

Space-time dispersion of graphene conductivity

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Abstract. We present an analytic calculation of the conductivity of pure graphene as a function of frequency ω , wave-vector k , and temperature for the range where the energies related to all these parameters are small in comparison with the band parameter $\gamma \simeq 3$ eV, but much larger than the collision rate τ^{-1} . The simple asymptotic expressions are given in various limiting cases. For instance, the conductivity for $kv_0 \ll T \ll \omega$ is equal to $\sigma(\omega, k) = e^2/4\hbar$ and independent of the band structure parameters γ and v_0 . Our results are also used to explain the known dependence of the graphite conductivity on temperature and pressure.

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Since the pioneering experimental investigations of a single atomic layer of graphite (graphene) [1, 2], its properties attract much attention. Among the various reasons for this interest, there is the following. Graphene can be wrapped into 0d fullerenes, rolled into 1d nanotubes, and stacked into 3d graphite [3]. Hence one has a possibility to study the dimensionality effects for the unique substance [4]. Unusual properties of graphene appeal for their explanation. Graphene exhibits Shubnikov-de Haas oscillations with the temperature dependence explained in terms of the standard Fermi-gas theory. Furthermore, while the carrier concentration is decreasing in the field gate experiment, the graphene conductivity at low temperatures goes to the finite minimal values of the order of $\sigma_{min} \simeq e^2/h$. Much theoretical efforts [5–11] have been devoted to evaluate the minimal conductivity in different approaches. The finite values of conductivity at low temperature means that 2d graphene turns out to be a metal (or a semimetal) in contradiction with the recent theoretical analysis [12]. On the other hand, it was found that the weak-localization corrections can have a different sign depending on the interaction range of impurity potentials [13] or can be strongly suppressed [14] because of the Dirac peculiarity of the electron spectrum. The problem of the carrier interaction with defects in graphene and in the underlying substrate was studied in references [8, 15, 16].

Two-dimensional graphene has a very simple band structure, which can be obtained with help of the symmetry consideration or in the tight-binding approximation.

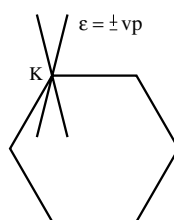


Fig. 1. The Brillouin zone of graphene and the electron spectrum in the vicinity of the K points.

It was shown in references [17, 18] that the energy bands of graphene are degenerated at the corners of the 2d Brillouin zone $K = (0, 4\pi/3\sqrt{3}a)$, where $a = 1.44$ Å is the interatomic distance (see Fig. 1). This is the Dirac-type spectrum but it is massless and two-dimensional. It was demonstrated that due to the symmetry arguments such a gapless spectrum with the conic point in the 3d case turns out to be stable with respect to the Coulomb interaction [19]. One can prove that this stability remains also for the 2d graphene spectrum with the conic point. Such simple band structure can be used in analytic calculations of various thermodynamic and transport properties of graphene. An example of such calculations was presented in reference [20] where the imaginary part of the dielectric function $\text{Im}\varepsilon(\omega)$ of graphite was calculated. The gapless band structure of graphene also results in the unusual behavior of conductivity. Despite the enormous number of papers devoted to carbon materials, the analytic expression of graphene conductivity $\sigma(\omega, k)$ was not yet derived to our best knowledge.

The standard diagrammatic approach to calculation of transport properties of impure metals is restricted by the fundamental requirement that the mean free path of

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carriers $\ell = v_0\tau$ must be much larger than the electron wavelength $\lambda = h/p_F$, i.e. $\ell p_F \gg 1$. This condition cannot evidently be satisfied for graphene when the Fermi surface degenerates to the points. We avoid this difficulty addressing the problem in the case that the graphene sample is clean enough but temperature is finite ($T \gg 1/\tau$). Then the temperature appears instead of the Fermi energy and electrons obey Boltzmann statistics.

In the present paper, we analytically calculate both the frequency and wave-vector dependencies of the graphene conductivity $\sigma_{ij}(\omega, k)$ at finite temperature T for the relatively low frequencies $\omega \ll 3$ eV when only the nearest π bands are taken into consideration. Let us emphasize that we obtain the definite conductivity in collisionless limit because the finite values of frequencies or wave-vectors are considered. In particular, the real part of conductivity appears as a result of the inter-band electron transitions in the alternative electric field. We found that the value of this inter-band contribution at frequencies $\omega > T$ agrees well with the minimal dc conductivity obtained in experiments [1].

