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Kramers–Krönig relation of graphene conductivity

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Abstract

Utilizing a complete Lorentz-covariant and local-gauge-invariant formulation, we discuss the response of graphene to arbitrary external electric fields. The relation, which we call here the Kramers–Krönig relation, between the imaginary part and the real part of ac conductivity is given. We point out that there exists an ambiguity in the conductivity computing, attributed to the ‘poor’ behavior in the ultraviolet region. We argue that to study the electrical response of graphene completely, the non-perturbational contribution should be considered.

1. Introduction

Graphene, a flat monolayer of carbon atoms tightly packed into a two-dimensional honeycomb lattice, has spawned many theoretical and experimental focuses. As stated in [1], graphene plays the role of a bridge between condensed physics and high energy physics. This is attributed to the massless Dirac fermion behavior of quasielectrons in graphene, i.e. we can treat the quasielectrons in graphene as ultimately relativistic particles.

This behavior also brings about many unusual properties of graphene, such as its ac and dc conductivity; much attention [2–5] has been given to such topics. However, there exist discrepancies in the problem, including the discrepancies between theories and experiments on dc conductivity, the famous missing ‘ $\frac{1}{\pi}$ factor’, and conflict between different theoretical calculations [6]. So far, different theories are mostly based on the perturbational approximation, even calculations may be performed by multi-loop diagrams [7].

We introduce a correlation function with respect to only one variable, the invariant amplitude of the spatial-time position, x , to study the graphene conductivity non-perturbationally. From the correlation function, we show that there is relation between the imaginary part and the real part of the ac conductivity. The function is very close to a spectral function and we find that the perturbational calculations for conductivity only include contributions from free valence-conduction electron pairs. Therefore, besides these contributions, to compute conductivity completely we should also consider other factors, such as excitation or impurity. To check the statement, we perform a perturbational calculation for the dc conductivity using quantum field theory.

This technique guarantees that the formulation is Lorentz-covariant and local-gauge-invariant. We point out that there exist discrepancies among different theoretical calculations, attributed to poor behavior in the ultraviolet vicinity of δ -functions.

We organize the paper as following: in section 2, we discuss the electrical response to arbitrary external electric field. A discussion on obtaining dc conductivity utilizing Kubo theory [8] is also given. The relation between the imaginary part and the real part of ac conductivity is listed in section 3. We show explicit perturbational computing for conductivity in section 4 and a brief discussion in section 5.

2. The conductivity under arbitrary external fields

To perform the calculation we first give the second quantization of graphene briefly. The Lagrangian density is

$$\mathcal{L} = \bar{\psi}(i\gamma_\mu \partial^\mu - m)\psi, \quad (1)$$

where $\partial^\mu = \frac{\partial}{\partial x_\mu}$, $\bar{\psi} = \psi^\dagger \gamma_0$, m is the mass of a quasiparticle (to clarify, we here endow the quasielectrons with nonzero mass), and γ s are

$$\gamma_0 = \beta = \tau_3, \quad \gamma_1 = \beta \tau_1, \quad \gamma_2 = \beta \tau_2,$$

where τ_1 , τ_2 , and τ_3 are three Pauli matrices. In this paper, the repeated indices are generally summed, unless otherwise indicated. Furthermore, $\hbar = v_F = e = 1$ are always set.

The Hamiltonian is then [5]

$$H = \int d^2\mathbf{r} \psi^\dagger(\mathbf{r}) \beta (-i\gamma_i \partial^i + m) \psi(\mathbf{r}). \quad (2)$$

Here, indices i, j , etc generally run over two spatial coordinate labels, 1, 2, (while Greek indices μ, ν , and so on, run over three spatial-time coordinate labels 0, 1, 2 with x_0 the time coordinate.)

