Diffusive transport in graphene

K. Ziegler

Institut für Physik, Universität Augsburg, D-86135 Augsburg, Germany

1. Introduction

Graphene, a sheet of graphite with a honeycomb structure, was discovered as a genuine two-dimensional electronic system [1–3]. The separation of a single sheet is possible in graphite because this material has an extreme anisotropy due to layers with an interlayer spacing of 3.4 Å and an interatomic distance within the layers of 1.4 Å. Among many other characteristic features, this material has surprisingly robust transport properties: It behaves like a metal with almost constant mobility over a large range of temperatures and charge densities. This raises questions about the relevant mechanism of transport and the role of scattering of the quasiparticles in graphene.

It has been suggested that transport in graphene is ballistic even at temperatures up to 300 K [4] due to its high mobility. However, recent studies have seen strong breaking of translational invariance due to ripples [5] which make ballistic transport unlikely. Moreover, an inhomogeneous charge-carrier distribution with an intrinsic disorder length scale of $l \approx 30\,\mathrm{nm}$ was seen in a scanning single-electron transistor study at $T = 0.3\,\mathrm{K}$ [6]. This also indicates that ballistic transport is unlikely. Although it is not clear, whether or not the charge inhomogeneities are caused by ripples, the latter present the main source of disorder in graphene.

In order to study transport in a two-dimensional (2D) system, a classical (Boltzmann) as well as a quantum (Kubo) approach can be applied. Quantum effects (i.e., the spectral properties of the quasiparticles) can be included in the Boltzmann approach, but for a consistent treatment the Kubo approach is favorable. The Kubo approach is sensitive if certain limits are applied (e.g., zero temperature or zero frequency (DC) limit [7]). Therefore, the following discussion will be restricted to the case where the zero-temperature limit is taken first. This allows us to concentrate on quantum effects in the transport mechanism of graphene. It is also motivated by the fact that the relevant energy scale in graphene is given by the nearest-neighbor hopping rate of about 3 eV [8]. Thus the energy of thermal fluctuations at typical temperature in the transport experiments is relatively small in comparison to the hopping energy.

In the following, we will study a model for quasiparticles in graphene, where weak and strong disorder is taken into account. The Boltzmann approach and its results for graphene near the Dirac point is briefly discussed. Then the Kubo approach is used to evaluate the DC conductivity at the Dirac point, applying different approximations. The main result is a diffusion propagator for the average

E-mail address: klaus.ziegler@physik.uni-augsburg.de

two-particle Green's function for weak as well as for strong disorder.

1.1. Boltzmann approach

The Einstein relation [9]

$$\sigma = e^2 \rho D \tag{1}$$

is a possible starting point for calculating the DC conductivity. Here the diffusion coefficient is proportional to the scattering time τ, and ρ is the density of states at the Fermi energy. An extension to frequency $\omega > 0$ leads to the Drude formula

$$\sigma(\omega) = \frac{\sigma_0 \tau}{1 - \mathrm{i}\omega\tau}.$$

The main problem is to evaluate τ, and a possible way to do that is provided by the Boltzmann approach. The latter, based on the classical Boltzmann equation, has been a very successful concept for the discussion of transport in solid-state physics. It was also successfully applied the case in graphene [10,11].

A special case in graphene, however, the observation of a minimal conductivity at the Dirac point requires some explanation [2]. At this point the density of states vanishes (i.e., there are no states at the Fermi energy). This implies that a statistical concept which uses the distribution of charges may experience some difficulties. Nevertheless, the Boltzmann approach can be applied away from the Dirac point and then the Dirac point is approached at the end. Then the density of states is $\rho \propto k_\mathrm{F}$, where k_F is the Fermi vector (at the Dirac point is $k_\mathrm{F} = 0$). Perturbation theory with short-range scatterers gives for the scattering time [10,12,13]

