Robust Transport Properties in Graphene

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Two-dimensional Dirac fermions are used to discuss quasiparticles in graphene in the presence of impurity scattering. Transport properties are completely dominated by diffusion. This may explain why recent experiments did not find weak localization in graphene. The diffusion coefficient of the quasiparticles decreases strongly with increasing strength of disorder. Using the Kubo formalism, however, we find a robust minimal conductivity that is independent of disorder. This is a consequence of the fact that the change of the diffusion coefficient is fully compensated by a change of the number of delocalized quasiparticle states.

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Recent experimental studies of single graphite layers (graphene) have revealed interesting transport properties [1–3]. A quantum Hall effect was found in the presence of an external magnetic field with Hall plateaus $\sigma_{xy} = \pm(2n+1)2e^2/h$ $(n = 0, 1, \ldots)$. This result can be explained by the band structure of graphene which has two nodes (or valleys) due to the hexagonal lattice and a linear dispersion around each of these nodes [4]. If the Fermi energy is near these nodes the quasiparticles can be described as fourfold degenerated (two valleys and two spins orientations) 2D Dirac fermions. Another interesting observation is the existence of a minimal conductivity $\sigma_{xx}^{\min}$ which occurs if the Fermi energy is exactly at the nodes. This quantity shows a remarkable stability with $\sigma_{xx}^{\min} = 3 \ldots 5\ e^2/h$, even if the mobility of the studied samples changes by almost a factor 6 from $\mu = 0.15\ \mathrm{m}^2/\mathrm{V\,s}$ to $\mu = 0.85\ \mathrm{m}^2/\mathrm{V\,s}$ [1]. The varying mobilities in different samples indicate a varying density of impurities. The transport mechanism must be related to diffusion of electrons and holes, caused by impurity scattering. The latter can formally be described by a random potential. Then, in terms of the Dirac fermions, the impurities can create gap fluctuations, i.e., a random Dirac mass, because a gap can easily be opened at the nodes of the band structure, for instance, by a staggered potential [5].

Existing theories of 2D Dirac fermions predicted the value $\sigma_{xx} = e^2/h\pi$ for a single Dirac node [6–10], (i.e., $\sigma_{xx}^{\min} = 4e^2/h\pi$) such that there is a quantitative discrepancy by a factor $1/\pi$ in comparison with the experimental observation, as discussed in Ref. [1]. In recent papers several authors applied the Landauer formula, instead of the Kubo formula used in previous studies, to determine the minimal conductivity also as $\sigma_{xx}^{\min} = 4e^2/h\pi$ for a rectangular system with aspect ratio $W/L \gg 1$ [11,12]. Nomura and MacDonald argued that $\sigma_{xx}^{\min}$ could be enhanced by Coulomb scattering, leading to $\sigma_{xx}^{\min} = 4e^2/h\pi$ [13]. Several possibilities for the value of $\sigma_{xx}^{\min}$, using different approaches to the linear response were also discussed in Ref. [14].

The effect of quantum interference due to impurity scattering was studied in a recent experiment [3]. It was found that there is no weak localization in a single graphene sheet. Multilayer graphite films, on the other hand, exhibit clearly weak localization. These observations indicate that graphene has special transport properties.

It will be shown in the following that (1) a calculation, based on linear response theory (Kubo formula), gives a conductivity of $\sigma_{xx}^{\min} = \pi e^2/h$ for the pure system, (2) weak scattering leads to a linear Boltzmann conductivity similar to what was observed experimentally, and (3) there are no weak (anti-)localization corrections due to a spontaneously broken supersymmetry which creates diffusive fermions.

Starting from the Kubo formula [15], the conductivity tensor $\sigma_{\mu\nu}$ of a system with Hamiltonian H at inverse temperature $\beta = 1/k_B T$ and for frequency ω reads

$$\frac{e}{i\hbar}\lim_{\alpha\to 0}\int_{-\infty}^{0} e^{(i\omega+\alpha)t}\mathrm{Tr}([e^{-\beta H}, r_\mu]e^{-iHt}j_\nu e^{iHt})dt. \quad (1)$$

