Magnetic barriers in graphene nanoribbons: Theoretical study of transport properties

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A theoretical study of the transport properties of zigzag and armchair graphene nanoribbons with a magnetic barrier on top is presented. The magnetic barrier modifies the energy spectrum of the nanoribbons locally, which results in an energy shift of the conductance steps towards higher energies. The magnetic barrier also induces Fabry – Pérot type oscillations, provided the edges of the barrier are sufficiently sharp. The lowest propagating state present in zigzag and metallic armchair nanoribbons prevent confinement of the charge carriers by the magnetic barrier. Disordered edges in nanoribbons tend to localize the lowest propagating state, which get delocalized in the magnetic barrier region. Thus, in sharp contrast to the case of two-dimensional graphene, the charge carriers in graphene nanoribbons cannot be confined by magnetic barriers. We also present a novel method based on the Green’s function technique for the calculation of the magnetosubband structure, Bloch states and magnetoconductance of the graphene nanoribbons in a perpendicular magnetic field. Utilization of this method greatly facilitates the conductance calculations, because, in contrast to excising methods, the present method does not require self-consistent calculations for the surface Green’s function.

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I. INTRODUCTION

The single planar sheet with carbon atoms densely packed in a honeycomb structure forms the so-called graphene, which demonstrates a variety of unique electronic transport properties and has the potential applications in the future nanoelectronics\[2\]. Theoretical studies have indicated that the special lattice structure of the graphene results in nearly linear dispersion relations around the K points (Dirac points) of the Brillouin zone\[3\]. This unique band structure is responsible for the distinct electronic properties of the graphene. Near the Dirac point, electrons manifest themselves the massless chiral fermions and can be described by the Dirac equation\[2,4,5\]. The electronic transport behaviors of the two-dimensional graphene subjected to an electrostatic potential or a magnetic barrier (MB) were studied on the basis of the Dirac equation, which indicate that the Dirac fermions can be transmitted perfectly through a classically forbidden region while confined effectively by the magnetic barrier. Moreover, the anomalous integer and fractional quantum Hall effects in two-dimensional graphene have been studied experimentally and theoretically by various groups\[6,7,8,9,10\].

The rolled-up graphene is known as the single-wall carbon nanotube whose electronic properties have been studied extensively in the past decades. The quantized conductance and Fabry – Pérot interference pattern were observed experimentally and interpreted by various theoretical approaches\[11\]. The other interesting effects including Coulomb blockade\[12\] and Kondo effects\[13\], and the electronic transport in ballistic\[14\] and disordered nanotubes\[15\] were studied. Another related carbon-based structure is the graphene nanoribbon (GNR), referred to the quasi-one-dimensional graphene with a finite width \(W\). Recent development of the experimental technique enable one to fabricate very narrow GNRs with ultrasmooth edges of the width \(W \leq 10\) nm\[16\]. The electrons propagate in such narrow systems very differently compared with the two-dimensional graphene where the edges are totally irrelevant. In graphene ribbons, the transport properties are strongly influenced by their edges along the transport direction which are distinguished into two types: zigzag and armchair. For armchair case, it is particularly interesting that the graphene ribbons may be metallic or semiconducting depending on their widths. There is a lot of theoretical effort devoted to the studies of the quantum transport in graphene ribbons. The conductance quantization in mesoscopic graphene\[10\] and coherent transport in graphene nanoconstrictions with or without defects\[17\] were reported recently.

The purpose of the present paper is twofold. First, we explore a possibility to control electron conductance of graphene nanoribbons with the help of magnetic barriers. MBs in the conventional quantum wires (QWRs) have been the subject of theoretical and experimental studies, which are driven by the MB’s potential ability of parametric spin filtering. The pioneering theoretical research by Peeters et al.\[18\] indicated that the magnetic barrier possesses the wave-vector filtering properties in QWRs and further work in graphene was also suggested\[1\]. Furthermore, recent theoretical studies have revealed further rich phenomenology of magnetic barriers in quantum wires, such as Fano-type resonances\[19\] and...
spin filtering. In two-dimensional graphene, theoretical work has shown the strong effects of the magnetic barrier on the direction-dependent transmission. Our studies will focus on the magnetic barrier effects on the quasi-one-dimensional GNRs.

Second, we present a detailed description of a novel method based on the Green’s function technique for the calculation of the magnetosubband structure, Bloch states and magnetoconductance of the graphene nanoribbons in a perpendicular magnetic field. Note that magnetoconductance calculations for the graphene nanoribbons based on the Green’s function technique has been reported previously. However, a distinct feature of the present method is a novel approach to calculation of the surface Green’s function $\Gamma$ for semi-infinite nanoribbons. In contrast to the Green’s functions for finite structures that can be easily calculated by adding slice by slice in a recursive way with the help of the Dyson’s equation, the calculation of the surface Green’s function of a semi-infinite structure represents a non-trivial problem. Such calculations are typically done self-consistently which makes conductance calculations very time-consuming. In the present paper we present a different method of computing $\Gamma$ which does not require self-consistent calculations. Instead, the surface Green’s function is expressed via the Bloch states of the graphene nanoribbons which in turn are simply obtained as solutions of the eigenvalue equation of the dimension $2N \times 2N$ (with $N$ being the width of the nanoribbon). Utilization of this method greatly facilitates the conductance calculations, making the present method far more efficient in comparison to the existing ones. Programming codes for calculation of the magnetosubband structure, the surface Green's function and the magnetoconductance based on the developed method are freely available in the AIP EPAPS electronic depository.

