Minimal longitudinal dc conductivity of perfect bilayer graphene

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We calculated the minimal longitudinal conductivity in prefect single-layer and bilayer graphene by extending the two methods developed for Dirac fermion gas by A. W. W. Ludwig *et al.* in Phys. Rev. B **50**, 7526 (1994). Using the Kubo formula which was originally applied for spintronic systems we obtain $\sigma_{xx}^{\min}=(J\pi/2)e^2/h$ while from the other formula used in the above-mentioned work we find $\bar{\sigma}_{xx}^{\min}=(4J/\pi)e^2/h$, where $J=1$ for single-layer and $J=2$ for bilayer graphene. The two universal values are different although they are numerically close to each other. Our two results are in the same order of magnitude as that of experiments and for the single-layer case one of our results agrees with many earlier theoretical predictions. However, for bilayer graphene only two studies are known with predictions for the minimal conductivity different from our calculated values. Similarly to the single-layer case, the physical origin of the minimal conductivity in bilayer graphene is also rooted back to the intrinsic disorder induced by the Zitterbewegung which is related to the trembling motion of the electron.

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Unusual and remarkable transport properties of graphene (single or stacks of atomic layers of graphite) have been proved by recent experiments.[1,2] Besides the unconventional quantum Hall effect, many new phenomena have been predicted and studied in graphene such as the Klein paradoxon,[3] the specular Andreev reflection,[4,5] the Josephson effect,[6] a new electric field effect,[7] the photon-assisted electron transport,[8] composite Dirac fermions,[9] quantum dots,[10] the *n-p* junction,[11] the fractional quantum Hall effect,[12] and the spin-orbit gap.[13]

In this work we study the longitudinal conductivity of graphenes which, according to experiments, takes the minimum values of orders of e^2/h. This is an intrinsic property in the sense that it persists even in perfect (impurity-free) carbon honeycomb lattice. Such a peculiar behavior can be related to the excitation spectrum of single-layer graphene described well by a Dirac-like dispersion relation (Dirac cones) of two-dimensional massless Dirac fermions.[14]

Much theoretical effort has been devoted to explain quantitatively the observed minimal longitudinal conductivity. However, at the theoretical side different predictions exist for the value of the minimal conductivity $\sigma_{xx}^{\min}$ even in prefect single-layer graphene. Actually, long before experimental evidence of minimal conductivity, it has already been considered theoretically[15–17] and Ludwig *et al.* found different values using two different approaches.[18] Similarly, in many recent works[19–22] it has been found that $\sigma_{xx}^{\min}=(4/\pi)e^2/h$, while Ziegler predicted[23] $\sigma_{xx}^{\min}=\pi e^2/h$, Falkovsky and Varlamov[24] obtained $\sigma_{xx}^{\min}=(\pi/2)e^2/h$, and Nomura and MacDonald obtain from numerical calculations of the Kubo formula $\sigma_{xx}^{\min}=(4/\pi)e^2/h$ for the short range scattering case and $\sigma_{xx}^{\min}=4e^2/h$ for the Coulomb scattering case.[25] Recently, Gusynin and Sharapov have derived analytical results for the ac and dc conductivity of Dirac fermions in graphene[26] which could be used for studying the minimal conductivity.

For bilayer graphene first studied experimentally[27] by Novoselov *et al.* and theoretically[28] by McCann and Fal'ko, the situation is not better regarding the minimal conductivity. Much less theoretical work considered the minimal conductivity in bilayer graphene. Recently, Koshino and Ando have investigated the transport in bilayer graphene in the self-consistent Born approximation[29] and they found that in the strong-disorder regime $\sigma_{xx}^{\min}=(8/\pi)e^2/h$, while in the weak-disorder regime $\sigma_{xx}^{\min}=(24/\pi)e^2/h$ which is six times larger than in single-layer graphene. Similarly, Katsnelson has also calculated the minimal conductivity in bilayers using the Landauer approach[29,30] and he obtained a different value $\sigma_{xx}^{\min}=2e^2/h$.

For massless Dirac fermion (corresponding to the single-layer graphene) Ludwig *et al.* calculated the conductivity[18] using two definitions: one is the Kubo formula ($\sigma_{xx}^{\min}$) and the other ($\bar{\sigma}_{xx}^{\min}$) is a definition often used in the sigma model literature.[31] The two definitions yield two different results (although numerically they are close to each other) for the longitudinal conductivity of perfect single-layer graphene, namely, $\sigma_{xx}^{\min}=n_v n_s(\pi/8)e^2/h$ and $\bar{\sigma}_{xx}^{\min}=n_v n_s(1/\pi)e^2/h$, respectively. Here the factors $n_v=2$ and $n_s=2$ correspond to the two valleys and the electron spin, respectively (for details see references below).