The current operator is given by the Hamiltonian as the commutator $j_\nu = -ie[H, r_\nu]$. For noninteracting fermions with single-particle energy eigenstates $|k\rangle$ (i.e., $H|k\rangle = \epsilon_k|k\rangle$) a lengthy but straightforward calculation yields

$$\sigma_{\mu\nu} = -i\frac{e^2}{\hbar}\sum_{k_1,k_2}\langle k_1|[H, r_\mu]|k_2\rangle\langle k_2|r_\nu|k_1\rangle \times \frac{f_\beta(\epsilon_{k_2}) - f_\beta(\epsilon_{k_1})}{\epsilon_{k_1} - \epsilon_{k_2} + \omega - i\alpha} \quad (2)$$

with Fermi function $f_\beta(\epsilon) = 1/(1 + e^{-\beta\epsilon})$. The identity $\langle k_2|[H, r_\nu]|k_1\rangle = (\epsilon_{k_2} - \epsilon_{k_1})\langle k_2|r_\nu|k_1\rangle$ and the Dirac delta function $\pi\delta(\epsilon_k - \epsilon) = \lim_{\eta\to 0}\eta/[(\epsilon_k - \epsilon)^2 + \eta^2]$ allow us to express the conductivity in Eq. (2) as a double integral with respect to two energies ϵ, ϵ':

$$\sigma_{\mu\nu} = i\frac{e^2}{\hbar}\iint \mathrm{Tr}\{[H, r_\mu]\delta(H-\epsilon')[H, r_\nu]\delta(H-\epsilon)\} \times \frac{1}{\epsilon-\epsilon'+\omega-i\alpha}\frac{f_\beta(\epsilon')-f_\beta(\epsilon)}{\epsilon-\epsilon'} d\epsilon d\epsilon'. \quad (3)$$

An alternative expression is obtained by writing the Dirac delta functions in terms of the Green's function $G(z) = (H-z)^{-1}$. Using the identity

$$G(z)[H, r_\mu]G(z') = r_\mu G(z') - G(z) r_\mu + G(z) r_\mu (z-z') G(z'),$$

the diagonal elements of the conductivity tensor read

$$\sigma_{\mu\mu} = i\frac{e^2}{\hbar}\frac{1}{8\pi^2}\lim_{\eta_1,\eta_2\to 0}\iint \sum_{r,r'}(r_\mu - r'_\mu)^2 \times \sum_{s_1,s_2=\pm 1} s_1 s_2[\epsilon' - \epsilon + i(s_1\eta_1 - s_2\eta_2)] \times \mathrm{Tr}_n[G_{rr'}(\epsilon' + is_1\eta_1)G_{r'r}(\epsilon + is_2\eta_2)] \times \frac{f_\beta(\epsilon')-f_\beta(\epsilon)}{\epsilon-\epsilon'+\omega-i\alpha} d\epsilon d\epsilon', \quad (4)$$

where Tr_n is the trace related to n additional degrees of freedom (e.g., $n = 2$ for the spinor index of 2D Dirac fermions).

In the special case of graphene the Hamiltonian reads in sublattice representation [4,5]

$$H = \sigma_1 h_1 + \sigma_2 h_2, \quad (5)$$

where σ_j $(j = 1, 2, 3)$ are Pauli matrices. In Fourier representation with wave vector $\vec{k} = (k_1, k_2)$ the coefficients of the Pauli matrices in a pure system are

$$h_1 = -t\sum_{j=1}^{3}\cos(\vec{a}_j\cdot\vec{k}), \qquad h_2 = -t\sum_{j=1}^{3}\sin(\vec{a}_j\cdot\vec{k}),$$

with the lattice vectors of the honeycomb lattice $\vec{a}_1 = (-\sqrt{3}/2, 1/2)$, $\vec{a}_2 = (0, -1)$, and $\vec{a}_3 = (\sqrt{3}/2, 1/2)$. H can be diagonalized as $H = \mathrm{diag}(e_k, -e_k)$ with $e_k = \sqrt{h_1^2 + h_2^2}$. The current operator transforms under Fourier transformation as $-ie[H, r_\mu] \to e\partial H/\partial k_\mu$.