Under the second quantization, we have

$$\begin{aligned}\psi(\mathbf{x}) &= \int \frac{d^2\mathbf{p}}{(2\pi)^2\sqrt{2p_0}} [a_p u(\mathbf{p}) e^{-i\mathbf{p}\cdot\mathbf{x}} + b_p^\dagger v(\mathbf{p}) e^{i\mathbf{p}\cdot\mathbf{x}}], \\ \bar{\psi}(\mathbf{x}) &= \int \frac{d^2\mathbf{p}}{(2\pi)^2\sqrt{2p_0}} [a_p^\dagger \bar{u}(\mathbf{p}) e^{i\mathbf{p}\cdot\mathbf{x}} + b_p \bar{v}(\mathbf{p}) e^{-i\mathbf{p}\cdot\mathbf{x}}],\end{aligned}$$

where $p_0 = \sqrt{m^2 + \mathbf{p}^2} > 0$. Solutions to positive energy $u(\mathbf{p})$ and to negative energy $v(\mathbf{p})$ satisfy respectively

$$\begin{aligned}u^\dagger u &= 2p_0, & \bar{u}u &= 2m, & u\bar{u} &= \not{p} + m, \\ v^\dagger v &= 2p_0, & \bar{v}v &= -2m, & v\bar{v} &= \not{p} - m.\end{aligned}\quad (3)$$

The explicit forms of u and v are irrelevant. For simplification, we call the operator a_p^\dagger (a_p), which creates (annihilates) quasielectrons in the conduction band, the creation (annihilation) operator which creates (annihilates) electrons, at the same time, we call the operator b_p^\dagger (b_p), which annihilates (creates) electron in the valence band, the creation (annihilation) operator which creates (annihilates) hole. Both electron and hole have positive energy, p_0 .

Since in the perturbational ground state, the valence band is completely filled while the conduction band is empty, the energy of the ground state is nonzero, $E_{\text{gnd}} = -\int d^2\mathbf{p} \sqrt{m^2 + \mathbf{p}^2}$. To obtain a Lorentz invariant ground state, we perform a subtraction for all the states, $E \rightarrow E - E_{\text{gnd}}$. Under such subtraction, each physics quantity, such as energy, current, etc should be in its normal form [9].

With the substitution $i\partial_\mu \rightarrow p_\mu$, we read the Hamiltonian operator eventually as

$$H = \int d^2\mathbf{p} p_0 (a_p^\dagger a_p + b_p^\dagger b_p). \quad (4)$$

When concerning electromagnetic interactions we should make a substitution of $p_\mu \rightarrow p_\mu - eA_\mu$ in equation (2). Denoting $A_\mu = g_{\mu\nu} A^\nu$ with metric matrix $g = \text{diag}\{1, -1, -1\}$, the interacting Lagrangian density is $\mathcal{L}_{\text{int}} = -e\bar{\psi}\gamma_\mu\psi A^\mu = -J_\mu A^\mu$ and the corresponding Hamiltonian is

$$H_{\text{int}} = -\int d^2\mathbf{x} \mathcal{L}_{\text{int}} = \int d^2\mathbf{x} J_\mu(\mathbf{x}) A^\mu(\mathbf{x}), \quad (5)$$

where, just as pointed out above, $J_\mu(x)$ is in the normal form:

$$\begin{aligned}J_\mu(x) &= : \bar{\psi}\gamma_\mu\psi(x) : \\ &= \int \frac{d^2\mathbf{p} d^2\mathbf{p}'}{(2\pi)^4\sqrt{2p_0 p_0'}} \{ a_p^\dagger a_{p'} e^{i(p-p')x} \bar{u}(\mathbf{p}) \gamma_\mu u(\mathbf{p}') \\ &\quad + a_p^\dagger b_{p'}^\dagger e^{i(p+p')x} \bar{u}(\mathbf{p}) \gamma_\mu v(\mathbf{p}') \\ &\quad + b_p a_{p'} e^{-i(p+p')x} \bar{v}(\mathbf{p}) \gamma_\mu u(\mathbf{p}') \\ &\quad - b_p^\dagger b_{p'} e^{-i(p-p')x} \bar{v}(\mathbf{p}) \gamma_\mu v(\mathbf{p}') \}.\end{aligned}$$

Unlike some papers, we here introduce a factor $\frac{1}{\sqrt{2p_0}}$ associated with momentum integration, which is attributed to the Lorentz-covariant [9, 10]. Both the electron number and the

hole number are conserved without interaction. However, the only conserved quantity is their difference when interactions are included,

$$N = \int d^2\mathbf{x} : \psi^\dagger \psi : = \int \frac{d^2\mathbf{p}}{(2\pi)^2} (a_p^\dagger a_p - b_p^\dagger b_p). \quad (6)$$

Generally, the interacting Hamiltonian of graphene in external field $A^\mu(x_0, \mathbf{x})$ is described by equation (5). The density operator is $\rho = \rho_0 + \delta\rho$, where ρ_0 is the equilibrium density operator and $\delta\rho$ is the leading order correction with respect to the external field.

