Minimal conductivity of graphene: Nonuniversal values from the Kubo formula

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The minimal conductivity of graphene is a quantity measured in the dc limit. It is shown, using the Kubo formula, that the actual value of the minimal conductivity is sensitive to the order in which certain limits are taken. If the dc limit is taken before the integration over energies is performed, the minimal conductivity of graphene is $4/\pi$ (in units of e^2/h) and it is $\pi/2$ in the reverse order. The value π is obtained if weak disorder is included via a small frequency-dependent self-energy. In the high-frequency limit, the minimal conductivity approaches $\pi/2$ and drops to zero if the frequency exceeds the cutoff energy of the particles.

INTRODUCTION

The conductivity $\sigma_{\mu\mu}$ of graphene varies with the density of quasiparticles almost linearly with a minimal value $\sigma^{\min} \approx 4e^2/h$.[1,2] In terms of theoretical calculations, there has been some confusion about the actual value of the minimal conductivity $\sigma^{\min}$. This confusion is twofold: one originates from the experimentally observed value that is roughly three times as big as most of the calculated values, and the other one is related to the theoretical calculations that produced different values of $\sigma^{\min}$ (calculated per spin and per valley):

$$\sigma_1^{\min} = \frac{1}{\pi}\frac{e^2}{h} \quad \text{(Refs. 3–11)},$$

$$\sigma_2^{\min} = \frac{\pi}{8}\frac{e^2}{h} \quad \text{(Refs. 3, 9, and 12)},$$

$$\sigma_3^{\min} = \frac{\pi}{4}\frac{e^2}{h} \quad \text{(Ref. 13)}. \tag{1}$$

$\sigma_1^{\min}$ was obtained from the Kubo formula[3,4,6,7,10,11] as well as from the Landauer formula,[5,8,11] whereas $\sigma_{2,3}^{\min}$ were obtained from the Kubo formula only. All these results were calculated near the ballistic regime of the quasiparticles. The possibility of reaching the experimentally observed values of the minimal conductivity by including long-range disorder due to charged impurities was also discussed recently.[14] The latter will not be considered in the subsequent discussion. Instead, it shall be explained that all the results in Eq. (1) can be obtained from the standard Kubo formula of nearly ballistic quasiparticles by taking limits in different order. When a nonzero temperature T is considered, the conductivity is a function $\sigma^{\min}(\omega/T, \eta/T)$, for frequency ω and scattering rate η.

FREQUENCY-DEPENDENT CONDUCTIVITY

The conductivity $\sigma_{\mu\nu}$ is given by the Kubo formula as a response to an external field with frequency ω. Here, the representation given in Ref. 13 is used,

$$\sigma_{\mu\nu} = i\frac{e^2}{\hbar} \int \int \text{Tr}\{[H, r_\mu]\delta(H-\epsilon')[H, r_\nu]\delta(H-\epsilon)\}$$
$$\times \frac{1}{\epsilon - \epsilon' + \omega - i\alpha}\frac{f_\beta(\epsilon') - f_\beta(\epsilon)}{\epsilon - \epsilon'}d\epsilon d\epsilon', \tag{2}$$

where $f_\beta(\epsilon) = 1/[1 + \exp(\beta\epsilon)]$ is the Fermi function at temperature $T = 1/(k_B\beta)$. For the minimal conductivity, only the real part of the diagonal conductivity $\sigma'_{\nu\nu} = \text{Re}(\sigma_{\nu\nu})$ is of interest. After taking the limit $\alpha \to 0$, the ϵ' integration can be performed and gives

$$\sigma'_{\nu\nu} = \pi\frac{e^2}{\hbar} \int \text{Tr}\{[H, r_\nu]\delta(H-\epsilon-\omega)[H, r_\nu]\delta(H-\epsilon)\}$$
$$\times \frac{f_\beta(\epsilon+\omega) - f_\beta(\epsilon)}{\omega}d\epsilon. \tag{3}$$

In the zero-temperature limit $\beta \to \infty$, this becomes

$$\sigma'_{\nu\nu} = -\pi\frac{e^2}{\hbar}\frac{1}{\omega}\int_{-\omega/2}^{\omega/2} \text{Tr}\{[H, r_\nu]\delta(H-\omega/2-\epsilon)[H, r_\nu]$$
$$\times \delta(H+\omega/2-\epsilon)\}d\epsilon. \tag{4}$$

The minimal conductivity $\sigma^{\min}$ is obtained by taking the limit $\omega \to 0$ of $\sigma'_{\nu\nu}$. It is tempting to ignore the ω dependence of the integrand and replace the right-hand side by the integrand at $\epsilon = \omega = 0$. It will be shown subsequently that this does not agree with the result when we perform the energy integration first and take the limit $\omega \to 0$ later.