As can be seen from the above-reviewed literature, several predictions of the exact value of the minimal conductivity even in perfect single-layer and bilayer graphene exist although they are consistent at least in order of magnitude. In this work we extend the Ludwig *et al.* approach to calculate the longitudinal conductivity for bilayer graphene. We find that, similarly to the case of single-layer graphene, the two definitions of the conductivity used in Ref. 18 yield also different results for perfect bilayer graphene. More interestingly, we find that the conductivity obtained from both approaches is *doubled* compared to that for single-layer graphene. Thus, our results show that obtaining the exact value of the minimal conductivity is a rather subtle task and needs further investigation.

Regarding the technical details of our calculations we note that when we used the Kubo formula, instead of following the approach of Ludwig *et al.* we applied an *equivalent* method developed by Bernevig[32] for spintronic systems. In this method the conductivity is calculated in "bubble" ap-

proximation using the one-particle noninteracting Green's function for finite temperature. This approach results in the same conductivity for single-layer graphene as that obtained from the Ludwig *et al.* method and, as can be seen below, it is more convenient to extend to bilayer graphene.

In order to treat the single-layer and bilayer graphene simultaneously we start from the Hamiltonian given in a unified form as[1,28]

$$H_J = g\begin{pmatrix} 0 & (p_x - ip_y)^J \\ (p_x + ip_y)^J & 0 \end{pmatrix}, \tag{1}$$

where $J=1$ for single-layer and $J=2$ for bilayer graphene, and g is a constant depending on J. In what follows, it is more convenient to use the following equivalent form of Eq. (1):

$$H_J = \mathbf{\Omega}(\mathbf{p})\boldsymbol{\sigma}, \tag{2}$$

where $\boldsymbol{\sigma}=(\sigma_x,\sigma_y)$ are the Pauli matrices representing the "pseudospin" acting on the spinor states with components corresponding to the wave function's amplitudes at the two nonequivalent basis atoms in the unit cell of the honeycomb lattice, $\mathbf{\Omega}(\mathbf{p})=gp^J(\cos J\varphi, \sin J\varphi)$ and φ is the polar angle of $\mathbf{p}$, i.e., $\mathbf{p}=p(\cos\varphi,\sin\varphi)$ with $p=|\mathbf{p}|$. The eigenstates of the Hamiltonian H_J with plane wave solutions $e^{i\mathbf{kr}}$ have eigenvalues

$$E_\pm(\mathbf{k}) = \pm\Omega(\hbar\mathbf{k}), \tag{3}$$

where $\Omega=\sqrt{\mathbf{\Omega}^2(\hbar\mathbf{k})}$ is the magnitude of the vector $\mathbf{\Omega}(\hbar\mathbf{k})$.

The Green's function of a Hamiltonian H is defined by $\hat{G}(z)=(z-\hat{H})^{-1}$ and its position representation reads $G(\mathbf{r},\mathbf{r}',z)=\langle\mathbf{r}|\hat{G}(z)|\mathbf{r}'\rangle$. Using the Hamiltonian (2) one finds

$$G(\mathbf{r},\mathbf{r}',z) = \langle\mathbf{r}|G(z)|\mathbf{r}'\rangle = \int \frac{d^2k}{(2\pi)^2} e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')} \frac{z+\mathbf{\Omega}(\mathbf{k})\boldsymbol{\sigma}}{z^2-\mathbf{\Omega}^2(\mathbf{k})}, \tag{4}$$

where z is a complex number.

To calculate the conductivity from the Kubo formula we apply the result derived first by Bernevig[32] for spintronic systems using the Green's function (4):

$$\sigma_{ij}(\omega) = -\frac{e^2}{\hbar}\lim_{\omega\to 0}\frac{\mathrm{Im}\{\Pi_{ij}^{\mathrm{ret}}(\omega)\}}{\omega}, \tag{5a}$$

where

$$\Pi_{ij}(\omega) = \frac{2}{A}\sum_{\mathbf{k}}\frac{n_F(E_+)-n_F(E_-)}{\omega^2-4\Omega^2}\Omega^2 \times (i\omega\epsilon_{\alpha\beta\gamma}F_{i\alpha}F_{j\beta}\hat{\Omega}_\gamma - 2\Omega F_{i\alpha}F_{j\alpha}), \tag{5b}$$

$$F_{i\alpha} = \frac{\partial\hat{\Omega}_\alpha}{\partial k_i}, \quad \hat{\Omega}_\alpha = \frac{\Omega_\alpha}{\Omega}, \tag{5c}$$

