Graphene nanoribbons in criss-crossed electric and magnetic fields

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Graphene nanoribbons (GNRs) in mutually perpendicular electric and magnetic fields are shown to exhibit dramatic changes in their band structure and electron-transport properties. A strong electric field across the ribbon induces multiple chiral Dirac points, closing the semiconducting gap in armchair GNRs. A perpendicular magnetic field induces partially formed Landau levels as well as dispersive surface-bound states. Each of the applied fields on its own preserves the even symmetry \( E_k = E_{-k} \) of the sub-band dispersion. When applied together, they reverse the dispersion parity to be odd, which gives \( E_{e,k} = -E_{h,-k} \), and mix the electron and hole sub-bands within the energy range corresponding to the change in potential across the ribbon. This leads to oscillations of the ballistic conductance within this energy range. The broken time-reversal symmetry provides dichroism in the absorption of the circularly polarized light. As a consequence, one can observe electrically enhanced Faraday rotation, since the edges of the ribbon provide formation of the substantial density of states.

Keywords: graphene; nanoribbons; ballistic transport

1. Introduction

Recent advantages in the fabrication techniques of graphene nanoribbons (GNRs), together with the long electron mean free path, have stimulated considerable interest in their potential applications as interconnects in nano circuits. Near the \( K \) and \( K' \) Dirac points for infinite graphene, the electrons are massless and chiral (Neto et al. 2009). The electronic properties of GNRs are sensitive to the geometry of their edges and the number of carbon atoms \( N \) across the ribbon. The GNRs are thus classified as armchair (ANR), zigzag (ZNR) nanoribbons for even \( N \) and their counterpart anti-armchair (AANR), anti-zigzag (AZNR) for odd \( N \). The armchair confinement mixes \( K \) and \( K' \) valleys creating chiral electrons around the \( \Gamma \) point. Chirality is the key ingredient for...
unimpeded electron transport (Klein effect). Depending on $N$, modulo 3, the ANR/AANR can be either metallic or semiconducting, making them suitable candidates for use as field-effect transistors. By contrast, the zigzag confinement does not mix the valleys but rather intertwines their longitudinal and transverse momenta, creating edges-bound quasi-particles between the $K$ and $K'$ points. For ZNR/AZNR, the electrons are not chiral (in the sense of projection of the pseudo-parity on the particle momentum), and the electron transmission through a potential barrier is determined by the electron pseudo-parity (Rainis et al. 2009). This quantity redefines the Klein effect as the suppressed transmission through the barrier in ZNR, also known as the valley-valve effect (Roslyak et al. 2010). The latter is the basis for the proposed valley filters. The electron confinement in GNRs causes their properties to be quite sensitive to an applied electric (Novikov & Levitov 2006; Novikov 2007; Raza & Kan 2008) or magnetic (Brey & Fertig 2006; Perfetto et al. 2007; Golizadeh-Mojarad et al. 2008; Ritter et al. 2008) field. These changes are reflected in measurable quantities such as the ballistic conductivity, local/joined density of states (LDOS, JDOS) and optical conductivity (Lyo & Huang 2004; Li et al. 2009).

In this article, we report on the individual and combined effects of an electric and magnetic field on the band structure and conductance of GNRs. If only one of the fields is applied, it is well known that the time-reversal symmetry\(^1\) (Simon et al. 2009) of the energy bands for electrons and holes is preserved for all the types of GNRs we listed above. However, the combined effect of an electric and magnetic field on the energy dispersion is to break the time-reversal symmetry for both electrons and holes and mix the energy bands. The effect of mixing on the differential conductance and LDOS is presented below, and our results are compared with those obtained when only one of the two external fields is applied to an ANR with quantum point contacts, as illustrated schematically in figure 1.

\(^1\)Since we neglect spin, the action of the time-reversal operator $\hat{T}$ amounts to reversing the direction of the wavevector propagation. The even/odd particle energy symmetry may be defined as $E_{n,k} = \pm \hat{T} E_{n,-k} = \pm E_{n,-k}$.
and \( V \) is the bias potential) and serves as the source. We choose coordinate axes so that the nanoribbon is along the \( x \)-axis in the \( xy \)-plane. Mutually perpendicular static electric field \( \mathbf{E}_y \) along the \( y \)-axis and magnetic field \( \mathbf{B}_z \) along the \( z \)-axis are applied, as shown in figure 1.