This paper is organized as follows: In Sec. II we sketch the geometry of the devices and briefly introduce the model for the conductance for our calculations. In Sec. III, we describe the tight-binding model for the graphene, theory of the Green’s function method, as well as the formalism for the computation of surface Green’s functions. This is followed by the presentation and discussion of the numerical results in Sec. IV. Summary and conclusion constitute the Sec. V.

II. FORMULATION OF THE PROBLEM

The geometries under consideration for graphene nanoribbons with zigzag and armchair edges are illustrated in Fig. 1(b) and (c), respectively, where the left and right leads are made of semi-infinite graphene. The nanoribbons are subjected to a magnetic barrier whose shapes may be rectangular or smooth as shown in Fig. 1(a) with zero magnetic field in leads. (Note however that the theory presented in the next section is not restricted to the case of zero field in the leads). The magnetic barrier represents a strongly localized magnetic field that is oriented perpendicular to the surface of the ribbon. Magnetic barriers with amplitudes up to 1 T have been realized experimentally by ferromagnetic films on top of a graphene sheet: magnetizing the ferromagnetic film in the transport direction results in a magnetic fringe field with a perpendicular component localized at the edge of the film that extends along the transverse direction. Alternatively, magnetic barrier formation has been demonstrated by placing two-dimensional electron gases with a step in an external magnetic field an approach which conceptually allows much larger barrier amplitudes. Both concepts should be in principle adaptable to graphene nanoribbons.

We model the leads and the device in the middle by the standard tight-binding Hamiltonian on the honeycomb lattice, see below, Eq. [3]. The conductance $G$ can be calculated using the Landauer-Büttiker formalism which gives the conductance of the system in terms of the electron transmission coefficient $T$, expressed as

$$G = \frac{2e^2}{h} \int dE \ T(E) \frac{\partial f_{FD}(E - E_F)}{\partial E},$$

(1)
We define the Bloch states in the infinite periodic graphene ribbons,

\[ |\psi\rangle = \sum_{i,j} \psi_{i,j} a_{i,j}^\dagger |0\rangle, \quad \psi_{i,j} = e^{ikx_i} \varphi_{i,j}, \]  

where \( a_{i,j}^\dagger \) (\( a_{i,j} \)) is a standard creation (annihilation) operator on the site \((i, j)\); \( \psi_{i,j} \) is the amplitude of the wave function on the site \((i, j)\); \( x_i \) is the coordinate of the \(i\)-th slice, \( k\) is the Bloch wave vector in the direction of the translational invariance \( x\), and the summation runs over all sites of the graphene lattice (see Fig. 2). Note that this form of the wave function does not distinguish between sublattices A and B of the graphene lattice. An explicit distinction between these sublattices is not necessary when using the Green’s function technique, where, instead, it is more convenient to define the wave function on slices of the lattice (see Sec. IIIB).

The standard tight-binding Hamiltonian has the form

\[ H = \sum_r V_r a_r^\dagger a_r - \sum_{r,\Delta} t_{r,r+\Delta} a_r^\dagger a_{r+\Delta}, \]  

where \( V_r \) describes the electrostatic potential on the site \( r = i, j \) and summation in the second term is performed over all available nearest neighbors with \( t_{r,r+\Delta} \) being the nearest-neighbor hopping integral. In the absence of a magnetic field the nearest-neighbor hopping integral is \( t_{r,r+\Delta} = t_0 \approx 2.7 \text{ eV} \). In the presence of an external perpendicular magnetic field \( B \) the hopping integral acquires the Peierls phase factor, \( t_{r,r+\Delta} = t_0 \exp(i\theta_{r,r+\Delta}) \), where \( \theta_{r,r+\Delta} = 2\pi \phi_{r,r+\Delta}/\phi_0 \), with \( \phi_{r,r+\Delta} \) being the line integral of the vector potential \( A \) from site \( r \) to a neighboring site \( r + \Delta \),

\[ \phi_{r,r+\Delta} = \int_r^{r+\Delta} A \cdot dl \]  

and \( \phi_0 = h/e \) is the flux quantum (in our calculations we use the Landau gauge, \( A = (-By, 0) \)). (In calculation of hopping integral \( 11 \) we use the carbon-carbon bond length \( a = 0.142 \text{ nm} \), see Appendix). Note that the Hamiltonian operator \( H \) is convenient to write down in the form

\[ H = \sum_i [h_i] + U, \]  

where \( h_i \) describes the Hamiltonian of the \( i\)-th slice, and \( U \) describes hopping between all neighboring slices (explicit forms of \( h_i \) and \( U \) can be easily obtained from Eq. (3)).

The Green’s function of the operator \( H \) is defined in a standard way\( 27,28 \),

\[ (E - H + i\varepsilon) G = I \]  

where \( I \) is the unitary operator.

