Edge states interferometry and spin rotations in zigzag graphene nanoribbons

Gonzalo Usaj

Centro Atómico Bariloche and Instituto Balseiro, Comisión Nacional de Energía Atómica, 8400 S. C. de Bariloche, Argentina and Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), Argentina

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An interesting property of zigzag graphene nanoribbons is the presence of edge states, extended along its borders but localized in the transverse direction. Here we show that because of this property, electron transport through an externally induced potential well displays two-path-interference oscillations when subjected either to a magnetic or a transverse electric field. This effect does not require the existence of an actual “hole” in the nanoribbon’s geometry. Moreover, since edge states are spin polarized, having opposite polarization on opposite sides, such interference effect can be used to rotate the spin of the incident carriers in a controlled way.

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Graphene, a two-dimensional array of carbon atoms in a honeycomb lattice, is a very interesting material with unusual electronic properties. It has attracted much attention since its first experimental realization as it offers great potential for technological applications while, at the same time, it has led to the observation of new physical phenomena such as an anomalous quantization of the Hall effect, observable at room temperature, or the manifestation of the Klein tunneling paradox in transport among others. The key to understand graphene’s peculiarities relies on its band structure: electronic excitations around the Fermi energy can be described by an effective Hamiltonian that mimics the Dirac equation for massless chiral fermions where the spin is described by an effective Hamiltonian that mimics the honeycomb lattice.

Since the resulting edge states are then spin polarized, several groups have proposed to use them for spintronics applications such as creating pure spin currents or inducing half-metallic behavior with electric fields.

Here, we analyze electron transport through a ZGNR with a potential well created by external gates and tuned in such a way that transport inside the well is governed only by the edge states. In this case, while the current flow is essentially homogeneous outside the PW region, it flows along the edges inside it. We show then that the system behaves as a two-path interferometer even though the ZGNR is structurally homogeneous, an effect unique to the ZGNR band structure. Interference between the two paths can be tested by either using a magnetic or a transverse electric field to tune the orbital phase difference between the two branches.

Furthermore, since the ground state corresponds to an antiferromagnetic ordering of the polarization of the two edges, each path corresponds to a different spin orientation. Then, if the spin polarization of the incoming electron, set for instance by a ferromagnetic contact, is perpendicular to the intrinsic spin-quantization axis of the ribbon, the two-path interference leads to a rotation of the carrier’s spin. Its angle can be controlled externally, offering an interesting potential for spintronics.

FIG. 1. (Color online) (a) Scheme of a ZGNR. The energy of a 32-ZGNR as a function of the wavevector along the δ axis is shown for: (b) $B_δ=0$; (c) $µ_δ B_δ=\pi/2$; (d) $µ_δ B_δ=\pi'$; and (e) $µ_δ B_δ=1.2\pi'$. The bands connecting the two nonequivalent Dirac points correspond to the edge states.
We describe the ZGNR in the tight-binding approximation. The Hamiltonian then reads as \( H = H_{\text{GNR}}^0 + H_{\text{ext}} + H_{\text{int}} \), where
\[
H_{\text{GNR}}^0 = -t \sum_{\langle i,j \rangle, \sigma} b_{i}^\dagger a_{i\sigma}^\dagger a_{j\sigma} b_{j}^\dagger + t' \sum_{\langle \langle i,j \rangle \rangle, \sigma} (a_{i\sigma}^\dagger b_{j\sigma}^\dagger + b_{i\sigma} a_{j\sigma}) + H. \c.
\]
describes the ribbon. Here, \( a_{i\sigma}^\dagger \) (\( b_{i\sigma}^\dagger \)) creates an electron on a Wannier orbital centered at site \( r_i \) of the sublattice \( A \) (\( B \)) with spin \( \sigma \), \( t = 2.8 \text{ eV} \) and \( t' = -0.1t \) are the nearest- and next-to-nearest-neighbor hopping parameters, respectively. The symbols \( \langle ... \rangle \) and \( \langle \langle ... \rangle \rangle \) restrict the sum to the corresponding neighboring sites. The borders contain \( A \) sites on one edge and \( B \) sites on the other. \( H_{\text{ext}} \), which describes the action of external gates, is defined below. Finally, \( H_{\text{int}} \) describes the electron-electron interaction. Because of the high density of states induced by the edge states, the system is magnetically unstable. Density functional theory and Hartree-Fock calculations show that the ground state corresponds to an antiferromagnetic ordering of the sublattices’ magnetization. Since the latter is mainly localized at the edges, we take such interaction into account by introducing an effective magnetic field only at the edges sites,
\[
H_{\text{int}} = -\mu_B B_{\alpha} \sum_{\alpha \sigma} \sigma a_{\alpha \sigma}^\dagger a_{\alpha \sigma} - \mu_B B_{\beta} \sum_{\beta \sigma} \sigma b_{\beta \sigma}^\dagger b_{\beta \sigma},
\]
where \( \alpha (\beta) \) labels the top (bottom) edge. We take this field to be perpendicular to the plane of the ZGNR (\( \hat{z} \) axis). In the ground state the two edges have opposite magnetizations, \( B_{\alpha} = -B_{\beta} \). The value of \( B_{\alpha} \) should, in principle, be determined by a self-consistent calculation. Since its precise value depends on the chemical passivation of the edges, and in order to discuss different situations, we take it here as a free parameter.\(^{28}\)

