Conductance quantization in graphene nanoconstrictions with mesoscopically smooth but atomically stepped boundaries

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We present the results of million-atom electronic quantum transport calculations for graphene nanoconstrictions with edges that are smooth apart from atomic-scale steps. We find conductances quantized in integer multiples of $2e^2/h$ and a plateau at $\sim 0.5 \times 2e^2/h$ as in recent experiments [N. Tombros et al., Nat. Phys. 7, 697 (2011)]. We demonstrate that, surprisingly, conductances quantized in integer multiples of $2e^2/h$ occur even for strongly nonadiabatic electron backscattering at the stepped edges that lowers the conductance by one or more conductance quanta below the adiabatic value. We also show that conductance plateaus near $0.5 \times 2e^2/h$ can occur as a result of electron backscattering at stepped edges even in the absence of electron-electron interactions.

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Electrical conductances quantized in integer multiples of the fundamental quantum $2e^2/h$ are the hallmark of ballistic quantum transport in nanostructures such as semiconductor quantum point contacts,1,2 gold atomic wires,3 and carbon nanotubes.4 These quantized conductances are explained theoretically in terms of the Landauer theory of transport.5 However, in the case of graphene nanostructures, quantum transport calculations have shown the conductance quantization to be easily destroyed by disorder6–14 that is ubiquitous in these systems or by abrupt bends in the quantum wire geometry.15 Accordingly, there have been only a few reports16–18 of conductance quantization being observed experimentally in graphene nanostructures: Lin et al.16 and Lian et al.17 demonstrated conductance quantization experimentally in graphene nanoribbons. However, the conductance steps that they observed were a few orders of magnitude smaller than the ballistic conductance quantum $2e^2/h$. This phenomenon16,17 has been explained theoretically,19,20 as arising from strong electron backscattering at the edges of the electronic subbands of the ribbons due to the presence of random defects. More recently, Tombros et al.18 have reported the experimental observation of conductance quantization in integer multiples of $2e^2/h$, as well as a fractional conductance plateau at $\sim 0.6 \times 2e^2/h$, in a graphene nanoconstriction (GNC) at zero magnetic field. To minimize the effects of disorder on transport in their device, Tombros et al.18 studied a short suspended GNC whose width was similar to its length and estimated to be $\sim 300$ nm. Their sample was annealed by Joule heating, which resulted in the constriction being formed with curved boundaries that were smooth on the mesoscopic length scale of $\sim 100$ nm. The atomic-scale structure of the boundaries was not determined experimentally, however, the curvature of the constriction’s boundaries implies the presence of large numbers of atomic-scale steps (and possibly also other defects) along the boundaries. In this respect the GNC of Tombros et al.18 differs from the well-known semiconductor quantum point contacts (SQPCs),1,2 where the transverse electron confinement is achieved electrostatically and thus the constriction boundaries are effectively smooth on the atomic scale as well as on the much larger (submicrometer) length scale of the overall dimensions of the constriction. In the limit of extremely slow spatial variation of the confining potential, electrons are adiabatically transmitted through the SQPC or adiabatically reflected. As was pointed out by Glazman et al.,21 such adiabatic transport results in quantized conductances; each electronic subband that is adiabatically transmitted through the narrowest part of the SQPC at the Fermi energy contributes a quantum $2e^2/h$ to the measured conductance. If the confining potential of the SQPC varies smoothly but not adiabatically, conductance quantization may still occur, each electronic subband transmitted through the narrowest part of the SQPC at the Fermi energy again contributing a quantum $2e^2/h$ to the total conductance.22 However, to the best of our knowledge, to date there have been no theoretical studies of conductance quantization in constrictions with boundaries exhibiting large-scale smoothness but atomic-scale steps, as in the GNC of Tombros et al.18. For this reason a definitive understanding of the conductance quantization in integer multiples of $2e^2/h$ observed by Tombros et al.18 has been lacking. Furthermore, it has also been unclear whether the conductance plateau observed by Tombros et al.18 at $\sim 0.6 \times 2e^2/h$ was the result of electron-electron interactions (as is widely believed of the $0.7 \times 2e^2/h$ plateau in SQPCs23,24) or whether it can be accounted for instead by strong single-electron scattering at steps in the constriction’s boundaries.