**B. Bloch states and velocities in the graphene nanoribbons.**

We continue by describing a method for calculation of the Bloch states and their group velocities in the zigzag and armchair graphene nanoribbons in the presence of a perpendicular magnetic field. The method is based on the technique developed for calculation of the band structure of a mesoscopic antidot lattice in confined geometries\( 29 \) and has been used for calculation of the Bloch states in photonic structures\( 30 \) and in the interacting quantum wires in the integer quantum Hall regime\( 31 \).

Consider an infinite ideal graphene ribbon with \( N \) sites in the transverse \( j\)-direction, Fig. 2. A unit cell of the structure consists of \( M \) slices, where \( M = 2 \) for the zigzag graphene and \( M = 4 \) for the armchair graphene.
The Hamiltonian of an ideal infinitely long graphene ribbon can be written in the form
\[ H = H_{\text{cell}} + H_{\text{out}} + U, \tag{7} \]
where the operators \( H_{\text{cell}} \) and \( H_{\text{out}} \) describe respectively the unit under consideration \( (1 \leq i \leq M) \), and the outside region including all other slices \( -\infty < i \leq 0 \) and \( M + 1 \leq i < \infty \), and \( U \) is the hopping operator between the cell and slices \( i = 0 \) and \( i = M + 1 \) (an explicit form for these operators can be easily obtained from Eq. \( \text{(3)} \)). We write the total wave function, Eq. \( \text{(4)} \), in the form
\[ |\psi\rangle = |\psi_{\text{cell}}\rangle + |\psi_{\text{out}}\rangle, \tag{8} \]
where \( |\psi_{\text{cell}}\rangle \) and \( |\psi_{\text{out}}\rangle \) are respectively wave functions in the cell and in the outside region. Substituting Eqs. \( \text{(17)} \), \( \text{(23)} \) into the Schrödinger equation \( H|\psi\rangle = E|\psi\rangle \) and using the definition of the Green’s function, Eq. \( \text{(6)} \), we obtain \( |\psi_{\text{cell}}\rangle = G_{\text{cell}}U|\psi_{\text{out}}\rangle \), where \( G_{\text{cell}} \) is the Green’s function of the operator \( H_{\text{cell}} \). Taking the matrix elements of the wave functions in the real space representations, \( \psi_{i,j} = \langle 0_{a_{i,j}}|\psi \rangle \) for the first \( (i = 1) \) and the last \( (i = M) \) slices of the unit cell, this equation can be written in the matrix form,
\[ \begin{pmatrix} \psi_1 \\ \vdots \\ \psi_M \end{pmatrix} = G_{\text{cell}}^{11} U_{1,0} \begin{pmatrix} \psi_0 \\ \vdots \\ \psi_{M-1} \end{pmatrix}, \tag{9} \]
where \( \psi_i \) is the vector column describing the wave function for the slice \( i \),
\[ \psi_i = (\psi_{i,1}; \ldots; \psi_{i,N})^T \tag{10} \]
and \( U_{1,0} \) and \( G_{\text{cell}}^{i,i'} \) denote the matrixes with the matrix elements
\[ (U_{1,0})_{jj'} = \langle 0_{a_{1,j}}|U|0_{a_{1,j'}}\rangle, \tag{11} \]
\[ (G_{\text{cell}}^{i,i'})_{jj'} = \langle 0_{a_{i,j}}|G_{\text{cell}}|0_{a_{i',j'}}\rangle. \]
Explicit expressions for the matrix elements of the matrix \( U \) are given in the Appendix. In the derivation of Eq. \( \text{(9)} \) we used \( U_{M,M+1} = U_{0,1} \) (because of the periodicity of the ribbons) and \( U_{0,1} = U_{1,0}^+ \) (‘+’ stands for Hermitian conjugate).

It is convenient to rewrite Eq. \( \text{(9)} \) in a compact form
\[ T_1 \begin{pmatrix} \psi_{M+1} \\ \psi_M \end{pmatrix} = T_2 \begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix}, \tag{12} \]
with \( I \) being the unitary matrix. The wave function of the periodic structure has the Bloch form,
\[ \psi_{m+M} = e^{ikM} I \psi_m. \tag{13} \]
Combining Eqs. \( \text{(12)} \) and \( \text{(13)} \), we arrive at the eigenequation,
\[ T_1^{-1} T_2 \begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix} = e^{ikM} \begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix}, \tag{14} \]
determining the set of Bloch eigenvectors \( k_\alpha \) and eigenfunctions \( \psi_\alpha \), \( 1 \leq \alpha \leq N \). It should be stressed that this eigenequation provides a set of the Bloch states \( \{k_\alpha\} \) for a fixed energy \( E \), which includes both propagating and evanescent states. The latter can be easily identified by a non-zero imaginary part.

In order to separate right- and left-propagating states, \( k_1^+ \) and \( k_1^- \), we compute the group velocities of the Bloch states \( v_\alpha = \frac{\partial E}{\partial k} \), whose signs determine the direction of propagation (‘+’ stands for the right-propagating and ‘−’ for the left propagating states). The group velocities can be computed directly by numerical differentiation of the dispersion relation. This is however not an efficient approach because for each energy the eigensolver gives eigenstates \( \alpha \) in different order. We instead derive below a simple formula which gives the group velocities of the Bloch states based on the eigenfunctions of Eq. \( \text{(14)} \).

