. (24) with C defined in Eq. (36) and introducing the variable $\zeta = \hbar \xi$, one obtains

$$-\frac{2\omega}{\pi} \int_{0}^{\infty} \frac{\operatorname{Re}\sigma(\xi,0)}{\xi^{2}-\omega^{2}} d\xi + \frac{\sigma_{0}}{\pi} \frac{(2\mu)^{2}-\Delta^{2}}{\hbar\mu\omega}$$
$$= -\frac{2\sigma_{0}}{\pi} \hbar\omega \left[\int_{2\mu}^{\infty} \frac{d\zeta}{\zeta^{2}-\hbar^{2}\omega^{2}} + \Delta^{2} \int_{2\mu}^{\infty} \frac{d\zeta}{\zeta^{2}(\zeta^{2}-\hbar^{2}\omega^{2})} \right],$$
$$+ \frac{\sigma_{0}}{\pi} \frac{(2\mu)^{2}-\Delta^{2}}{\hbar\mu\omega}.$$
(37)

Calculating the integrals in Eq. (37), we arrive at

$$-\frac{2\omega}{\pi} \int_{0}^{\infty} \frac{\operatorname{Re}\sigma(\xi,0)d\xi}{\xi^{2}-\omega^{2}} + \frac{\sigma_{0}}{\pi} \frac{(2\mu)^{2}-\Delta^{2}}{\hbar\mu\omega}.$$
$$= \frac{\sigma_{0}}{\pi} \left[\frac{4\mu}{\hbar\omega} - \frac{(\hbar\omega)^{2}+\Delta^{2}}{(\hbar\omega)^{2}} \ln \left| \frac{\hbar\omega+2\mu}{\hbar\omega-2\mu} \right| \right] = \operatorname{Im}\sigma(\omega,0)$$
(38)

in accordance with Eq. (24).

Now we verify the first Kramers-Kronig relation in Eq. (24), when C(T) is replaced with C(0) from Eq. (36). It is more illustrative to consider first the case $\omega \neq 0$ when C(0) can be simply omitted due to Eq. (22). Substituting the second line of Eq. (34) in the right-hand side of the first Kramers-Kronig relation in Eq. (24), we find

$$\sigma_{0} + \frac{2}{\pi} \int_{0}^{\infty} \frac{\xi \operatorname{Im}\sigma(\xi, 0)}{\xi^{2} - \omega^{2}} d\xi = \sigma_{0} - \frac{2\sigma_{0}}{\pi^{2}} \int_{0}^{\infty} \frac{\xi}{\xi^{2} - \omega^{2}} \\ \times \left[\ln \left| \frac{\hbar\xi + 2\mu}{\hbar\xi - 2\mu} \right| + \frac{\Delta^{2}}{(\hbar\xi)^{2}} \ln \left| \frac{\hbar\xi + 2\mu}{\hbar\xi - 2\mu} \right| \right] d\xi.$$
(39)

The first integral on the right-hand side of this equation is calculated like in Eq. (29) with $y = \hbar \xi/(2\mu)$ and $b = \hbar \omega/(2\mu)$ using Eq. (28). The result is given by Eq. (29) where Δ is replaced with 2μ . The second integral is calculated like in Eq. (30). It is equal to zero when $\hbar \omega < 2\mu$ and to $-(\pi \Delta)^2/(2\hbar^2 \omega^2)$ when $\hbar \omega > 2\mu$. Substituting the values of both integrals in Eq. (39) and taking into account the first line in Eq. (34), one finds

$$\sigma_{0} + \frac{2}{\pi} \int_{0}^{\infty} \frac{\xi \mathrm{Im}\sigma(\xi, 0)}{\xi^{2} - \omega^{2}} d\xi = \begin{cases} 0, & \hbar\omega < 2\mu, \\ \sigma_{0} \frac{(\hbar\omega)^{2} + \Delta^{2}}{(\hbar\omega)^{2}}, & \hbar\omega > 2\mu. \end{cases}$$
$$= \mathrm{Re}\sigma(\omega, 0). \tag{40}$$

Thus, with account of Eq. (22), the first Kramers-Kronig relation in Eq. (24) is proven for all $\omega \neq 0$.

