Spatial distribution of local currents of massless Dirac fermions in quantum transport through graphene nanoribbons

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Abstract – We employ the formalism of bond currents, expressed in terms of the nonequilibrium Green functions, to image the charge flow between two sites of the honeycomb lattice of graphene ribbons of few nanometers width. In sharp contrast to nonrelativistic electrons, current density profiles of quantum transport at energies close to the Dirac point in clean zigzag graphene nanoribbons (ZGNR) differ markedly from the profiles of charge density peaked at the edges due to zero-energy localized edge states. For transport through the lowest propagating mode induced by these edge states, edge vacancies do not affect current density peaked in the center of ZGNR. Furthermore, the long-range potential of a single impurity placed in the center of ZGNR acts to reduce local current around it while concurrently increasing the current density along the zigzag edge, so that ZGNR conductance remains perfect $G = 2e^2/h$.

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Introduction. – The recent experimental discovery of a two-dimensional (2D) allotrope of carbon, termed graphene, has ushered unforeseen avenues to explore transport and interactions of low-dimensional electron system, build quantum-coherent carbon-based nanoelectronic devices, and probe high-energy physics of “charged neutrinos” in table-top experiments [1,2]. Graphene represents one-atom–thick layer of carbon atoms tightly packed into a honeycomb crystal lattice whose symmetries impose linear energy-momentum dispersion of the low-energy quasiparticles [3]. Moreover, in the continuum limit sublattice degree of freedom can be regarded as an internal “pseudospin” degree of freedom which connects electrons and holes through “pseudochirality” (projection of pseudospin on the direction of motion) of opposite sign. Thus, the effective mass equation for graphene turns into the Weyl equation for massless Dirac fermions (familiar from neutrino physics) [3].

Relativistic energy spectrum, pseudospin, and zero gap with linearly vanishing density of states in the bulk graphene, have been probed in transport experiments unveiling the “chiral” quantum Hall effect, “minimal conductivity” at the charge-neutrality (Dirac) point $E_F = 0$, and weak-localization–type of quantum interference effects [1]. The intriguing concept of pseudochirality, whose conservation would be responsible for the suppression [3] of backscattering from smooth (on the scale of the lattice constant) disorder and Klein tunneling [2] through high and wide electrostatic potential barriers, has also led to a number of theoretical predictions [4] for esoteric micrometer-size graphene-based devices.

On the other hand, recent experiments on graphene wires of nanoscale width have demonstrated the existence of a gap in their energy spectrum [5], which would allow graphene nanoribbons (GNR) to replace semiconductor single-wall carbon nanotubes while making possible easy integration into nanoelectronic circuits via standard lithography and etching techniques. Direct STM imaging of the states localized at the edges of realistic GNR [6], as well as possible pseudochirality non-conserving scattering off the GNR edges, requires to examine the effects of the edge-topology–dependent transverse subband structure [7,8], the structure of edge states, impurities, and potential barriers in tailoring quantum transport properties of GNR-based devices.

The effects of zero-energy quantum states localized at the edges of ZGNR shown in fig. 1 (which originate from the gauge field generated by lattice deformation [9] and reflect the topological order in the bulk of bipartite honeycomb lattice [10]), as well as the energy gaps in armchair graphene nanoribbons (AGNR) controllable by their width, have been studied theoretically for more than a decade, both in equilibrium [11–13] and in conduction properties [7,8,14–18] of GNRs. However, very little is known about local features of charge transport through GNR. Moreover, the application of recently advanced...
scanning probe techniques (developed to image local charge flow in quantum transport through 2D electron gases buried inside semiconductor heterostructures [19]) to graphene samples is eagerly awaited [1]. Many interesting findings are anticipated [1] when 2D electron states exposed on graphene surface are directly accessed by tunneling and local probes. Also, such transport experiments, going beyond traditional measurements of macroscopically averaged quantities, are becoming increasingly important for the development of nanoelectronic devices. For example, recent imaging [20] of the charge flow in conventional $p-n$ junctions suggests that in structures shrunk below 50 nm individual positions of scarce dopants will affect their function, thereby requiring to know precisely how charge carriers propagate on the nanoscale.