Consider a unit cell of an infinite graphene nanoribbon consisting of \( M \) slices. The wavefunction of the \( \alpha \)-th Bloch state \( |\varphi_\alpha \rangle \) can be conveniently rewritten in the form
\[ |\psi_i\rangle = e^{ikx}|\varphi_i\rangle \tag{15} \]
where \( |\psi_i\rangle \) is the wave function for the \( i \)-th slice.

[To simplify our notations we have dropped the Bloch index \( \alpha \).] Starting from the Schrödinger equation and calculating the matrix element of the Hamiltonian of the unit cell, we obtain for each slice \( i \), \( \langle \psi_i|H|\psi_i\rangle = E|\psi_i\rangle = E|\varphi_i\rangle \). Performing summation over all slices of the unit cell and using a definition of the group velocity, we obtain
\[ v = \frac{\partial E}{\partial k} = \frac{1}{M} \sum_{i=1}^M \frac{\partial}{\partial k} \left[ \frac{\langle \psi_i|H|\psi_i\rangle}{|\psi_i|^2} \right], \tag{16} \]
where the summation is performed over all slices \( i \) of the unit cell, and
\[ \varphi_\alpha = (\varphi_{\alpha,1}; \ldots; \varphi_{\alpha,N})^T, \tag{17} \]

is a vector composed of the matrix elements \( \varphi_{ij} = \langle 0_{a_{i,j}}|\varphi \rangle \). (Note that according to Eq. \( \text{(10)} \) and \( \text{(15)} \), vectors \( \varphi_i \) can be obtained from \( \psi_i \) via the relation \( \psi_i = e^{ikx}|\varphi_i\rangle \).)

Representing the Hamiltonian of the unit cell in the form \( \text{(14)} \), the matrix elements \( \langle \psi_i|H|\psi_i\rangle \) can be easily evaluated, which gives
\[ v = \frac{-i}{M} \sum_{i=1}^M \frac{\varphi_i^T}{|\varphi_i|^2} \left[ (x_i - x_{i-1}) U_{i,i-1} \varphi_{i-1} e^{-ik(x_i-x_{i-1})} \right. \]
\[ - (x_{i+1} - x_i) U_{i+1,i} \varphi_{i+1} e^{-ik(x_{i+1}-x_i)} \left. \right], \tag{18} \]
where the matrixes \( U_{i,j} \) are defined by Eq. \( \text{(11)} \) [explicit expressions for these matrix elements are given in the Appendix].
C. Surface Greens function $\Gamma$.

Here, we describe an efficient method for calculation of the surface Green’s function $\Gamma$ in the magnetic field.\(^{27,28}\) Note that most of the methods for calculation of the Green’s function reported to date require searching for a self-consistent solution for $\Gamma$ which makes these calculation very time consuming.\(^{27,28}\) In contrast, our method does not require self-consistent calculations, and the surface Greens function is simply given by multiplication of matrices composed of the Bloch states of the graphene lattice (see below, Eqs. \((21),(22)\)). The calculations described in this section are based on the method developed in Ref.\(^{26}\) for periodic photonic crystals which is adapted here for the case of the graphene nanoribbons.

Consider a semi-infinite periodic ideal graphene ribbon extended to the right in the region $-m \leq i < \infty$. Suppose that an excitation $|s\rangle$ is applied to its surface slice $i = -m$. Introducing the Green’s function of the semi-infinite ribbon, $G_{\text{rib}}$, one can write down the response to the excitation $|s\rangle$ in a standard form\(^{27}\)

\[
|\psi\rangle = G_{\text{rib}}|s\rangle,
\]

where $|\psi\rangle$ is the wave function that has to satisfy the Bloch condition\(^{2}\). Consider a unit cell of a graphene lattice, $1 \leq i \leq M$ ($M = 2$ and $4$ for the zigzag and armchair lattices, see Fig. \(2\)). Applying Dyson’s equation between the slices $0$ and $1$ we obtain

\[
G_{\text{rib}}^{1,-m} = \Gamma L U_{1,0} \delta_{r,0}^{1,-m},
\]

where $\Gamma L \equiv G_{\text{rib}}^{1,1}$ is the right surface Green’s function (i.e. the surface function of the semiinfinite ribbon open to the right), and the definition of the matrices $U$ and $G$ in the real space representation are given by Eq. \((11)\). Evaluating the matrix elements $\langle \alpha | a_{j} | \psi \rangle$ of Eq. \((11)\) and making use of Eq. \((20)\), we obtain for each Bloch state $\alpha$, $\psi_{\alpha}^{r} = \Gamma_{L} U_{1,0} \phi_{\alpha}^{0}$. The latter equations can be used for determination of $\Gamma_{L}$,

\[
\Gamma_{L} U_{1,0} = \Psi_{L} \Psi_{0}^{-1},
\]