Figure 1 shows the energy dispersion of a 32-ZGNR (Ref. 29) for different values of \( B_{\alpha} \). Several bands originated from the quantization along the \( \hat{y} \) axis are clearly visible. The bands in the range \( k_x a \in [2 \pi /3, 4 \pi /3] \) that are close to the Dirac point, \( E = t' \), are the ones that correspond to the edge states with a characteristic localization length \( \lambda(k_x) = -3a_0/2 \ln[2 \cos(k_{\alpha}a/2)] \). Here, \( a_0 = 3a_0 \) is the lattice parameter with \( a_0 \) the C-C bond length. For \( B_{\alpha} = 0 \) [Fig. 1(b)], there are two of those bands (for each spin orientation) that are almost degenerated; there is an exponentially small splitting between them. They essentially correspond to the symmetric and antisymmetric combinations of the exponentially decaying solutions of each individual edge.\(^{5,13} \) For \( B_{\alpha} \neq 0 \) [Figs. 1(c)–1(e)], both the spatial and the spin degeneracies are broken. For each spin orientation, each band now corresponds to states localized on a different edge. The energy dispersion is approximately given by \( E(k_x) = E_{\text{HN}} + t' + \nu_B B_{\alpha} \) \( 2 \cos(k_{\alpha}a+/2) \). Note that it is nonzero due to the nonzero value of \( t' \) or \( B_{\alpha} \). The key point is to notice that, for a given energy, the states with opposite spin polarization in the \( \hat{z} \) direction are localized on opposite edges of the ZGNR.

Let us now consider the transport properties of a ZGNR in the presence of an electrostatic potential created by external gates,\(^{30}\) where \( f(x) \) is a smooth function describing a PW of height \( V_g \) [see Fig. 2(a)]. For simplicity, we use a sum of Fermi functions, with the parameter \( \Delta \) playing the role of the temperature, to set the spatial profile of \( f(x) \) (which depends only on \( x \)). We assume that \( E_F < 3t' < 0 \) far from the PW which ensures that the current carrying states in that region are extended throughout the entire width of the ribbon. On the other hand, \( V_g < 0 \) can be tuned in such a way that \( E_F - V_g \) corresponds to the energy of an edge state. For the sake of simplicity, we discuss first the conceptually simpler case \( B_{\alpha} = 0 \). Then, if \( f(x) \) changes smoothly, the electrons’ wave function will adiabatically change from extended to localized, while keeping its band index and having a position dependent wave vector \( k_x(x) \). Correspondingly, the charge flow will “split” in two paths inside the well and merge again afterwards, creating a “hole” in its spatial distribution [Fig. 2(a)]. In this way, we have created an interferometer, which can be tested by introducing a relative phase difference between the two paths.