In this letter we extend the bond current formalism for square lattices [21–23] to a graphene honeycomb lattice, which allows us to predict the spatial profiles of nonequilibrium charge and current densities. This imaging of charge flow provides direct insight into how massless Dirac fermions propagate between two neighboring lattice sites. The two-terminal device setup is shown in fig. 1 where the finite GNR sample is attached to two semi-infinite GNR leads. When the sample is clean, the whole structure represents infinite ZGNR (illustrated by fig. 1) or AGNR. The disordered sample is created by introducing vacancies at its edges or a short-range or long-range impurity potential within its interior. The whole structure is described by the tight-binding Hamiltonian

$$\hat{H} = - \sum_{\mathbf{m}\mathbf{m}'} t_{\mathbf{m}\mathbf{m}'} \hat{c}_{\mathbf{m}}^\dagger \hat{c}_{\mathbf{m}'} + \sum_{\mathbf{m}} V_{\mathbf{m}} \hat{c}_{\mathbf{m}}^\dagger \hat{c}_{\mathbf{m}},$$

with single $\pi$-orbital per site. Here $\hat{c}_{\mathbf{m}}$ creates (annihilates) an electron in the $\pi$-orbital at the site $\mathbf{m} = (m_x, m_y)$, and $t_{\mathbf{m}\mathbf{m}'} = \gamma_0 \approx 2.84$ eV is a hopping parameter between nearest-neighbor orbitals (which allows to reproduce the ab initio [24] computed structure of the conduction and valence bands in the vicinity of $K$ and $K'$ Dirac points located in two inequivalent corners of the hexagonal Brillouin zone where the bands touch conically). The impurity potential at site $\mathbf{m}$ is denoted by $V_{\mathbf{m}}$.

Bond current formalism on graphene honeycomb lattice. – The central quantity of the steady-state local transport formalism on tight-binding lattices is the nonequilibrium lesser Green function [25]

$$G_{\mathbf{m}\mathbf{m}'}^<(\tau = 0) = \frac{i}{\hbar} \langle \hat{c}_{\mathbf{m}}^\dagger \hat{c}_{\mathbf{m}'} \rangle = \frac{1}{\hbar} \int_{-\infty}^{\infty} dE G_{\mathbf{m}\mathbf{m}'}^<(E),$$

where $\langle \ldots \rangle$ is the nonequilibrium statistical average with respect to the density matrix at time $t' = 0$. It yields the magnitude of the bond current

$$J_{\mathbf{m}\mathbf{m}'} = \frac{2e}{\hbar} \int_{E_F - eV/2}^{E_F + eV/2} dE \left[ t_{\mathbf{m}\mathbf{m}'} G_{\mathbf{m}\mathbf{m}'}^<(E) - t_{\mathbf{m}'\mathbf{m}} G_{\mathbf{m}'\mathbf{m}}^<(E) \right],$$

between the lattice sites $\mathbf{m}$ and its nearest neighbor site $\mathbf{m}'$, and the nonequilibrium charge density at site $\mathbf{m}$

$$n_{\mathbf{m}} = \frac{e}{2\pi \hbar} \int_{E_F - eV/2}^{E_F + eV/2} dE G_{\mathbf{m}\mathbf{m}}^<(E).$$

These are the expectation values of the corresponding operators, $J_{\mathbf{m}\mathbf{m}'} = \langle \hat{J}_{\mathbf{m}\mathbf{m}'} \rangle$ and $n_{\mathbf{m}} = \langle \hat{N}_{\mathbf{m}} \rangle$, which satisfy the charge continuity equation on the lattice, $e dN_{\mathbf{m}}/dt + \sum_{\mathbf{m}'} (J_{\mathbf{m}\mathbf{m}'} - J_{\mathbf{m}'\mathbf{m}}) = 0$, where $\mathbf{m}'$ are the three nearest neighbor sublattice B sites of site $\mathbf{m}$ belonging to sublattice A, and vice versa. Thus, the bond current $J_{\mathbf{m}\mathbf{m}'}$ can be visualized as a bundle of flow lines bunched together along a link joining the two sites.

The connection between the bond current vector $J_{\mathbf{m}\mathbf{m}'}$, outflowing current $J_{\mathbf{m}\mathbf{m}}$ from site $\mathbf{m}$ and total current $I = \sum_{\mathbf{m}'} |J_{\mathbf{m}\mathbf{m}'}| = \sum_{\mathbf{m}'} |J_{\mathbf{m}'}\mathbf{m}|$ is illustrated by fig. 1(b). That is, when magnitudes of all vectors $J_{\mathbf{m}\mathbf{m}'}$ (where length of the arrow is proportional to local current) on the bonds connecting supercells in fig. 1(a) are summed up to get $I$, then $G = I/V$ gives the linear response conductance for small applied voltage bias $V = 0.001\gamma_0/e$. For zero-temperature quantum transport of electrons injected at the Fermi energy $E_F = 0.01\gamma_0$ there is only one open conducting channel, so that $G = I/V = 2e^2/h = G_Q$. 47001-p2
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(GQ is the conductance quantum) for spatial distribution of local currents within ZGNR of fig. 1(a).

