Impurity and edge roughness scattering in graphene nanoribbons: the Boltzmann approach

Hengyi Xu and Thomas Heinzel

Condensed Matter Physics Laboratory, Heinrich-Heine-Universität, Universitätsstraße 1, D-40225 Düsseldorf, Germany

E-mail: hengyi.xu@hhu.de

Received 25 July 2012, in final form 5 October 2012
Published 23 October 2012
Online at stacks.iop.org/JPhysCM/24/455303

Abstract

The conductivity of graphene nanoribbons in the presence of bulk impurities and edge roughness is studied theoretically using the Boltzmann transport equation for quasi-one-dimensional systems. As the number of occupied subbands increases, the conductivity due to bulk impurities converges towards the two-dimensional case. It is shown that the dependence of the conductivity generated by edge roughness scattering depends in a distinctly different way on the sample parameters than the conductivity due to bulk scattering. The Boltzmann model furthermore predicts the amplitude of the edge-roughness-induced magnetoconductance dip as a function of the amplitude and the correlation length of the edge roughness.

(Some figures may appear in colour only in the online journal)

1. Introduction

The theoretical description of electron transport in graphene sheets with various scattering sources, such as charged impurities in substrates, microscopic corrugations or short-range resonant scatterers, has frequently been based on the Boltzmann approach. Such studies, in particular the electron density dependence of the conductivity, are of fundamental interest since they help in identifying the dominant scattering sources [1, 2]. It has been verified systematically that the Boltzmann approach is well suited to describe the transport in a broad range of parameters for both single and double layer graphene [3]. As the width of the graphene strips is decreased, graphene nanoribbons (GNRs) are formed, where size-dependent effects, for example the inhomogeneous electron density [4] or the edge roughness, become relevant for the transport properties. In this case, the transport has so far been described within the framework of the Landauer–Büttiker model with the aid of Green’s function techniques [5, 6]. It is well established that in GNRs, edge disorder can contribute significantly to the scattering [7–10], which in wide structures is governed by a combination of scattering at charged impurities and resonant scattering at short-range defects. Edge disorder has been suggested as the source of the transport gap in narrow GNRs around the charge neutrality point [10–13]. Furthermore, a typical size effect, the so-called edge-roughness-induced magnetoconductance dip (ERID), in GNRs has been studied by numerical quantum simulations; it is interpreted as magnetic-field-enhanced diffusive scattering when the electron trajectory grazes the edges [14]. This structure, also known as the wire peak [15], has recently been observed by Masubuchi et al [16] in quasi-ballistic GNRs. The Boltzmann approach has been applied to treat a variety of scattering sources in conventional quasi-one-dimensional (Q1D) systems, for example quantum wires [17–19]. On the other hand, only a few aspects of transport in GNRs have so far been studied within the Boltzmann model [20, 21].

In this paper, we apply the linear Boltzmann equation to armchair GNRs and determine their transport properties in the presence of both δ-type short-range impurities and edge roughness. Both contributions to the total conductivity are studied as a function of various sample parameters. The model suggests that the two scattering mechanisms show...
different parametric dependences, most strikingly with respect to the GNR width. Furthermore, an analytic expression for the amplitude of the ERID is derived and the applicability of the model to interpret experimental data is discussed.

2. Model and theory

We start with the Dirac Hamiltonian

$$H = \hbar v_F (\sigma_x k_x + \sigma_y k_y),$$

(1)

with Fermi velocity $v_F \approx 10^6 \text{ m s}^{-1}$ and Pauli matrices $\sigma_{x,y}$ and $\sigma_z$ acting on the $A/B$ sublattice and $K/K'$ valley spaces, respectively. The energy spectra of GNRS depend on the nature of their edges, namely zigzag or armchair. Within this work, we restrict ourselves to metallic armchair GNRS for computational reasons. We choose a GNR of length $L$ oriented along the $y$-direction with size quantization established in the $x$-direction (width $W$). For this system, the boundary conditions imposed on the wavefunction, namely $\Psi_A(x = 0) = \Psi_B(x = 0) = \Psi_A(x = W) = \Psi_B(x = 0) = 0$, give rise to the allowed transverse wavevectors as

$$k_n = \frac{n \pi}{W} - \frac{4 \pi}{3a},$$

(2)

with $a = 0.246 \text{ nm}$ being the lattice constant of graphene. $W$ is the width of the armchair GNR. The integer $n$ is of the order of $W/a$ for the energetically lowest modes. Throughout this text we denote the energy $\epsilon$ normalized to $\hbar v_F$ as $\tilde{\epsilon} = \epsilon / (\hbar v_F)$ with $\tilde{\epsilon}^2 = k_n^2 + k_x^2$. The normalized wavefunction for the $n$th subband reads [22, 23]

$$\Psi(r) = \frac{e^{ik_y x}}{\sqrt{4WL}} \begin{pmatrix} e^{ik_n x} \\ k_n + ik \tilde{\epsilon} e^{ik_n x} \\ -e^{-ik_n x} \\ k_n + ik \tilde{\epsilon} e^{-ik_n x} \end{pmatrix},$$

(3)

which is a mixture of two Dirac points $K = (4\pi/(3a), 0) = (K, 0)$ and $K' = (-4\pi/(3a), 0) = (-K, 0)$ (see appendix A for a discussion).

