Transport in a Clean Graphene Sheet at Finite Temperature and Frequency

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We calculate the conductivity of a clean graphene sheet at finite temperatures starting from the tight-binding model. We obtain a finite value for the dc-conductivity at zero temperature. For finite temperature, the spontaneous electron-hole creation, responsible for the finite conductivity at zero temperature, is washed out and the dc-conductivity yields zero. Our results are in agreement with calculations based on the field-theoretical model for graphene.

Keywords: Electronic properties of graphene; Kubo formula; minimal conductivity.

1. Introduction

The recent achievements of isolating and locating a single layer of graphene and performing transport measurements have tremendously stimulated the research on carbon-based electronics.\(^1\) By applying an external gate voltage, the system can be switched from \(n\)-type to \(p\)-type carriers, thus controlling the electronic properties and giving rise to carbon-based devices. At the crossover from \(n\)- to \(p\)-type carriers, i.e., at the charge neutrality point where no carriers are present, experiments nevertheless report a minimal finite, “universal” conductivity.\(^2\)

A first understanding of this result is already obtained from the band structure of the system. Within a two-band tight-binding approach\(^3\) and in the long-wavelength limit, single-layer graphene is described by two-dimensional Dirac Fermions (see e.g. Ref.\(^4\)). At zero doping, the density-of-states (DOS) at the Fermi energy is zero and the system is a zero-band gap semiconductor or semi-metal. Graphene thus lies at the borderline of a semiconductor and a metal which gives rise to a number of new phenomena. E.g., in contrast to the zero (infinite) conductivity for a clean semiconductor (metal), the conductivity of a clean graphene sheet at zero temperature is finite and of order \(e^2/h\).

Already Ludwig et. al.\(^5\) pointed out that there are two possible prefactors to the conductance quantum \(e^2/h\). Calculating, e.g., the dc-conductivity via the Kubo-formula using the polarizability for undoped graphene of Ref.\(^6\) yields \(\sigma = \frac{\pi \epsilon}{4 \pi} \), where the dielectric constant \(\epsilon\) is usually omitted (\(\epsilon = 1\)).\(^7\) Introducing a finite scattering amplitude \(\Gamma\) due to impurities and performing the limit \(\Gamma \rightarrow 0\) in the end leads to \(\sigma = \frac{\pi \epsilon^2}{4}\).\(^8\)
Besides using the Kubo formula, there were also calculations based on the Landauer formula for a rectangular system with aspect ratio $W/L \gg 1$. Independent from the explicit boundary conditions, the conductivity was given by $\sigma = \frac{4\pi e^2}{h}$, corresponding to the physical limit procedure (first $\omega \to 0$ and then $\Gamma \to 0$) in the case of the infinite system without contacts. In Ref. [11], Ryu et al. thoroughly discuss the crossover between the two values depending on the different dc-limits. But taking the dc-limit after the integration over energies is performed, one obtains a third finite value for the minimal conductivity, i.e., $\sigma = \frac{\pi e^2}{h}$ which is closest to the experimentally measured value given by $\sigma \approx 4e^2/h$.

The above works are based on a ballistic transport model which predicts a universal conductivity. But Mishchenko pointed out that electron-electron interaction may lead to a non-universal correction. Also diffusive transport models can account for a minimal, but non-universal conductivity via midgap states, Coulomb scatterers, or electron-hole puddles.

This paper shall focus on the transport properties of clean graphene sheets at finite temperature and frequency. For an overview on ac conductivity in graphene see Ref. [17]. The effect of temperature was also discussed in Ref. [11], which can have two contrary effects as outlined below.

On the one hand, one can see temperature as some effective finite chemical potential which would lead to an enhancement of the conductivity. This is suggested by the results by Vafek on the plasmon dispersion for graphene at zero doping and at finite temperature. He finds that the collective plasmon excitations are only weakly damped even though they lie in the region where electron-hole excitations are allowed. In the case of finite doping and zero temperature, electron-hole excitations are forbidden due to the Pauli principle, thus leading to undamped plasmon excitations within the RPA approximation.

On the other hand, the finite conductivity at $T = 0$ can be related to the spontaneous electron-hole creation at zero energy. These quantum fluctuations can be washed out at finite temperature, thus rendering the mechanism for finite conductivity for clean graphene to zero. It is this scenario which prevails and the dc-conductivity for graphene is indeed zero if the energy scale set by the carrier density is smaller than the temperature.