At $\omega = 0$ the validity of this Kramers-Kronig relation is achieved by the subtraction of C(0) in the first line of Eq. (39). To see this, we substitute Im $\sigma(\omega, 0)$ from Eq. (34) and C(0) from Eq. (36) in the right-hand side of the first Kramers-Kronig relation of Eq. (24) at $\omega = 0$ and obtain

$$\sigma_{0} + \frac{2}{\pi} \int_{0}^{\infty} \frac{\xi \operatorname{Im}\sigma(\xi, 0) - C(0)}{\xi^{2}} d\xi = \sigma_{0} + \frac{2\sigma_{0}}{\pi^{2}} \int_{0}^{\infty} d\xi \\ \times \left[\frac{\Delta^{2}}{\hbar\mu\xi^{2}} - \frac{1}{\xi} \ln \left| \frac{\hbar\xi + 2\mu}{\hbar\xi - 2\mu} \right| - \frac{\Delta^{2}}{(\hbar\xi)^{3}} \ln \left| \frac{\hbar\xi + 2\mu}{\hbar\xi - 2\mu} \right| \right].$$
(41)

Calculation of all the three integrals on the right-hand side of this equation (see Appendix B) results in

$$\sigma_0 + \frac{2}{\pi} \int_0^\infty \frac{\xi \text{Im}\sigma(\xi, 0) - C(0)}{\xi^2} d\xi = \sigma_0 - \sigma_0 = 0, \quad (42)$$

as it should be because in accordance to the first line of Eq. (34)

$$\operatorname{Re}\sigma(0,0) = 0. \tag{43}$$

This concludes the proof of the Kramers-Kroniog relations for the conductivity of graphene at zero temperature and validates the fact that expressions (9) for $\Delta > 2\mu$ and (34) for $\Delta < 2\mu$ satisfy the condition of causality. In some particular cases Eqs. (9) and (34) have been derived using various models and phenomenological approaches (see, for instance, Refs. [47,62,63]). Note, however, that the additional terms in the conductivity of graphene at zero temperature containing the δ function of ω , which were obtained within some approaches (see, e.g., Refs. [47,64]), are not obtainable in our formalism based on the first principles of quantum electrodynamics. Such terms would violate the Kramers-Kronig relations and, thus, lead to contradiction with the principle of causality [65].

IV. KRAMERS-KRONIG RELATIONS AT NONZERO TEMPERATURE

At first, we prove the validity of the Kramers-Kronig relations for the temperature-dependent part of the conductivity of graphene $\sigma^{(1)}(\omega, T)$ defined in Eq. (15). As usual, we start from the second Kramers-Kronig relation in Eq. (23). Substituting the first line of Eq. (15) in the right-hand side of the second Kramers-Kronig relation in Eq. (23), one obtains

$$-\frac{2\omega}{\pi} \int_{0}^{\infty} \frac{\operatorname{Re}\sigma^{(1)}(\xi,T)}{\xi^{2}-\omega^{2}} d\xi + \frac{C(T)}{\omega}$$
$$= \frac{2\omega\sigma_{0}}{\pi\hbar^{2}} \int_{\frac{\Lambda}{\hbar}}^{\infty} \frac{(\hbar\xi)^{2}+\Delta^{2}}{\xi^{2}(\xi^{2}-\omega^{2})} F(\xi,T) d\xi + \frac{C(T)}{\omega}. \quad (44)$$

Introducing the new integration variable $v = \hbar \xi / \Delta$ and using the second line of Eq. (15), we find

$$-\frac{2\omega}{\pi} \int_{0}^{\infty} \frac{\operatorname{Re}\sigma^{(1)}(\xi,T)}{\xi^{2}-\omega^{2}} d\xi + \frac{C(T)}{\omega}$$
$$= \frac{2\sigma_{0}}{\pi} \hbar\omega \Delta \int_{1}^{\infty} dv \frac{v^{2}+1}{v^{2}[(v\Delta)^{2}-(\hbar\omega)^{2}]} F\left(\frac{v\Delta}{\hbar},T\right) + \frac{C(T)}{\omega}$$
$$= \operatorname{Im}\sigma^{(1)}(\omega,T), \tag{45}$$

i.e., the second Kramers-Kronig relation in Eq. (23) is satisfied.