and $\Pi_{ij}^{\mathrm{ret}}(\omega)$ is the retarded correlation function obtained by analytic continuation $\omega\to\omega+i\eta$ of function $\Pi_{ij}(\omega)$, $n_F(E)=1/(e^{\beta(E-\mu)}+1)$ is the Fermi function with Fermi energy μ, the indices take the values 1,2,3, and summation over repeated indices is assumed. Here A is the area of the two-dimensional system, $\epsilon_{\alpha\beta\gamma}$ is the Levi-Civita symbol, and the two energy bands $E_\pm(\mathbf{k})$ are given by Eq. (3). This result is valid for ballistic systems (note that this result is slightly rewritten to make it more transparent and useful for further calculations).

We now evaluate the conductivity for undoped single-layer and bilayer graphene at zero temperature using Eq. (5). The Fermi energy for undoped graphene is $\mu=0$, i.e., the negative energy band is fully occupied and the positive one is empty at zero temperature. Thus, in Eq. (5b) $n_F(E_+)-n_F(E_-)=-1$ for all occupied states with Fermi wave number $\mathbf{k}$. For dc conductivity we need to find $\sigma(\omega)$ in the limit $\omega\to 0$. Therefore, the integration over $\mathbf{k}$ can safely be extended to infinity since the contribution comes from the integrand close to $k\approx 0$ [see the denominator of $\Pi_{ij}(\omega)$]. Using Eq. (5b) and $\Sigma_{\mathbf{k}}\to A\int d^2k/(2\pi)^2$ (no contribution comes from the term containing the Levi-Civita symbol $\epsilon_{\alpha\beta\gamma}$) we find

$$\Pi_{xx}^{\mathrm{ret}}(\omega) = \lim_{\eta\to 0^+}\int_0^\infty \frac{dk}{2\pi}\frac{2g^3J^2k^{3J-1}}{(\omega+i\eta)^2-4g^2k^{2J}}. \tag{6}$$

The imaginary part of the above integral can be evaluated analytically and it yields

$$\mathrm{Im}\{\Pi_{xx}(\omega)\} = -\frac{J\omega}{16}. \tag{7}$$

Thus, from (5a) the longitudinal dc conductivity (per valley per spin) for single-layer ($J=1$) and bilayer ($J=2$) graphene becomes

$$\sigma_{xx} = \frac{J\pi}{8}\frac{e^2}{h}. \tag{8}$$

Note that the conductivity obtained from the Kubo formula is universal depending only on the type of graphene but not the constant g.

We now apply the other definition used by Ludwig *et al.* for calculating the conductivity [see Eq. (55) in Ref. 18] which reads as

$$\bar{\sigma}_{xx} = \frac{e^2}{h}\lim_{\eta\to 0^+}\eta^2\int d^2r r^2\mathrm{Tr}[G(0,\mathbf{r},i\eta)G(\mathbf{r},0,-i\eta)], \tag{9}$$

where the Green's function is given by Eq. (4). The conductivity $\bar{\sigma}_{xx}$ can be rewritten as[18,31]

$$\bar{\sigma}_{xx} = -\frac{8e^2}{h}\lim_{\eta\to 0^+}\eta^2\left.\frac{\partial}{\partial q^2}\right|_{q=0} K(\mathbf{q},\eta), \tag{10a}$$

$$K(\mathbf{q},\eta) = \frac{1}{2}\int d^2r e^{i\mathbf{qr}}\mathrm{Tr}[G(0,\mathbf{r},i\eta)G(\mathbf{r},0,-i\eta)], \tag{10b}$$

and the trace is taken over the "pseudospin space."

Using the Green's function given by Eq. (4) and performing the trace over the "pseudospin space" in (10b) we find

$$K(\mathbf{q},\eta) = \int\frac{d^2k}{(2\pi)^2}\frac{\mathbf{\Omega}_+\mathbf{\Omega}_- + \eta^2}{(\mathbf{\Omega}_+^2+\eta^2)(\mathbf{\Omega}_-^2+\eta^2)}, \tag{11a}$$

$$\mathbf{\Omega}_{\pm} = \mathbf{\Omega}(\mathbf{k} \pm \mathbf{q}/2). \tag{11b}$$