All calculations on the conductivity of clean graphene cited above are based on the long-wavelength approximation, i.e., start from relativistic Dirac Fermions. Here, we want to discuss the conductivity of a clean graphene sheet starting from the tight-binding model. We will further include finite temperature since the order of limits $\omega \to 0$ and then $T \to 0$ corresponds to the physical realization of an experiment.
2. Tight-binding model with vector potential

The simplest Hamiltonian describing non-interactive electrons on graphene in the presence of a time dependent vector potential $A(t)$ reads

$$H = - \sum_{R, \sigma, \delta} \left[ t_{R,R+\delta} a^\dagger_\sigma(R) b_\sigma(R + \delta) + \text{H.c.} \right],$$

where $R$ runs over all unit cells and $\delta$ runs over all three nearest neighbors with

$$\delta_1 = \frac{a}{2} (-1, \sqrt{3}, 0),$$

$$\delta_2 = \frac{a}{2} (-1, -\sqrt{3}, 0),$$

$$\delta_3 = a (1, 0, 0).$$

The bare tunnel-matrix element $t$ is thus modified by the time dependent vector potential $A(t)$ as

$$t_{R,R+\delta} = t \exp \left( i \frac{2 \pi e}{\hbar} \int_{R+\delta}^R d\mathbf{l} \cdot A(t) \right) = t \exp \left( i \frac{2 \pi e}{\hbar} A(t) \cdot \delta \right).$$

The current operator in the presence of the vector potential is defined as

$$j = -\nabla A H.$$

In linear response one needs the current operator up to first order in $A(t)$, which gives

$$j = t \sum_{R, \sigma, \delta} \left( \frac{ie}{\hbar} \left( u_x \delta_x + u_y \delta_y \right) a^\dagger_\sigma(R) b_\sigma(R + \delta) \right. \left. - \frac{e^2}{h} \left( u_x A_x \delta_x^2 + u_y A_y \delta_y^2 \right) a^\dagger_\sigma(R) b_\sigma(R + \delta) + \text{H.c.} \right).$$

The Maxwell equation

$$E = -\frac{\partial A(t)}{\partial t}$$

allows for a simple relation between the vector potential and the electric field, which is needed for the calculation of the electrical conductivity. If one introduces the Fourier representation for the operators as

$$a_\sigma(R) = \frac{1}{\sqrt{N_c}} \sum_k e^{-ik \cdot R} a_\sigma(k),$$

and the equivalent expression for the operators $b(R)$, the Hamiltonian, for $A = 0$, reads

$$H = -t \sum_{k, \sigma} [\phi(k) a^\dagger_\sigma(k) b_\sigma(k) + \text{H.c.}],$$

where

$$\phi(k) = \frac{1}{\sqrt{N_c}} \sum_{\alpha} e^{-ik \cdot R} \phi_{\alpha}(R).$$
where
\[ \phi(k) = \sum_\delta e^{-i k \cdot \delta}. \] (11)

It proves useful to redefine \( \phi(k) \) as
\[ \phi(k) = \sum_\delta e^{-i k \cdot (\delta - 3)}, \] (12)
and introduce the transformation \( a_{k}^\dagger \rightarrow e^{-i k \cdot 3} a_{k}^\dagger \). After these transformations, the single particle Green’s functions for the Hamiltonian (10) are given by
\[ G_{AA}^0(\omega_n, k) = \frac{i \omega_n + \mu / \hbar}{(i \omega_n + \mu / \hbar)^2 - t^2 |\phi(k)|^2 / \hbar^2}, \] (13)
\[ G_{BA}^0(\omega_n, k) = -\frac{t \phi^*(k)}{i \omega_n + \mu / \hbar - t^2 |\phi(k)|^2 / \hbar^2}, \] (14)
\[ G_{BB}^0(\omega_n, k) = \frac{i \omega_n + \mu / \hbar}{(i \omega_n + \mu / \hbar)^2 - t^2 |\phi(k)|^2 / \hbar^2}, \] (15)
\[ G_{AB}^0(\omega_n, k) = -\frac{t \phi(k)}{i \omega_n + \mu / \hbar - t^2 |\phi(k)|^2 / \hbar^2}, \] (16)
where we also introduced the chemical potential \( \mu \).