In the Heisenberg picture we have

$$i\delta\rho(x_0) = [H_{\text{int}}, \rho_0]. \quad (7)$$

Therefore [2],

$$\delta\rho(x_0) = -i \int_{-\infty}^{x_0} dx'_0 dx' J_\mu(x'_0 \mathbf{x}') A^\mu(x'_0 \mathbf{x}'). \quad (8)$$

Due to the spatial and time translation invariant, at zero temperature, on fixed time x_0^0 , the current density at arbitrary position is

$$\begin{aligned}\langle J_\mu(x_0^0) \rangle &= \text{Tr}(\delta\rho(x_0^0) J_\mu(x_0^0 \mathbf{0})) \\ &= \int_{-\infty}^0 dx_0 d^2\mathbf{x} T_{\mu\nu}(x_0 \mathbf{x}) A^\nu(x_0 + x_0^0 \mathbf{x}),\end{aligned}\quad (9)$$

where

$$T_{\mu\nu}(x_0 \mathbf{x}) = i \langle [J_\nu(x_0 \mathbf{x}), J_\mu(\mathbf{00})] \rangle \quad (10)$$

with the notation of the ground state $|\rangle$.

Noticing in equations (9) and (10), that the variable x_0 is defined on $(-\infty, 0)$, we expand the range of x_0 to $(-\infty, \infty)$ as

$$\begin{aligned}T_{\mu\nu}(x) &= i\theta(x_0) \langle [J_\mu(0), J_\nu(x)] \rangle \\ &\quad + i\theta(-x_0) \langle [J_\nu(x), J_\mu(0)] \rangle,\end{aligned}\quad (11)$$

where $\theta(x_0)$ is a step function: $\theta(x_0) = 1$ for $x_0 \geq 0$, $\theta(x_0) = 0$ for $x_0 \leq 0$. Tensor $T_{\mu\nu}(x)$ is vanishing for space-like x , i.e. the support of tensor $T_{\mu\nu}$ is a time-like three-dimensional vector x .

Our expansion is different to the one in [2], where $T_{\mu\nu}$ has only a forward term or backward term.

The conductivity should be independent of the gauge transformation. This means that, under a local gauge transformation $A^\nu \rightarrow A'^\nu = A^\nu - \partial^\nu f$, where f is an arbitrary function with $f(x_0 = x_0^0) = f(x_0 = -\infty) = 0$, the current density in equation (9) should be invariant. Integrating equation (9) by parts we find that this requirement is satisfied provided $\partial^\nu T_{\mu\nu} = 0$ everywhere. The statement can be proven by the following: (1) charge conservation, i.e. $\partial^\nu J_\nu \equiv 0$; (2) $\frac{\partial}{\partial x_\mu} \theta(x_0) = -\frac{\partial}{\partial x_\mu} \theta(-x_0) = \delta_{0\mu} \delta(x_0)$; (3) the equal time commutation relation $[J_0(\mathbf{x}), J_\mu(\mathbf{y})] = 0$.

$T_{\mu\nu}(x)$ is written as

$$T_{\mu\nu}(x) = -(\partial_\mu \partial_\nu - g_{\mu\nu} \square) \Pi(x), \quad (12)$$

where $\square \equiv \partial^\mu \partial_\mu = \frac{\partial^2}{\partial x_0^2} - \frac{\partial^2}{\partial x_1^2} - \frac{\partial^2}{\partial x_2^2}$, $\Pi(x)$ is a scalar function with respect to only one variable, the invariant amplitude of

the three-dimensional spatial-time vector x . After defining the Fourier transformation of function $f(x)$ as $f(q) = \int dx dt f(x) e^{iqx}$ with $qx \equiv q_\mu x^\mu$, we have, then,

$$T_{\mu\nu}(q) = (q_\mu q_\nu - q^2 g_{\mu\nu}) \Pi(q^2), \quad (13)$$

where $\Pi(q^2)$ is the only function with respect to the invariant amplitude of q .

