

Rough edges in quantum transport of Dirac particles

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We consider Dirac particles confined to a thin strip, e.g., graphene nanoribbon, with *rough* edges. The confinement is implemented by a large mass in the Hamiltonian or by imposing boundary conditions directly on the graphene wave-functions. The scattering of a rough edge leads to a transverse channel-mixing and provides crucial limitation to the quantum transport in narrow ribbons. We solve the problem perturbatively and find the edge scattering contribution to the conductivity, which can be measured experimentally. The case of Schrödinger particles in a strip is also addressed, and the comparison between Schrödinger and Dirac transport is made. Anomalies associated with quasi-one dimensionality, such as Van Hove singularities and localization, are discussed. The violation of the Matthiessen rule is pointed out.

Recent discovery of graphene [1, 2] has spurred much interest. The honeycomb structure of the graphene lattice implies that carbon orbitals are sp^2 hybridized, leaving one free (p_z) electron orbital per atom. Unlike the majority of systems in condensed matter physics, at low energies these electrons effectively obey Dirac equations of motion for massless fermions [3], with the Fermi velocity being the speed of light. Another example is a d-wave superconductor whose electrons behave relativistically in the vicinity of nodal points [4]. The “relativistic” character of graphene implies that its properties should be essentially different when compared to more traditional systems, whose electrons obey Schrödinger equation [5].

The central problem addressed in this Letter concerns transport properties of narrow graphene ribbons (strips). In general, the transport in thin and narrow structures is limited due to the restrictions imposed by quantum mechanics [6]. Classically, a beam of particles may be collimated as finely as desired so that it does not interact with the boundaries of a sample. As a consequence – in absence of ordinary impurity scattering – the mean free path of an electron is infinite, leading to vanishing resistivity. Due to the quantum mechanical uncertainty, however, a beam of particles must have a finite width: as the lateral dimensions of a sample shrink toward and below this width, the transport exhibits a crossover from the quasiclassical to the purely quantum regime, governed by boundary scattering [6]. This is true both for Schrödinger and Dirac particles. We expect our results to have broad implications for graphene based electronics.

We use the Kubo formalism [7] to derive the expression for the conductivity. Similar approach was used in Refs. [8, 9, 10, 11, 12], although these authors were interested in other issues. Alternatively, the conductivity can be derived from the dielectric function [13], or equivalently [14] from the Landauer formula [15, 16, 17, 18, 19, 20]. The quantum limitations to the transport properties of graphene strips with *smooth* edges were considered in Ref. [15]; obviously, this is a different problem, exploring *ballistic* transport, in contrast to the present paper, where the electrons are subject to a weak random scattering

(impurities, phonons, etc.), and have a *finite* mean free path. The transverse channel mixing due to rough edge scattering in graphene junctions was numerically examined in Ref. [20], however, this study too is centered on ballistic transport.

The confinement of Dirac fermions is a subtle issue due to the Klein paradox [21]. This problem can be circumvented by using a large mass term outside the strip in lieu of a static potential [22]. We employ this general method and refer to strips with such boundaries as the Dirac strips or ribbons. The boundary conditions in graphene are sensitive to the details of the edge [3], and can also be formulated on the microscopic level [23]. For definiteness, we consider the special case of a graphene strip with *metallic* armchair edges, i.e., armchair strips/ribbons. and assume the variations in its width do not change the metallicity at the boundary [3, 24]. The spectrum of metallic armchair strips is exceptional since it contains a band with zero transverse momentum. Consequently, the armchair strips are anomalously good conductors, especially in the vicinity of the Dirac point, where all the other boundary conditions yield a finite gap. At a finite chemical potential these differences subside but the aforementioned zero-band remains special as it does not get scattered from the edges [25]. Our boundary conditions assume “clean” edges, i.e., the dangling carbon bonds at the edges are inert and do not absorb environmental impurities that might cause the current redistribution [27] or localization of charge carriers [28].