Now we substitute the second line of Eq. (15) to the right-hand side of the first Kramers-Kronig relation in Eq. (23). Taking into account that in the second line of Eq. (15) the pole term is already separated, one can consider both cases $\omega \neq 0$ and $\omega = 0$ simultaneously. The result is

$$J = \frac{2}{\pi} \int_{0}^{\infty} \frac{\xi \text{Im}\sigma^{(1)}(\xi, T) - C(T)}{\xi^{2} - \omega^{2}} d\xi$$

$$= \frac{4\sigma_{0}}{\pi^{2}} \hbar \Delta \int_{0}^{\infty} \frac{\xi^{2} d\xi}{\xi^{2} - \omega^{2}} \int_{1}^{\infty} dv \frac{(v^{2} + 1)F(\frac{v\Delta}{\hbar}, T)}{v^{2}[(v\Delta)^{2} - (\hbar\omega)^{2}]}$$

$$= \frac{4\sigma_{0}}{\pi^{2}} \int_{0}^{\infty} \frac{y^{2} dy}{y^{2} - b^{2}} \int_{1}^{\infty} dv \frac{v^{2} + 1}{v^{2}} \frac{F(\frac{v\Delta}{\hbar}, T)}{v^{2} - y^{2}}, \qquad (46)$$

where the integration variable $y = \hbar \xi / \Delta$ was introduced and $b = \hbar \omega / \Delta$.

Note that if b < 1, i.e., $\hbar \omega < \Delta$, then $v \neq b$ holds over the entire integration region from unity to infinity. Taking into account that

$$\int_{0}^{\infty} \frac{y^2 dy}{(y^2 - b^2)(y^2 - v^2)} = 0 \quad \text{for } b \neq v, \qquad (47)$$

one immediately concludes that J = 0.

It remains to consider the case b > 1, i.e., $\hbar \omega > \Delta$. To deal with this case, we present our integral (46) in the form

$$J = -\frac{2\sigma_0}{\pi^2} \int_0^\infty \frac{y dy}{y^2 - b^2} \int_1^\infty \frac{v^2 + 1}{v^2} F\left(\frac{v\Delta}{\hbar}, T\right) d\ln\left|\frac{v + y}{v - y}\right|.$$
(48)

Integrating here by parts we find

$$J = -\frac{2\sigma_0}{\pi^2} \int_0^\infty \frac{y dy}{y^2 - b^2} \\ \times \left\{ \left[\frac{v^2 + 1}{v^2} F\left(\frac{v\Delta}{\hbar}, T\right) \ln \left| \frac{v + y}{v - y} \right| \right] \right|_1^\infty \\ - \int_1^\infty \ln \left| \frac{v + y}{v - y} \right| d \left[\frac{v^2 + 1}{v^2} F\left(\frac{v\Delta}{\hbar}, T\right) \right] \right\}.$$
(49)

Taking into account that in accordance to Eq. (12) $F(x, T) \rightarrow 0$ when $x \rightarrow \infty$, Eq. (49) leads to

$$J = \frac{4\sigma_0}{\pi^2} F\left(\frac{\Delta}{\hbar}, T\right) \int_0^\infty \frac{y dy}{y^2 - b^2} \ln\left|\frac{1+y}{1-y}\right| + \frac{2\sigma_0}{\pi^2} \int_0^\infty \frac{y dy}{y^2 - b^2} \int_1^\infty \ln\left|\frac{v+y}{v-y}\right| d\left[\frac{v^2+1}{v^2} F\left(\frac{v\Delta}{\hbar}, T\right)\right].$$
(50)