From equation (9) it seems that J_μ is time dependent in the time-invariant external electric field. But this is not true. It is enough to illustrate it by a special gauge, $A^v = (0, E x^0, 0)$ or $A_v = (0, -E x_0, 0)$, where A is a three-dimensional potential and E is the external electric field, $E_v = (E, 0)$. It is easy to see that

$$J_\mu(x_0^0) = -E \int_{-\infty}^0 \frac{dx_0 dq_0}{2\pi} e^{-iq_0 x_0} g_{\mu 1} q_0^2 \Pi(q_0) (x_0 + x_0^0), \quad (14)$$

where $\Pi(q_0) \equiv \Pi(q_0^2, \mathbf{q} = \mathbf{0})$. J_0 (charge density) and J_2 are both vanishing and only $J_1 \neq 0$:

$$\begin{aligned} J_1(x_0^0) &= E \int \frac{dq_0}{2\pi} q_0^2 \Pi(q_0^2) \int_{-\infty}^{x_0^0} dx_0 x_0 e^{iq_0 x_0 + \epsilon x_0} e^{iq_0 x_0^0} \\ &= E \int \frac{dq_0}{2\pi} \Pi(q_0^2) \frac{q_0^2}{q_0^2 + iq_0 \epsilon} (1 + iq_0 x_0^0) \\ &\equiv E \sigma(x_0^0), \end{aligned} \quad (15)$$

where the additional factor $e^{\epsilon x_0}$ (ϵ is a positive infinitesimal) is to guarantee that the external field is introduced adiabatically. When $\epsilon \rightarrow 0$, $\frac{q_0^2}{q_0^2 + iq_0 \epsilon} \rightarrow 1$, we can replace $\frac{q_0^2}{q_0^2 + iq_0 \epsilon}$ by unity. Furthermore, since $\Pi(q_0^2)$ is an even function of q_0 , $\int \frac{dq_0}{2\pi} \Pi(q_0^2) iq_0 x_0 \equiv 0$. We finally have a time-independent conductivity

$$\sigma = \int \frac{dq_0}{2\pi} \Pi(q_0^2) \equiv \Pi(x_0 = 0, \mathbf{q} = \mathbf{0}), \quad (16)$$

where, to obtain a meaningful quantity, we should perform a subtraction of Π , i.e. we make a substitution: $\Pi(x_0 = 0, \mathbf{q} = \mathbf{0}) \rightarrow \Pi(x_0 = 0, \mathbf{q} = \mathbf{0}) - \Pi(x_0 = -\infty, \mathbf{q} = \mathbf{0})$. In Fourier space, this subtraction is the substitution $\Pi(q_0, \mathbf{q}) \rightarrow \Pi(q_0, \mathbf{q}) - \Pi(q_0 = 0, \mathbf{q})$. In this paper, we always make such a subtraction for all the physical quantities.

As expected, we obtain a time-independent current density for a steady external field.

It is not difficult to deduce the response to arbitrary external fields. Supposing the external electric field is ac with frequency ω , $A = (0, E_0 e^{i\omega x_0}, 0) e^{\epsilon x_0}$ and substituting the potential into expression (9), we find that only the x -component of current density is nonvanishing,

$$J_1(x_0) = E_0 e^{i\omega x_0} \int \frac{dq_0}{2\pi} \Pi(q_0^2, \mathbf{0}) \frac{iq_0^2}{q_0 - \omega + i\epsilon}. \quad (17)$$

Since this potential stands for external electric field (E_1, E_2) = $(i\omega E_0 e^{i\omega x_0}, 0)$, the complex conductivity is

$$\sigma = \int \frac{dq_0}{2\pi} \Pi(q_0^2, \mathbf{0}) \frac{q_0^2}{\omega(q_0 - \omega + i\epsilon)} \quad (18a)$$

$$\begin{aligned} &= \frac{1}{\omega} \int \frac{dq_0}{2\pi} \Pi(q_0^2, \mathbf{0}) q_0 + \int \frac{dq_0}{2\pi} \Pi(q_0^2, \mathbf{0}) \\ &\quad \times \frac{q_0}{q_0 - \omega + i\epsilon}. \end{aligned} \quad (18b)$$