DIRAC FERMIONS

The Hamiltonian of Dirac fermions in two dimensions with wave vector (k_1, k_2),

$$H = \sigma_1 k_1 + \sigma_2 k_2, \tag{5}$$

describes the low-energy quasiparticles in graphene. σ_j ($j = 1, 2, 3$) are Pauli matrices. H can be diagonalized as $\text{diag}(k, -k)$ with $k = \sqrt{k_1^2 + k_2^2}$. The current operator transforms under Fourier transformation as

$$j_\mu = -ie[H, r_\mu] \rightarrow e \frac{\partial H}{\partial k_\mu}.$$

This means that the current operators for the Hamiltonian H in Eq. (5) is a 2×2 matrix with vanishing diagonal elements. The representation of j_2 in terms of energy eigenstates reads

$$j_2 = \frac{e}{k} \begin{pmatrix} k_2 & ik_1 \\ -ik_1 & -k_2 \end{pmatrix}. \tag{6}$$

Thus, the current j_2 does not depend on k but only on the polar angle. The trace term in the conductivity of Eq. (4) reads

$$T(\epsilon) = -\text{Tr}\{[H, r_\mu] \delta(H - \omega/2 - \epsilon)[H, r_\mu] \delta(H + \omega/2 - \epsilon)\}$$

$$= \int \text{Tr}_2 \left\{ \frac{\partial H}{\partial k_\mu} \delta\left(H - \frac{\omega}{2} - \epsilon\right) \frac{\partial H}{\partial k_\mu} \delta\left(H + \frac{\omega}{2} - \epsilon\right) \right\} \frac{d^2k}{(2\pi)^2}, \tag{7}$$

where Tr_2 is the trace with respect to 2×2 matrices. After diagonalizing H, this becomes, together with the current in Eq. (6),

$$T(\epsilon) = \int \frac{k_1^2}{k^2} \left[\delta\left(k + \frac{\omega}{2} + \epsilon\right) \delta\left(k + \frac{\omega}{2} - \epsilon\right) \right.$$

$$\left. + \delta\left(k - \frac{\omega}{2} - \epsilon\right) \delta\left(k - \frac{\omega}{2} + \epsilon\right) \right] \frac{dk_1 dk_2}{(2\pi)^2}$$

$$+ \int \frac{k_2^2}{k^2} \left[\delta\left(k - \frac{\omega}{2} - \epsilon\right) \delta\left(k + \frac{\omega}{2} - \epsilon\right) \right.$$

$$\left. + \delta\left(k + \frac{\omega}{2} + \epsilon\right) \delta\left(k - \frac{\omega}{2} + \epsilon\right) \right] \frac{dk_1 dk_2}{(2\pi)^2}, \tag{8}$$

which is a symmetric function with respect to ϵ.

Now, a soft Dirac delta function $\delta_\eta(x)$ is considered with

$$\delta_\eta(x) = \frac{1}{\pi} \frac{\eta}{x^2 + \eta^2} = -\frac{1}{2i\pi} \left[\frac{1}{x + i\eta} - \frac{1}{x - i\eta} \right]. \tag{9}$$

The parameter η (a scattering rate) can be understood as the imaginary part of the self-energy, created, for instance, by random fluctuations due to disorder.[4] With the energy cutoff λ for the Dirac fermions and $\eta \sim 0$, the integral of the double product of soft Dirac delta functions reads

$$\int_0^\lambda \delta_\eta(k-a) \delta_\eta(k-b) k \, dk \sim (a+b) \delta_\eta(a-b) \frac{1}{8} [\Theta(\lambda - a)$$

$$+ \Theta(a) + \Theta(\lambda - b) + \Theta(b) - 2]$$

$$- \frac{\eta}{a-b} \frac{1}{2\pi} [\Theta(\lambda - b) + \Theta(b)$$

$$- \Theta(\lambda - a) - \Theta(a)].$$

Returning to Eq. (8), we restrict the variable ϵ to $-\omega/2 < \epsilon < \omega/2$, since for low temperature the term