Let us briefly remind properties of the graphene electron spectrum. The tight-binding approximation allows to write down the following effective Hamiltonian 2×2 matrix

$$H(\mathbf{p}) = \begin{pmatrix} 0 & h(\mathbf{p}) \\ h^*(\mathbf{p}) & 0 \end{pmatrix}, \quad (1)$$

where $h(\mathbf{p}) = \gamma \{ e^{ip_x a} + 2e^{-ip_x a/2} \cos(p_y a \sqrt{3}/2) \}$ and $\gamma = \langle \psi(a, 0) | H_0 | \psi(0, 0) \rangle$ is the $pp\pi$ transfer integral. The dispersion law of graphene, $\varepsilon_{1,2}(\mathbf{p})$ can be obtained by means of its diagonalization:

$$\varepsilon_{1,2}(\mathbf{p}) = \pm \gamma \left\{ 1 + 4 \cos(3p_x a/2) \cos(p_y a \sqrt{3}/2) + 4 \cos^2(p_y a \sqrt{3}/2) \right\}^{1/2}. \quad (2)$$

In the vicinity of the K point, the matrix element can be expanded as

$$h(\mathbf{p}) = v_0(ip_x - p_y),$$

where $v_0 = 3\gamma a/2$. This results in the linear dispersion relation $\varepsilon_{1,2}(\mathbf{p}) = \pm v_0 p$.

Let us pass to the calculation of the electric current, following the paper by Abrikosov [21], where the dielectric function of Bi-type metals was considered. We assume that the external field is described by the vector potential A_j . The current operator has the form

$$j_i(x) = e\tilde{\psi}^+(x')v_{x'x}^i\tilde{\psi}(x) - \frac{e^2}{c}\tilde{\psi}^+(x')(m^{-1})_{x'x}^{ij}\tilde{\psi}(x)A_j, \quad (3)$$

where $x' \rightarrow x$, $v_{x'x}^i$ and $(m^{-1})_{x'x}^{ij}$ are the velocity and mass operators correspondingly, the tilde in the notation $\tilde{\psi}$ means that the operator is taken in the interaction representation with

$$V = -\frac{e}{c} \int \psi^+(x')v_{x'x}^i\psi(x)A_i(x)d^4x. \quad (4)$$

The matrix of the velocity $\mathbf{v} = \partial H(\mathbf{p})/\partial \mathbf{p}$ near the point K in the band representation is determined by the

Hamiltonian (1). By the use of the unitary transformation, which transforms the Hamiltonian from the band representation to the diagonal one, we obtain the matrix of the velocity in the same representation:

$$\mathbf{v} = \frac{v_0}{p} \begin{pmatrix} \mathbf{e}_x p_x + \mathbf{e}_y p_y & i(\mathbf{e}_x p_y - \mathbf{e}_y p_x) \\ -i(\mathbf{e}_x p_y - \mathbf{e}_y p_x) & -\mathbf{e}_x p_x - \mathbf{e}_y p_y \end{pmatrix}, \quad (5)$$

where \mathbf{e}_i are unit vectors along the coordinate axis directions.

We calculate the current in the linear approximation in $A_i(x)$. Therefore, the second term in equation (3) can be taken in zeroth approximation with respect to the interaction (4). Expanding the first term to the first order in $A_i(x)$, we get the retarded correlator of four ψ operators which has to be averaged over the Gibbs ensemble. At finite temperatures, the Fourier component (with respect to the spatial coordinates and imaginary time) of this correlator

$$\mathcal{P}(\omega_l, \mathbf{k}) = T \sum_{\omega_n} \int \frac{d^2 \mathbf{p}}{(2\pi)^2} Tr \{ v^i \mathcal{G}(p_+) v^j \mathcal{G}(p_-) \} \quad (6)$$

is expressed in terms of the temperature Green's functions:

$$\mathcal{G}(p) = [i\omega_n - H(\mathbf{p})]^{-1}.$$

In equation (6) the notations $p_{\pm} = (\omega_n \pm \omega_l/2, \mathbf{p} \pm \mathbf{k}/2)$ are used, the summation is carried out over the fermionic frequencies $\omega_n = 2\pi T(n + 1/2)$, while the trace operation is performed over the band index of the Hamiltonian (1). The latter can be easily carried out in the representation where the Hamiltonian has diagonal form:

$$Tr \{ v^i \mathcal{G} v^j \mathcal{G} \} = v_{11}^i \mathcal{G}_{11} v_{11}^j \mathcal{G}_{11} + v_{22}^i \mathcal{G}_{22} v_{22}^j \mathcal{G}_{22} + v_{12}^i \mathcal{G}_{22} v_{21}^j \mathcal{G}_{11} + v_{21}^i \mathcal{G}_{11} v_{12}^j \mathcal{G}_{22}.$$