The matrix $\mathbf{G}^<(E)$ contains information about the occupied states in the central region, and can be obtained by solving the Keldysh equation $\mathbf{G}^<(E) = \mathbf{G}^r(E) \Sigma^<(E) \mathbf{G}^a(E)$. In the single-particle approximation, where interactions are of the mean-field type, this equation can be solved exactly by evaluating the retarded $\mathbf{G}^r(E) = [\mathbf{E} - \mathbf{H} - \mathbf{U}_m - \Sigma^r(E)]^{-1}$ and the advanced $\mathbf{G}^a(E) = \mathbf{G}^r(E)^\dagger$ Green function matrices. In the absence of inelastic scattering, the retarded self-energies $\Sigma^r(E - eV/2)$ and $\Sigma^r(E + eV/2)$ introduced by the left and the right lead [26], respectively, determine $\Sigma^<(E) = -2i[\text{Im } \Sigma^r(E + eV/2) f_L(E - eV/2) + \text{Im } \Sigma^r(E + eV/2) f_R(E + eV/2)]$ [27]. The gauge invariance of $\Sigma^r$ depends explicitly on the applied bias voltage $V$, while $\mathbf{G}^r(E)$ has to include the electric potential landscape $U_m$ within the sample.

The key issue in the study of transport through nanodevices attached to graphene leads is an efficient algorithm to compute the retarded surface Green function at the terminating edge of the semi-infinite GNR. For this purpose we employ the Ando algorithm [27], which constructs this Green function from the left and right transverse propagating exact Bloch eigenmodes. The original algorithm [27] has to be generalized [28] to handle the non-invertible Hamiltonian $\mathbf{H}_1$ connecting supercells consisting of atoms described by the Hamiltonian $\mathbf{H}_0$ (see fig. 1 for illustration).

Imaging charge flow in clean GNRSs. – In ZGNRs localized edge states arise at energies close to the Fermi level $E_F = 0$ of undoped graphene. Thus, they manifest as edge peaks in the local density of states (DOS) $\rho(E, \mathbf{m}) = -\text{Im } G_{\mathbf{mm}}^r(E)/\pi$ in fig. 1 at $E = 0.01 \gamma_0$, as well as the peak in the total DOS $D(E) = \sum \rho(E, \mathbf{m})$ at $E = 0$ (in contrast to the bulk graphene where $D(E = 0) \equiv 0$ shown in the inset. They correspond to non-bonding molecular orbitals, where electrons are strongly localized near the zigzag edge composed on sublattice A sites (bottom) or sublattice B sites (top), and, therefore, cannot carry current. However, the overlap of two edge states from the top and bottom edge of a ZGNR yields bonding and anti-bonding states ensuring single conducting channel (with partially flat energy-momentum dispersion [7,8]) at energies arbitrarily close to the Dirac point. Therefore, ZGNR are metallic for all widths (as long as possible ferromagnetic ordering along the zigzag edges is not taken into account [12]). This channel, together with 2n right-moving propagating modes crossing the Fermi energy for $0 < |E_F| < \gamma_0$ yields odd-number conductance quantization $G(E_F) = (2n + 1)G_Q$ in clean ZGNR [14–16].

The Fermi energy of undoped GNR is at half-filling $E_F = 0$ due to perfect electron-hole symmetry. In narrow ZGNR the gap $\Delta_{12} \sim 1/N_z$ between the second subband and $E_F = 0$ is so large (e.g., $\Delta_{12} = 0.4 \gamma_0$ for $N_z = 10$) that transport would remain within the single channel regime $E_F < \Delta_{12}$ for presently achievable densities of extra carriers that can be injected into the ZGNR. Therefore, we focus on single-channel transport at $E_F = 0.01 \gamma_0$ with maximum conductance $G = G_Q$ in the rest of the paper, while also using multichannel transport ($E_F = 0.8 \gamma_0$) with maximum conductance $G = 5G_Q$ for comparison.

Figure 2 contrasts spatial profiles of $J_{\text{out}}$ and $n_m$ for single-channel transport through 10-ZGNR, 20-AGNR, and quantum wire modeled on a conventional square tight-binding lattice with 10 sites (hosting single s-orbitals) over its cross-section. Following previous convention, the width of $N_z$-ZGNR is measured by the number of zigzag chains $N_z$, while $N_a$-AGNR have $N_a$ dimer lines across the ribbon width [12]. In fig. 2, 10-ZGNR corresponds to 20-AGNR and square lattice wires with $N = 10$ sites per cross-section in the sense that all three quantum wires support maximum of 10 open conducting channels.