In order to calculate the transport properties of GNRS, we adopt the linearized Boltzmann equation

$$-\frac{eE_F}{\hbar} \frac{\partial f_n(\epsilon_n)}{\partial \epsilon} = \sum_{n'} \sum_{k} W_{nk'nk} [f_{nk'} - f_{nk}],$$

(4)

describing the general Q1D system, where $E_F$ is the applied electric field along the transport direction, $f_{nk}$ is the distribution function of a state with wavevector $k$ and energy $\epsilon_n$ in the $n$th subband, and the superscript '0' denotes the equilibrium distribution. According to Fermi’s golden rule, the scattering probability due to the perturbation potential is given by

$$W_{nk'nk} = \frac{2\pi}{\hbar} \langle n', k'|U|n, k \rangle^2 \delta(\epsilon_{n'k'} - \epsilon_n).$$

(5)

The nonequilibrium distribution function can be written as

$$f_n(\epsilon_n) = f_{n0}^\mu(\epsilon_n) - eE_F v_n(\epsilon_n) \tau_n(\epsilon_n) \delta(\epsilon_n - E_F),$$

(6)

with Fermi energy $E_F$ and relaxation time $\tau_n$ for a state in the $n$th subband. The corresponding velocity $v_n$ is given by $v_n = (1/\hbar)\partial \epsilon_n/\partial k = v_F k_0/\sqrt{(k_0^2 + k_z^2)}$. Inserting equation (6) into (4), the Boltzmann equation at zero temperature can be written as

$$\frac{k}{\epsilon_n} \delta(\epsilon_n - E_F) = \sum_{n', k'} W_{n'k'nk} \left[ \frac{k}{\epsilon_n} \tau_n(\epsilon_n) \delta(\epsilon_n - E_F) - \frac{k'}{\epsilon_{n'k'}} \tau_{n'}(\epsilon_{n'k'}) \delta(\epsilon_{n'k'} - E_F) \right].$$

(7)

Multiplying both sides of equation (7) by $e$ and summing over $k$, we obtain after some algebra

$$\tau_n(E_F) = \frac{\hbar}{2\pi} \sum_{n'}(T^{-1})_{nk'}^\mu,$$

(8)

where $E_F$ is the Fermi wavevector in the $n$’th subband. The transition matrix element $T_{nk'}^\mu$ is defined as

$$T_{nk'}^\mu = \frac{\pi \hbar v_F}{L} \sum_{k''} \sum_{\mu} \left[ \delta_{n\mu} \sum_{|U|n, k|F} k^2 \frac{F_{n}^{\mu}}{\epsilon_{n}^{\mu}} \delta(\epsilon_{nk} - E_{F}) - \epsilon_{n'k'} \delta(\epsilon_{n'k'} - E_{F}) \right],$$

(9)

with the summation running over the mode index $\mu$. The Boltzmann conductivity for GNRS can then, according to appendix B, be written as

$$\sigma(E_F) = \frac{2e^2 \hbar v_F^2}{h^2} \frac{1}{\pi E_F W} \sum_{n,n'} \frac{\delta_{nk}^{\mu} k_{nk}^{\mu}}{(T^{-1})_{nk'}^\mu}.$$ (10)

For nonzero temperature, the conductivity is obtained from

$$\sigma = \int d\epsilon \left( -\frac{\partial f(\epsilon)}{\partial \epsilon} \right) \sigma(\epsilon).$$

(11)

We proceed by describing the implementation of scattering potentials in this formalism. For methodological purposes, we first consider $\delta$-type impurities (this model may be ill-defined according to the Lippmann–Schwinger equation [11]) in the form of

$$U = \gamma \sum_{j=1}^{N_{I}} \delta(x - x_j) \delta(y - y_j),$$

(12)

where $\gamma$ and $N_{I}$ are the strength and the number of impurities, respectively. Thus the matrix element squared of the perturbation is evaluated as

$$\langle n'k'|U|n,k \rangle^2 = \frac{\gamma^2}{4W^2L^2} \sum_{j=1}^{N_{I}} \cos^2 \left( \frac{(n - n')\pi x_j}{W} \right) \left[ 1 + \frac{(k_{n'} - ik')(k_{n} + ik)}{\epsilon_{n'k'} \epsilon_{nk}} \right]^2.$$
equation (15) converges to the well-known result for the conductivity. To describe the effect of strong short-range scatterers on the conductivity, it has been argued [1] that this insensitivity of the conductivity does depend on the carrier concentration. In recent quantum simulations, we have used this model to study the effects of bulk disorder [14]. The squared matrix element of the Gaussian disorder is given by

\[ |\langle n' | U | n \rangle|^2 = \frac{K_0 (hv_F)^2}{4WL} \left( 1 + \frac{\delta_{nn'} e^{-\frac{(r_{nn'}^2)^2}{2}}}{2} \right) \]

where the dimensionless impurity strength is described by the parameter \( K_0 \approx 40.5 \sqrt{n_{\text{imp}}(\delta)^2} / \xi^2 \), with \( n_{\text{imp}} \) being the relative concentration of impurities. In this approximation, the transition matrix is given by

\[ \mathcal{T}_{nn'} = \frac{K_0 (hv_F)^2}{4\pi W} \left( 1 + \frac{\delta_{nn'} e^{-\frac{(r_{nn'}^2)^2}{2}}}{2} \right) \]

