Zitterbewegung, chirality, and minimal conductivity in graphene

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Abstract. It has been recently demonstrated experimentally that graphene, or single-layer carbon, is a gapless semiconductor with massless Dirac energy spectrum. A finite conductivity per channel of order of e^2/h in the limit of zero temperature and zero charge carrier density is one of the striking features of this system. Here we analyze this peculiarity based on the Kubo and Landauer formulas. The appearance of a finite conductivity without scattering is shown to be a characteristic property of Dirac chiral fermions in two dimensions.

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Graphene, or single layer carbon [1], demonstrates unique electronic properties. It has been shown recently [2,3] that the charge carriers in graphene are massless Dirac fermions with effective "velocity of light" of order of 10^6 ms^{-1}. Graphene provides unexpected connections between condensed matter physics and quantum field theory; in particular, a new kind of quantum Hall effect observed in graphene, that is, half-integer quantum Hall effect [2,3,4,5] can be considered as a consequence of the famous Atiyah-Singer index theorem [2]. The latter guarantees the existence of macroscopically large number of chiral states with zero energy in external magnetic field.

Another amazing property of graphene is the finite minimal conductivity which is of the order of the conductance quantum e^2/h per valley per spin; it is important to stress that this is a "quantization" of the conductivity rather than of the conductance [2]. This is not only very interesting conceptually but also important in light of potential applications of graphene for ballistic field-effect transistors [1]. Therefore the physical origin of the minimal conductivity is worth the special consideration which is a subject of this Note.

Numerous considerations of the conductivity of a two-dimensional massless Dirac fermion gas do give this value of the minimal conductivity with the accuracy of some factor of order of unity [6,7,8,9,10,11,12,13]. It is really surprising that in this case there is a final conductivity for an *ideal* crystal, that is, without any scattering processes [8]. This fact is important since without complete understanding of the ideal crystal case one can hardly hope to have a reliable answer for the realistic case with disorder and electron-electron interactions. Here we use the Landauer formula [14] to clarify the physical meaning of this anomaly.

We start with the Hamiltonian of a two-dimensional gapless semiconductor

$$H = v \sum_{\mathbf{p}} \Psi_{\mathbf{p}}^{\dagger} \sigma \mathbf{p} \Psi_{\mathbf{p}} \tag{1}$$

and the corresponding expression for the current operator [15]

$$\mathbf{j} = ev \sum_{\mathbf{p}} \Psi_{\mathbf{p}}^{\dagger} \sigma \Psi_{\mathbf{p}} = \sum_{\mathbf{p}} \mathbf{j}_{\mathbf{p}} \tag{2}$$

where v is the electron velocity, $\sigma = (\sigma_x, \sigma_y)$ are Pauli matrices, $\mathbf{p}$ is the momentum, and $\Psi_{\mathbf{p}}^{\dagger} = \left(\psi_{\mathbf{p}1}^{\dagger}, \psi_{\mathbf{p}2}^{\dagger} \right)$ are pseudospinor electron operators. Here we omit spin and valley indices (so, keeping in mind applications to graphene, the results for the conductivity should be multiplied by 4 due to two spin projections and two conical points per Brillouine zone). Straightforward calculations give for the time evolution of the electron operators

$$\Psi_{\mathbf{p}}(t) = \frac{1}{2} \left[e^{-i\epsilon_{\mathbf{p}}t} \left(1 + \frac{\mathbf{p}\sigma}{p} \right) + e^{i\epsilon_{\mathbf{p}}t} \left(1 - \frac{\mathbf{p}\sigma}{p} \right) \right] \Psi_{\mathbf{p}} \tag{3}$$

and for the current operator

$$\mathbf{j}(t) = \mathbf{j}_0(t) + \mathbf{j}_1(t) + \mathbf{j}_1^{\dagger}(t)$$

$$\mathbf{j}_0(t) = ev \sum_{\mathbf{p}} \Psi_{\mathbf{p}}^{\dagger} \frac{\mathbf{p}(\mathbf{p}\sigma)}{p^2} \Psi_{\mathbf{p}}$$