As the Aharonov-Bohm (AB) effect provides the simplest way to do this, we introduce a magnetic field \( B_\perp \) perpendicular to the ZGNR (via a Peierls substitution in the hoppings) and calculate the zero-temperature conductance using the Landauer approach.\(^{31} \) For that, we separate the system into a central region (containing the PW) and the leads’ regions and use the standard recursive method to obtain the lattice Green’s functions and the transmission coefficient from them. Figure 2(b) shows the conductance \( G \) of a 32-ZGNR as a function of the \( V_g \) for different values of \( B_\perp \). It is ap-
parent that $G$ changes with $B_{\perp}$ only when $V_{g}$ is below the threshold where the edge states participate on transport (indicated by the arrow). The inset shows the oscillatory behavior of $G$ as function of $B_{\perp}$ for three different values of $V_{g}$. The period is roughly $\phi_{0}/A' \approx 1.3$ T with $\phi_{0}$ the flux quantum and $A' = L_{\text{eff}} W$ with $L_{\text{eff}} = (L - 4 \times 3.5 \Delta)$. An increment of the period, due to the reduction in the effective “hole” area, is difficult to see since the visibility of the oscillations is rapidly lost. In addition, and despite this seemingly simple picture, the behavior of the conductance is more involved as it shows pronounced narrow dips when $B_{\perp} \neq 0$. This is related to the fact that bonding and antibonding bands are mixed by $B_{\perp}$ (recall that for $B_{\perp}=0$ the splitting is exponentially small) and then both bands get involved in transport, which in turns leads to Fano-like interference between them and a reduction in the visibility of the AB oscillations.33

A more interesting situation occurs for $B_{\perp} \neq 0$. As we mentioned above, in this case, both the spatial and the spin degeneracies are broken. Therefore, an incoming electron mentioned above, in this case, both the spatial and the spin projection remains on the plane of the ZGNR. The probability for an electron to keep its spin orientation is cos$^{2}$ (16).36

\[ |\text{in}| = \sqrt{2} \left| \frac{|\hat{\epsilon}| + e^{i\phi}|\hat{\epsilon}|}{\sqrt{2}} \right| \rightarrow |\text{out}| = \sqrt{2} \left| \frac{|\hat{\epsilon}| + e^{i\phi}|\hat{\epsilon}|}{\sqrt{2}} \right|, \tag{4} \]

where $\hat{\epsilon}$ is the relative phase of the transmission amplitude of the two paths. Due to the symmetry of the setup, the spin projection remains on the plane of the ZGNR. The probability for an electron to keep its spin orientation is cos$^{2}$ (16) and so we expect the conductance between two collinear ferromagnetic leads34 to oscillate as a function of $\hat{\epsilon}$. Note that we have assumed that $L \ll L_{\text{corr}}$, where $L_{\text{corr}}$ is the spin-correlation length of the ferromagnetic order along each edge.35

Figure 3 shows the spin-resolved transmission probability $T_{\epsilon\nu}$ for an incident electron with spin $|\uparrow\rangle = |\hat{\epsilon}\rangle$ to be transmitted with spin $\sigma = \pm$ (in the same axis) as a function of $V_{g}$ and $B_{\perp}$. The relative phase of the two paths is $\hat{\epsilon} = 2\pi\phi/\phi_{0}$, where $\phi = B_{\perp} A_{\text{eff}}$ is the magnetic flux enclosed by the current flow and $A_{\text{eff}} = L_{\text{eff}} W_{\text{eff}}$ is the effective area. For our geometry, the latter depends mainly on the effective width $W_{\text{eff}}(V_{g})$, which is a function of $V_{g}$ through the energy dependence of $\lambda(k_{zz})$ ($W_{\text{eff}} = W(\coth(W/\lambda) - \lambda/W)$) for $\lambda/W \approx 1$). As expected, the transmission is a simple oscillatory function of $B_{\perp}$. Note that the shorter period corresponds to the maximum effective area, $\phi_{0}/(L_{\text{eff}} W) = 1.5$ T and that for $V_{g} > V'_{c} = -0.5\delta t$ (threshold for the participation of the edge states) there are no oscillations. The total transmission $T = T_{\uparrow\uparrow} + T_{\uparrow\downarrow}$ is constant, implying that the effect of the field is to produce a pure spin rotation. The features that are apparent in the figure for $V_{g} \leq -0.5\delta t$, are related to the presence of the “w-shaped” edge states band (see discussion below). It is worth pointing out that $B_{\perp}$ cannot be too large to avoid a transition to a ferromagnetic state [$B_{\perp} \leq 2$ T (9 T) for a 32-ZGNR (16-ZGNR)].36