The first integral on the right-hand side of this equation is equal to zero due to Eq. (28) and, changing the integration order with respect to y and v, we have

$$J = \frac{2\sigma_0}{\pi^2} \int_{-1}^{\infty} d\left[\frac{v^2 + 1}{v^2} F\left(\frac{v\Delta}{\hbar}, T\right)\right] \int_{-0}^{\infty} \frac{ydy}{y^2 - b^2} \ln\left|\frac{v + y}{v - y}\right|.$$
(51)

Now we introduce the integration variable t = y/v in the last integral and obtain

$$J = \frac{2\sigma_0}{\pi^2} \int_{-1}^{\infty} d\left[\frac{v^2 + 1}{v^2} F\left(\frac{v\Delta}{\hbar}, T\right)\right] \int_{-0}^{\infty} \frac{tdt}{t^2 - \tilde{b}^2} \ln\left|\frac{t+1}{t-1}\right|,$$
(52)

where $\tilde{b} = b/v$ can be both larger and less than unity. According to Eq. (28), the last integral on the right-hand side of Eq. (52) is equal to zero if $\tilde{b} > 1$ (i.e., v < b) and to $\pi^2/2$ if $\tilde{b} < 1$ (i.e., v > b). As a result, Eq. (52) is simplified to

$$J = \sigma_0 \int_{-b}^{\infty} d\left[\frac{v^2 + 1}{v^2} F\left(\frac{v\Delta}{\hbar}, T\right)\right]$$

= $-\sigma_0 \frac{b^2 + 1}{b^2} F\left(\frac{b\Delta}{\hbar}, T\right) = -\sigma_0 \frac{(\hbar\omega)^2 + \Delta^2}{(\hbar\omega)^2} F(\omega, T).$ (53)

Combining together the results for b < 1 (i.e., $\hbar \omega < \Delta$) and b > 1 (i.e., $\hbar \omega > \Delta$) and using the first line of Eq. (11), we conclude from Eq. (46) that

$$J = -\sigma_0 \theta(\hbar \omega - \Delta) \frac{(\hbar \omega)^2 + \Delta^2}{(\hbar \omega)^2} F(\omega, T) = \operatorname{Re}\sigma^{(1)}(\omega, T),$$
(54)

i.e., the first Kramers-Kronig relation in Eq. (23) is satisfied.

The total conductivity of graphene at nonzero temperature is given by Eq. (8). Using Eqs. (9) and (15), one obtains

$$\begin{aligned} \operatorname{Re}\sigma(\omega,T) &= \sigma_0 \theta(\hbar\omega - \Delta) \frac{(\hbar\omega)^2 + \Delta^2}{(\hbar\omega)^2} [1 - F(\omega,T)], \\ \operatorname{Im}\sigma(\omega,T) &= \frac{\sigma_0}{\pi} \bigg\{ \bigg[\frac{2\Delta}{\hbar} + \frac{\pi C(T)}{\sigma_0} \bigg] \frac{1}{\omega} \\ &- \frac{(\hbar\omega)^2 + \Delta^2}{(\hbar\omega)^2} \ln \bigg| \frac{\hbar\omega + \Delta}{\hbar\omega - \Delta} \bigg| \\ &+ 2\hbar\omega \Delta \int_{-1}^{\infty} dv \frac{v^2 + 1}{v^2 [(v\Delta)^2 - (\hbar\omega)^2]} F\bigg(\frac{v\Delta}{\hbar}, T \bigg) \bigg\}. \end{aligned}$$
(55)

Note that $\text{Re}\sigma(\omega, T)$ can be rewritten in especially simple and transparent equivalent form. For this purpose we use the definition of *F* in Eq. (12) and the following identity:

$$\frac{1}{2} - \frac{1}{e^y + 1} = \frac{1}{2} \tanh \frac{y}{2}.$$
 (56)