$$f_\beta\left(\epsilon + \frac{\omega}{2}\right) - f_\beta\left(\epsilon - \frac{\omega}{2}\right) = -\frac{\sinh(\beta\omega/2)}{\cosh(\beta\omega/2) + \cosh(\beta\epsilon)}$$

in the conductivity is exponentially small for $|\epsilon| > \omega/2$. If it is further assumed that $\eta, \omega \ll \lambda$, and we obtain

$$T(\epsilon) \sim \frac{\pi}{(2\pi)^2} \left(\frac{\omega}{4} \delta_\eta(\epsilon) + \frac{\eta}{\pi\omega} \right) \Theta\left(\lambda - \frac{\omega}{2}\right), \tag{10}$$

where the prefactor π is a result of the angular integration of k_j^2/k^2. The first term describes interband scattering (i.e., scattering between states with different energies $\pm\epsilon$) and the second term intraband scattering (i.e., scattering between states with the same energy ϵ or $-\epsilon$). The intraband scattering term increases linearly with the scattering rate η, in contrast to the η-independent interband scattering. The frequency dependence is also different for the two types of scattering: the interband term increases with ω, whereas the intraband term decreases.

The temperature-dependent conductivity can be calculated from Eqs. (3) and (7) as

$$\sigma'_{22} = -\pi \frac{e^2}{\hbar} \int T(\epsilon) \frac{f_\beta(\epsilon + \omega/2) - f_\beta(\epsilon - \omega/2)}{\omega} d\epsilon. \tag{11}$$

Thus, Eq. (10) implies

$$\sigma'_{22} \sim -\frac{\pi e^2}{8h} \left[f_\beta\left(\frac{\omega}{2}\right) - f_\beta\left(-\frac{\omega}{2}\right) \right]$$

$$+ \frac{e^2}{2h} \frac{\eta}{\omega^2} \int_{-\omega/2}^{\omega/2} \frac{\sinh(\beta\omega/2)}{\cosh(\beta\epsilon) + \cosh(\beta\omega/2)} d\epsilon \tag{12}$$

for $\omega < 2\lambda$ and a vanishing conductivity for $\omega > 2\lambda$. The integral in the second term gives

$$\frac{1}{\omega} \int_{-\omega/2}^{\omega/2} \frac{\sinh(\beta\omega/2)}{\cosh(\beta\epsilon) + \cosh(\beta\omega/2)} d\epsilon$$

$$= \frac{4}{\beta\omega} \text{arctanh}\left[\tanh^2\left(\frac{\beta\omega}{4}\right) \right].$$

Moreover, the relation

$$\text{arctanh}(x) = \frac{1}{2} \log\left[\frac{1+x}{1-x} \right]$$

can be used to get

$$\sigma'_{22} \sim \frac{\pi e^2}{8h} \tanh\left(\frac{\beta\omega}{4}\right) + \frac{e^2}{h} \frac{\beta\eta}{(\beta\omega)^2} \log\left[\frac{1 + \tanh^2(\beta\omega/4)}{1 - \tanh^2(\beta\omega/4)} \right]. \tag{13}$$

This is the main result of this Brief Report. It shows that the conductivity depends on two parameters, $\beta\omega$ and $\beta\eta$. Experimentally interesting is the case where $\beta\eta$ is fixed and $\beta\omega$ is varied (cf. Fig. 1). This is motivated by two facts. The first one is related to the origin of η (the scattering rate or inverse scattering time). It grows with increasing disorder. An important source of disorder in graphene are "ripples" in the carbon sheet,[15,16] which are created by thermal fluctuations. Therefore, a simple estimate gives a linear growth of the scattering rate with temperature. The other support for a con-
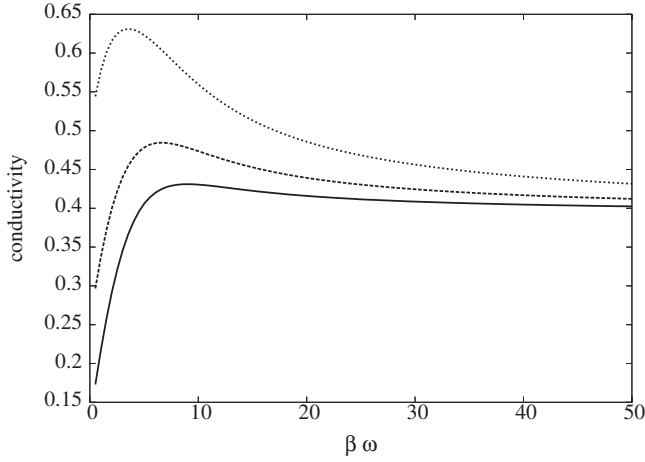
FIG. 1. Conductivity of Dirac fermions vs $\beta\omega$ (β is the inverse temperature and ω the frequency) in units of e^2/h. The conductivity increases with the rate $\beta\eta = 1, 2, 4$ (η the scattering rate). It is assumed that $\beta\eta$ does not depend on β [from Eq. (13)].