3. Current operator and Kubo formula

Let us now concentrate on the current operator \( j_x \), which is composed of the paramagnetic and diamagnetic contribution \( j_x = j_x^P + A_c(t)j_x^D \), each of them given by
\[ j_x^P = -\frac{itea}{2 \hbar} \sum_{k, \sigma} [(\phi(k) - 3)a_{\sigma}^\dagger(k)b_{\sigma}(k) - (\phi^*(k) - 3)b_{\sigma}^\dagger(k)a_{\sigma}(k)], \] (17)
and
\[ j_x^D = -\frac{te^2a^2}{4 \hbar^2} \sum_{k, \sigma} [(\phi(k) + 3)a_{\sigma}^\dagger(k)b_{\sigma}(k) + (\phi^*(k) + 3)b_{\sigma}^\dagger(k)a_{\sigma}(k)]. \] (18)

The Kubo formula for the conductivity is given by
\[ \sigma_{xx}(\omega) = \frac{< j_x^D >}{i A_s (\omega + i 0^+)} + \frac{\Lambda_{xx}(\omega + i 0^+)}{i \hbar A_s (\omega + i 0^+)}, \] (19)
with \( A_s = N_c A_c \) the area of the sample, and \( A_c \) the area of the unit cell, from which it follows that
\[ \Re \sigma(\omega) = D\delta(\omega) + \frac{3 \Lambda_{xx}(\omega + i 0^+)}{\hbar \omega A_s}, \] (20)
where \( D \) is the charge stiffness which reads
\[ D = -\pi < j_x^D > A_s - \pi \frac{\Re \Lambda_{xx}(\omega + i 0^+)}{\hbar A_s}. \] (21)
where in the Dirac cone approximation one has
\[ \Lambda_{xx}(i\omega_n) = \int_0^{\hbar \beta} d\tau e^{i\omega_n \tau} < T_x j_x^B(\tau) j_x^B(0) > . \] (22)

The \( f \)-sum rule, giving the oscillator strength, reads
\[ \int_0^\infty \sigma_{xx}(\omega) d\omega = -\pi < j_x^D > , \] (23)
where we have used \( \int_0^\infty \delta(\omega) d\omega = 1/2 \), see also Ref. \[23\].

Within this model, the several quantities read
\[ < j_x^D > = -\frac{t e^2 a^2}{\hbar^2} \sum_k \phi(k)[|n_F(-t|\phi(k)| - \mu) - n_F(t|\phi(k)| - \mu)] , \] (24)
\[ \Re \Lambda_{xx}(0 + i0^+) = \frac{t e^2 a^2}{8\hbar^2} \sum_k f[\phi(k)] \left[ n_F(-t|\phi(k)| - \mu) - n_F(t|\phi(k)| - \mu) \right] , \] (25)
\[ \Im \Lambda_{xx}(\omega + i0^+) = \frac{t e^2 a^2}{8\hbar^2} \sum_k f[\phi(k)] \left[ n_F(-t|\phi(k)| - \mu) - n_F(t|\phi(k)| - \mu) \right] \times \left[ \pi \delta(\omega - 2t|\phi(k)|/\hbar) - \pi \delta(\omega + 2t|\phi(k)|/\hbar) \right] , \] (26)
and
\[ f[\phi(k)] = 18 - 4|\phi(k)|^2 + 18 \frac{|\Re \phi(k)|^2 - |\Im \phi(k)|^2}{|\phi(k)|^2} . \] (27)