Obtaining the dc conductivity from equations (18a) and (18b) corresponds to the results obtained from the famous Kubo theory. However, it is not obvious whether we can obtain dc conductivity (16) from the limit of equation (18a): firstly, to obtain equation (18b) from (18a) we need not only convergence of all the integrations, such as $\int \frac{dq_0}{2\pi} \Pi(q_0^2, \mathbf{0}) \frac{q_0^2}{\omega(q_0 - \omega + i\epsilon)}$, etc but also proper subtraction of physical quantities. Secondly, when we choose $\omega = 0$ directly in equation (18b), we meet an uncomfortable situation: the first term in equation (18b) is an ambiguous $\frac{0}{0}$. To obtain the correct dc conductivity we should perform the computation as follows: we calculate the ac conductivity in the course of nature from equation (18) at $\omega \neq 0$, with proper subtraction. At last we read the dc conductivity utilizing the limit of $\omega \rightarrow 0$. This was pointed out by Kubo [8], which implies that, compared to results in [3], the results in [4] are correct. Of course, all the results in [3, 4] are obtained by a perturbational approach.

After suitable subtraction, the ac conductivity is

$$\sigma = \int \frac{dq_0}{2\pi} \Pi(q_0^2, \mathbf{0}) \frac{q_0}{q_0 - \omega + i\epsilon}. \quad (19)$$

Generally, $\Pi(q_0^2, \mathbf{0})$ is not convergent or well defined, as will be shown by perturbative calculation in section 4. This is relevant to the wick definition of the δ -function. Therefore, in order to obtain a meaningful physical result, we need to perform subtraction to cancel divergence. For instance, in [6] the author has proposed a soft δ -function. The subtraction should meet some physical criteria. For instance, as found in the above paragraph, to obtain the result in equation (19) from equations (18), after the subtraction Π is still a function of q_0^2 rather than a function of q_0 in Fourier space. In section 4 we shall show an explicit subtraction for $\Pi(x_0, q)$.

3. Kramers–Krönig relation of graphene conductivity

In this section we show a relation between the imaginary part and the real part of graphene conductivity.

We first give a non-perturbational proof that $\Pi(q^2)$ is real. $\Pi(q^2)$ is real at $q^2 < 0$ obviously, the only need is to prove that $\Pi(q^2)$ is also real at $q^2 > 0$.

At $q^2 > 0$, after inserting the completed intermediate states $\sum_\Gamma |\Gamma\rangle \langle \Gamma|$, we have for $T \equiv T_\mu^\mu(q)$,

$$\begin{aligned} T &= \int \frac{d^3x d^3p e^{iqx}}{(2\pi)^2} i(\theta(x_0) - \theta(-x_0)) \\ &\quad \times (e^{ipx} - e^{-ipx}) s(p) \theta(p_0), \end{aligned}$$

where the spectral function $s(p)$ is defined as

$$2\pi s(p) = \sum_\Gamma (|J^\mu(0)| \Gamma) \langle \Gamma | J_\mu(0) | \rangle (2\pi)^3 \delta^3(p - p_\Gamma). \quad (20)$$

The spectral function $s(p)$, which is very close to the state density, includes not only perturbational contributions, but also non-perturbational contributions. To study the non-perturbational contributions, one should consider, for instance, excitations.

Inserting $\int_0^\infty dt \delta(p^2 - t) \equiv 1$ at $p^2 > 0$, we obtain

$$T = \int_0^\infty dt s(t) \int d^3x e^{iqx} i(\theta(x_0) - \theta(-x_0))I, \quad (21)$$

where

$$\begin{aligned} I &= \int \frac{d^3p}{(2\pi)^2} \theta(p_0) \delta(p^2 - t) (e^{ipx} - e^{-ipx}) \\ &= \int \frac{d^3p}{(2\pi)^2} e^{-ipx} \delta(p^2 - t) (\theta(-p_0) - \theta(p_0)). \end{aligned}$$