Then one can perform the summation over ω_n in standard way. For instance, for the cross product of the Green functions one finds

$$T \sum_{\omega_n} \mathcal{G}_{11}(p_+) \mathcal{G}_{22}(p_-) = \frac{f_0[\varepsilon_1(\mathbf{p}_-)] - f_0[\varepsilon_2(\mathbf{p}_+)]}{i\omega_l - \varepsilon_2(\mathbf{p}_+) + \varepsilon_1(\mathbf{p}_-)}, \quad (7)$$

where we have taken into account that the photon frequencies $\omega_l = 2\pi T$ are "even" in the Matsubara technique; f_0 is the Fermi distribution function. Analytic continuation of the expressions similar to equation (7) into the upper half plane of the complex frequency can be performed by simple substitution $i\omega_l \rightarrow \omega + i\delta$ with $\delta \rightarrow 0$.

Let us notice that the current has to vanish when the vector potential does not vary in time. Since the second term in equation (3) is time independent, one can omit it, subtracting from the first term its value at $\omega = 0$. In result, we obtain

$$\sigma_{ij}(\omega, k) = \frac{ie^2}{\pi^2} \times \left\{ \sum_{a=1,2} \int \frac{d^2 p v^i v^j \{ f_0[\varepsilon_a(\mathbf{p}_-)] - f_0[\varepsilon_a(\mathbf{p}_+)] \}}{[\varepsilon_a(\mathbf{p}_+) - \varepsilon_a(\mathbf{p}_-)] [\omega - \varepsilon_a(\mathbf{p}_+) + \varepsilon_a(\mathbf{p}_-)]} + 2\omega \int \frac{d^2 p v_{12}^i v_{21}^j \{ f_0[\varepsilon_1(\mathbf{p}_-)] - f_0[\varepsilon_2(\mathbf{p}_+)] \}}{[\varepsilon_2(\mathbf{p}_+) - \varepsilon_1(\mathbf{p}_-)] [\omega^2 - [\varepsilon_2(\mathbf{p}_+) - \varepsilon_1(\mathbf{p}_-)]^2]} \right\}. \quad (8)$$

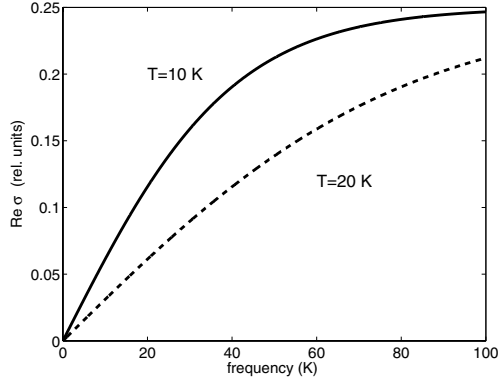


Fig. 2. The real part of conductivity $\sigma(\omega, k \rightarrow 0)$ in units e^2/\hbar for two temperatures vs frequency ω in units of temperature.

Hitherto we did not use any peculiarities of the graphene spectrum besides the number of bands. Thus our main result (8) has a general character. The expression acquired only the factor 4 due to summation over spin and over six points of the K type (two per each Brillouin zone).

The first term in equation (8) corresponds to the intra-band electron-photon scattering processes. In the limit of the high carriers concentration (T, E_F) $\gg kv_0$, it coincides with the usual Drude expression

$$\sigma_{xx}^{intra}(\omega, 0) = \frac{e^2}{\pi^2} \sum_{a=1,2} \int \frac{d^2 p v_{ax}^2}{i\omega - \tau^{-1}} \frac{df_0[\varepsilon_a(\mathbf{p})]}{d\varepsilon}, \quad (9)$$

if the transport scattering time is large enough, $\tau\omega \gg 1$. The second term in equation (8) owes its origin to the inter-band electron transitions. The real part of this contribution (let us recall, that $i\omega_l \rightarrow \omega + i\delta$) at $k \rightarrow 0$ is reduced to the well-known expression for the absorbed energy due to the direct inter-band transitions.