The scattering matrix due to rough edges is [6]

$$\hat{V} \propto [\lambda(\hat{x})\{\hat{y}, \hat{p}_y\}, \hat{H}_y], \quad (1)$$

where x and y are the propagating and the transverse direction, respectively, \hat{H}_y is the transverse part of the Dirac Hamiltonian (straight edge), and $\lambda(x)$ parametrizes the width profile. In contrast to the Schrödinger case, the matrix Eq. (1) is *not* separable. The matrix elements for a single rough edge can be found in Ref. [29], and it appears that the only way to proceed requires inverting dense matrices of $n_c \times n_c$ size, with n_c being the number of transverse channels. To overcome

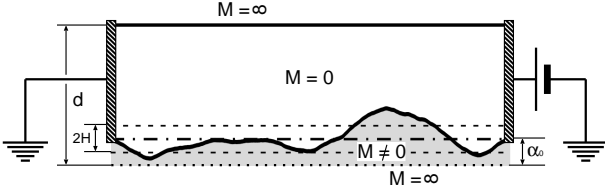


FIG. 1: A thin strip of width d , whose bottom edge is rough (the thick lines represent the physical edges). A buffer layer (light gray) with large, but finite mass is attached to the rough edge of the sample.

this sensitivity of the Dirac fermions to rough edges, we implement varying width boundary through an alternative construction, which mimics the confinement of the Dirac fermions. In place of an infinite mass jump at the edge, we allow the mass parameter to change in two steps. At the edge the mass becomes large but finite, followed by the infinite mass jump (Fig. 1). This buffer layer of variable width suppresses the wave-function outside the strip while it simultaneously allows us to recast the equivalent of the scattering matrix Eq. (1) in a *quasi-separable* form, amenable to analytic treatment.

The Letter is organized as follows: first, we consider Dirac states of a thin strip, and derive the Kubo formula for these Dirac states. The Kubo formula is tested on a case of a *smooth* finite-width strip, whose resistivity is needed in what follows. Next, the buffer layer is introduced and the corresponding matrix elements that mix transverse channels are found. The exact mass parameter appearing in the matrix elements is determined by demanding that the first-order perturbative corrections to the conductivity from a buffer layer with a straight edge are in agreement with the physical result. The effects of rough edges appear in the second-order perturbative corrections to the energy. This leads to our main result, the conductivity due to rough edge scattering. Finally, we find the conductivity of a thin strip whose electrons obey the Schrödinger equation [6]. The comparison is made between the conductivities of two identical strips, one containing Dirac, and the other Schrödinger particles.

The 4-component Dirac equation

$$(v \gamma_0 \boldsymbol{\gamma} \cdot \mathbf{p} - \mu) \Psi = \epsilon \Psi, \quad (2)$$

with $\gamma_0 = \text{diag}(\sigma_3, \sigma_3)$, $\gamma_1 = \text{diag}(-i\sigma_2, i\sigma_2)$, and $\gamma_2 = \text{diag}(i\sigma_1, i\sigma_1)$, has solutions in form of plane waves

$$\Psi_{km\xi,a}(\mathbf{r}) = e^{ikx} \left[u_{k,m,\xi,a}^{(+)} e^{iq_m y} + u_{k,m,\xi,a}^{(-)} e^{-iq_m y} \right]. \quad (3)$$

In our notation, k is the momentum in the propagating direction, and q_m is the transverse momentum. The boundary conditions discretize the latter, yielding $q_m = (m + 1/2)\pi/d$, and $q_m = m\pi/d$ in the case of a Dirac, and an armchair strip respectively. m is taken nonnegative. ξ is ± 1 corresponding to conductance and valence Dirac cones. The elements of spinors $u_{k,m,\xi,a}^{\pm}$ are determined through the boundary conditions [3] and the Dirac

equation Eq. (2). Index $a = 1, 2$ denotes two decoupled valleys for a Dirac strip, and two orthogonal states which admit the valleys for an armchair strip. The energy of state Eq. (3) is $\epsilon_{km\xi} = -\mu + \xi v \sqrt{k^2 + q_m^2}$, with μ being the chemical potential (equivalent to the gate voltage). The unperturbed propagator is given by $\mathcal{G}_{n\zeta b}^{m\xi a}(i\omega_n; k) = \mathcal{G}_{m\xi a}^{(0)}(i\omega_n; k) \delta_{mn} \delta_{\xi\zeta} \delta_{ab} = \delta_{mn} \delta_{\xi\zeta} \delta_{ab} / (i\omega_n - \epsilon_{km\xi})$.