Utilizing

$$\begin{aligned} i \int \frac{d^3p e^{-ipx}}{(2\pi)^2} [\theta(x_0)\theta(p_0) + \theta(-x_0)\theta(-p_0)] \delta(p^2 - t) \\ = - \int \frac{d^3p}{(2\pi)^3} \frac{e^{-ipx}}{p^2 - t + i\epsilon}, \\ i \int \frac{d^3p e^{-ipx}}{(2\pi)^2} [\theta(-x_0)\theta(p_0) + \theta(x_0)\theta(-p_0)] \delta(p^2 - t) \\ = \int \frac{d^3p}{(2\pi)^3} \frac{e^{-ipx}}{p^2 - t - i\epsilon}, \end{aligned}$$

we finally get

$$T = 2P \int_0^\infty dt s(t) \frac{1}{q^2 - t} \quad (22)$$

with identity $\frac{1}{f \pm i\epsilon} = P \frac{1}{f} \mp i\pi \delta(f)$. Since $s(t) \geq 0$ is real, $T(q)$ and therefore $\Pi(q)$ are both real. The spectral density is in fact a very important function, which will be studied elsewhere [11].

Thus, from equation (19), we obtain an important relation between the real part and the imaginary part of conductivity σ

$$\begin{aligned} \text{Im } \sigma(\omega) &= -\frac{\omega \Pi(\omega^2, \mathbf{0})}{2}, \\ \text{Re } \sigma(\omega) &= P \int \frac{ds}{\pi} \frac{\text{Im } \sigma(s)}{\omega - s}. \end{aligned} \quad (23)$$

This relationship between the real part and the imaginary part of conductivity is beyond the perturbation approach and can be considered as a Kramers–Krönig relation of graphene conductivity. We hope an advanced study of graphene will check this relation.

Equation (23) is one of the main results of this paper. It points out that the electrical response of graphene can never be considered as a pure resistance, but a resistance connected in parallel with a capacitor with capacitivity $\Pi(\omega^2, \mathbf{0})/2$. Furthermore, due to the obvious relation between $\text{Im } \sigma$ and Π , $\text{Im } \sigma$ reflects the state structure of graphene. $\text{Im } \sigma$ is therefore a non-perturbational probe to detect the state structure of graphene. From this viewpoint, $\text{Im } \sigma$ is a more basic quantity than $\text{Re } \sigma$. Furthermore, equation (23) is irrelevant to the idiographic interactions, which means that, the equation holds under very general conditions, such as the existence of impurities or excitations in graphene.

More recent works reveal that graphene is rarely flat, i.e. there are always ripples in graphene. The nonvanishing curvature, raised by ripples, will lead to two main effects:

altering the group velocity of quasiparticles and introducing effective gauge fields. The first effect possibly makes a global correction to conductivity, which may be absorbed into the redefinition of spectral function, Π . Furthermore, since the holding of equation (23) is irrelevant to idiographic interactions, we conclude that the Kramers–Krönig relation is still valid for corrugated graphene.

Equation (23) supplies one possible way to study the discrepancy of dc conductivity between theory and experiment. One may first perform perturbational computing to the imaginary part of ac conductivity and then compare the perturbational result with experiments at different frequencies. The discrepancy between these results reveals a contribution which cannot be ascribed to perturbational theory. Furthermore, the complete contributions to dc conductivity are not only from the Dirac nodal point, but from the spectral structure of carriers.

4. Perturbational calculation of dc conductivity

We here deduce the dc conductivity in a perturbational approximation. After that we shall discuss an ambiguity besides the one pointed out in [6].

We begin with a perturbational calculation of $T_{\mu\nu}$. Noticing that $\langle 0 | b_{p_f} a_{p_f} a_{p_i}^\dagger b_{p_i}^\dagger | 0 \rangle = (2\pi)^4 \delta^2(\mathbf{p}_f - \mathbf{p}_i) \delta^2(\mathbf{p}'_f - \mathbf{p}'_i)$ and that we have normal ordering of operators in current density, we have, for the perturbational ground state,

$$\langle 0 | J^\mu(x) J_\mu(0) | 0 \rangle = \int \frac{d^2\mathbf{p} d^2\mathbf{p}'}{(2\pi)^4 2p_0 2p'_0} F_\mu^\mu e^{-i(p+p')x}, \quad (24)$$

where $F_\mu^\mu = \bar{v}(\mathbf{p}') \gamma^\mu u(\mathbf{p}) \bar{u}(\mathbf{p}) \gamma_\mu v(\mathbf{p}')$. Taking advantage of equation (3), one finds,

$$F_\mu^\mu = -2\mathbf{p} \cdot \mathbf{p}' - 6m^2 = -(p + p')^2 - 4m^2. \quad (25)$$