The disorder-averaged conductivity of graphene for Gaussian-type impurities is given by

\[ \sigma = \frac{8e^2}{\hbar} \frac{1}{\gamma^2 n_i} \left( \sum_{n,m} \left( 1 + \delta_{nm} \right) (\mathcal{E}_F^2 + k_n^2 k_m^2) \right) e^{-\frac{(r_{nm}^2)^2}{2}} \]

where \( \mathcal{E}_F \) is the Fermi energy. This expression diverges at \( k_n, k_m \ll \mathcal{E}_F \), which is typical for scattering by short-range impurities. A more realistic and well-defined model of impurities is obtained by introducing a length scale via the Gaussian-type disorder, which is defined as

\[ V(\mathbf{r}_j) = \sum_{i=1}^{N_{\text{imp}}} U_i \exp \left( -\frac{|\mathbf{r}_j - \mathbf{r}_i|^2}{2\xi^2} \right) \]

with \( n_i = N_i / WL \). In the second step of this derivation, the summation over the random impurity positions has been replaced by an integral over \( x \). The transition matrix elements are finally given by

\[ \mathcal{T}_{nn'} = \frac{8e^2}{\hbar} \frac{(hv_F)^2}{\gamma^2 n_i} \left( \sum_{\mu} \left( 1 + \delta_{mn} \right) \left( \mathcal{E}_F^2 + k_n^2 k_m^2 \right) \right) e^{-\frac{(r_{nn'}^2)^2}{2}} \]

where \( \mathcal{E}_F \) is the Fermi energy.
length of the edge roughness. Furthermore, \( \langle \cdots \rangle \) denotes position averaging.

To evaluate the perturbation matrix element, we define the function \( \Xi \) related to the \( x \)-components of the wavefunctions as

\[
\Xi_{n'n} = \frac{1}{W} \int_{0(W)}^{\infty} \frac{x}{\Phi_W} \frac{dV(x)}{dx} \phi_n(x),
\tag{22}
\]

where \( \phi_n(x) \) denotes one of the components of the wavefunction in equation (3). Note that in our notation \( W \) denotes the width of the unperturbed ribbon with perfect edges, and the disordered stripes are added to both edges. For the hard wall confinement potential present in GNRs, this function can be expressed as

\[
\Xi_{n'n} = \frac{1}{W} \frac{\hbar v_F}{2E_F} \left[ \frac{\partial \Phi_{n'n}}{\partial x} \right]_{x=0,W}.
\tag{23}
\]

It is noteworthy that a linear form for the matrix elements of the edge roughness perturbation has been used elsewhere, which, however, neglects the interband scattering [31, 21]. As shown in more detail in appendix C, by using equation (23), the square of the matrix element for the edge roughness can be written as

\[
|\left\langle n', k'|U|n, k \right\rangle|^2 = \frac{\pi^{3/2} n^2 \hbar^2 v_F^2}{8W^6 E_F^2} \left( 1 + \frac{k_{n,k} k_{n',k'}}{\epsilon_{n,k} \epsilon_{n',k'}} \right) \times \frac{\Lambda^2}{L} \exp(-\Lambda^2 (k - k')^2 / 4),
\tag{24}
\]

where we have used the Gaussian integral in the evaluation of the part in the \( y \)-direction. In the case of a small correlation length, \( \Lambda \ll \lambda_F \), the transition matrix element has the form (see appendix C for details)

\[
\mathcal{T}_{nn'} = \frac{\pi^{3/2} \Lambda^2 \hbar v_F}{8W^6 E_F^2} \times \left[ \sum_\mu \mu^2 \left( 1 + \frac{k_{n,k_\mu}}{E_F} \right) \frac{k_{n',k_\mu}}{E_F} \delta_{nn'} - n^2 \frac{k_{n,k} k_{n',k}}{E_F^2} \right].
\tag{25}
\]

This results in a conductivity given by

\[
\sigma = \frac{16e^2}{3} \frac{W^5}{h} \pi^{3/2} \Lambda^2 \sum_{n,n'} k_{n,k} k_{n',k'} \times \left[ \mu^2 \sum_\mu \mu^2 \left( 1 + \frac{k_{n,k_\mu}}{E_F} \right) \frac{k_{n',k_\mu}}{E_F} \delta_{nn'} - n^2 \frac{k_{n,k} k_{n',k}}{E_F^2} \right]^{-1}.
\tag{26}
\]

Regarding the diagonal elements of the transition rate matrix, it is convenient to write the inverse of the relaxation time for the \( n \)th subband as

\[
\frac{1}{\tau_n} = \frac{\pi^{3/2}}{4W^6 E_F} \Lambda^2 \sum_\mu \mu^2 \left[ \frac{1}{E_F} + \frac{k_{n,k_\mu}/k_{n',k_\mu}}{E_F^2} \right].
\tag{27}
\]

For a large number of occupied subbands \( N \gg 1 \), the second term in the bracket can be neglected since \( k_{n,k} \ll E_F \), and the summation can be replaced by an integral. Equation (27) can then be written as

\[
\frac{1}{\tau_n} \approx \frac{\pi^{5/2}}{16W^3} \Lambda^2 v_F E_F n^2,
\tag{28}
\]

which shows a striking similarity to the corresponding results reported for semiconductor quantum wires [17]. Furthermore, this relaxation time results in a conductivity in the limit \( N \gg 1 \) of

\[
\sigma_{\text{Boltzmann}}(B = 0) \approx \frac{32e^2}{h} \frac{1}{3 \pi^{1/2}} \frac{W^2}{\Lambda^2 E_F}.
\tag{29}
\]

Up to now, we have looked at the transport with edge roughness in the absence of a magnetic field \( B \). We continue by including it and discuss its effects within the semiclassical picture. A weak magnetic field tends to homogenize the contributions of the occupied subbands to the overall conductivity and results in a reduction of the magnetoconductivity for cyclotron radii of \( r_c \approx W / E_F [17] \). This effect has been quantified numerically by quantum calculations of GNRs [14], while its experimental observation has been reported recently [16]. Here, the maximum reduction of the relaxation time \( \tau \) in a magnetic field can be roughly estimated by averaging over all occupied modes, resulting in

\[
\frac{1}{\tau(B > 0)} \approx \frac{\pi^{1/2}}{48W} \Lambda^2 v_F E_F.
\tag{30}
\]

Here, all modes enter with the same weight.