stant $\beta\eta$ with respect to temperature comes from the experimentally observed constant minimal conductivity found for a wide range of temperatures.[1] It will be shown below that the minimal conductivity at $\omega = 0$ and $\beta < \infty$ is proportional to $\beta\eta$.

DISCUSSION OF THE RESULTS

Zero temperature

With expression (10), the conductivity σ'_{22} in Eq. (4) eventually reads

$$\sigma'_{22} = \frac{e^2}{4\hbar} \frac{1}{\omega} \int_{-\omega/2}^{\omega/2} \left(\frac{\omega}{4} \delta_\eta(\epsilon) + \frac{\eta}{\pi\omega} \right) d\epsilon = \frac{\pi}{8} \left(1 + \frac{4\eta}{\pi\omega} \right) \frac{e^2}{h}.$$

(14)

The linear increase with the scattering rate η is in agreement with the Drude formula

$$\sigma' = \frac{\sigma_0/\eta}{1 + (\omega/\eta)^2}$$

for large ω, except for the different power in ω. This dependence on η is in qualitative agreement with the reduction of the minimal conductivity after annealing (i.e., effectively reducing η), which was observed in a recent experiment by Geim and Novoselov.[15]

The expression of the conductivity σ'_{22} can be studied in several limits. As a first example, in Eq. (8), the limit $\omega \to 0$ is taken first and then the limit $\eta \to 0$. Then, the conductivity in Eq. (4) reads

$$\sigma_1^{\min} = \frac{e^2}{\hbar} \frac{\eta^2}{\pi^2} \int_0^\infty \frac{1}{(k^2 + \eta^2)^2} k \, dk \approx \frac{1}{\pi} \frac{e^2}{h}.$$

(15)

In the next example, the result in Eq. (14) is considered. This yields, for $\eta \ll \omega$, the minimal conductivity

$$\sigma_2^{\min} \approx \frac{\pi}{8} \frac{e^2}{h} \quad \text{for } \eta \approx 0$$

(16)

and

$$\sigma_3^{\min} \approx \frac{\pi}{4} \frac{e^2}{h} \quad \text{for } \eta \approx \omega.$$

(17)

The last result agrees reasonably well with the experimental observation of Ref. 1 if it is multiplied by 4, the factor that is taking care of the twofold spin and the twofold valley degeneracy of graphene.

Frequency and temperature dependence

There are two asymptotic regimes with

$$\frac{1}{(\beta\omega)^2} \log\left[\frac{1 + \tanh^2(\beta\omega/4)}{1 - \tanh^2(\beta\omega/4)} \right] \sim \begin{cases} 1/8 & \text{for } \beta\omega \sim 0 \\ 1/2\beta\omega & \text{for } \beta\omega \sim \infty, \end{cases}$$

which implies for the conductivity

$$\sigma'_{22} \sim \frac{e^2}{8h} \begin{cases} \beta\eta & \text{for } \beta\omega \sim 0 \\ \pi + 4\beta\eta/\beta\omega & \text{for } \beta\omega \sim \infty. \end{cases}$$

(18)

The result of Eq. (14) is reproduced when the temperature is sent to zero first. Experimentally, however, it is more realistic to study the dc conductivity at a nonzero temperature. Then, the conductivity depends on the scattering rate as $\sigma'_{22} \propto \beta\eta$. Remarkable is the frequency-dependent conductivity in comparison with the Drude formula. The Drude conductivity vanishes for large frequencies like $\propto \omega^{-2}$, in contrast to the almost constant behavior in Eq. (18) for $\omega < 2\lambda$ and an abrupt vanishing of the conductivity if the frequency exceeds the energy cutoff of the Dirac fermions 2λ.

In conclusion, the Kubo formula produces a nonuniversal value for the minimal conductivity in graphene. Depending on the order of the limits, this quantity can vary over a wider range in units of e^2/h. The frequency-dependent conductivity of graphene at the Dirac point is exceptional, since it is almost constant and drops to zero when the frequency reaches the energy cutoff of the Dirac fermions.

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