In this Rapid Communication we report the results of quantum transport calculations that address these issues. We consider a noninteracting electron tight-binding model of graphene constrictions having similar dimensions to the GNC of Tombros et al.18 and having boundaries that are smooth on the length scale of the constriction but with large numbers of steps on the atomic scale.25 We show that this model exhibits integer and fractional conductance plateaus similar to those that were observed experimentally.18 Our results depend qualitatively on both the width of the constriction and its orientation. For the armchair orientation, the calculated integer quantized conductances of the constrictions have smaller integer values than those of uniform armchair graphene ribbons with the same width as the narrowest part of the constriction. This differs qualitatively from the well-known behavior of SQPCs where the adiabatic and nonadiabatic quantized conductance values are equal to those of a uniform quantum wire whose width equals that of the narrowest part of the constriction.21,22 We find plateaus with conductance values $\sim 0.5 \times 2e^2/h$ as...
well as the integer plateaus. For the zigzag orientation the
calculated integer quantized conductances of the constrictions
are either the same as or lower than those of uniform ribbons
of the same width as the constriction. We also find integer
and fractional quantized conductances for constrictions whose
narrowest parts are neither zigzag nor armchair.

We describe GNCs by the standard tight-binding Hamilto-
nian on a honeycomb lattice,

$$H = \sum_i \epsilon_i a_i^\dagger a_i - \sum_{i,j} t_{ij} (a_i^\dagger a_j + H.c.),$$  \hspace{1cm} (1)$$
where $\epsilon_i$ is the on-site energy and $t_{ij} = t = 2.7$ eV is the
matrix element between nearest-neighbor atoms. This Hamiltonian
is known to describe the $\pi$-band dispersion of graphene well
at low energies.\textsuperscript{26} Spin and electron interaction effects
are outside of the scope of our study. The nanoconstriction and
any random edge disorder and bulk vacancies that are present
are introduced by removing carbon atoms from a uniform
ribbon and setting appropriate hopping elements $t_{ij}$ to zero. It
is assumed that atoms at the edges are always attached to two
other carbon atoms and all dangling bonds are passivated by a
neutral chemical ligand, such as hydrogen, so that the bonding
between the carbon atoms at the edge and around vacancies
is similar to that in bulk graphene. Random bulk and edge
disorders (when present) are characterized by the probability
of the carbon atoms being removed, $p^b$ and $p^e$, respectively.$p^b$ is normalized relative to the whole sample, while $p^e$ is
defined relative to an edge only. The long-range potential due
to charged impurities is approximated by a Gaussian form\textsuperscript{9,11}
of range $d$: $\epsilon_i = \sum_n V_0 \exp(-|r_i - r_n|^2/d^2)$, where both the
amplitude $V_0$ and coordinate $r_n$ are generated randomly.

In the linear response regime the conductance of the GNC
is given by the Landauer formula\textsuperscript{5}

$$G = \frac{2e^2}{h} \sum_{ji} T_{ji},$$  \hspace{1cm} (2)$$
$T_{ji}$ is the transmission coefficient from subband $i$ in the left
lead to the subband $j$ in the right lead, at the Fermi energy. $T_{ji}$
is calculated by the recursive Green’s function method—see
Ref. 27 for details. The average conductance ($G$) for samples
with random disorder was calculated by averaging over an
ensemble of samples with different realizations of the disorder.
For the results presented below, averaging was carried out over
ten realizations for each disorder type.

To investigate the transport properties of GNCs we chose
graphical geometries similar to those studied experimentally.\textsuperscript{18}
The shape of the constriction was modeled by a cosine function
so that its edges were smooth apart from atomic-scale steps.
The width of the narrowest part of the GNC was varied in the
range $W = 150 \ldots 250$ nm. The GNC was attached at its two
ends to semi-infinite leads represented by ideal nanoribbons
of width $W_{\text{lead}} = 300$ nm. This guarantees that for any $W$
the leads supply more states for propagation than can pass
through the narrowest part of the constriction. The region of
the constriction itself in our tight-binding quantum transport
calculations included up to $\sim 1500000$ carbon atoms. In our
modeling of the effects of random disorder we assumed it to
be present only in a finite region of width $300$ nm and length
$L = 300$ nm; the semi-infinite leads were free from disorder.