The (longitudinal) current operator for a Dirac particle is $j_x(\mathbf{r}) = ev\Psi(\mathbf{r})^\dagger \gamma_0 \gamma_1 \Psi(\mathbf{r})$. Starting with the Kubo formula, and invoking the Lehmann representation for the propagators [7], we find the one-loop contribution to the dc conductivity for Dirac particles

$$\sigma_{dc} = \frac{e^2 v^2}{2\pi d} \int \mathfrak{d}k \sum_{m\zeta\xi ab} \sum_{n\eta\rho cd} \mathcal{A}_{m\zeta a}^{n\eta c}(0, k) \mathcal{A}_{n\eta d}^{m\xi b}(0, k) \times \frac{(k\sigma_3 + q_m\sigma_2)_{\zeta\xi} (k\sigma_3 + q_n\sigma_2)_{\eta\rho}}{\sqrt{(k^2 + q_m^2)(k^2 + q_n^2)}}. \quad (4)$$

Here, $\mathcal{A}_{n\zeta b}^{m\xi a}(E, k) = -2 \text{Im} \mathcal{G}_{n\zeta b}^{m\xi a}(E + i\delta; k)$ is the spectral function matrix.

The Kubo formula Eq. (4) reproduces the Dirac point conductivity, both the Gaussian [8] and the universal values [30], depending on the spectral function used. We use the Eq. (4) to find the conductivity of a straight strip of width d , where particles weakly scatter with an average lifetime $\tau = 1/(2\Gamma)$. A straightforward calculation yields

$$\sigma_0 = \frac{e^2}{2\pi} \frac{4v}{d\Gamma} \sum_m^* \sqrt{1 - Y_m^2}, \quad (5)$$

where $Y_m = vq_m/|\mu|$, and the star indicates summation over all m -s with $Y_m < 1$. When a strip is wide (or μ large), the conductivity converges to $\sigma = \frac{e^2}{2\pi} (\mu/\Gamma)$ regardless the edge type.

We now implement the confinement of the Dirac particles by means of a *finite* mass buffer layer. The basic idea is that in a lattice system, it suffices for the wave-function to fall-off faster than the lattice spacing to effectively prohibit hopping between the sites at the edge and their (non-existing) neighbours. Hence, mass M has to be large, and its precise value will be determined shortly. Since the buffer layer serves as an extension of the strip exterior, this mass should be of the same type as the infinite mass confining the fermions to the strip [31]. For a Dirac strip that is the *chiral* mass, and a buffer layer of variable width $\alpha(x)$ introduces a perturbation $\hat{V} = Mv^2\gamma_0$, for $0 \leq y \leq \alpha(x)$. The armchair boundary conditions are instead recreated via a $\gamma_3 = \begin{pmatrix} 0 & -i\sigma_2 \\ -i\sigma_2 & 0 \end{pmatrix}$ “mass term”; the buffer layer perturbation for this edge is $\hat{V} = Mv^2\gamma_0\gamma_3$. Using $t = -i\gamma_2$, the matrix elements to the leading order in α are

$$V_{km\xi b}^{ln\zeta a} = \frac{Mv^2}{4d} [\widetilde{\alpha(x)^2}]_{k-l} [(f_{ln\zeta a}^*)^\nu t_{\nu\mu} (f_{km\xi b})^\mu], \quad (6)$$