The minimum conductivity due to edge roughness located at \( B = B_{\text{min}} \) is then given by

\[
\sigma_{\text{Boltzmann}}(B_{\text{min}}) \approx \frac{48e^2}{h} \frac{1}{3 \pi^{1/2}} \frac{W}{\Lambda^2 E_F},
\tag{31}
\]

which again holds for \( N \gg 1 \).

3. Numerical results and discussion

In figure 1, the conductivity for Gaussian-type impurities according to equation (21) is shown as a function of the Fermi energy. Note that the one-dimensional conductivity is obtained by multiplying \( \sigma \) by \( W \). First of all, \( \sigma \) increases in a superlinear manner with \( E_F \), resembling the extended case [2, 3]. Furthermore, prominent conductivity oscillations are observed, i.e., the conductivity drops rapidly as a new scattering channel is opened and increases again until the Fermi energy hits the next subband at larger energies. As the temperature is increased, these oscillations get suppressed. The conductivity oscillations are smeared by nonzero temperatures. It should be noted that these oscillations are not related to quantum fluctuations and solely reflect the oscillating density of states at the Fermi level. Moreover, for different degrees of disorder, the conductivity shows very similar features, while the amplitude of the conductivity depends on the disorder parameters (not shown).

Figure 2 shows the conductivity of armchair GNRs with edge roughness as a function of the Fermi energy in the absence of bulk disorder, as calculated from equation (26).
Figure 1. The numerical conductivity of Gaussian-type impurities in armchair GNRs with $W = 180$ nm plotted versus the Fermi energy for two different temperatures $T$. The parameter values are $n_{\text{imp}} = 4 \times 10^{12}$ cm$^{-2}$, $\xi = 12a$ and $\delta = 0.01t$, where $t$ is the hopping energy.

Figure 2. The Boltzmann conductivity as a function of the Fermi energy for different edge roughnesses in armchair GNRs (bold solid lines). The dashed and solid lines correspond to zero temperature and a temperature of $T = 10$ K, respectively. The fine solid lines are calculated from equation (29) in the limit of $N \gg 1$.

Figure 3. The magnetoconductivity around the ERID as a function of the width for different Fermi energies at a finite temperature of $T = 10$ K. (Note the logarithmic scale.) The zero-field conductivity with $E_F = 200$ meV is also plotted at the top. The solid and dashed lines correspond to the results from equations (26) and (31) for $N \gg 1$, respectively.

The parameter values chosen for $\Lambda$ and $\Delta$ correspond to short-range defects, which, for instance, represent a few atoms being missing at the GNR edges without long-range correlations, as widely assumed in simulations of edge disorder [8, 32, 9, 14]. The correlation length chosen ensures that $\Lambda \ll \lambda_F$ over the whole range of Fermi energies. The Boltzmann conductivity at nonzero temperature (indicated by the solid lines) shows suppressed fluctuations in comparison with the zero-temperature cases (dashed lines). Hence, in the case of edge disorder, the overall conductivity decreases as the Fermi energy increases. Since $\Lambda$ and $\Delta$ increase relative to the Fermi wavelength as $E_F$ is increased, this behavior is similar to that found in conventional quantum wires [17, 19]. In the case of a large number of subbands, $N \gg 1$, the results from equation (29) (thin, black solid lines) exhibit the same overall trend and agree well with the exact solution while the oscillatory component is absent.

The Fermi energies in figures 1 and 2 correspond to the numbers of occupied subbands between 10 and 30. The sizes of the matrices to be inverted are therefore between $10 \times 10$ and $30 \times 30$. For smaller Fermi energies, i.e. a few occupied modes (not shown), $\sigma$ shows more prominent fluctuations and may deviate considerably from the asymptotic expressions. Moreover, it should be noted that our calculations based on the Boltzmann approach are valid for rather strong interband scattering. This is the case when the mean free path is considerably shorter than the length of the GNR.

We continue by estimating the conductivity of a GNR with edge roughness in a magnetic field with a strength close to the position of the ERID, i.e., $r_c \approx W$, which is modeled by a mode-independent scattering time (equation (30)). A more exact calculation would have to rely upon a calculation of the wavefunctions in magnetic fields, which can be obtained by solving the eigenvalue equation of the Dirac Hamiltonian with magnetic fields included [33, 34]. This, however, should have only a marginal effect and we limit ourselves to the qualitative properties of the system close to the ERID.

In figure 3, the conductivity at $T = 10$ K is shown for magnetic fields close to the ERID for different Fermi energies. The parameters for edge roughness are fixed to $\Lambda = 0.3$ nm and $\Delta = 6$ nm. For comparison, the corresponding conductivity in the absence of a magnetic field with $E_F = 200$ meV is plotted as well. The conductivity around the ERID increases linearly with the GNR width, in contrast to the parabolic dependence in the absence of a magnetic field. This linear relationship can be easily identified from equation (31) and is also illustrated by the dashed lines in figure 3. As a consequence, the ERID can be expected to be more pronounced in wider GNRs. This feature is in qualitative agreement with our previous quantum simulations [14].