Let us pass to the discussion of the pure graphene conductivity in absence of gate voltage, when the chemical potential is equal to zero. The integral (8) can be analytically performed for various limiting cases.

(i) *Small spatial dispersion* $kv_0 \ll \omega, T$

Putting $k = 0$ and integrating over angle, one can find that the off-diagonal elements of conductivity vanish, while the diagonal ones shown in Figures 2 and 3 are equal to

$$\sigma(\omega, 0) = -\frac{i e^2 \omega}{\pi} \times \left[\frac{2}{\omega^2} \int_0^\infty \varepsilon d\varepsilon \left(\frac{df_0(\varepsilon)}{d\varepsilon} \right) - \int_0^\infty d\varepsilon \frac{f_0(-\varepsilon) - f_0(\varepsilon)}{\omega^2 - 4\varepsilon^2} \right].$$

The first (intra-band) contribution reads:

$$\sigma^{intra}(\omega, k) = 2 \ln 2 \frac{i e^2 T}{\pi \hbar \omega}, \quad kv_0 \ll \omega, T \quad (10)$$

(we restore the Planck constant in the final expressions, T and ω are in the common units). This result was obtained in reference [17] using the Drude expression, equation (9).

The second (inter-band) term consists of the real and imaginary parts (the last one due to the pole of the

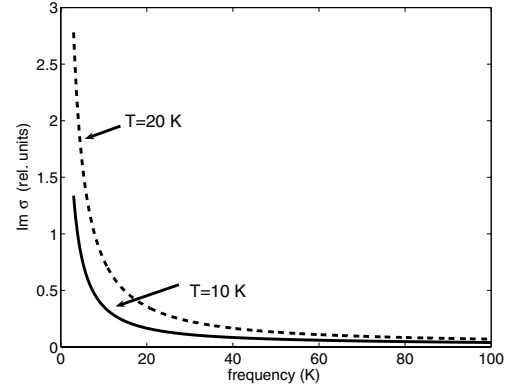


Fig. 3. The same as in Figure 2 but for the imaginary part of conductivity.

integrand). We obtain

$$\sigma^{inter}(\omega, k) = \frac{e^2}{4\hbar} \tanh \frac{\omega}{4T} - \frac{2ie^2}{\pi\hbar} \times \begin{cases} (T/\omega)[\ln 2 + 6\zeta(3)(T/\omega)^2], & kv_0 \ll T \ll \omega, \\ (\omega/16T) \ln(T/\omega), & kv_0 \ll \omega \ll T, \end{cases} \quad (11)$$

where $\zeta(3) = 1.20$. One can see that the term with $\ln 2$ in the first line of equations (11) cancels the intra-band contribution (10).

(ii) *Large spatial dispersion* $\omega \ll kv_0, T$

Let us consider the limit of large dispersion $kv_0 \gg \omega$. The longitudinal and transversal components (with respect to the \mathbf{k} -direction) of the intra-band contribution are different now. For instance, the transversal one, which is important in the optical range, is equal to

$$\sigma_{\perp}^{intra}(\omega, k) = \frac{e^2}{\pi\hbar} \times \begin{cases} (4T/kv_0) \ln 2, & \omega \ll kv_0 \ll T, \\ \sqrt{\pi kv_0/T} \exp(-kv_0/2T), & \omega \ll T \ll kv_0. \end{cases}$$

What concerns the inter-band contribution, we obtain for both components

$$\sigma_{\perp}^{inter}(\omega, k) = \sigma_{\parallel}^{inter}(\omega, k) = -\frac{i e^2 \omega}{2\pi\hbar} \times \begin{cases} (1/4T) \ln(4T/kv_0), & \omega \ll kv_0 \ll T, \\ 1/kv_0, & \omega \ll T \ll kv_0. \end{cases}$$

Finally, we make several remarks. Equations (10) and (11) allows us to estimate the conductivity of pure graphene when $\tau^{-1} = 0$. For small k and at low temperatures, when $\tanh \omega/T \rightarrow 1$, the first term in equation (11) plays the leading role and the conductivity reads:

$$\sigma(\omega, k) = \frac{e^2}{4\hbar}, \quad kv_0 \ll T \ll \omega. \quad (12)$$