$$\tau \propto \frac{1}{k_\mathrm{F}} \sim \infty.$$

A divergent scattering time at the Dirac point does not describe a realistic situation because quasiparticles are scattered, e.g., by the ripples or charge inhomogeneities. However, the conductivity is constant because the wave vectors k_F cancel each other. This would agree with a nonzero minimal conductivity for $k_\mathrm{F} = 0$. Unfortunately, the constant conductivity is in disagreement with experiments, where a linearly increasing conductivity was observed away from the Dirac point [2]. This problem can be cured by the assumption of charged (i.e., long-range correlated) scatterers. They give indeed a linear conductivity [10]. The price is that the conductivity vanishes at the Dirac point. So, the classical Boltzmann approach is not capable to describe transport near the Dirac point properly, and it must be replaced by a more microscopic approach, based on the Kubo formula for linear response to an external electric field. We will discuss subsequently that the Kubo formula, averaged with respect to disorder, recovers the Einstein relation Eq. (1) with a disorder dependent diffusion coefficient D.

2. Model

The lattice Hamiltonian

$$H = h_1\sigma_1 + h_2\sigma_2 + m\sigma_3 \tag{2}$$

with Pauli matrices σ_j and a (Dirac mass) term $m\sigma_3$ is considered in this paper. 2D Dirac fermions (2DDF) is a special case of this Hamiltonian, the tight-binding Hamiltonian on a honeycomb lattice (TBHL) is another one. In a translational-invariant system the Fourier representation with wavevector $\vec{k} = (k_1, k_2)$ reads

$$h_j = k_j \text{ (2DDF)}; \quad h_1 = -t\sum_{j=1}^{3} \cos(\vec{a}_j \cdot \vec{k}),$$

$$h_2 = -t\sum_{j=1}^{3} \sin(\vec{a}_j \cdot \vec{k}) \text{ (TBHL)}$$

with the lattice vectors of the honeycomb lattice

$$\vec{a}_1 = (-\sqrt{3}/2, 1/2), \quad \vec{a}_2 = (0, -1), \quad \vec{a}_3 = (\sqrt{3}/2, 1/2).$$

H can be diagonalized as $H = \mathrm{diag}(e_k, -e_k)$ with $e_k = \sqrt{m^2 + h_1^2 + h_2^2}$. In graphene usually we have $m = 0$. However, in a bilayer of two graphene sheets it is possible to create a weak term with $m \neq 0$ due to its internal structure (i.e., A and B sublattice are not equivalent in a bilayer).

2.1. Disorder

Disorder due to ripples can be described by quenched randomly distributed bonds. In terms of our Hamiltonian H this leads to a random "gauge field". This means that a random term $v_1\sigma_1 + v_2\sigma_2$ appears in H [11,14,15]. It is not a real gauge field, because it does not appear in a Peierls phase factor but can be understood as a gauge field in the continuum limit of the Dirac fermions [16]. Another source of disorder is doping with impurity atoms or bilayers. This is represented by a random $m\sigma_3$ term in H which corresponds with a random mass term in the case of Dirac fermions. Moreover, it is assumed that randomness due to disorder has an uncorrelated Gaussian distribution with mean zero and variance $\langle v^2 \rangle = \langle m^2 \rangle = g$.

2.2. Kubo approach

Starting from a Hamiltonian, in our case from H in Eq. (2), the current operator is

$$j_k = -\mathrm{i}e[H, r_k].$$

On the other hand, the average current induced by an external electric field E reads in terms of linear response as Ohm's law

$$\langle j_k \rangle = \sigma_{kl} E_l$$

with conductivity (we use the notation of Ref. [18] here)

$$\sigma_{kk} = -\frac{e^2}{h}\frac{\omega^2}{2}\int \sum_r r_k^2 K(r;\varepsilon,\omega) \times \frac{f_\beta(\varepsilon+\omega/2)-f_\beta(\varepsilon-\omega/2)}{\omega}\,\mathrm{d}\varepsilon. \quad (3)$$