The result is

$$\operatorname{Re}\sigma(\omega,T) = \sigma_0 \theta(\hbar\omega - \Delta) \frac{(\hbar\omega)^2 + \Delta^2}{2(\hbar\omega)^2} \times \left(\tanh \frac{\hbar\omega + 2\mu}{4k_BT} + \tanh \frac{\hbar\omega - 2\mu}{4k_BT} \right).$$
(57)

As to $\text{Im}\sigma(\omega, T)$, simple asymptotic expressions for it in different regions of parameters and the results of numerical computations can be found in Refs. [50–52]. Although in

the general case of gapped graphene with nonzero chemical potential Eqs. (55) and (57) were derived in Ref. [52], in different special cases similar dependences have been obtained previously using various approaches based on the Kubo formalism and two-dimensional Drude model (see, e.g., Refs. [66–71]).

The Kramers-Kronig relations (24) for the total conductivity of graphene (55) are satisfied automatically, because they are obtained by the combination of already proven Kramers-Kronig relations (21) and (23) satisfied for $\sigma^{(0)}(\omega)$ and $\sigma^{(1)}(\omega, T)$, respectively.

V. CONCLUSIONS AND DISCUSSION

In the foregoing, we have investigated the problem of causality for the conductivity of graphene in the framework of the Dirac model. Until recently, only some partial results for the conductivity of graphene have been obtained using some models and phenomenological approaches. To investigate the problem of causality, we use the complete results for the spatially local conductivity found on the basis of first principles of thermal quantum field theory using the polarization tensor of graphene in (2 + 1)-dimensional space-time [50–52]. The spatially nonlocal corrections to these results were shown to be of the order of 10^{-5} of the local contributions and, thus, are of no physical significance in the framework of Dirac's model.

General discussion of causality presented in the paper leads to the conclusion that both the total conductivity of graphene and contributions to it $\sigma^{(0)}(\omega)$, depending on the band gap, and $\sigma^{(1)}(\omega, T)$, depending on the band gap and chemical potential, are the analytic functions in the upper half-plane of complex frequencies and possess all the standard symmetry properties. Hence it follows that the real and imaginary parts of the conductivity of graphene derived in any specific formalism must satisfy the Kramers-Kronig relations. The form of these relations, as shown above, depends on the presence of a pole at zero frequency and takes into account an existence of the universal conductivity. There is no pole for the conductivity of graphene at zero temperature under the condition that the band gap is larger than twice the chemical potential, and there is such a pole in all remaining cases. The fulfilment of the Kramers-Kronig relations can be considered as a basic guideline in deciding which specific expression for the conductivity of graphene is correct.

We have shown through the direct analytic calculations that the real and imaginary parts of the conductivity of graphene, found in Ref. [52] in the most general case of nonzero temperature, band gap and chemical potential on the basis of first principles of thermal quantum field theory, satisfy both Kramers-Kronig relations precisely. In the process, the values of two important integrals in the widely used tables have been corrected, which might be useful in the context of dispersion relations for the scattering amplitudes in quantum field theory. One can conclude that the obtained results are not of only fundamental theoretical character, but they also open fresh opportunities for the use of Kramers-Kronig relations in different fields of physics and for the interpretation of experimental data.

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APPENDIX A: CALCULATION OF IMPORTANT INTEGRALS

Here, we calculate the integral (28) and correct relevant integrals in Ref. [58] which are important for various applications in a wide context of dispersion relations in different branches of physics.

The integral in Eq. (28) can be presented in the form

$$I(b) = \frac{1}{2} [I_{+}(b) + I_{-}(b)], \qquad (A1)$$

where

$$I_{+}(b) = \int_{0}^{\infty} \frac{dy}{y+b} \ln \left| \frac{y+1}{y-1} \right|,$$

$$I_{-}(b) = \int_{0}^{\infty} \frac{dy}{y-b} \ln \left| \frac{y+1}{y-1} \right|.$$
 (A2)

We consider the case $b \ge 0$, $b \ne 1$. It is easily seen that the integrals in Eq. (A2) converge at the points y = 1, y = b. Integrating by parts in Eq. (A2), one obtains

$$I_{\pm}(b) = 2 \int_{0}^{\infty} dy \frac{\ln|y \pm b|}{y^{2} - 1},$$
 (A3)

where the out-of-integral terms vanish and the lower indices \pm correspond to plus and minus on the right-hand side, respectively.