where $\Psi_{L}$ and $\Psi_{0}$ are the square matrices composed of the matrix-columns $\psi_{\alpha}^{r}$ and $\psi_{\alpha}^{0}$, $1 \leq \alpha \leq N$, Eq. \((14)\), i.e. $\Psi_{L} = (\psi_{1}^{r}, ..., \psi_{N}^{r})$; $\Psi_{0} = (\psi_{1}^{0}, ..., \psi_{N}^{0})$. The expression for the left surface Greens function $\Gamma_{L}$ (i.e. the surface function of the semiinfinite ribbon open to the right) is derived in a similar fashion,

\[
\Gamma_{L} U_{1,0}^{+} = \Psi_{M} \Psi_{M+1}^{-1},
\]

where the matrices $\Psi_{M}$ and $\Psi_{M+1}$ are defined in a similar way as $\Psi_{L}$ and $\Psi_{0}$ above. Note that matrices $\Psi_{M}$ and $\Psi_{M+1}$ can be easily obtained from $\Psi_{L}$ and $\Psi_{0}$ using the relation \((12)\). Note also that when the magnetic field is restricted to zero, the right and left surface Greens functions are identical, $\Gamma_{L} = \Gamma_{R}$.

D. Magnetococonductance of the graphene nanoribbons

In order to calculate the transmission coefficient $T(E)$ we divide the structure into three regions, two ideal semi-infinite leads of the width $N$ extending in the regions $i \leq 0$ and $i \geq L$ respectively, and the central device region (where scattering occurs), see Fig. \(1\). We assume that the left and right leads are identical. The incoming, transmitted and reflected states in the leads, $|\psi_{\alpha}^{L}\rangle$, $|\psi_{\alpha}^{R}\rangle$ and $|\psi_{\alpha}^{T}\rangle$, have the Bloch form\(^{2}\),

\[
|\psi_{\alpha}^{L}\rangle = \sum_{i \leq 0} e^{ik_{x}x_{i}} \phi_{i,j}^{\alpha} a_{i,j}^{+}|0\rangle
\]

(23)

\[
|\psi_{\alpha}^{R}\rangle = \sum_{i \geq L} e^{ik_{x}x_{i}} \phi_{i,j}^{\alpha} a_{i,j}^{+}|0\rangle
\]

(24)

\[
|\psi_{\alpha}^{T}\rangle = \sum_{i \leq 0} e^{ik_{x}x_{i}} \phi_{i,j}^{\alpha} a_{i,j}^{+}|0\rangle
\]

(25)

where $t_{\beta \alpha}$ ($r_{\beta \alpha}$) stands for the transmission (reflection) amplitude from the incoming Bloch state $\alpha$ to the transmitted (reflected) Bloch state $\beta$, and we choose $x_{0} = 0$. The transmission and reflection coefficients are expressed through the corresponding amplitudes and the Bloch velocities\(^{26}\),

\[
T = \sum_{\alpha,\beta} \frac{v_{\beta\alpha}^{\prime}}{v_{\alpha\beta}^{\prime}} |t_{\beta\alpha}|^{2}; \quad R = \sum_{\alpha,\beta} \frac{v_{\beta\alpha}^{\prime}}{v_{\alpha\beta}^{\prime}} |r_{\beta\alpha}|^{2},
\]

where the summation runs over propagating states only. The transmission and reflection amplitudes can be calculated from the equations\(^{26}\),

\[
\Phi_{1} T = -G_{L,0}^{L,0}(U_{0,1} \Phi_{1} K_{1} - \Gamma L^{-1} \Phi_{0})
\]

(26)

\[
\Phi_{0} R = -G_{0,0}^{L,0}(U_{0,1} \Phi_{1} K_{1} - \Gamma L^{-1} \Phi_{0}) - \Phi_{0}
\]

(27)

where the matrices $T$ and $R$ of the dimension $N \times N_{\text{prop}}$ are composed of the transmission and reflection amplitudes $T_{\beta\alpha}$, $R_{\beta\alpha}$; (with $N_{\text{prop}}$ being the number of propagating modes in the leads); $G_{L,0}^{L,0}$ and $G_{0,0}^{L,0}$ are the Green’s function matrixes with matrix elements defined according to Eq. \((11)\); $U_{0,1}$ is the hopping matrix between the left lead and the device region; $K_{1}$ is the diagonal matrix with the matrix elements $(K_{1})_{\alpha\beta} = \exp(ik_{x}x_{1}) \delta_{\alpha\beta}$. The square matrices $\Phi_{1}$ and $\Phi_{0}$ describe the Bloch states on the slices $1$ and $0$ of a ribbon unit cell (see Fig. \(2\)) and are composed of matrix-columns $\phi_{\alpha}^{0}$ and $\phi_{\alpha}^{1}$, $1 \leq \alpha \leq N$, Eq. \((17)\), i.e. $\Phi_{1} = (\phi_{1}^{1}, ..., \phi_{N}^{1})$; $\Phi_{0} = (\phi_{1}^{0}, ..., \phi_{N}^{0})$.

Calculation of the Green’s functions $G_{L,0}^{L,0}$ and $G_{0,0}^{L,0}$ is performed in a standard way\(^{26}\). We start from the Greens function of the first slice in the device region and, using the Dyson’s equation, add recursively slice by slice up to the last slice of this region is reached. Finally, we apply the Dyson’s equation two more times adding the
left and right semi-infinite ribbons whose surface Green's functions are given by Eqs. (21), (22).