$f_\beta(x) = (1+e^{\beta x})^{-1}$ is the Fermi distribution at temperature $T = 1/k_B\beta$, $K(r;\varepsilon,\omega)$ is the average two-particle Green's function (2PGF)

$$K(r;\varepsilon,\omega) = \lim_{\delta\to 0}\langle Tr_2[G(r,0;\varepsilon-\omega/2+\mathrm{i}\delta)G(r,0;\varepsilon+\omega/2-\mathrm{i}\delta)]\rangle$$

and G is the one-particle Green's function (1PGF):

$$G(r,0;z) = (z-H)^{-1}_{r,0}.$$

Off-diagonal terms of σ_{kl} vanish because we do not consider a magnetic field here. $\langle\ldots\rangle$ means averaging with respect to quenched disorder. In the case of zero temperature the factor $-(f_\beta(\varepsilon+\omega/2)-f_\beta(\varepsilon-\omega/2))/\omega$ in the Kubo formula becomes a Dirac delta function with respect to ε. Thus the conductivity reduces to the expression

$$\sigma_{kk} = \omega^2\left[\frac{\partial^2 K(q;0,\omega)}{\partial q_k^2}\right]_{q=0}\frac{e^2}{h}. \quad (4)$$

2.3. Approximations

A common approximation is to use a one-particle average in the average 2PGF, where the average of the 2PGF is replaced by the product of two average 1PGFs [12,13]:

$$K(r;\varepsilon,\omega) \approx \lim_{\delta\to 0} Tr_2[\langle G(r,0;\varepsilon-\omega/2+\mathrm{i}\delta)\rangle \times\langle G(r,0;\varepsilon+\omega/2-\mathrm{i}\delta)\rangle]. \quad (5)$$

This allows us to apply the self-consistent Born approximation to the average 1PGF [13], where a self-energy $\mathrm{i}\eta$ is introduced to shift the Hamiltonian $H_0 \equiv \langle H\rangle$ as $H_0 \to H_0 - \mathrm{i}\eta$. η is given by the self-consistent condition

$$\eta = \mathrm{i}gTr_2[(z-H_0+\mathrm{i}\eta)^{-1}_{rr}]. \quad (6)$$

η can be interpreted as an effective scattering rate, or $1/\eta = \tau$ can be interpreted as a scattering time. The average 1PGF then reads

$$\langle G(r,0;z+\mathrm{i}\delta)\rangle \approx (z+\mathrm{i}\eta+\mathrm{i}\delta-H_0)^{-1}_{r,0}$$

and $\eta \propto e^{-\pi/g}/g$ for $z=0$. Moreover, the average 2PGF of Eq. (5) is

$$K(q=0;\varepsilon=0,\omega) \approx -\frac{1}{2\pi}\log(-(\omega-\mathrm{i}\eta)^2)$$

and

$$\left[\frac{\partial^2 K(q;0,\omega)}{\partial q_k^2}\right]_{q=0} \approx \frac{1}{\pi(\omega-\mathrm{i}\eta)^2},$$

such that with Eq. (4) the conductivity reads

$$\sigma_{kk} = \omega^2\left[\frac{\partial^2 K(q;0,\omega)}{\partial q_k^2}\right]_{q=0}\frac{e^2}{h} \approx \frac{e^2}{h}\frac{\omega^2}{\pi(\omega-\mathrm{i}\eta)^2}. \quad (7)$$

This result gives a minimal conductivity for $\eta \ll \omega$, i.e., in the perturbative regime of disorder. However, the conductivity of Eq. (4) would vanish in the limit $\omega \to 0$ if $\eta > 0$. In other words, the DC limit does not make sense in this approximation. The result is also in disagreement with the Drude formula.

2.4. Nonlinear sigma model

It is possible to avoid the approximation of Eq. (5) and to evaluate the average 2PGF directly [19]. The reason is that the 2PGF preserves an intrinsic symmetry. After averaging over disorder, the symmetry leads to a special nonlinear sigma model which gives for the Fourier components of the 2PGF a diffusion propagator

$$K(q;0,\omega) = \frac{K_0}{\mathrm{i}\omega + Dq^2}.$$

The prefactor K_0 and the diffusion coefficient D depend in general on the strength of disorder g and on the frequency ω. We have (up to some numerical constants) for weak bond disorder [18] or for a weak random $m\sigma_3$ term in H [19]

$$K_0 = \frac{\mathrm{i}\omega+\eta}{g}, \quad D \propto \frac{g}{\mathrm{i}\omega+\eta}$$

and for strong disorder [15]

$$K_0 \propto \frac{1}{\sqrt{g}}, \quad D \propto \frac{1}{\sqrt{g}}.$$

Eq. (4) implies the Einstein relation of Eq. (1) with

$$\sigma_{kk} = \omega^2\left[\frac{\partial^2 K(q;0,\omega)}{\partial q_k^2}\right]_{q=0}\frac{e^2}{h} \propto K_0 D\frac{e^2}{h} = \frac{e^2}{h}\begin{cases}1 & \text{weak disorder,}\\ g^{-1} & \text{strong disorder.}\end{cases} \quad (8)$$

Thus, there is a non-vanishing minimal conductivity even in the presence of strong disorder, although it is suppressed by $1/g$ in comparison with the case of weak disorder.