The calculated conductances of GNCs with different
constriction widths $W$ are shown in Fig. 1(a) for the armchair
orientation of the graphene host and edges of the ideal leads.
Note, however, that the edge orientation along most of the
constriction itself is neither armchair nor zigzag; see the
inset in Fig. 1. The conductance shows faint quantization
steps in integer multiples of $2e^2/h$, similar to those observed
experimentally by Tombros et al.\textsuperscript{18} For better visualization
we plot the energy derivative of the conductance $dG/dE$ in
Fig. 1(b). Here a dip in $dG/dE$ indicates a plateau in the
conductance. The prominent dips in $dG/dE$ in Fig. 1(b)
cluster around conductance values that are integer multiples
of $2e^2/h$, including both odd and even integer multiples.
The conductance of the GNC decreases as constriction becomes
narrower, a feature expected theoretically and observed\textsuperscript{2,3}
in conventional semiconductor quantum point contacts: As the
constriction width shrinks, the number of propagating states
for a given Fermi energy decreases. Interestingly, although the
conductance plateaus occur near integer multiples of $2e^2/h$, in
each case the integer has a smaller value than that for the
ideal infinite ribbon of uniform width whose width equals the
width $W$ of the narrowest part of the constriction, for the same
electron Fermi energy, calculated with the same tight-binding
approach. This can be seen by comparing the conductances of
the GNC’s in Fig. 1(a) with those of the corresponding uniform
ideal ribbons\textsuperscript{28,29} that are shown as the dotted lines of the
same color in Fig. 1(a). We also found no correlation between
the calculated GNC conductances and the semiconductor or
metallic property of uniform ideal armchair ribbons. These
findings show that the conductance quantization that we find
for the armchair-oriented host and leads is not due to adiabatic
transmission of individual eigenmodes of the ideal leads
through the constriction, but that additional scattering along
the constriction edges plays an important role.

For $W = 200$ nm, we find an additional conductance step at $\sim 0.5 \times 2e^2/h$ [see Fig. 1(b) and the inset of Fig. 1(a)]. This
agrees with the experimental findings in Ref. 18. Whether or
not this feature is present in the results of our quantum transport
calculations depends on the width $W$ of the constriction; note
that experiments have been reported for only a single sample.\textsuperscript{18}
However, as can be seen in Fig. 1, this fractional plateau
coexists with integer conductance plateaus at higher electron
Fermi energies for the same GNC and occurs for both electron
and hole transport (not shown), as in the experimental data.\textsuperscript{18}

Our results for GNCs with the zigzag orientation\textsuperscript{30,31} of
the graphene host and edges of the leads are shown in Fig. 2.
A comparison of Figs. 1 and 2 reveals significant differences
between quantized conductance plateaus in GNCs with the
host and leads in the zigzag and armchair orientations: For the
zigzag orientation the quantized conductance plateaus are
more pronounced than for the armchair case. Also for the
zigzag case the calculated values of the quantized
conductances of the GNCs in many (but not all) cases are
close to the values of the quantized conductances of ideal
uniform zigzag ribbons having the same width as the narrowest
part of the GNC and the same electron Fermi energy. By
contrast, as we have already mentioned, all of the integer
quantized GNC conductances for the armchair case are smaller
than those of the corresponding uniform ideal ribbons by
integer multiples of $2e^2/h$. Thus in many cases nonadiabatic
plateaus. In the dashed rectangle whose width equals that of the leads black solid line shows the conductance of a 300-nm-wide ribbon, GNCs whose conductances are plotted in the same colors. The armchair ribbons of the same widths as the narrowest parts of the leads is armchair. The dotted lines show conductances of uniform on the atomic scale. Host and edge orientation of the semi-infinite shape follows the cosine function and is smooth apart from steps only. Temperature $T$ energy derivative $dG/dE$. The dips in $dG/dE$ indicate conductance plateaus. In the dashed rectangle $dG/dE$ is shown for $W = 200$ nm only. Temperature $T = 0$, $t = 2.7$ eV. The subband spacing is an order of magnitude larger than $k_BT$ even at 4.2 K as in Ref. 18.

electron backscattering is much weaker for GNCs in the zigzag orientation than for those in the armchair orientation. This difference may be attributed to the current densities being much lower near zigzag graphene edges than near armchair edges, so that the conductances are less affected by edge imperfections for zigzag ribbons.