Having calculated the transmission and reflection amplitudes that give the wave functions on slices \( i = 0 \) and \( i = L \), we can easily restore the wave function inside the device region using the relation between the wave functions on slices \( i, i' \) and \( i + 1, i' - 1 \) (we assume that \( i' > i \))

\[
\psi_{i+1} = G^{i+1,i+1}_{\text{inner}} U_{i+1,i} \psi_i + G^{i+1,i'-1}_{\text{inner}} U_{i',i-1}^{i+1} \psi'_{i'}
\]

\[
\psi_{i'-1} = G^{i'-1,i+1}_{\text{inner}} U_{i+1,i} \psi_i + G^{i'-1,i'-1}_{\text{inner}} U_{i',i-1}^{i'-1} \psi'_{i'},
\]

where \( G^{i,m}_{\text{inner}} \) is the Green's function of the internal region only (extending from the slice \( i \) to the slice \( m \)). (Equation (28) is derived in a similar way as Eq. (30).) Removing slice by slice from the inner region and repeatedly using Eq. (28) on each step, we restore the wave function in the entire region \( 0 < i < L \).

The diagonal elements of the total Green's function for each slice \( i \) give the local density of states (LDOS) at the site \( i, j \)

\[
\rho(i, j, E) = \sum_{j} \left( G^{i,i}_{\text{inner}} \right)_{jj} \frac{1}{\pi} \Im \left( \epsilon_{ij} \right).
\]

The LDOS can be used to calculate the local electron density at the site \( i, j \),

\[
n(i, j) = \int dE \rho(i, j, E) f(E - E_F). \tag{29}
\]

For quasi-one dimensional structures considered in this study it is convenient to introduce the local density of states integrated in the transverse direction,

\[
\rho(i, E) = \sum_{j} \rho(i, j, E). \tag{30}
\]

IV. RESULTS AND DISCUSSION

In this section we discuss the conductance properties of two-terminal GNRs with MBs using the formalism described above. GNRs with both zigzag and armchair edges are considered. The electronic properties of armchair GNRs depend strongly on its width \( W \). The armchair GNRs are metallic when \( 2N + 1 \) is a multiple of 3, and otherwise they are semiconducting. Metallic armchair GNRs behave similarly to zigzag GNRs regarding the effects discussed here, even though the origin of the first subband is different, and are not presented separately.

Figure 3 shows the Fermi energy dependence of the conductance for the zigzag and armchair ribbons with \( N = 151 \) and 150, respectively, corresponding to a width of \( W \approx 32 \) nm. The rectangular magnetic barrier has a length of 120 nm. The smooth magnetic barrier has the standard shape realized in experiments\(^{25,33}\) and a full width at half maximum of 120 nm. For the case of the smooth barrier the central (device) region has a length of 360 nm. The shapes of the smooth and sharp barriers are depicted schematically in the insets to Fig. 3. We present the conductance calculations for the maximum magnetic field strength in the barrier in the interval of \( 0 \) to 8 T. While inhomogeneous fields up to \( \approx 3.4 \) T have been achieved in the laboratory by using etch facets,\(^{26}\) we consider such high fields in order to address the regime when the magnetic length \( l_B = \sqrt{\hbar/eB} \) (\( = 26 \) nm at 1 T) is smaller than the ribbon width. Alternatively, this could have been achieved by increasing the ribbon width, which is however rather impractical from the computational point of view.

In the absence of MBs, the ballistic conductance of the GNRs is simply proportional to the number of subbands \( N_0 \) at the Fermi energy at zero magnetic field, see Fig. 3. The conductance shows plateaus and increases as a function of Fermi energy, in analogy to the case of QWRs.

Figures 3(a), (b) show the conductance of the semiconducting armchair GNR for the rectangular and smooth magnetic barriers. The dashed lines indicate the number of propagating states \( N_B \) in the corresponding GNR in the homogeneous magnetic field whose amplitude is equal to the maximum field \( B \) in the barrier region. As the magnetic field increases the subbands depopulate and hence the corresponding number of available propagating states \( N_B \) decreases. Because the magnetic field provides an additional confinement in the ribbon, at a given Fermi energy the number of the magnetosubbands \( N_B \) is always smaller than \( N_0 \). Because of this, \( N_B \) represents the limiting factor for the conductance of the magnetic barrier structure such that \( N_0 \) incoming states in the leads are redistributed among \( N_B \) available states in the magnetic barrier. This is clearly seen in Figs. 3(a), (b) where the conductance of the structure at hand approximately follows \( N_B \). Note that the magnetic field reduces the energy gap in the vicinity of \( E = 0 \). Despite of this the conductance of the magnetic barrier is always zero below the energy threshold of \( E_{th} \approx 0.006 \text{eV} \) regardless of the strength of the magnetic barrier. This simply reflects the fact that propagating states are injected from the leads where the magnetic field is absent and the threshold propagation energy \( E_{th} \approx 0.006 \text{eV} \) is not affected by the strength of the barrier in the central region of the device. In addition, transmission resonances are superimposed on the conductance plateaus. They are well pronounced for the rectangular barriers, but get heavily suppressed as the magnetic barrier becomes more realistic, soft shape.