From Eq. (A3) we find the derivative of I_{\pm} with respect to b

$$\frac{dI_{\pm}(b)}{db} = \pm 2 \int_{0}^{\infty} dy \frac{1}{(y \pm b)(y^{2} - 1)}.$$
 (A4)

Calculating this integral, we obtain the result

$$\frac{dI_{\pm}(b)}{db} = \pm 2 \frac{\ln b}{1 - b^2}.$$
 (A5)

From this it follows that

$$\frac{dI(b)}{db} = \frac{1}{2} \left[\frac{dI_{+}(b)}{db} + \frac{dI_{-}(b)}{db} \right] = 0,$$
 (A6)

i.e., I(b) takes the constant values in the intervals [0, 1) and $(1, \infty)$, where it is a continuous function.

Let us consider first the interval [0,1) and find the values

$$I_{+}(0) = I_{-}(0) = \int_{0}^{\infty} \frac{dy}{y} \ln \left| \frac{y+1}{y-1} \right|$$

= $\int_{0}^{1} \frac{dy}{y} \ln \frac{1+y}{1-y} + \int_{1}^{\infty} \frac{dy}{y} \ln \frac{y+1}{y-1}.$ (A7)

Changing the integration variable according to y = 1/x in the second integral on the right-hand side of Eq. (A7), one obtains

$$I_{\pm}(0) = 2 \int_0^1 \frac{dy}{y} \ln \frac{1+y}{1-y} = 4 \sum_{k=1}^\infty \frac{1}{2k-1} \int_0^1 y^{2k-2} dy.$$
(A8)

Calculating this integral and taking into account that [72]

$$\sum_{k=1}^{\infty} \frac{1}{(2k-1)^2} = \frac{\pi^2}{8},$$
 (A9)

we find

$$I_{\pm}(0) = \frac{\pi^2}{2}.$$
 (A10)

Then from Eq. (A1) it follows that $I(b) = \pi^2/2$ under the condition $0 \le b < 1$ in agreement with the first line of Eq. (28).

Note that it is also possible now to find the values of integrals $I_{\pm}(b)$ at any *b*. By integrating Eq. (A5) with respect to *b* for b < 1, we have

$$I_{\pm}(b) = \pm \ln b \ln \frac{1+b}{1-b} \mp \text{Li}_{2}(b) \pm \text{Li}_{2}(-b) + \frac{\pi^{2}}{2},$$
(A11)

where $Li_n(x)$ is the polylogarithm function. This equation can be checked by differentiation taking into account that

$$\frac{d\mathrm{Li}_2(\pm b)}{db} = -\frac{\ln(1 \mp b)}{b}.$$
 (A12)

The value of the arbitrary integration constant in Eq. (A11), $C = \pi^2/2$, is determined from Eq. (A10) taking into account that $\text{Li}_2(0) = 0$.

The result (A11) is in disagreement with the formula 2.6.14.27 of Ref. [58] where the independent on *b* value of the integrals $I_{\pm}(b)$ equal to π is indicated leading to an incorrect result $I(b) = \pi$. This formula is also in contradiction with the formula 2.6.14.24. The latter is in agreement with our result (A10).

Now we consider the case when *b* varies in the interval $(1, \infty)$, where the dilogarithm function has a cut. Using Eq. (A12), one can easily check that the integration of Eq. (A5) results in

$$I_{\pm}(b) = \pm \ln b \ln \frac{b+1}{b-1} \pm \operatorname{Li}_2\left(\frac{1}{b}\right) \mp \operatorname{Li}_2\left(-\frac{1}{b}\right). \quad (A13)$$

The integration constant C = 0 is found from the fact that $I_{\pm}(b) \rightarrow 0$ when $b \rightarrow \infty$. From Eqs. (A1) and (A13) we have I(b) = 0 over the entire interval $(1, \infty)$ which concludes the proof of Eq. (28).