These model calculations illustrate that edge roughness in GNRs generates characteristic dependences on the GNR
width and Fermi energy, which makes it qualitatively distinguishable from bulk disorder. Several conclusions regarding the observability of the ERID can be drawn. The ERID amplitude has been calculated and predicted to increase with the GNR width. The GNR length, on the other hand, is irrelevant in the present treatment since diffusive transport has been assumed. It has furthermore emerged that the characteristic edge-disorder-induced behavior requires a sufficiently low density of scattering centers in the bulk in order not to mask the scattering from edge roughness. Finally, we have restricted ourselves to the case of rather small correlation lengths for the edge roughness. It is self-evident that a large correlation length suppresses the ERID in view of the reduced diffusiveness of the scattering at the edges. We moreover expect that qualitatively the ERID does not depend much on the type of edges, even though numerical simulations suggest that zigzag GNRs are more robust with respect to edge disorder [14]. Similar analytical expressions for zigzag GNRs are possible in principle but more complicated, due to the presence of edge states and the interdependence of the transverse and longitudinal wavevectors.

According to the above analysis, GNR samples of low bulk disorder are indispensable for an observation of the ERID. On the other hand, in order to be diffusive, the GNR length should be much longer than the mean free path. We are not aware of any experiment carried out in the range of validity of our model. Very recently, however, Masubuchi et al [16] have reported the observation of an ERID in magnetoresistance measurements performed on GNRs deposited on top of boron nitride [35]. These authors investigated GNRs of length and width $L = 2.3 \, \mu m$, $W = 1.0 \, \mu m$ and $L = 3.1 \, \mu m$, $W = 1.5 \, \mu m$, respectively, at rather large Fermi energies around $E_F \approx 180$ meV. The edge roughness parameters of their ribbons were estimated from topographical pictures to be $\Delta \approx 2.5$ nm and a correlation length of the same order of magnitude [36].

The mean free path is comparable to the wire width, hence these GNRs are clearly not diffusive. Nevertheless, a discussion of these data in terms of our model does provide some insight. Figure 4 shows a magnetoresistance measurement on a GNR of $L = 3.1 \, \mu m$ and $W = 1.5 \, \mu m$ at a gate voltage of $V_g = -37$ V from [16], transformed to conductivity. Applying the technique described in [14], we have performed numerical simulations of the magnetoconductivity of GNRs with edge roughness based on the tight-binding model in combination with the recursive Green’s function technique, where the standard recursive technique is used to compute the total Green’s function related to the transmission amplitude. The perpendicular magnetic field is incorporated via the Peierls’ substitution. The edge disorder is modeled by removing atoms around the defect centers following the Gaussian-type shape [14]. A comparison of the experimental data with the numerical results in the absence of bulk disorder shows that the parameters for the edge roughness amplitude and correlation length give good agreement (figure 4). Also, the observation of the ERID position at $W/r_c \approx 0.8–1$ is well reproduced for the full interval of carrier densities in which the ERID has been observed (inset of figure 4). This ratio is larger than for conventional semiconductor wires and may be understood within a semiclassical argument as a consequence of the difference in the confinement potential. In graphene, the potential is hard wall and $r_c$ is independent of $x$. In a parabolic confinement potential, the local cyclotron radius decreases as the edge is approached, which results in a decreased average $r_c$ as compared to the bulk value, such that the ratio $W/r_c$ at the ERID minimum drops when the bulk value is used for $r_c$. It should be emphasized that in these model calculations the bulk scattering was set to zero, which is justified from the observation that the shape of the ERID structure depends only slightly on the bulk disorder, which generates an offset instead [14].

On the other hand, by comparing the experimental data ($\sigma(B) \approx 8.5$ mS, $\sigma(B_{\min}) = 120$ mT) with equations (29) and (31), we obtain values of $\Delta^2 \Delta \approx (60 \, \text{nm})^3$ and $\approx (14 \, \text{nm})^3$, respectively, which are unrealistically large. Besides the sample not being in the diffusive limit, an additional reason for this deviation may be that bulk scattering as well as other effects which reduce the conductivity like weak localization and a possible coupling resistance at the interface [37] between the two-dimensional graphene and the GNR are not included. This increases the apparent value of $\Delta^2 \Delta$. We note that both the 2D–quasi 1D interface resistance and the weak localization drop as $B$ is increased, which is consistent with a more realistic value of $\Delta^2 \Delta$ at $B_{\min}$.

In summary, we have studied the transport properties of armchair GNRs with bulk impurities and edge roughness within the framework given by the Boltzmann equation. An edge-roughness-induced magnetoconductivity minimum suggested by recent quantum calculations is confirmed by the Boltzmann results. The model suggests that for diffusive GNRs, the ERID should become more visible as the GNR width is increased. Furthermore, analytic expressions are derived for the conductivity at $B = 0$ and at the minimum.
of the ERID. In order to confirm the expressions derived quantitatively, the magnetoconductivity of GNRs with high bulk mobility and with a mean free path which is not only dominated by edge disorder but also short compared to the GNR length should be measured.

Acknowledgments

HX and TH acknowledge financial support from Heinrich-Heine-Universität Düsseldorf. The authors thank T Machida and S Masubuchi for making their experimental data available to us and for the permission to use them in this manuscript.