There are six points at $\vec{k} = (\pm 4\pi/3\sqrt{3}, 0)$, $(2\pi/3\sqrt{3}, \pm 2\pi/3)$, and $(-2\pi/3\sqrt{3}, \pm 2\pi/3)$ where e_k vanishes, corresponding with the two nodes. The commutators are in the diagonal representation of H

$$[H, r_\mu]_{12}[H, r_\mu]_{21} = \frac{1}{e_k^2}\left(h_2\frac{\partial h_1}{\partial k_\mu} - h_1\frac{\partial h_2}{\partial k_\mu}\right)^2, \quad (6)$$

whose value is $9/4$ at all nodes. The 2D k integration at each node can be expressed by an integration with respect to h_1 and h_2 as $d^2k = J dh_1 dh_2$, where the Jacobian is $J = 4/9$ at all nodes. Therefore, after the angular integration around the nodes the integration is given by

$$J(2\pi/3)e_k de_k = (8\pi/27)e_k de_k (0 \le e_k \le \lambda).$$

This can be inserted in the conductivity of Eq. (3) and after the summation over all nodes the conductivity $\sigma_{\mu\mu}$ reads at low temperatures $(\beta \sim \infty)$

$$-i\frac{e^2}{h}\frac{12}{27}\int_0^\lambda\left\{\frac{[H, r_\mu]_{12}[H, r_\nu]_{21}}{2e_k+\omega-i\alpha} + \frac{[H, r_\mu]_{21}[H, r_\nu]_{12}}{-2e_k+\omega-i\alpha}\right\} de_k.$$

Inserting the commutators from Eq. (6) yields eventually

$$\mathrm{Re}\,(\sigma_{22}) = \frac{e^2}{h}\int_0^\lambda \pi\delta(2e_k-\omega)de_k = \frac{\pi}{2}\frac{e^2}{h}. \quad (7)$$

Another factor of 2 comes from the spin-1/2 degeneracy of the quasiparticles. Thus our calculation gives for the minimal conductivity $\sigma_{xx}^{\min} = \pi e^2/h$.

In a pure graphene sheet there is only ballistic transport. Consequently, the diffusion coefficient D is infinite. On the other hand, if the Fermi energy is exactly at the nodes, the related density of states ρ vanishes. From this point of view, the conductivity, expressed by the Einstein relation as $\sigma_{xx}^{\min} \propto \rho D$, depends very sensitively on the limits of the model parameters (e.g., the dc limit $\omega \to 0$). A more instructive situation is a system with randomly distributed scatterers that may lead to diffusion (i.e., $D < \infty$) or even to Anderson localization (i.e., $D = 0$) [16–19]. A source of disorder in the tight-binding Hamiltonian H of Eq. (5) is a randomly fluctuating nearest-neighbor hopping rate. For a qualitative discussion of random scattering, the Hamiltonian is approximated by the 2D Dirac Hamiltonian

$$H_D = i\sigma_1\nabla_1 + i\sigma_2\nabla_2 + m\sigma_3.$$

A randomly fluctuating gap is introduced by a random Dirac mass m with Gaussian distribution of zero mean and variance g. The transformation property of the tight-binding Hamiltonian

$$H^T = -\sigma_2 H \sigma_2 \quad (8)$$

is also obeyed by the random Dirac Hamiltonian H_D after rotating $\sigma_1 \to \sigma_2$ and $\sigma_2 \to \sigma_1$. This property is crucial for the formation of a diffusion mode in two dimensions [10]. Models which violate this property, e.g., by an additional term proportional to a 2×2 unit matrix, may lead to localization of states near the Fermi energy [18,19]. Intervalley scattering is ignored by the approximation $H \approx H_D$ such that we have only independent Dirac cones. The effect of the random mass can be studied by applying a perturbation theory, using a partial summation of an infinite series of most relevant contributions. On the level of the averaged single-particle Green's function this leads to a self-energy term η in the Green's function: $G_\pm(i\epsilon) \equiv G(i\epsilon \pm i\eta)$. This is formally equivalent to a mean-field approximation of a supersymmetric functional-integral approach, where the random Dirac mass is replaced by a random supermatrix [10]. Then η is obtained as a solution of

$$\eta = g(\eta + \epsilon) \int [(\eta + \epsilon)^2 + k^2]^{-1} k dk/\pi. \quad (9)$$

The Green's function can be expressed again by a perturbation expansion, now in terms of fluctuations around the mean-field approximation $G_{\pm}(i\epsilon)$. This expansion can be inserted into the conductivity (3). The leading term for $i\epsilon = E_F$ (Fermi energy) is the Boltzmann conductivity

$$\mathrm{Re}(\sigma_{\mu\mu}) \approx \frac{e^2 \bar{\sigma} \eta^2}{\hbar \pi} \int \{[(e_k - E_F)^2 + \eta^2]^{-2} + [(e_k + E_F)^2 + \eta^2]^{-2}\} \rho(e_k) de_k. \quad (10)$$