$$\mathbf{j}_1(t) = \frac{ev}{2} \sum_{\mathbf{p}} \Psi_{\mathbf{p}}^{\dagger} \left[\sigma - \frac{\mathbf{p}(\mathbf{p}\sigma)}{p^2} + \frac{i}{p} \sigma \times \mathbf{p} \right] \Psi_{\mathbf{p}} e^{2i\epsilon_{\mathbf{p}}t} \tag{4}$$

where $\epsilon_{\mathbf{p}} = vp/\hbar$ is the particle frequency. The last term in Eq.(4) corresponds to the "Zitterbewegung", a phenomenon connected with the uncertainty of the position

of relativistic quantum particles due to the inevitable creation of particle-antiparticle pairs at the position measurement [16,17]. Classical models for this phenomenon are discussed, e.g., in Ref.[18] and references therein.

In terms of condensed matter physics, the Zitterbewegung is nothing but a special kind of inter-band transitions with creation of virtual electron-hole pairs. The unitary transformation generated by the operator $U_{\mathbf{p}} = 1/\sqrt{2}(1 + i\mathbf{m_p}\sigma)$, where $\mathbf{m_p} = (\cos\phi_{\mathbf{p}}, -\sin\phi_{\mathbf{p}})$ and $\phi_{\mathbf{p}}$ is the polar angle of the vector $\mathbf{p}$, diagonalizes the Hamiltonian $H_{\mathbf{p}} = diag\,(-vp, vp)$ and thus introduces electron and hole states; after this transformation the oscillating term in Eq.(4) corresponds to the inter-band transitions, e.g.

$$U_{\mathbf{p}}^{\dagger} j_{\mathbf{p}}^{x} U_{\mathbf{p}} = ev \begin{pmatrix} -\cos\phi_{\mathbf{p}} & -i\sin\phi_{\mathbf{p}} e^{-i\phi_{\mathbf{p}}+2i\epsilon_{\mathbf{p}}t} \\ i\sin\phi_{\mathbf{p}} e^{i\phi_{\mathbf{p}}-2i\epsilon_{\mathbf{p}}t} & \cos\phi_{\mathbf{p}} \end{pmatrix}. \tag{5}$$

To calculate the conductivity $\sigma(\omega)$ we will try first to use the Kubo formula [19] which reads for two-dimensional isotropic case:

$$\sigma(\omega) = \frac{1}{2A} \int\limits_{0}^{\infty} dt e^{i\omega t} \int\limits_{0}^{\beta} d\lambda \, \langle \mathbf{j}(t - i\lambda)\mathbf{j} \rangle \tag{6}$$

where $\beta = T^{-1}$ is the inverse temperature, A is the sample area. In the static limit $\omega = 0$ taking into account Onsager relations and analyticity of the correlators $\langle \mathbf{j}(z)\mathbf{j} \rangle$ for $-\beta < \mathrm{Im}z \le 0$ one has [19]

$$\sigma = \frac{\beta}{4A} \int\limits_{-\infty}^{\infty} dt \, \langle \mathbf{j}(t)\mathbf{j} \rangle. \tag{7}$$

Usually, for ideal crystals, the current operator commutes with the Hamiltonian and thus $\mathbf{j}(t)$ does not depend on time. In that case, due to Eq.(6) the frequency-dependent conductivity contains only the Drude peak

$$\sigma_D(\omega) = \frac{\pi}{2A} \lim_{T \to 0} \frac{\langle \mathbf{j}^2 \rangle}{T} \delta(\omega) \tag{8}$$