![FIG. 3. (Color online) (a) Density plot of the spin-resolved transmission $T_{\epsilon\nu}$ as a function of the depth of the potential well $V_{g}$ and the perpendicular magnetic field $B_{\perp}$ for a 32-ZGNR and $\mu B_{\parallel} = t'/2$, $E_{g} = -0.8\Delta$, $L = 2400a$, and $\Delta = 30\Delta$; (b) same for $T_{\downarrow\uparrow}$; (c) magnetic field dependence of $T_{\uparrow\uparrow}$ (open symbols); and $T_{\downarrow\uparrow}$ (filled symbols) for $V_{g}/t = -0.53$ (□, ■), -0.515 (○, ●), and -0.51 (△, ▲).](image-url)

Interestingly enough, there is also a way to produce a controlled spin rotation using an all-electrical setup. The key is to change $\hat{\epsilon}$ by inducing a difference between the wave vectors of the two paths, and therefore changing their relative plane-wave phase. This can be achieved by applying a small transverse electrical field that changes the energy of the two paths, and then the wave vectors, in a small fraction and in opposite directions. Note that only a change $\delta k_{zz} = 2\pi/L$ is required. The transverse potential is described by adding a term $V_{g}(\gamma_{y} - W/2) / L / f(x_{e})$ to $V_{g}(x_{e})$ in Eq. (3). Figure 4 shows the spin-dependent transmission for this setup. As for the previous case, there are clear oscillations indicating the rotation of the spin of the carriers, even for a very small transverse field $E_{T} = 2\gamma_{y}/W = 2 \mu V / A$ for $V_{g} = 5 \times 10^{-2}\tau$. Again, the rotation disappears for $V_{g} > V'_{c}$. The period of the oscillations is in good agreement with the estimated value...
the transverse potential in the corresponding edge state ing in one direction but extended states for those moving in the “w-shaped” band involves edge states for electrons mov-
80 sible due to a resonant mechanism that involves the upper
318 well and are then reflected. However, transport is still pos-
87 ability with
Figs. 3 and 4. We note that in Fig. 3, they present a period of the resonances increases as the potential profile is more
81 kx
adiabatic transport is not possible for
318
VT
\mu_B B_a > t' as electrons reach a point where \nu_x=0 before they penetrate the well and are then re
defined as the electrons in that case follow a
216803 single path. This is, however, not true as each minimum of the “w-shaped” band involves edge states for electrons moving in one direction but extended states for those moving in the opposite direction — another unique characteristic of the ZGNR band structure. The phase difference is then related to half the area of the PW. A detailed analysis\(^{33}\) shows that the spin rotation is still possible for some of the resonances, showing that the effect is robust against the precise value of \(B_a\).
In summary, we showed that ZGNRs present interesting interference phenomena in the presence of a PW. Moreover, the spin-dependent structure of the edge states allows for a controlled rotation of the spin of the carriers by either magnetic or electric fields. Since the characteristic of the zigzag termination seems to be generic\(^ {37}\) and robust against disorder,\(^ {19}\) we expect these effects to manifest in less ideal samples, opening an alternative for spintronics in graphene.

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29. Following the standard notation, we identify a given GNR by the number \(N\) of zigzag chains it contains in the transverse direction. See Ref. 4 for details.
30. For ferromagnetic order between edges, \(B_{\sigma}=B_{\beta}\), there is a spin splitting of the bands but the spatial symmetry is not broken. Oscillations similar to the ones discussed below for \(B_{\sigma}=0\) should also appear in this case.
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