Here $\bar{\sigma}$ is an approximation of the two commutators in Eq. (3) and ρ is the density of states of pure Dirac fermions: $\rho(E) = \rho_0 |E|$, where ρ_0 depends on the cutoff λ of the spectrum of H. This is a classical result for the conductivity of Dirac fermions that was already anticipated by Fradkin [6] and discussed in the context of d-wave superconductors by Lee [7] and for graphene by Peres *et al.* [8]. The conductivity at $E_F = 0$ is $\sigma_{xx}^{\min} \approx 2e^2 \bar{\sigma} \rho_0 / h$ and does not depend on η. Thus $\sigma_{xx}^{\min}$ is independent of the strength of impurity scattering g. Sufficiently away from $E_F = 0$ the conductivity becomes linear, as shown in Fig. 1. This behavior agrees well with the experimentally observed linear conductivity [1].

The next question is whether or not quantum interference effects are important. The corresponding corrections in the conductivity are given by the next order terms of the expanded Green's function. This includes a logarithmic term (Cooperons) due to a massless mode of the fluctuations around the mean-field approximation. Previous studies found that the corrections give an antilocalization effect for conventional scatterers, i.e., an increase of the conductivity due to quantum interference effects [20]. Additional terms in the Hamiltonian of second order in the momentum can suppress weak antilocalization [21].

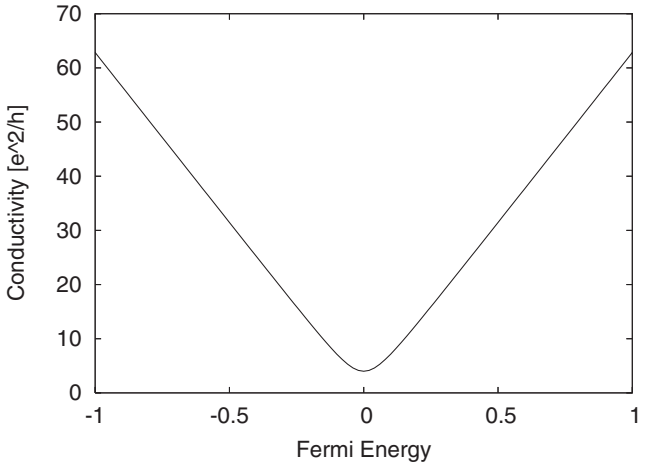

FIG. 1. Conductivity of graphene calculated in mean-field approximation [from Eq. (10)].

A crucial question, implied by the antilocalization effect and the absence of weak-localized corrections in experiments [3], is whether or not the states in graphene are localized. The conductivity in Eq. (3) does not directly address localization, in contrast to the alternative expression in Eq. (4): The long-distance behavior of the Green's functions is directly related to the behavior of the quantum states. For this purpose we return to Eq. (4), consider the minimal conductivity (i.e., $E_F = 0$), and take the limits $\alpha \to 0$ and $\beta \to \infty$ (η_1, $\eta_2 \to 0$ are implicit) to obtain

$$\sigma_{xx}^{\min} = -\frac{e^2}{\hbar} \frac{\omega}{8\pi} \int_{-\omega/2}^{\omega/2} \sum_{r,r'} (r_\mu - r'_\mu)^2 \times \sum_{s_1, s_2 = \pm 1} s_1 s_2 \mathrm{Tr}_2[G_{rr'}(\epsilon + \omega/2 + i s_1 \eta_1) \times G_{r'r}(\epsilon - \omega/2 + i s_2 \eta_2)] d\epsilon. \quad (11)$$

Assuming that the integrand is finite for $0 < \omega \ll 1$ it can be pulled out of the integral for $\epsilon = 0$. The major contribution comes from $s_1 \neq s_2$, where the poles of the Green's function are on different sides of the real axis. A finite factor σ' takes care of a correction in comparison with the exact value of the integral

$$\sigma_{xx}^{\min} \approx \frac{e^2}{\hbar} \frac{\sigma'}{2\pi} \omega^2 \sum_{r,r'} (r_\mu - r'_\mu)^2 \mathrm{Tr}_2[G_{rr'}(\omega/2 + i\eta_1) \times G_{r'r}(-\omega/2 - i\eta_1)]. \quad (12)$$

For localized states the sum, averaged with respect to randomness, is finite due to the exponential decay for $|r - r'| \gg 1$. In the dc limit $\omega \to 0$ this would lead to a vanishing $\sigma_{xx}^{\min}$.