Appendix A. Derivation of equation (3)

The Dirac Hamiltonian, equation (1), including two different valleys \( K \) and \( K' \) can written as

\[
H = \hbar v_F \begin{pmatrix} \sigma \xi x + \sigma \xi y & 0 \\ 0 & -\sigma \xi x + \sigma \xi y \end{pmatrix}.
\]  

(A.1)

The eigenfunction of this Hamiltonian contains four components corresponding to the sublattices A and B from the two valleys, namely \( \Psi (r) = [\Psi_A(r), \Psi_B(r), \Psi'_A(r), \Psi'_B(r)]^T \). The total wavefunction containing the fast oscillations from the \( K \) and \( K' \) points is then of the form

\[
\Psi (r) = e^{iKx} \begin{pmatrix} \Psi_A(r) \\ \Psi_B(r) \end{pmatrix} + e^{iK'x} \begin{pmatrix} \Psi'_A(r) \\ \Psi'_B(r) \end{pmatrix}.
\]

(A.2)

To calculate the eigenfunctions of GNRs explicitly, we first use Dirac equation (1) for the \( K \) valley, which is given by

\[
\hbar v_F \begin{pmatrix} 0 & k_x - ik_y \\ k_x + ik_y & 0 \end{pmatrix} \begin{pmatrix} \Psi_A(r) \\ \Psi_B(r) \end{pmatrix} = \epsilon \begin{pmatrix} \Psi_A(r) \\ \Psi_B(r) \end{pmatrix}.
\]

(A.3)

where \( \Psi_A \) and \( \Psi_B \) are the scalar wavefunctions of the sublattices A and B, respectively. For GNRs with armchair edges along the y-direction, the translational symmetry guarantees that the spinor wavefunction can be further written as

\[
\begin{pmatrix} \Psi_A(r) \\ \Psi_B(r) \end{pmatrix} = e^{ik_y y} \begin{pmatrix} \phi_A(x) \\ \phi_B(x) \end{pmatrix},
\]

(A.4)

with quantized wavevectors \( k_n \) in the \( x \)-direction due to the boundary conditions. Substituting equation (A.4) into equation (A.3), we obtain the two linear differential equations

\[
\begin{align*}
-\imath(k_y + \partial_x) \phi_B(x) &= \bar{\epsilon} \phi_A(x), \\
\imath(k_y - \partial_x) \phi_A(x) &= \bar{\epsilon} \phi_B(x),
\end{align*}
\]

(A.5)

with \( \bar{\epsilon} = \epsilon / (\hbar v_F) \). Similarly, we obtain the two differential equations for the \( K' \) valley as

\[
\begin{align*}
-\imath(k_y - \partial_x) \phi'_B(x) &= \bar{\epsilon} \phi'_A(x), \\
\imath(k_y + \partial_x) \phi'_A(x) &= \bar{\epsilon} \phi'_B(x).
\end{align*}
\]

(A.6)

By applying the operator \((k_y \pm \partial_x)\) to the second equations in (A.5) and (A.6), respectively, we obtain

\[
(k_y^2 - \bar{\epsilon}^2) \phi_A(x) = \bar{\epsilon}^2 \phi_A(x).
\]

(A.7)

For the valleys \( K \) and \( K' \), the solutions of (A.7) have the form

\[
\begin{align*}
\phi_A(x) &= Ae^{ik_y x} + Be^{-ik_y x}, \\
\phi'_A(x) &= Ce^{ik_y x} + De^{-ik_y x}.
\end{align*}
\]

(A.8)

The boundary conditions require

\[
\begin{align*}
A + B + C + D &= 0, \\
Ae^{i(k_y + K)W} + Be^{-i(k_y - K)W} + Ce^{i(k_y - K)W} + De^{-i(k_y + K)W} &= 0.
\end{align*}
\]

(A.9)

We choose \( B = C = 0 \) and \( A = -D \). This leads to the quantized wavevectors of equation (2) and \( \bar{\epsilon} = \sqrt{k_x^2 + k_y^2} \). We have dropped the subscript of \( k_n \) in the main text. From the second equations in (A.5) and (A.6), we can determine \( \phi_B(x) \) and \( \phi'_B(x) \) from \( \phi_A(x) \) and \( \phi'_A(x) \), respectively. Finally, we arrive at the four-component wavefunction up to a normalization factor as

\[
\Psi (r) = \frac{e^{ik_y y}}{\sqrt{4WL}} \begin{pmatrix} e^{ik_x x} \\ k_n + ik \epsilon e^{ik_x x} \\ \frac{k_n + ik}{\bar{\epsilon}_n} e^{-ik_x x} \end{pmatrix},
\]

(A.10)

which is equal to equation (3). The first two components of equation (A.10) correspond to the contribution from the \( K \) point, while the last two components correspond to the contribution from the \( K' \) point. To fulfil the boundary conditions, the armchair GNRs mix states from the two Dirac points as expressed in equation (A.2). After inserting the surface values, the contributions from the two Dirac points cancel each other and the total wavefunction vanishes.