The above formulas were derived using the fact that
\[ \sum_k \phi(k) g(|\phi(k)|) = \sum_k \phi^*(k) g(|\phi(k)|) \]
\[ = \frac{1}{3} \sum_k |\phi(k)|^2 g(|\phi(k)|) \] (28)
where \( g(|\phi(k)|) \) is an arbitrary function of the absolute value of \( \phi(k) \), and the fact that in the Dirac cone approximation one has
\[ \frac{\phi^2(k)}{|\phi(k)|^2} \approx e^{2\pi/\hbar^2} \left[ \cos(2\theta) - i \sin(2\theta) \right] , \] (29)
and a similar expression for the complex conjugate expression \( |\phi^*(k)|^2 / |\phi(k)|^2 \). One can also show that the following relation holds true
\[ \sum_k |\phi(k)| = \frac{1}{8} \sum_k \left| \frac{f[\phi(k)]}{|\phi(k)|} \right| , \] (30)
which proves that the charge stiffness is zero at zero temperature and for zero chemical potential (half-filling). As a consequence, the system can only show d.c. conductivity at half filling and zero temperature if
\[ \sigma_{d.c.} = \lim_{\omega \to 0} \frac{3 \Lambda_{xx}(\omega + i0^+)}{\hbar \omega A_s} \] (31)
is finite.

The calculation is simple to do within the Dirac cone approximation. The term in $f[\phi(k)]$ proportional to $[\Re\phi(k)]^2 - [\Im\phi(k)]^2$ gives zero in this approximation. Let us first introduce the density of states per unit area $\rho(\epsilon)$

$$\rho(\epsilon) = \frac{1}{4\pi^2} \int_0^{\epsilon_c} 2\pi q dq \delta(\epsilon - \frac{3}{2}aq) = \frac{4\epsilon}{18\pi a^2}. \tag{32}$$

Using $\rho(\epsilon)$ we can calculate

$$\frac{1}{A_s} \sum_k f[\phi(k)] \delta(\omega - 2t|\phi(k)|/\hbar) \simeq \int_0^{\epsilon_c} d\epsilon \rho(\epsilon)(18 - 4\epsilon^2)\delta(\omega - 2\epsilon/\hbar)$$

$$= \frac{h^2}{\pi a^2 \omega^2} \left[ 1 - \left( \frac{\hbar \omega}{3\sqrt{2}t} \right)^2 \right]. \tag{33}$$

The contribution just computed corresponds to the value of a single Dirac cone. The optical conductivity is (the two Dirac cone contributions included)

$$\sigma(\omega) = \frac{\pi e^2}{2\hbar} \left[ 1 - \left( \frac{\hbar \omega}{3\sqrt{2}t} \right)^2 \right], \tag{34}$$

which gives a d.c. value of

$$\sigma_{d.c.} = \frac{\pi e^2}{2\hbar}. \tag{35}$$

This is the result which one obtains if a finite damping term is not included.\[11\]

The above result holds only at zero temperature. For finite temperature, which is the case in any experiment, the conductivity, at half filling and within the Dirac cone approximation, is (note that due to particle-hole symmetry the chemical potential is zero for any temperature)

$$\sigma(\omega, T) = \frac{\pi e^2}{2\hbar} \left[ 1 - \left( \frac{\hbar \omega}{3\sqrt{2}t} \right)^2 \right] \tanh \left( \frac{\hbar \omega}{4k_B T} \right), \tag{36}$$

leading to

$$\sigma_{d.c.}(T) = 0, \tag{37}$$

which should be interpreted as the correct result at zero frequency instead of result\[35\]. This is shown in Fig. 11 where the optical conductivity as function of frequency is plotted for various temperatures for $t = 3eV$. Only the $T = 0$ curve yields a finite d.c conductivity whereas for finite temperature all curves eventually become zero for $\omega \to 0$. E.g. at $T = 70K$, the universal value is only reached for frequencies $\omega > 0.075eV$, at $T = 4K$ for $\omega > 0.01eV$. 

4. Summary

Starting from the tight-binding model, we have calculated the conductivity of clean graphene as a function of the frequency and temperature. Depending on the order of the limits $\omega \rightarrow 0$ and $T \rightarrow 0$, we obtain either the finite value $\sigma = \frac{\pi}{2} \frac{e^2}{h}$ or zero in agreement with field-theoretical calculations. The universal value of the conductivity of a clean graphene at finite frequencies was recently confirmed experimentally.

Our calculations start from the tight-binding model to complement the current discussion on the conductivity of clean graphene and we believe that the explicit calculation based on the lattice model will be useful to a wide audience. An obvious extension is to include the next-nearest neighbor coupling and corrections to the Dirac cone approximation. Also, the effect of out-of-plane phonons and other scattering mechanisms on the optical conductivity of clean graphene can easily be assessed within the presented formalism.

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