where summation over μ, ν is assumed, and $[\widetilde{\alpha(x)^2}]$ is the Fourier transform of $\alpha(x)^2$. Defining $z_{km\xi} = \xi(k + iq_m)/\sqrt{k^2 + q_m^2}$, we have $f_{km\xi 1}^D = (-iq_m(1 + z_{km\xi}), 1 - z_{km\xi}, 0, 0)^T$, and $f_{km\xi 2}^D = (0, 0, -iq_m(1 - z_{km\xi}^*), (1 + z_{km\xi}^*))^T$ for Dirac strips, while for armchair strips $f_{km\xi 1}^A = (-iq_m z_{km\xi}, 1, iq_m, z_{km\xi})^T$, and $f_{km\xi 2}^A = (f_{km\xi 1}^A)^*$. Importantly, the channel mixing matrix Eq. (6) is quasi-separable.

Now, consider a buffer layer of a uniform and small width α_0 . Both M and α_0 enter Eq. (6) as free parameters. It is, however, clear that the first order corrections to the conductivity will be proportional to $M\alpha_0^2$, while, according to Eq. (5), they should be proportional to α_0 . The conclusion is that the product $M\alpha_0$ has to be a well defined constant. This is rather natural: as the buffer layer shrinks, the suppression of the wave function, driven by the inverse mass, is enhanced. To find this constant, we recall that the change of the conductivity by an infinitesimally thin buffer layer should satisfy:

$$\delta\sigma = \sigma(d) - \sigma(d - \alpha) \approx \alpha d\sigma(d)/dd. \quad (7)$$

The right hand side of Eq. (7) follows from Eq. (5). The left hand side can be found from Dyson equation

$$\mathcal{G}_{m\xi b}^{n\zeta a} = \mathcal{G}_{n\zeta a}^{(0)} \delta_{nm} \delta_{\zeta\xi} \delta_{ab} + \mathcal{G}_{n\zeta a}^{(0)} (1 - V_{k\zeta a}^{kn\zeta a} \mathcal{G}_{spc}^{(0)})^{-1} V_{km\xi b}^{k\zeta a} \mathcal{G}_{m\xi b}^{(0)}, \quad (8)$$

where argument $(i\omega_n; k)$ is assumed. The self-energy following from Eq. (8) is real, yielding the “effective” dispersion $\epsilon'_{km\xi} = \epsilon_{km\xi} + \xi M v^2 \alpha_0^2 q_m^2 / (d\sqrt{k^2 + q_m^2})$ for both Dirac and armchair strips. The corrections to the conductivity caused by this dispersion are now substituted in (7), implying that the mass in (6) has the channel dependent form $M = 1/(v\alpha_0 Y_m Y_n)$. Thus, an infinitesimally thin buffer layer perturbatively – at the lowest order – reproduces the physical behavior expected from a layer of infinite mass. A *metallic* armchair ribbon needs special attention: the coupling for scattering into its *lowest* energy channel ($Y_0 = 0$) appears infinite, thus rendering the perturbative approach invalid. This is reflective of an anomalous character of such a state, stemming from special boundary conditions. Since this state is impervious to the mass term, we ask how it is affected by the change of the strip width *exactly*, i.e., we directly examine the matrix elements V_{0m} , Eq. (1). They all vanish and hereinafter we ignore the scattering to/from this channel.

We are now ready to find the second-order self-energy. Due to the quasi-separability of the scattering potential Eq. (6), we use the following ansatz $W_{n\zeta a, m\xi b}(i\omega_n; k) = (f_{kn\zeta a}^*)^\nu \hat{W}_{\nu\mu}(i\omega_n; k) (f_{km\xi b})^\mu$. The self energy and the

propagator equations are cast as

$$\begin{aligned} \hat{W}(i\omega_n; k) &= \left(\frac{Mv^2\alpha_0}{2d}\right)^2 \int d\mathbf{l} \langle \tilde{w}_{k-l} \tilde{w}_{l-k} \rangle \times \\ & t g^{(0)}(i\omega_n; l) [\hat{1} - \hat{W}(i\omega_n) g^{(0)}(i\omega_n; l)]^{-1} t, \\ \mathcal{G}_{m\xi b}^{n\zeta a} &= \mathcal{G}_{n\zeta a}^{(0)} \delta_{nm} \delta_{\zeta\xi} \delta_{ab} + \\ & \mathcal{G}_{n\zeta a}^{(0)} (f_{n\zeta a})^\dagger [\hat{1} - \hat{W} g^{(0)}]^{-1} \hat{W} (f_{m\xi b}) \mathcal{G}_{m\xi b}^{(0)}. \end{aligned} \quad (9)$$