In order to evaluate the expression in Eq. (12) it is convenient to return to the functional integral of Ref. [10]. It was found that the underlying supersymmetry of the integral is spontaneously broken by the mean-field solution of Eq. (9). The main consequence of this effect is a diffusive fermionic mode, similar to the Goldstone mode in systems with a rotational symmetry, that can be formally described by a complex Grassmann field Ψ_r. This allows us to write

$$\langle \mathrm{Tr}_2[G_{rr'}(i\epsilon) G_{r'r}(-i\epsilon)] \rangle = \frac{-4\eta^2}{g^2} \int \bar{\Psi}_r \Psi_{r'} e^{-S''} \mathcal{D}[\psi], \quad (13)$$

where the action depends on the solution η of Eq. (9):

$$S'' = \frac{4\eta^2}{g(\eta + \epsilon)} \int \left[\epsilon + \frac{g}{4\pi(\eta + \epsilon)} k^2 \right] \bar{\Psi}_k \Psi_{-k} d^2 k. \quad (14)$$

The latter contains the diffusion coefficient

$$D = \frac{g}{4\pi(\eta + \epsilon)} \quad (15)$$

that depends strongly on the variance g of the distribution of random scatterers.

The minimal conductivity is obtained from Eq. (13) for small $\epsilon = i\omega/2$, together with Eq. (12), as

$$\sigma_{xx}^{\min} = \sigma' \frac{e^2}{h\pi}. \tag{16}$$

This agrees with the result of the mean-field approximation in Eq. (10), except for the (undetermined) prefactors. The variation of σ' with g for $0 \leq g \leq 1$ can be neglected. Comparing it with the result in Eq. (7) we conclude that the renormalization factor is $\sigma' = \pi^2$. Thus, in contrast to the diffusion coefficient D the minimal conductivity $\sigma_{xx}^{\min}$ does not depend on g. This implies the absence of corrections due to quantum interference on characteristic length scales, in agreement with recent experimental observations [3].

The fact that $\sigma_{xx}^{\min}$ is so robust with respect to impurity scattering can be understood in terms of the Einstein relation $\sigma_{xx}^{\min} \propto \rho D$, where the conductivity is separated into the diffusion coefficient D and the averaged density of states ρ at the Fermi energy $E_F = 0$. The latter is calculated from a functional integral similar to Eq. (13) as $\rho = \eta/\pi g$ [10]. Then with D of Eq. (15) the minimal conductivity reads

$$\sigma_{xx}^{\min} \propto \rho D \propto \frac{\eta}{\eta + \epsilon} = \frac{\eta}{\eta + i\omega/2}.$$

For small ϵ the mean-field Eq. (9) gives $\eta \approx e^{-\pi/g}$, which implies for D and ρ

$$D \approx g e^{\pi/g}/4\pi, \qquad \rho \approx e^{-\pi/g}/\pi g. \tag{17}$$

Thus, moving away from the ballistic limit $g = 0$, the conductivity should fall rapidly with increasing random potential fluctuations due to a decreasing D in the Einstein relation. On the other hand, the density of states ρ increases correspondingly so that in $\sigma_{xx}^{\min}$ the influence of random scattering is compensated. This is in agreement with the direct evaluation of $\sigma_{xx}^{\min}$ in Eq. (16). The results for ρ and D in Eq. (17) describe a nonperturbative effect of disorder which is not visible within an expansion in powers of g.

Strong potential scattering by charged impurities in the substrate, for instance, can lead to a destruction of the massless fermion mode used in Eq. (14). This can cause localization and a vanishing $\sigma_{xx}^{\min}$, at least at very low temperatures. The localized regime cannot be treated within a conventional field theory but would require either a numerical finite-size scaling approach [22] or a strong-disorder expansion.

In conclusion, we have studied the conductivity of graphene, using a model of 2D Dirac fermions. In the case of a pure system the ballistic transport leads to a minimal conductivity $\sigma_{xx}^{\min} = \pi e^2/h$. In the case of impurity scattering we found pure diffusion for any strength of Gaussian distributed scatterers, where the diffusion coefficient depends strongly on the distribution. The minimal conductivity $\sigma_{xx}^{\min}$, on the other hand, does not depend on the strength of impurity scattering because the change of the diffusion coefficient is completely compensated by a change of the density of diffusive states.

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