After simple algebra the integrand I in Eq. (11a) can be calculated explicitly:

$$I = \frac{g^2[(k^2 + q^2/4)^2 - (\mathbf{kq})^2]^{J/2}\cos(J\Phi) + \eta^2}{\Sigma_+\Sigma_-}, \tag{12a}$$

$$\Sigma_{\pm} = g^2\left(k^2 + \frac{q^2}{4} \pm \mathbf{kq}\right)^J + \eta^2, \tag{12b}$$

$$\cos\Phi = \frac{k^2 - q^2/4}{\sqrt{(k^2 + q^2/4)^2 - (\mathbf{kq})^2}}. \tag{12c}$$

Here Φ is the angle between vector $\mathbf{k}+\mathbf{q}/2$ and $\mathbf{k}-\mathbf{q}/2$. Expanding I for small q we obtain

$$I \approx \frac{1}{g^2k^{2J} + \eta^2} - q^2g^2Jk^{2J-2}\frac{J(g^2k^{2J} + 3\eta^2) - [g^2(J+1)k^{2J} - (J-1)\eta^2]\cos(2\varphi - 2\gamma)}{4(g^2k^{2J} + \eta^2)^3}, \tag{13}$$

where φ and γ are the polar angle of $\mathbf{k}$ and $\mathbf{q}$, i.e., $\mathbf{k} = k(\cos\varphi, \sin\varphi)$ and $\mathbf{q} = q(\cos\gamma, \sin\gamma)$. As can be seen below γ will be dropped out in the final result.

Integrating the integrand I in (13) over $\mathbf{k}$ and taking the derivation with respect to q^2 we have the following simple result:

$$\left.\frac{\partial}{\partial q^2}\right|_{q=0} K(\mathbf{q}, \eta) = -\frac{J}{8\pi\eta^2}, \tag{14}$$

where γ has been dropped out after the integration over φ. Similarly, the first term disappears in I since it is independent of q. Now using Eq. (10a) the conductivity (per valley per spin) becomes

$$\bar{\sigma}_{xx} = \frac{J}{\pi}\frac{e^2}{h}. \tag{15}$$

Discussion. We calculated the minimal conductivity for perfect single-layer ($J=1$) and bilayer ($J=2$) graphene using the Kubo formula and the definition (9). Taking into account the two valleys ($n_v=2$) and the electron spin ($n_s=2$) we find from Eqs. (8) and (15) that the minimal conductivities take the universal values:

$$\sigma_{xx}^{\min} = \frac{J\pi}{2}\frac{e^2}{h}, \tag{16a}$$

$$\bar{\sigma}_{xx}^{\min} = \frac{4J}{\pi}\frac{e^2}{h}. \tag{16b}$$

Note that these results are independent of the constant g in the Hamiltonian (1). Just like in the case of single-layer graphene we also find different values for the conductivity when the two methods in Ref. 18 are extended to bilayer graphene. Moreover, the minimal conductivity in perfect bilayer graphene calculated from Eqs. (5) and (9) is doubled compared to that in single-layer graphene. One can also see that for perfect single-layer graphene our result (16b) agrees with that obtained in Refs. 19–22.

As pointed out by Katsnelson,[21,30] the reason for the different results (16a) and (16b) is related to the "trembling" or oscillatory motion of the center of a free wave packet called *Zitterbewegung* which has recently been reconsidered in Ref. 33. The Zitterbewegung induces an intrinsic disorder in perfect graphenes which has indirectly been confirmed by Tworzydlo *et al.*[22] by calculating the Fano factor of the shot noise in single-layer graphene, and they found that it has the same value (1/3) as in disordered metals.

In our calculation the energy dispersion of bilayer graphenes was assumed to be purely parabolic in $\mathbf{k}$ [see Eq. (1)]. Koshino and Ando studied the conductivity when the energy dispersion includes both k-linear and k-square terms[29] which results in a trigonally warped Fermi surface.[28] To clarify the role of the k-linear term it would be interesting to extend our work along this line.

Similarly, extending the theoretical efforts to study multilayer graphenes would be desirable in order to have a better understanding of the unusual transport in graphenes. Recently, the electronic states in stacks of graphene layers have been studied.[34] However, it is not clear whether in the case of trilayers the Hamiltonian can be described simply by Eq. (1) with $J=3$.

The single-layer and bilayer graphene are zero-gap semiconductors but this gap can open up due to impurities or the presence of interaction. Then, graphenes mapped to the massless Dirac fermion gas transform to random mass Dirac fermion systems. In this case, to calculate the conductivity it is useful to start from the definition (9) as it was demonstrated by Ludwig *et al.*[18] Recently, Gusynin *et al.* proposed theoretically that microwaves could be an experimental tool to understand the role of the impurities and the presence of interaction in graphene systems.[35]

In summary, our work shows that the physical explanation of the existence of the minimal conductivity in graphene systems still remains a theoretical challenge in the future.

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