Either the spectral weight of the Drude peak is finite and, thus, the static conductivity is infinite, or it is equal to zero. It is easy to check that for the system under consideration the spectral weight of the Drude peak is proportional to the modulus of the chemical potential $|\mu|$ (cf. Eq.(44) of Ref.[13]) and thus vanishes at zero doping ($\mu = 0$). It is the Zitterbewegung, i.e. the oscillating term $\mathbf{j}_1(t)$ which is responsible for nontrivial behavior of the conductivity for zero temperature and zero chemical potential (that is, the gapless semiconductor case). A straightforward calculation gives a formal result

$$\sigma = \frac{\pi e^2}{2h} \int\limits_{0}^{\infty} d\epsilon \epsilon \delta^2(\epsilon) \tag{9}$$

where one delta-function originates from the integration over t in Eq.(7) and the second one - from the derivative

of the Fermi distribution function appearing at the calculation of the average over product of Fermi-operators. Of course, the square of the delta function is not a well-defined object and thus Eq.(9) is meaningless before specification of the way how one should regularize the delta-functions. After regularization the integral in Eq.(9) is finite, but its value depends on the regularization procedure. It is not surprising therefore that two different ways of calculations in Ref.[8] led to two different answers. Our derivation, at least, clarifies the origin of these difficulties: it is the Zitterbewegung, or, physically, the impossibility to localize ultrarelativistic particles and to measure their coordinates.

At finite frequency and finite chemical potential the Zitterbewegung contribution to the expression (6) coincides with the result for inter-band conductivity found in Ref.[13].

Despite this derivation cannot give us a correct numerical factor, it opens new way to qualitative understanding of more complicated situations. For example, the minimal conductivity of order of e^2/h per channel has been observed experimentally also for the bilayer graphene [20] with the energy spectrum drastically different from that for the single-layer case. The bilayer graphene is a zero-gap semiconductor with *parabolic* touching of the electron and hole bands described by the single-particle Hamiltonian [20,21]

$$H_{\mathbf{p}} = \begin{pmatrix} 0 & (p_x - ip_y)^2/2m \\ (p_x + ip_y)^2/2m & 0 \end{pmatrix} \tag{10}$$

(here we ignore some complications due to large-scale hopping processes which are important for a very narrow range of the Fermi energies [21]). The Hamiltonian (10) can be diagonalized by the unitary transformation $U_{\mathbf{p}}$ with the replacement $\phi_{\mathbf{p}} \to 2\phi_{\mathbf{p}}$. Thus, the current operator after the transformation takes the form (5) with the replacement $v \to p/m$, $e^{-i\phi_{\mathbf{p}}} \to e^{-2i\phi_{\mathbf{p}}}$. In contrast with the single-layer case, the density of electron states for the Hamiltonian (10) is finite at zero energy but the square of the current is, vice versa, linear in energy. As a result, we have the same estimation (9), with the accuracy of additional factor 2.

To circumvent the problem of ambiguity in the expression for σ in Eq.(9) we now follow the alternative Landauer approach. Let us assume that our sample is a ring of length L_y in y direction; we will use Landauer formula to calculate the conductance in x direction (see Fig. 1). There is still an uncertainty in the sense that the conductivity turns out to be dependent on the shape of the sample. To have a final transparency we should keep L_x finite. On the other hand, periodic boundary conditions in y direction are nonphysical and we have to choose L_y as large as possible to weaken their effects. Thus, for two-dimensional situation one should choose $L_x \ll L_y$.

In the coordinate representation the Dirac equation at zero energy takes the form

$$(K_x + iK_y)\psi_1 = 0 \tag{11}$$
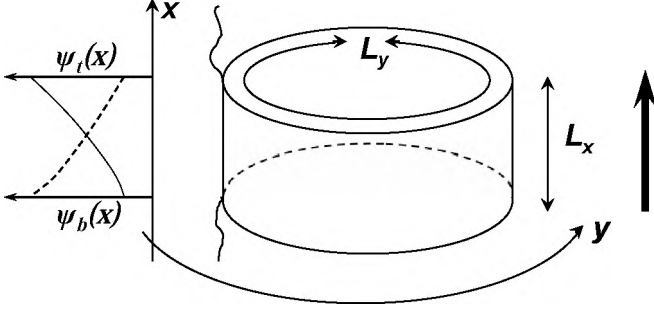$$(K_x - iK_y)\psi_2 = 0$$