As the strength of the barrier increases, the resonances become more prominent.

In the zigzag GNR with a MB, the conductance steps also move towards higher energies and follow \( N_B \) vs energy as \( B \) increases, see Fig. 3(c), (d). This, as in the case of the armchair GNRs, simply reflects the magnetic field induced shifts of the GNR modes in the barrier region. Around \( E = 0 \), an energy interval exists in which only the lowest propagating state contributes to the conductance. This state evolves from the dispersionless edge state present in the zigzag GNRs at zero energy. The MB is thus able to reduce the number of current carrying states in certain energy intervals, e.g.
between $E \approx 0.03t_0$ and $E \approx 0.037t_0$ for the MBs with strengths of 8 T. Note that for the zigzag GNR the conductance changes in steps of $2 \times 2e^2/h$, whereas for the armchair GNR it changes in steps of $2e^2/h$. This reflects the difference in evolution of the subband structure of corresponding homogeneous armchair and zigzag GNRs, where the number of states at the given energy depends on the wire width $N$ and on whether the ribbon is metallic or insulating. (The conductance quantization for armchair and zigzag GNRs was discussed by Peres et al.)

In addition, as in the case of the armchair GNR, transmission resonances are observed for the rectangular MBs. These resonances are completely suppressed for the case of the smooth barriers. Both the frequency and the amplitude of the oscillations become higher as the strength of the MBs is increased (Fig. 3). Furthermore, the frequency decreases as the length of the MB is decreased (not shown). This behavior is similar to the conductance resonances in quantum point contacts with abrupt openings and originates from multiple reflections at the edges of the MB along the transport direction. The multiple reflections at the edges lead to the Fabry – Pérot type oscillations, as can be seen in Fig. 4 for the case of a GNR with zigzag edges where the number of maxima in the LDOS along the transport direction changes by one for successive resonances. Similar to the case of a smooth quantum point contact, a gradual change of the magnetic field reduces the reflection probabilities and suppresses the resonances, resulting in smaller oscillation amplitudes.

The dependence of the conductance on the magnetic barrier suggests that complete confinement by magnetic barriers is not possible due to the presence of the low-
on the barrier boundaries the edge state circulates inside of the homogeneous channel. Note that due to reflection region is directly related to the corresponding eigenstate patterns demonstrates that the wave function in the barrier maximum is formed close to the center of the GNR. As at this energy. At \( B = 8 \, \text{T} \), its probability density has

\[ |\psi|^2 \text{ at } x \text{ in the } \text{zigzag GNR} \]

The LDOS plot shows the localized states form inside the magnetic barrier. The position of the localized states in relation to the corresponding conductance.

The effect of the magnetic field is therefore to delocalize the lowest propagating state which have been localized \( B \text{ MB, move in energy while their amplitude is suppressed.} \) presumably those originating from defects underneath the MB, move in energy while their amplitude is suppressed. The effect of the magnetic field is therefore to delocalize the lowest propagating state which have been localized by the edge defects. These results suggest that a magnetic barrier can in fact be used to switch the conductance in a GNR, but the mechanism differs from that one to be expected for magnetic barriers in two-dimensional graphene. Activation of the MB is able to delocalize the lowest propagating state in GNRs with disorder, thereby switching the conductance from zero to one.

V. SUMMARY AND CONCLUSIONS

We have provided an extensive theoretical study of the transport through graphene nanoribbons under the influence of magnetic barriers. The magnetic barrier modifies the energy spectrum of the nanoribbon locally, which results in an energy shift of the conductance steps. In addition, multiple reflections along the transport direction between the entrance and the exit of the magnetic barrier generate Fabry–Pérot resonances, the magnitude of which depends on the gradient of the magnetic field. These Fabry–Pérot resonances are strongly suppressed in the case of magnetic barriers with smooth confinement. The lowest propagating state present in zigzag metallic armchair GNRs is only weakly modified by magnetic barriers of realistic strengths. However, localization of

![Graph showing LDOS](image_url)
FIG. 5: Spatial distributions of local density of states in the zigzag GNR with $N = 151$ (left column) without a magnetic barrier (a), with a rectangular barrier of strength $B = 8$ T (b) and $B = 100$ T (c) extending from $x = -60$ nm to $x = 60$ nm. The gray scales (indicated by the bars on top) give the LDOS in units of $t_0^{-1}$ nm$^{-2}$. The Fermi energy is $E_F = 0.01t_0$ corresponding to the case when only the lowest propagating state is occupied. The corresponding probability densities of the lowest Bloch state (in arbitrary units) in an infinite homogeneous wire are shown in the right column.

FIG. 6: The Fermi energy dependence of the conductance of defective graphene ribbons with and without the rectangular MB of strengths 8 T. The edge defect concentration is 30%.

The lowest propagating state by disorder can be lifted by a perpendicular magnetic field, which offers a concept for magnetic barrier induced conductance switching in GNRs with disordered edges.