Appendix B. Derivation of equation (10)

The conductivity is defined as

\[
\sigma = j_y / E_y = -\frac{2e}{E_y WL} \sum_n \sum_k v_{nk} f_{nk},
\]

(B.1)

where \( W \) and \( L \) are the width and length of the system. \( E_y \) is the electric field and \( e \) is the electron charge. The factor of 2 accounts for the spin degeneracy. Inserting equation (6) into (B.1) and neglecting the equilibrium part, we obtain

\[
\sigma = \frac{2e^2}{WL} \sum_n \sum_k v_{nk}^2 \frac{\partial f_0^R(\epsilon_{nk})}{\partial \epsilon_{nk}} \tau_n(\epsilon_{nk}).
\]

(B.2)

After approximating the sum by an integral, i.e., \( \sum_k \rightarrow L/(2\pi) \int dk \), and a transformation of the wavevector integral to an energy integral, the conductivity at zero temperature can
be expressed as

\[ \sigma = \frac{2e^2}{h} \sum_n \int d\epsilon_n v_n \delta(\epsilon_n - E_F) \tau_n(\epsilon_n) \]  
\[ = 4e^2 \frac{1}{h} \sum_n v_n \tau_n(E_F) \]  
\[ = \frac{2e^2}{h} \frac{\hbar^2}{\pi E_F} \sum_{k,k'} \frac{k^2_F k^2_F'}{(T^{-1})_{nn'}} \]  
\[ = \frac{2e^2}{h} \frac{\hbar^2}{\pi E_F} \sum_{k,k'} \frac{k^2_F k^2_F'}{(T^{-1})_{nn'}} \]  
where we have used \( v_n = v_F k / \sqrt{k^2 + \mu^2 / \ell^2} \) and equation (8). This is equation (10) of the main text.

Appendix C. Derivations of equations (24) and (25)

We start with equation (23). Inserting the four-component wavefunction (12), some straightforward algebra gives us

\[ |\Xi_{n}\rangle^2 = |\Xi_{n}(x = 0)|^2 + |\Xi_{n}(x = W)|^2 \]  
\[ = \frac{2n^2\pi^4}{W^6} \frac{\langle \Delta(\epsilon_n) \rangle}{E_F} \left( 1 + \frac{k^2_n k^2_{n'}}{E_F k^2_{n'}} \right). \]  
where both boundaries contribute equally to the matrix element. For the term in the \( y \)-direction, one finds

\[ \left\langle \frac{1}{L} \int \frac{d\gamma}{L} \int \frac{d\gamma}{L} \int \frac{d\gamma}{L} \int \frac{d\gamma}{L} \right\rangle^{2} \]  
\[ = \frac{1}{L^2} \int_{0}^{L} dy_1 \int_{0}^{L} dy_2 \int_{0}^{L} dy_3 \int_{0}^{L} dy_4 \]  
\[ = \frac{\Delta^2}{L} e^{-\frac{\Delta^2}{L}} \int_{-\infty}^{\infty} dy e^{-\frac{\Delta^2}{L} + i u y + (\frac{\Delta^2}{L})^2} \]  
\[ = \frac{\Delta^2}{L} \Delta \sqrt{\pi} e^{-\frac{\Delta^2}{L}}, \]  
with \( q = k - k' \). Here, the Gaussian integral has been used. The extension of the integration range to \( \pm\infty \) is justified if the correlation length is much smaller than \( L \). We thus obtain

\[ |\langle n', k' | U | n, k \rangle|^2 = \frac{\pi^{3/2} n^2 \ell^2}{8W^6} \left( \frac{\langle \Delta(\epsilon_n) \rangle}{E_F} \right)^2 \times \left( 1 + \frac{k^2_n k^2_{n'}}{E_F k^2_{n'}} \right) \frac{\Delta^2}{L} e^{-\frac{\Delta^2}{L} + i u y + (\frac{\Delta^2}{L})^2} \]  
\[ = \frac{\pi^{3/2} n^2 \ell^2}{8W^6} \left( \frac{\langle \Delta(\epsilon_n) \rangle}{E_F} \right)^2 \times \left( 1 + \frac{k^2_n k^2_{n'}}{E_F k^2_{n'}} \right) \frac{\Delta^2}{L} e^{-\frac{\Delta^2}{L} + i u y + (\frac{\Delta^2}{L})^2} \]  
which is identical to equation (24) of the main text.

We proceed with the derivation of equation (25). The transition matrix element has the form

\[ \mathcal{T}_{nn'} = \frac{\pi \hbar^2 v_F}{L} \sum_{k,k'} \left| \langle n, k' | U | n, k \rangle \right|^2 \]  
\[ \times \frac{k^2_F}{\epsilon_{nk'}} \delta(\epsilon_{nk} - E_F) \delta(E_{kk'} - E_F) \]  
\[ - \left| \langle n', k' | U | n, k \rangle \right|^2 \frac{k^2_F}{\epsilon_{nk'}} \delta(\epsilon_{nk} - E_F) \delta(\epsilon_{nk'} - E_F) \]  
The first term in the bracket can be written as

\[ \frac{\pi \hbar^2 v_F}{L} \sum_{k,k'} \frac{k^2_F}{\epsilon_{nk'}} \delta(\epsilon_{nk} - E_F) \tau_n(\epsilon_n) \]  
\[ = \frac{4e^2}{h} \sum_n v_n \tau_n(E_F) \]  
\[ = \frac{2e^2}{h} \frac{\hbar^2}{\pi E_F} \sum_{k,k'} \frac{k^2_F k^2_F'}{(T^{-1})_{nn'}} \]  
\[ = \frac{2e^2}{h} \frac{\hbar^2}{\pi E_F} \sum_{k,k'} \frac{k^2_F k^2_F'}{(T^{-1})_{nn'}} \]  
where the summations over \( k \) and \( k' \) have been transformed into the corresponding integrals. It is convenient to convert the wavevector integral to an energy integral by using \( dk = \frac{dk}{h} \). The second term in the bracket can be reformulated as