Fig. 1. Geometry of the sample. Thick arrow shows the direction of current. ψ_t (solid line) and ψ_b (dashed line) are wave functions of the edge states localized near the top and the bottom of the sample, correspondingly.

where $K_i = -i\frac{\partial}{\partial x_i}$. General solutions of these equations are just arbitrary analytical (or complex conjugated analytical) functions:

$$\psi_1 = \psi_1\,(x + iy)\,, \tag{12}$$
$$\psi_2 = \psi_2\,(x - iy)\,.$$

Due to periodicity in y direction both wave functions should be proportional to $\exp(ik_y y)$ where $k_y = 2\pi n/L_y, n = 0, \pm 1, \pm 2, \dots$. This means that the dependence on x is also fixed: the wave functions are proportional to $\exp(\pm 2\pi n x/L_y)$. They correspond to the states localized near the bottom and top of the sample (see Fig. 1).

To use the Landauer formula, we should introduce boundary conditions at the sample edges ($x = 0$ and $x = L_x$). To be specific, let us assume that the leads are made of doped graphene with the potential $V_0 < 0$ and the Fermi energy $E_F = vk_F = -V_0$. The wave functions in the leads are supposed to have the same y-dependence, that is, $\psi_{1,2}\,(x,y) = \psi_{1,2}\,(x)\exp(ik_y y)$. Thus, one can try the solution of the Dirac equation in the following form:

$$\psi_1\,(x) = \begin{cases} e^{ik_x x} + re^{-ik_x x}, & x < 0 \\ ae^{k_y x}, & 0 < x < L_x \\ te^{ik_x x}, & x > L_x \end{cases}$$

$$\psi_2\,(x) = \begin{cases} e^{ik_x x+i\phi} - re^{-ik_x x-i\phi}, & x < 0 \\ be^{-k_y x}, & 0 < x < L_x \\ te^{ik_x x+i\phi}, & x > L_x \end{cases} \tag{13}$$

where $\sin\phi = k_y/k_F, k_x = \sqrt{k_F^2 - k_y^2}$. From the conditions of continuity of the wave functions, one can find the transmission coefficient

$$T_n = |t\,(k_y)|^2 = \frac{\cos^2\phi}{\cosh^2(k_y L_x) - \sin^2\phi}. \tag{14}$$

Further, one should assume that $k_F L_x \gg 1$ and put $\phi \simeq 0$ in Eq.(14). Thus, the trace of the transparency which is just the conductance (in units of e^2/h) is

$$TrT = \sum_{n=-\infty}^{\infty} \frac{1}{\cosh^2(k_y L_x)} \simeq \frac{L_y}{\pi L_x}. \tag{15}$$

Assuming that the conductance is equal to $\sigma\frac{L_y}{L_x}$ one finds the contribution to the conductivity equal to $e^2/(\pi h)$. Experimentally [2], it is close to e^2/h, that is, roughly, three times larger than our estimation. The same result has been found earlier in Ref.[8] by one of the ways of derivation (the other one gives, instead, a factor $\pi/8$). Note also that for the case of nanotubes ($L_x \gg L_y$) one has a conductance e^2/h per channel, in accordance with known results [22,23].

The result $\sigma = e^2/(\pi h)$ per valley per spin is found here for the case of ideal crystal. If one calculates in the simplest "bubble" approximation the conductivity in the presence of weakly scattering impurities and then put $T = \mu = 0$ it leads to the same value [4,5,7,11,12]. However, one can hope that more transparent physical understanding of the origin of finite conductivity in ideal crystals which is provided by the Landauer formula will be useful to consider more complicated situations, such as the case of bilayer [20].

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Note added: After this work was basically finished (cond-mat/0512337, revised version) I have become aware of a relevant work by J. Tworzydlo, B. Trauzettel, M. Titov, A. Rycerz, and C. W. J. Beenakker (cond-mat/0603315) where a similar result for the transmission coefficient (14) has been obtained, with a bit different choice of boundary conditions. They have found also a sub-Poissonian shot noise in *ideal* graphene similar to that in disordered metals which gives a beautiful example of the importance of electron Zitterbewegung.

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