The charge density (fig. 2) of low-energy states is proportional to $n(y) \propto |\phi_A|^2 + |\phi_B|^2$, which in ZGNR (fig. 1) is peaked at its edges. On the other hand, the current density $j_z(y) \propto v(\Phi x, \sigma_x, \Phi)$ (where $\sigma_x$ is the Pauli matrix representing the $x$-component of the pseudospin operator acting on the AB space) of Dirac fermions, which are described in the low-energy (i.e., long-wavelength) limit by continuum theory for the two-component wave functions $\Phi = (\phi^+ \phi^-)$ (defining relative contribution of the A and B sublattice in the make-up of quasiparticles), reaches its maximum in the center of the ribbon. This,
together with the imaging of the local charge flow $J_m^{\text{out}}$ shown in fig. 3(a), explains why isolated edge vacancies have very little effect on the Landauer conductance $G \approx 0.98G_Q$ of single-channel transport through ZGNR [16]. When more channels are open for zero-temperature quantum transport, the vacancy affects not only the local current at the zigzag edge as in fig. 3(a), but also the magnitude and the direction of $J_m^{\text{out}}$ within the bulk of ZGNR in fig. 3(b), so that its conductance drops from $G \approx 5G_Q$ (when the vacancy is absent) to $G \approx 4G_Q$.

In contrast to ZGNR, spatial profiles of charge and current density in AGNR are highly inhomogeneous in both single and multichannel transport regimes. It is also instructive to compare $n_m$ vs. $J_m^{\text{out}}$ profiles in GNRs with those of non-relativistic electrons in quantum wires defined on the square lattice (third column in fig. 2). Their scalar wave function $\phi(x, y) = \phi_{\text{trans}}(y)e^{ikx}$ yields the charge density $n(y) \propto |\phi(y)|^2$ which has the same profile as the corresponding current density $j_\phi(y) = e\phi_\phi\phi^* - \phi^*\phi_\phi \propto kn(y)$.

**Imaging charge flow in GNRs with a single impurity.** – In the recent intense efforts to understand the experimentally observed properties of the conductivity of bulk graphene (such as its linear dependence on carrier concentration; minimal value $\sim e^2/h$ at the Dirac point; and absence of weak antilocalization, expected due to pseudochiral nature of electrons in graphene, or suppression of standard weak localization corrections [1,2]), the analysis of the scattering problem of massless Dirac fermions from different types of impurities has played an essential role [29]. In particular, even a single impurity can generate unusual transport effects in graphene [30], where the exceptional sensitivity required to detect a single absorbed molecule due to the change of graphene resistivity has recently been demonstrated experimentally [31].

The quantum scattering theory of free particles in infinite space is a textbook subject, which has been recently scrutinized for massless Dirac fermions in infinite 2D space [2,32]. However, it has been known since the advent of mesoscopic semiconductor structures that scattering from a single impurity in a quasi–one-dimensional electron gas (Q1DEG), which represents a quantum wire realized using two-dimensional electron gas and split gates, requires special treatment due to the fact that asymptotic scattering states have to satisfy different boundary conditions and symmetries imposed by semi-infinite leads [33,34].

Since the energy-momentum dispersion $\varepsilon(k_x)$ of transverse propagating modes in GNRs strongly depends on the confinement effects and topology of their edges, the investigation of the disorder effects in transport properties of mesoscopic graphene structures requires to re-examine the conditions for the absence of backscattering due to conservation of pseudochirality [3]. For example, it has been argued recently [7] that the large momentum difference between two valleys [8] of GNRs at $k_x = 2\pi/3a$ and $k_x = -2\pi/3a$ (which originate from the Dirac points $K$ and $K'$ of bulk graphene) prevents inter-valley scattering by long-range disorder, so that the special conducting channel generated by the edges states remains a “chiral” propagating mode in the sense that ZGNR has perfect conductance $G(E_F) = 2e^2/h$ for $|E_F| < \Delta_{12}$ that does not decay as the length of the wire is increased [7]. This special channel is comprised of states belonging to only one valley (unlike higher-energy modes where both valleys contribute), switching to the opposite one when changing the direction of propagation and allowing for the valley filter devices [8]. The Landauer-formula-computed conductance does decay exponentially due to Anderson localization in the single or multichannel transport regimes when the impurity potential is short-ranged [7].