Let us underline that this conductivity results from the electron transitions between two intersecting bands at the K points of the Brillouin zone. Remarkable fact is that its value is independent of any parameter of graphene, like γ_0 or v_0 . Indeed, the universal conductivity behavior for the samples with different carrier concentrations was

found in reference [1]. In spite of the fact that the experiment was performed in conditions $\omega \ll T$, different from equation (12), the minimal value of measured conductivity $\sigma_{min} = 2e^2/\pi\hbar$ was found close to our estimation.

At high temperatures, when the conditions $kv_0 \ll \omega \ll T$ are fulfilled, the conductivity is governed by the intra-band contribution depending on temperature, equation (10). This behavior can be examined in experiments with the plasmon modes. We obtain the dispersion law of $2d$ plasmon modes in graphene

$$\omega = \sqrt{\kappa k}, \quad \kappa = \frac{4e^2 T \ln 2}{\hbar^2 \varepsilon_\infty},$$

where ε_∞ is the lattice dielectric constant.

So far we considered the $2d$ graphene sheet. No experimental data on the temperature dependence of graphen conductivity have published up to now. But our results can be immediately applied to the $3d$ graphite where the interaction between layers is known to be weak. Then the integration with respect to the p_z component of the quasi-momentum in the Brillouin zone gives just the additional factor $1/c_z$, where c_z is the distance between the layers in the z -direction. In the low-frequency limit $\omega \ll 1/\tau$, the in-plane conductivity can be estimated as

$$\sigma_a(\omega, k \rightarrow 0) = \frac{e^2 T \tau}{\pi \hbar c_z}, \quad (13)$$

where τ depends on the energy variable ε or temperature. Using the Fermi golden rule, one can find the collision rate for scattering by defects $1/\tau_{imp}(\varepsilon) = n_{imp} a^2 |\varepsilon| \simeq n_{imp} a^2 T$, where n_{imp} is the defect concentration per the plane unit and a is the interatomic distance. Thus, with the help of equation (13), we obtain the independent of temperature residual conductivity.

The temperature dependence arises due to scattering by phonons. The number of phonons in the $2d$ system at low temperatures ($T \ll T_D$, T_D is the Debye temperature) is proportional to T^2 . Since the Fermi surface (or the chemical potential) is assumed to be small ($\varepsilon_F \sim T \ll T_D$), all scattering angles are essential in this region of temperatures. For the electron collision rate determined by the electron-phonon interaction, one can write $1/\tau_{el-ph} = \alpha T^2/T_D$ with the constant α of the order of unity. Thus the in-plane resistivity increases linearly with temperature (see Fig. 2):

$$\rho_a = \frac{\pi \hbar c_z}{e^2} \left(n_{imp} a^2 + \frac{\alpha T}{T_D} \right). \quad (14)$$

This expression answers the question discussed in references [22,23] on the pressure dependence of the graphite resistivity. We see that the resistivity decreases under the pressure because the inter-layer distance c_z decreases and the Debye temperature T_D grows.

In summary, we found a simple analytical expression for the graphen conductivity which consists of the inter- and intra-band contributions. At low temperatures and for small carrier concentration, the first one plays a leading role (because of the gapless electron dispersion in grapene) and its estimate agrees with the value obtained in reference [1]. The second one (temperature dependent intra-

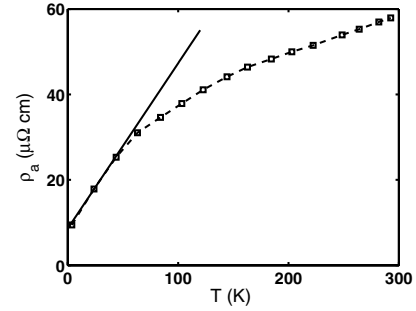


Fig. 4. In-plane electrical resistivity vs T for a graphite single crystal; experimental points reference [22] are fitted at low temperatures to the theory (solid line) equation (14) with the atomic concentration of defects $n_{imp} a^2 = 0.02$ and the Debye factor $T_D/\alpha = 1100$ K.

band contribution) can be observed in the transport as well as in experiments with plasmon modes.

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