The open red squares in Fig. 3 show the calculated conductance of an asymmetric GNC with the armchair orientation of the host and leads. As shown in the inset, the geometry in this case is similar to the $W = 200$ nm armchair-oriented constriction in Fig. 1 except that the upper and lower regions where the carbon atoms have been removed are now offset from each other laterally by 80 nm. Thus the edges of the narrowest part of the constriction have neither the armchair nor the zigzag orientation. We find that the electron backscattering is somewhat stronger (the conductance lower) in this case than for the symmetric $W = 200$ nm armchair-oriented constriction in Fig. 1; the calculated conductance for the latter is replotted as the solid black squares in Fig. 3 for comparison. However the first few quantized conductance plateaus (as well as the plateau at $\sim 0.5 \times 2e^2/h$) are still clearly visible for the asymmetric GNC.

The effects of disorder of different types are shown in Fig. 4. As a test system we chose a GNC of width $W = 200$ nm having the armchair orientation. The effect of disorder on the conductance of the GNC is similar to that for graphene nanoribbons. However, the conductance quantization is strongly degraded for every disorder type, including bulk vacancies. This may be attributed to the varying width of the GNC along the transport direction that precludes the existence of well-defined subband edges for the whole structure. We find each type of disorder to suppress the conductance and to result in universal conductance fluctuations.

In conclusion, we have carried out million-atom electronic quantum transport calculations for graphene nanoconstrictions with boundaries that are smooth except for steps on the atomic scale and have dimensions similar to those of the graphene nanoconstrictions that have been found to exhibit conductances quantized in integer multiples of $2e^2/h$ in recent experiments. Our results demonstrate quantized conductances similar to those observed experimentally in a tight-binding model with noninteracting electrons. We find...
FIG. 4. (Color online) (a) Effect of different disorder types on the conductance of armchair-oriented GNCs. (b) Conductance averaged over ten realizations of disorder. Constriction width \( W = 200 \) nm. The red line with filled circles is for edge disorder with \( p^e = 0.2 \). The blue line with filled squares is for bulk vacancy disorder with \( p^b = 10^{-5} \). The green line with rhombuses is for long-range potentials due to charged impurities with effective parameters \( |V| \leq 0.2t, \rho = 5 \times 10^{15} \text{ m}^{-2}, d = 10a \). The black solid line shows the conductance for an ideal, uniform ribbon 300 nm wide, and is given as a reference.

Conductances quantized in integer multiples of \( 2e^2/h \) to occur in graphene nanoconstrictions, even in the presence of strong electron backscattering, at the stepped constriction edges that depresses the quantized conductance values by \( \text{one or more} \ 2e^2/h \) conductance quanta below the quantized conductance values of uniform graphene ribbons with the same width and electron Fermi energy as those of the narrowest part of the constriction. This integer conductance quantization in the presence of such strong backscattering has no known analog in either adiabatic or nonadiabatic semiconductor quantum point contacts. It may explain why, based on their transport measurements, Tombros \textit{et al.}\cite{tombros} estimated the width of their GNC to be smaller (200–275 vs 300 nm) at zero magnetic field than at higher magnetic fields where electron backscattering at the edges of the constriction is reduced.\cite{tombros} We also find that conductance plateaus at \( \sim 0.5 \times 2e^2/h \) need not be the result of electron-electron interactions in these systems, but can result instead from nonadiabatic backscattering of electrons at atomically stepped constriction boundaries. However, the plateau observed experimentally at \( \sim 0.6 \times 2e^2/h \) by Tombros \textit{et al.}\cite{tombros} resembles the plateau that is seen at \( \sim 0.7 \times 2e^2/h \) in SQPCs and is attributed to electron-electron interactions,\cite{tombros} in part because in SQPCs the potentials are smooth and there is no analog of the atomic steps present at the edges of GNCs. Therefore, further experimental studies are required to clarify whether electron-electron interactions or boundary scattering are primarily responsible for the fractional plateau observed by Tombros \textit{et al.}\cite{tombros} in the GNC. Our results (see Fig. 1) suggest that systematic experimental studies of GNCs having differing widths may answer this question. Our quantum transport calculations also show random defects to strongly degrade the conductance quantization in graphene nanoconstrictions.

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24See also the special section on the 0.7 feature and interactions in one-dimensional systems, edited by M. Pepper and J. Bird, J. Phys. Condens. Matter 20, 160301–164217 (2008).