\[ \frac{\pi \hbar^2 v_F}{L} \sum_{k,k'} \frac{k^2_F}{\epsilon_{nk'}} \delta(\epsilon_{nk} - E_F) \tau_n(\epsilon_n) \]  
\[ \times \delta(\epsilon_{nk} - E_F) \delta(\epsilon_{nk'} - E_F) \]  
\[ \times \frac{2n^2\pi^4}{W^6} \frac{\langle \Delta(\epsilon_n) \rangle}{E_F} \left( 1 + \frac{k^2_n k^2_{n'}}{E_F k^2_{n'}} \right) \frac{\Delta^2}{L} \]  
\[ \times \left[ \left( \begin{array}{c} \frac{k^2_F}{E_F} \delta(\epsilon_{nk} - E_F) \delta(\epsilon_{nk'} - E_F) \end{array} \right) \right] \]  
which corresponds to equation (25).

References

[1] Peres N M R 2010 Rev. Mod. Phys. 82 2673
[2] Sarma S D, Adam S, Hwang E H and Rosso E 2011 Rev. Mod. Phys. 83 407
[3] Xu H, Heinzl T and Zozoulenko I V 2011 Phys. Rev. B 84 115409
[4] Xu H, Heinzl T, Shylau A A and Zozoulenko I V 2010 Phys. Rev. B 82 115311
[5] Lewenkopf C H, Mucciolo E R and Castro Neto A H 2008 Phys. Rev. B 77 081410
[6] Xu H, Heinzl T, Evaldsson M and Zozoulenko I V 2008 Phys. Rev. B 77 245401
[7] Areshkin D A, Gunlycke D and White C T 2007 Nano Lett. 7 204
[8] Evaldsson M, Zozoulenko I V, Xu H and Heinzel T 2008 Phys. Rev. B 78 161407
[9] Xu H, Heinzel T and Zozoulenko I V 2009 Phys. Rev. B 80 045308
[10] Han M Y, Ozyilmaz B, Zhang Y and Kim P 2007 Phys. Rev. Lett. 98 206805
[11] Stamplec C, Guettinger J, Hellmueller S, Molitor F, Ensslin K and Ihn T 2009 Phys. Rev. Lett. 102 056403
[12] Liu X L, Oostinga J B, Morpurgo A F and Vandersypen L M K 2009 Phys. Rev. B 80 0121407
[13] Todd K, Chou H T, Amasha S and Goldhaber-Gordon D 2009 Nano Lett. 9 416
[14] Xu H, Heinzel T and Zozoulenko I V 2012 Europhys. Lett. 97 28008
[15] Thornton T J, Roukes M L, Scherer A and van de Gaag B P 1989 Phys. Rev. Lett. 63 2128
[16] Masubuchi S, Iguchi K, Yamaguchi T, Onuki M, Arai M, Watanabe K, Taniguchi T and Machida T 2012 Phys. Rev. Lett. 109 036601
[17] Akera H and Ando T 1991 Phys. Rev. B 43 11676
[18] Bruus H, Flensberg K and Smith H 1993 Phys. Rev. B 48 11144–55
[19] Feilhauer J and Moško M 2011 Phys. Rev. B 83 245328
[20] Huang D and Gumbs G 2010 J. Appl. Phys. 107 103710
[21] Huang D, Gumbs G and Roslyak O 2011 Phys. Rev. B 83 115405
[22] Neto A H C, Guinea F, Peres N M R, Novoselov K S and Geim A K 2009 Rev. Mod. Phys. 81 109
[23] Wurm J, Winmer M, Adagideli, Richter K and Baranger H U 2009 New J. Phys. 11 095022
[24] Ferreira A, Viana-Gomes J, Nilsson J, Mucciolo E R, Peres N M R and Castro Neto A H 2011 Phys. Rev. B 83 165402
[25] Adam S, Brouwer P W and Sarma S D 2009 Phys. Rev. B 79 201404
[26] Rycerz A, Tworzydlo J and Beenakker C W J 2007 Europhys. Lett. 79 57003
[27] Bardarson J H, Tworzydlo J, Brouwer P W and Beenakker C W J 2007 Phys. Rev. Lett. 99 106801
[28] Goodnick S M, Ferry D K, Wilmesen C W, Liliental Z, Fathy D and Krivanek O L 1985 Phys. Rev. B 32 8171–86
[29] Ferry D K and Goodnick S M 1997 Transport in Nanostructures 1st edn (Cambridge: Cambridge University Press)
[30] Peres N M R, Rodrigues J N B, Stauber T and dos Santos J M B L 2009 J. Phys.: Condens. Matter 21 344202
[31] Fang T, Konar A, Xing H and Jena D 2008 Phys. Rev. B 78 205403
[32] Mucciolo E R, Castro Neto A H and Lewenkopf C H 2009 Phys. Rev. B 79 075407
[33] Brey L and Fertig H A 2006 Phys. Rev. B 73 195408
[34] De Martino A, Hütten A and Egger R 2011 Phys. Rev. B 84 155420
[35] Dean C R, Young A F, Meric I, Lee C, Wang L, Sorgenfrei S, Watanabe K, Taniguchi T, Kim P, Shepard K L and Hone J 2010 Nature Nanotechnol. 5 722
[36] Masubuchi S and Machida T 2012 private communication
[37] Choi K K, Tsui D C and Palmateer S C 1986 Phys. Rev. B 33 8216