$T_\mu^\mu \equiv T$ is given by a direct computing

$$T(x) = i(\theta(x_0) - \theta(-x_0))(\square - 4m^2)K'(x), \quad (26)$$

where

$$\begin{aligned} K'(x) &= \int \frac{d^2\mathbf{p} d^2\mathbf{p}'}{(2\pi)^4 2p_0 2p'_0} (e^{i(p+p')x} - e^{-i(p+p')x}) \\ &= \int \frac{d\mathbf{p}(e^{ipx} + e^{-ipx})}{(2\pi)^2 2p_0} \int \frac{d\mathbf{p}(e^{ipx} - e^{-ipx})}{(2\pi)^2 2p_0}. \end{aligned}$$

From

$$\begin{aligned} \int \frac{d\mathbf{p}(e^{ipx} + e^{-ipx})}{(2\pi)^2 2p_0} &= \int \frac{d^3p e^{-ipx}}{(2\pi)^2} \delta(p^2 - m^2), \\ \int \frac{d\mathbf{p}(e^{ipx} - e^{-ipx})}{(2\pi)^2 2p_0} &= \int \frac{d^3p e^{-ipx}}{(2\pi)^2} \delta(p^2 - m^2) \text{sgn}(p_0), \end{aligned}$$

the Fourier transformation of K' is

$$K'(p) = - \int \frac{d^3q}{2\pi} \delta((p-q)^2 - m^2) \delta(q^2 - m^2) \text{sgn}(q_0). \quad (27)$$

Here \underline{p} does not need to be on the mass shell, i.e. $p_0 = \sqrt{p^2 + m^2}$ is not needed, if the integrating factor is d^3p . We

focus on the case of $\mathbf{p} = 0$ (or p is a time-like vector). Letting $K(x) = (\square - 4m^2)K'(x)$ and $K(q_0) = K(q_0, \mathbf{q} = \mathbf{0})$, we get

$$K(q_0) = \frac{q_0^2 + 4m^2}{4q_0} \theta(q_0^2 - 4m^2). \quad (28)$$

The nonzero contribution to $K(q_0)$ is $|q_0|2m$. To simplify we let $m = 0$. Thus $T(x_0, \mathbf{p} = 0) = \frac{1}{4}(\theta(-x_0) - \theta(x_0))\delta'(x_0)$. Since $\Pi(q_0, \mathbf{q} = 0) = -\frac{1}{2q_0}T(q_0, \mathbf{q} = 0)$, we find the dc conductivity of graphene

$$\sigma = \frac{1}{8} \int_{-\infty}^0 dx_1 \int_{-\infty}^{x_1} dx_2 (\theta(-x_2) - \theta(x_2))\delta'(x_2), \quad (29)$$

utilizing equation (16). Notice that in the above equation we have made a subtraction $\Pi(x_0, \mathbf{p}) = \frac{\partial \Pi(x_0, \mathbf{p})}{\partial x_0} = 0$ at $x_0 \rightarrow -\infty$.

However, the functions, such as $\delta'(x)$ and $\theta(x)$, are not well defined. This means that there possibly exists ambiguity in equation (29). This ambiguity is different to the one pointed out in [6].

We consider dc conductivity here. First let $\delta(x)$ be the simplest form, $\delta_1(x) = 0$ for $|x| > \frac{a}{2}$ and $\delta_1(x) = 1/a$ for $|x| < \frac{a}{2}$. In this case we obtain $\sigma_1 = \frac{1}{16} = \frac{\pi}{8} \frac{1}{2\pi} \simeq \frac{0.39}{2\pi}$ utilizing equation (29). This is just the result obtained in [4]. Meanwhile, we can also let $\delta(x)$ be a somewhat complex form [6], $\delta_2(x) = \frac{1}{\pi} \frac{\eta}{x^2 + \eta^2}$. This time we get $\sigma_2 = \frac{4 + \pi^2}{16\pi} \frac{1}{2\pi} \simeq \frac{0.28}{2\pi}$. Finally, we can also set $\delta_3(x) = \frac{1}{4T_0} \cosh^2(\frac{x}{2T_0})$. We find $\sigma_3 = \frac{\pi(1/2 + \ln 2)}{12} \frac{1}{2\pi} \simeq \frac{0.31}{2\pi} \simeq \frac{1}{\pi} \frac{1}{2\pi}$, the numeric value of which is in agreement with that in [3].