The projected propagator is defined as

$$g^{(0)\nu\mu}(i\omega_n; k) = \sum_{m\xi a} (f_{km\xi a})^\nu \mathcal{G}_{m\xi a}^{(0)}(i\omega_n; k) (f_{km\xi a}^*)^\mu. \quad (11)$$

In (9), $w(x)$ is the deviation from the average buffer thickness α_0 . For simplicity, we assume the white noise edge profile characterized by $\langle w_k w_{-k} \rangle = aH^2$, where a is the lattice spacing, and H^2 measures the rms fluctuations in the strip width. Combining the self-energy from Eqs. (9, 10) and Kubo formula (4), yields the leading order conductivity expressed universally as

$$\begin{aligned} \sigma' &= \frac{e^2}{2\pi} \frac{4v^2 d}{\mu^2 a H^2} \sum_m^* \sqrt{1 - Y_m^2} \times \\ & \left\{ \sum_n^* \left(\frac{2 + \frac{1}{Y_m^2} + \frac{1}{Y_n^2}}{\sqrt{1 - Y_n^2}} - \sqrt{1 - Y_m^2} \left(\frac{1}{Y_n^2} + \frac{1}{Y_m^2} \right) \right) \right\}^{-1}. \end{aligned} \quad (12)$$

This is the main result of this Letter.

Unfortunately, the summation in Eq. (12) is difficult to carry out analytically and must instead be performed numerically for each μ and d . An example is plotted in Fig. 2a. Note sharp drops (to zero) of the conductivity each time a new channel is open. With μ at the bottom of a newly open band, the density of states experiences Van Hove singularity (absent in higher dimensions). As the number of states available for scattering increases, so does the self-energy, and the “effective” lifetime of excitations goes to zero. In Eq. (12), this corresponds to the situation when the highest Y_m is close to one.

For a wide strip, or large μ , one can estimate the asymptotic behavior of the maxima in the conductivity Eq. (12), i.e., its values just before the opening of a new channel. For a Dirac strip, the maxima converge to

$$\sigma_{max, D} \cong \frac{e^2}{2\pi} \frac{v^{11/4} d^{1/4}}{\mu^{11/4} a H^2} 4 \left(\frac{2\pi}{\pi - 2} \right)^{1/4}. \quad (13)$$

In the case of an armchair strip with the same width the result is $3^{3/4} \approx 2.28$ times larger. Although Fig. 2a shows approximately equal conductivity maxima at low chemical potential, as μ increases, so does the armchair strip become better conductor as compared to the Dirac strip. The conductivity converges slowly to Eq. (13), as shown in the inset of Fig. 2a.

For comparison, we consider the case of a strip with “Schrödinger” carriers. The Fermi energy is denoted

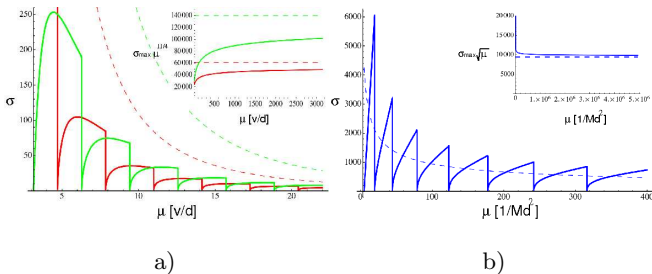


FIG. 2: The conductivities of a thin strip with a rough edge in units of e^2/h . We set $d = 1$, and $v = 1$ (Dirac, a), or $M = 1$ (Schrödinger, b). The roughness is $d^3/aH^2 = 10^4$. In all three cases, the Van Hove singularities appear; they are equidistant for Dirac particles, while their distance progressively grows in the Schrödinger case. The conductivity(ies) of the Dirac particles falls off considerably faster ($\mu^{-11/4}$) than that of the Schrödinger ones ($\mu^{-1/2}$). The inset shows the asymptotics: the dashed lines correspond to to Eqs. (13) and (15). The conductivity of an armchair strip (a; green) is on average greater by factor 2.28 than that of a Dirac strip (a; red).