In this paper we also present a novel method based on the Greens function technique for the calculation of the magnetosubband structure, Bloch states and magnetoconductance of the graphene nanoribbons in a perpendicular magnetic field. The non-trivial part of the method is the calculation of the surface Greens function $\Gamma$, which typically requires very time-consuming self-consistent calculations. We, however, introduced a novel way to calculate the surface Greens function that does not require self-consistent calculations and where $\Gamma$ is simply obtained from the solutions of the eigenvalue equation of the dimension $2N \times 2N$ (with $N$ being the width of the nanoribbon). Utilization of this method obviously greatly facilitates computations, making the present method by far more efficient in comparison to the existing methods based on the self-consistent calculations of $\Gamma$. The programming codes are freely available in the AIP EPAPS electronic depository.

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APPENDIX A: HOPPING MATRIXES $U$

In this appendix we provide explicit expressions for hopping matrixes $U_{i,j}$, Eq. (11), for armchair and zigzag ribbons in the Landau gauge $\mathbf{A} = (-By, 0)$. The numbering of slices and sites, $r = i,j$, within a unit cell is given in Fig. 2, and the definition of the phases $\theta_{r,r+\Delta} = 2\pi \phi_{r,r+\Delta} / \phi_0$ and the corresponding line integrals $\phi_{r,r+\Delta}$ are given by Eq. 4. In the expressions given below $y_{i,j}$ stands for the $y$-coordinate of the site $(i,j)$.

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a. Armchair graphene ribbon

$$(U_{1,0})_{j,j'} = -t_0 \exp(i\theta_{0,j+1,j})\delta_{j,j'}; \quad U_{0,1} = U_{1,0}^+$$  \hspace{1cm} (A1)

where $\phi_{0,j+1,j} = -By_{0,j}a$;

$$U_{2,1} = -t_0 \begin{pmatrix} e^{i\theta_1,2,1} & e^{i\theta_1,2,1} \\ e^{i\theta_1,2,2} & \ddots \\ \ddots & e^{i\theta_{1,N-2,2,N-1}} \\ 0 & e^{i\theta_{1,N-1,2,N-1}} & e^{i\theta_{1,N-1,1,2,N}} & e^{i\theta_{1,N,1,2,N}} \end{pmatrix}; \quad U_{1,2} = U_{2,1}^+$$  \hspace{1cm} (A2)

where $\phi_{1,j+2,j} = -\frac{B}{2} \left( y_{1,j+1}a + \frac{\sqrt{3}}{2}a^2 \right)$, $\phi_{1,j+1,j+2} = -\frac{B}{2} \left( y_{1,j+1}a - \frac{\sqrt{3}}{2}a^2 \right)$;

$$(U_{3,2})_{j,j'} = -t_0 \exp(i\theta_{2,j+3,j})\delta_{j,j'}; \quad U_{2,3} = U_{3,2}^+$$  \hspace{1cm} (A3)

where $\phi_{2,j+3,j} = -By_{2,j}a$;

$$U_{4,3} = -t_0 \begin{pmatrix} e^{i\theta_3,1,4,1} & e^{i\theta_3,1,4,1} \\ e^{i\theta_3,1,4,2} & \ddots \\ \ddots & e^{i\theta_{3,N-1,4,N-1}} \\ 0 & e^{i\theta_{3,N-1,4,N}} & e^{i\theta_{3,N,4,N}} \\ e^{i\theta_{3,1,4,2}} & \ddots & \ddots & \ddots & \ddots & e^{i\theta_{3,1,4,1}} \end{pmatrix}; \quad U_{3,4} = U_{4,3}^+$$  \hspace{1cm} (A4)

where $\phi_{3,j+4,j} = -\frac{B}{2} \left( y_{3,j}a - \frac{\sqrt{3}}{2}a^2 \right)$, $\phi_{3,j+4,j+1} = -\frac{B}{2} \left( y_{3,j}a + \frac{\sqrt{3}}{2}a^2 \right)$; and, because of periodicity,

$$U_{5,4} = U_{1,0}, U_{4,5} = U_{0,1}.$$  \hspace{1cm} (A5)

b. Zigzag graphene ribbon

$$(U_{1,0})_{j,j'} = -t_0 \exp(i\theta_{0,j+1,j})\delta_{j,j'}; \quad U_{0,1} = U_{1,0}^+,$$  \hspace{1cm} (A6)

where for odd $j$: $\phi_{0,j+1,j} = -\frac{\sqrt{3}}{2}B \left( y_{0,j}a + \frac{1}{2}a^2 \right)$, and for even $j$: $\phi_{0,j+1,j} = -\frac{\sqrt{3}}{2}B \left( y_{0,j}a - \frac{1}{2}a^2 \right)$

$$(U_{2,1})_{j,j'} = -t_0 \exp(i\theta_{1,j+2,j})\delta_{j,j'}; \quad U_{1,2} = U_{2,1}^+,$$  \hspace{1cm} (A7)

where for odd $j$: $\phi_{1,j+2,j} = -\frac{\sqrt{3}}{2}B \left( y_{1,j}a - \frac{1}{2}a^2 \right)$, and for even $j$: $\phi_{1,j+2,j} = -\frac{\sqrt{3}}{2}B \left( y_{1,j}a + \frac{1}{2}a^2 \right)$; and, because of periodicity,

$$U_{3,2} = U_{1,0}, U_{2,3} = U_{0,1}.$$  \hspace{1cm} (A8)

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