To develop a real-space local picture of transport through this special conducting channel of GNRs, we employ the Gaussian potential $V_m = U\exp(-|m - m_0|/d^2)$ of range $d$ centered at site $m_0$ that belongs to either sublattice A or B. Such single Gaussian potential can model an impurity within the wire or the effect of a tunable central gate [34]. The potential strength $U_0$ is defined by the normalization condition [7], $\sum_m U_0\exp(-|m - m_0|/d^2) = U_0$. The conductance of ZGNR as a function of $U_0$ for both short-range $d = 0.05a$ (i.e., Anderson-model-type of disorder) and long-range $d = 1.5a$ potential (which is short-ranged on the scale of the system size but varies smoothly on the atomic scale, corresponding to, e.g., screened charges in the substrate) is shown in fig. 4(a) in the single-channel ($E_F = 0.01\gamma_0$) and multichannel ($E_F = 0.8\gamma_0$) quantum-coherent transport regime. For long-range impurities, the
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Fig. 4: (a) The Landauer conductance of ZGNR with single impurity positioned in the center of the ribbon to generate short-range $d = 0.05a$ or long-range $d = 1.5a$ Gaussian potential as a function of the impurity potential strength. The electrons are injected from ZGNR lead through a single conducting channel ($E_F = 0.01\gamma_0$) in the main panel and through five conducting channels ($E_F = 0.8\gamma_0$) in the inset. The corresponding conductances for single channel and multi-channel (inset) electron transport through ZGNR within the nonrelativistic ($|E_F| > \gamma_0$) ladder regime (where conductance quantization of ballistic system is the same as in Q1DEG wires) or Q1DEG modeled by the square lattice are shown in panels (b) and (c), respectively.

The conductance remains perfect $G = 2e^2/h$ up to $U_0 \sim 0.2\gamma_0$ (and $G \approx 1.99e^2/h$ up to $U_0 \sim 8\gamma_0$), which is comparable to the energy difference between the transverse subbands.

The single-channel transport can also occur outside of the “Dirac ladder” [$G = (2n + 1)G_Q$ for $|E_F| < \gamma_0$] in conductance quantization for Fermi energies close to the bottom of the valence band or to the top of the conduction band. Although these regimes are experimentally inaccessible, they can be used for comparison — their single-channel conductance in fig.

Fig. 5: (Color online) The difference $J^{\text{out}}_{\text{m}}(\text{disorder}) - J^{\text{out}}_{\text{m}}(\text{clean})$ between the local currents at each site of a clean 10-ZGNR and the same ZGNR with disorder introduced as a single impurity positioned on the sublattice A or sublattice B site in its center. The Gaussian impurity potential of strength $U_0 = 5.0\gamma_0$ is short-range in (a) $d = 0.05a$ and long-range in (b) $d = 1.5a$. The value of the corresponding conductances of single-channel ($E_F = 0.01\gamma_0$) and five-channel ($E_F = 0.8\gamma_0$) quantum transport is marked by arrows in fig. 4 and its inset, respectively.
in the next higher-energy subband [33]. Unlike ZGNR, the dips are, therefore, absent for the repulsive potential $U_0 > 0$ on the square lattice wire, as shown in fig. 4(c).

The images of local charge flow through ZGNR corresponding to the conductance in fig. 4(a) are shown in fig. 5 by plotting the difference between local currents at each corresponding to the conductance in fig. 4(a) areshowninfig.5(b). Moreover, the edge being exploited by massless Dirac fermions to resist current degradation consists of the same sublattice sites as is the site on which the impurity is located.

Conclusions. – We have shown how to adapt the bond current formalism to a graphene honeycomb lattice, which makes it possible to predict spatial profiles of local currents of massless Dirac fermions between two sites of the lattice. The predicted current profiles for graphene nanoribbons suggest several interesting experiments that are within the reach of the present local probe-based direct charge imaging techniques [19]: i) in ZGNR with localized edge states the large part of current flows through the center of the ribbon which makes single-channel quantum transport largely insensitive to edge vacancies; ii) while both short-range and long-range impurities reduce current density within the region of their influence, in the single-channel transport (through the lowest transverse propagating mode generated by the edge states of ZGNR around the Dirac point) this reduction in the case of long-range impurities can be compensated by the increase of current density along the zigzag edge which ensures the perfectly conducting channel $G = 2e^2/h$ even in the presence of a potential barrier in the nanoribbon center.

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