by μ , the same as the chemical potential of the Dirac case. The dispersion in an unperturbed system is $\epsilon_{km} = -\mu + (k^2 + q_m^2)/(2M)$, M being the electron mass here. The formalism of Ref. [6] is readily adapted to a thin strip. Assuming the same parameters as before, the conductivity is

$$\sigma' = \frac{e^2}{2\pi} \frac{d}{aH^2 M \mu} \sum_m^* \frac{\sqrt{1 - Y_m^2}}{Y_m^2} \left\{ \sum_n^* \frac{Y_n^2}{\sqrt{1 - Y_n^2}} \right\}^{-1} \quad (14)$$

and is plotted in Fig. 2b. As in the previous case, $Y_m = q_m/\sqrt{2M\mu}$. Van Hove singularities are appearing here too; however, in contrast to the Dirac case, the singularities are not equidistant, and are instead distributed as squares of integers, due to the parabolic dispersion. The other qualitative difference is reflected in the asymptotic trend for the conductivity maxima. For wide strips, the conductivity peaks follow the envelope function

$$\sigma_{max,S} \cong \frac{e^2}{2\pi} \frac{4d^2}{3aH^2 \sqrt{2M\mu}}. \quad (15)$$

The conductivity has a sharp d^2 dependence (compare to d^3 for thin films [6]).

There is a notable qualitative difference between the asymptotic behaviors Eqs. (15) and (13). For a Schrödinger strip, the major contribution to the conductivity comes from the lowest bands, as these states scatter the least from rough edges. Accordingly, the sum in Eq. (15) is asymptotically proportional to the number of open channels, and the overall conductivity is proportional to $\mu^{-1/2}$. The Dirac states in the lowest bands are, on the other hand, the most susceptible to the edge scattering, and their contributions are largely suppressed. Hence, the conductivity Eq. (13) decreases rapidly ($\sim \mu^{-11/4}$) as the chemical potential increases. The high impact

of the edge scattering on the Dirac particles is also evident in the weak $d^{1/4}$ width dependence in Eq. (13). These peculiar power laws are the consequence of the conductivity-per-channel function in Eq. (12).

In quasi one-dimensional systems, one must be mindful of inevitable localization [32]. Its effects are discussed elsewhere [26]. Generally, one anticipates a certain localization length L for electrons. The results presented here should be valid for weak disorder, i.e. whenever the strip is shorter than L .

In thin films, the scattering from a rough surface yields a channel dependent mean free path, whereas the impurity scattering is channel independent, resulting in the violation of the Matthiessen rule [33]. In thin strips the situation is similar, the channel mean free path l'_m from Eq. (12) is not proportional to the impurity mean free path of a corresponding channel $l_m^0 = v\sqrt{1 - Y_m^2}/(d\Gamma k_F)$, Eq. (5), hence the Matthiessen rule is violated here, too.

In this Letter we have developed a perturbative approach to the problem of the edge scattering in Dirac strips. The particle confinement is implemented in the manner that allows us to solve the problem analytically. The conductivity is found to the leading order in the edge roughness. We also analyze thin strips with Schrödinger particles and compare the results to those for Dirac strips. In both cases, the conductivity develops Van Hove singularities; however, different dispersions mean that the singularities for Dirac particles are equidistant in the chemical potential, while those for the Schrödinger ones are not. The higher sensitivity of Dirac particles to the edge roughness suppresses the otherwise most conductive channels, and accordingly, the (average) conductivity fall off as a function of the chemical potential is much faster as compared to the Schrödinger case.

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