To see the physical meaning of T_0 in $\delta_3(x)$, we write out explicitly: $\theta(-x) = \frac{1}{1 + e^{x/T_0}}$. The role of T_0 is something like temperature, which means that T_0^{-1} symbolizes the disorder. a^{-1} in $\delta_1(x)$ and η in $\delta_2(x)$ [6] play a similar role. Since σ_1 , σ_2 and σ_3 are a -, η - and T_0 -independent respectively, we conclude that the dc conductivity is almost temperature-independent near zero temperature, although the conductivity value is ambiguous because of the ‘poor’ behavior of the δ -function. This is verified by experiments [12].

This is an unexpected occasion because the conductivity, a physical observable quantity, varies with different definitions of the δ -function. The ambiguity is associated with the different definitions of the δ -function in the ultraviolet region. One may argue that we can eliminate the ambiguity by a standard renormalization schedule in quantum field theory [9, 10], however, this elimination still contributes to the special definition of the δ -function in the ultraviolet region. We think that the ambiguity implies that the dc conductivity of graphene depends on the behavior of quasielectrons at high energy as well as the behavior at the Dirac nodal point. This is also pointed out by the Kramers–Krönig relation in equation (23). Unfortunately, the linear dispersion relation of quasielectrons does not hold at high energy, which means that different numeric values based on linear dispersion and perturbational approaches need correction. On the other hand, when we study the electrical response of graphene, we always perform calculations utilizing diagrams composed of different Green functions. To include higher corrections, we should use

loop diagrams. However, since coupling $g = 2\pi e^2 / \epsilon \hbar v_F$ is not small, i.e. $g \sim 1$, the loop corrections cannot be ignored compared to the leading order.

One possibly expects that the corrections to conductivity given above are not large. If this is the case, our computations and others [3, 4] indicate that about 30% of the full conductivity is from the perturbational contribution. A question is raised, then, as to where the other contributions to conductivity come from. A generalized version of equation (28) tells us that, from the definition of state density $s(q)$, the perturbational contribution to state density is

$$2\pi s^{pt}(q) = \frac{q^2 + 4m^2}{4q} \theta(q^2 - 4m^2), \quad (30)$$

at $q_0 > 0$. The θ -function in this equation reveals that, s^{pt} only includes the contribution from pairs of *free* quasielectrons and holes. However, since there are complex interactions between electrons and holes, electrons and holes may be combined into excitations [14, 15], or in other words, it is questionable whether we should consider quasielectrons in graphene as a two-dimensional electron gas with no interactions. To study the electrical responses completely, we must also consider the contribution of excitations (and impurities), attributed to equation (22). In standard field theory it is difficult to study the contribution perturbationally. We often nominate the contribution as being a non-perturbational one, such as we did in [13]. Since the coupling is large on graphene, such a contribution cannot be ignored when one consider electrical responses. Apparently, if m is large enough, the nonzero contribution from excitons appears before $q^2 = 4m^2$. We shall discuss such a contribution elsewhere [11].

5. Discussion

The relationship between the imaginary part, $\text{Im} \sigma$, and the real part, $\text{Re} \sigma$, of ac conductivity is given in this paper. $\text{Im} \sigma$ depends directly on details of state structure and one can study state structure from $\text{Im} \sigma$. We consider it to be a non-perturbational probe to detect the state structure of graphene and it is therefore a very important quantity. Our formulas are Lorentz-covariant and local-gauge-invariant.

We also perform an explicit perturbational calculation using quantum field theory. The computation shows that the conductivity is mainly manipulated by the momentum–energy relation and there is little nexus between the conductivity and the state density near the Dirac nodal point. The computation reveals that, due to the ‘wicked’ behavior of the δ -function, there is ambiguity in the graphene conductivity calculations. We argue that the full perturbational studies need two corrections: one is due to the incorrect value of carrier linear dispersion at high energy and the other is the higher order correction. Besides these corrections, however, there is a further correction which is called the non-perturbational correction in this paper. This correction comes from the contribution of excitations, which are attributed to electron–electron interactions.

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