The result (A13) contradicts to the formula 2.6.14.26 of Ref. [58], where instead of Eq. (A13) an incorrect value $I_{+}(b) = 0$ is indicated.

APPENDIX B: INTEGRALS NEEDED IN THE CASE OF ZERO FREQUENCY

Here, we calculate the integrals contained in Eq. (41). Introducing the new variable $y = \hbar \xi/(2\mu)$, the right-hand side of Eq. (41) takes the form

$$\sigma_0 + \frac{2\sigma_0}{\pi^2} (I_1 - I_2), \tag{B1}$$

where

$$I_{1} = \frac{\Delta^{2}}{(2\mu)^{2}} \int_{0}^{\infty} \left(\frac{2}{y^{2}} - \frac{1}{y^{3}} \ln \left| \frac{y+1}{y-1} \right| \right) dy,$$

$$I_{2} = \int_{0}^{\infty} \frac{dy}{y} \ln \left| \frac{y+1}{y-1} \right|.$$
 (B2)

Using Eq. (28) with b = 0, which is proven in Appendix A, one obtains $I_2 = \pi^2/2$. Because of this below we consider only I_1 . It is easily seen that this integral converges at y = 0. Really, for y < 1 it holds

$$\ln\left|\frac{y+1}{y-1}\right| = \ln\frac{1+y}{1-y} = 2\sum_{k=1}^{\infty} \frac{y^{2k-1}}{2k-1}$$
$$= 2y + 2\sum_{k=1}^{\infty} \frac{y^{2k+1}}{2k+1}.$$
(B3)

In a similar way, for y > 1 one obtains

$$\ln\left|\frac{y+1}{y-1}\right| = \ln\frac{y+1}{y-1} = \ln\frac{1+\frac{1}{y}}{1-\frac{1}{y}}$$
$$= 2\sum_{k=1}^{\infty} \frac{1}{(2k-1)y^{2k-1}}.$$
(B4)

Substituting Eqs. (B3) and (B4) in the first line of Eq. (B2), we find

$$I_{1} = \frac{\Delta^{2}}{(2\mu)^{2}} \left[\int_{0}^{1} \left(\frac{2}{y^{2}} - \frac{1}{y^{3}} \ln \frac{1+y}{1-y} \right) dy + \int_{1}^{\infty} \left(\frac{2}{y^{2}} - \frac{1}{y^{3}} \ln \frac{y+1}{y-1} \right) dy \right]$$
$$= -\frac{2\Delta^{2}}{(2\mu)^{2}} \left\{ \int_{0}^{1} \sum_{k=1}^{\infty} \frac{y^{2k-2}}{2k+1} dy - \int_{1}^{\infty} \left[\frac{1}{y^{2}} - \sum_{k=1}^{\infty} \frac{1}{(2k-1)y^{2k+2}} \right] dy \right\}.$$
(B5)

Integrating on the right-hand side of this equation, one arrives at

$$I_1 = -\frac{2\Delta^2}{(2\mu)^2} \left[\sum_{k=1}^{\infty} \frac{1}{4k^2 - 1} - 1 + \sum_{k=1}^{\infty} \frac{1}{4k^2 - 1} \right].$$
 (B6)

Taking into account that [72]

$$\sum_{k=1}^{\infty} \frac{1}{4k^2 - 1} = \frac{1}{2},\tag{B7}$$

we finally obtain that $I_1 = 0$. Substituting the values of both I_1 and I_2 in Eq. (B1), one finds

$$\sigma_0 + \frac{2\sigma_0}{\pi^2} (I_1 - I_2) = 0 \tag{B8}$$

in accordance with Eq. (42).

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