It is essential for these results that there is no random term proportional to σ_0 (random potential term) in the Hamiltonian of Eq. (2). Such a term would lead to Anderson localization, as discussed by Ludwig et al. [16]. Castro Neto and Kim [17] have shown recently that a random potential term can appear if next-nearest neighbor hopping is included in graphene with ripples. The experimental fact that Anderson localization has not been observed may indicate that there is a very large localization length.

3. Discussion and conclusions

Ballistic transport in graphene near the Dirac point can be ruled out on the basis of recent experiments [5,6]. In particular, the intrinsic disorder length scale $l \approx 30\,\mathrm{nm}$, which was found in a scanning single-electron transistor study [6], indicates that substantial disorder scattering must be present in graphene. Ripples might be the main source of disorder, whereas potential disorder due to impurities may not be so important. If ripples are approximated by random nearest-neighbor hopping rates, previous studies have found that an internal symmetry of the two-particle Green's function on the honeycomb lattice leads to a diffusion propagator, after averaging over disorder. It has been shown in this paper, that the usual self-consistent Born approximation misses this property. The fact that ripples lead to a diffusion mode, in contrast to impurity potential which causes localization [20], can explain the existence of the minimal conductivity.

Acknowledgments

I am grateful to A.K. Geim, M.I. Katsnelson, and S. Mikhailov for interesting discussions.

References

[1] K.S. Novoselov, et al., Science 306 (2004) 666.
[2] K.S. Novoselov, A.K. Geim, S.V. Morozov, D. Jiang, M.I. Katsnelson, I.V. Grigorieva, A.A. Firsov, Nature 438 (2005) 197.
[3] Y. Zhang, V.-W. Tan, H.L. Störmer, P. Kim, Nature 438 (2005) 201.
[4] A.K. Geim, K.S. Novoselov, Natur. Materials 6 (2007) 183.
[5] J.C. Meyer, A.K. Geim, M.I. Katsnelson, K.S. Novoselov, T.J. Booth, S. Roth, cond-mat/0701379.
[6] J. Martin, et al., cond-mat/0705.2180.
[7] K. Ziegler, Phys. Rev. B 75 (2007) 233407.
[8] A. Bostwick, T. Ohta, T. Seyller, K. Horn, E. Rotenberg, cond-mat/0609660.
[9] N.W. Ashcroft, N.D. Mermin, Solid State Physics, Holt, Rinehart and Winston, New York, 1976.
[10] K. Nomura, A.H. MacDonald, cond-mat/0606589.
[11] M.I. Katsnelson, A.K. Geim, cond-mat/0706.2490.
[12] P.A. Lee, Phys. Rev. Lett. 71 (1993) 1887.
[13] N.M.R. Peres, F. Guinea, A.H. Castro Neto, Phys. Rev. B 73 (2006) 125411.
[14] S.V. Morozov, et al., Phys. Rev. Lett. 97 (2006) 016801.
[15] K. Ziegler, cond-mat/0703628.
[16] A.W.W. Ludwig, M.P.A. Fisher, R. Shankar, G. Grinstein, Phys. Rev. B 50 (1994) 7526.
[17] A.H. Castro Neto, E. Kim, cond-mat/0702562.
[18] K. Ziegler, Phys. Rev. Lett. 97 (2006) 266802.
[19] K. Ziegler, Phys. Rev. B 55 (1997) 10661;
K. Ziegler, Phys. Rev. Lett. 80 (1998) 3113.
[20] I.L. Aleiner, K.B. Efetov, Phys. Rev. Lett. 97 (2006) 236801;
A. Altland, Phys. Rev. Lett. 97 (2006) 236802;
P.M. Ostrovsky, et al., Phys. Rev. B 74 (2006) 235443.