## 2. Model

In the appendix, we have calculated the energy bands for graphene with sublattices \( A \) and \( B \) in the super-symmetric form tight-binding model (Lin et al. 2009; Neto et al. 2009). These are then separated into hole \( \{ h \} = \{ 1 \leq n < N \} \) and electron \( \{ e \} = \{ N \leq n < 2N \} \) energy bands. The two-component wave function is a normalized \( 2N \) vector,

\[
\psi_{n,k}(y) = \begin{pmatrix} (A; n, k|y) \\ (B; n, k|y) \end{pmatrix}. \tag{2.1}
\]

Along the ribbon we have a plane wave \( \sim \exp(ikx) \), characterized by its wavevector \( k \). The electric field induces a potential across the ribbon \( U(y) = e\mathbf{E}_y/(y - W/2) = U_0[(y/W) - 1/2] \), where \( W \) is the ribbon width\(^2\) and \( U_0 = e\mathbf{E}_y W \). This potential is screened by the carriers. The screening potential is found self-consistently by solving the Poisson equation with the carrier density deviation from that of \( U_0 = 0 \) as the source. To assure convergence of the numerical simulation, the electric field is raised adiabatically to the desired value. In fact, owing to the absence of translational symmetry across the ribbon, the screening potential cannot be described by a mean field and varies across the ribbon. The magnetic field modifies the wavevector as \( k \rightarrow k - e\mathbf{B}_z y/\hbar \), which amounts to the Peierls phase in the hopping integrals (Liu et al. 2008a). The magnetic-field strength is assumed weak enough so that we could take the energy levels as spin degenerate. The dispersion curves can be experimentally observed via scanning tunnelling microscopy (Simon et al. 2009). The tunnelling current flowing through the microscope tip is proportional to the LDOS given by

\[
\text{LDOS}(E, y) = \sum_{n,k} |\psi_{n,k}(y)|^2 \delta(E - E_{n,k}). \tag{2.2}
\]

The energy dispersion determines the ballistic charge current \( I \) through the ribbon, at temperature \( T \), by

\[
I(V, \mu, \mathbf{E}_y, \mathbf{B}_z, T) = -2e \sum_n \int_{\text{BZ}} \frac{dk}{2\pi} v_{n,k} \left[ \theta(-v_{n,k}) f_{n,k}^>(1 - f_{n,k}^<) + \theta(v_{n,k}) f_{n,k}^<(1 - f_{n,k}^>) \right], \tag{2.3}
\]

where \( v_{n,k} = dE_{n,k}/d(\hbar k) \) is the carrier group velocity. At \( T = 0 \), the Fermi function at the source contact is \( f_{n,k}^> = 1 - \theta(E_{n,k} - \mu - eV) \) and for the drain, we have \( f_{n,k}^> = 1 - \theta(E_{n,k} - \mu) \). We note that equation (2.3) does not assume any symmetry for the energy-dispersion relation. If the energy satisfies \( E_{n,k} = E_{n,-k} \), we obtain the well-known Landauer–Büttiker formula (Büttiker 1988).

\(^2\)In the units of carbon–carbon distances, ANR width is given by \( W = (3N + 1)/2 \), and for ZNR it is \( W = (\sqrt{3}/2(N + 2)) \).
differential conductance $G(\mu, \mathcal{E}_y, B_z) = (\partial I / \partial V)_{V=0}$ is determined by the number of right-moving carriers through $n_{n,k}/|v_{n,k}| > 0$ at the chemical potential $E_{n,k} = \mu$. Alternatively, one may take the difference between the local minima and maxima below the chemical potential $E_{n,k} < \mu$ (Lyó & Huang 2004).

When the nanoribbon is illuminated by a linearly polarized light along the ribbon, the optical conductance can be calculated via the Kubo formula (Johnson & Dresselhaus 1973; Liu et al. 2008b). For the purpose of studying the symmetry breaking in external fields, the optical field can be represented as two circularly polarized waves, yielding the optical conductance in the following form:

$$
\sigma_{\pm}(\omega, \mu, \mathcal{E}_y, B_z) = -\frac{1}{i\omega W} \int_{BZ} \frac{dk}{2\pi} \sum_{n,n'} J^\pm_{n,n';k} J^\pm_{n',n;k} f^\prime_{n,k} - f^\prime_{n',k} / h \omega + E_{n,k} - E_{n',k} + i\gamma,
$$

(2.4)

where $\gamma$ is the inverse of the relaxation rate and $\pm$ stands for the optical conductance induced by the left/right polarized light whose frequency is in units of $\hbar \omega$. The optically induced current matrix elements are found from the gradient of the Hamiltonian (A.2),

$$
J^\pm_{n,n';k} = e \left\{ U^\pm_{n,k} \frac{\partial H^\pm_{n,k}}{\partial k} U^{-1}_{n',k} \right\}_{n,n';k},
$$

(2.5)

where $U_k$ is the unitary transformation that diagonalizes the Hamiltonian, whose columns are given by the wave functions (2.8), and $\pm$ subscripts stand for equations (A.5) and (A.6), respectively. If the current matrix elements are set to unity, equation (2.5) describes JDOS. The real part of the optical conductance is proportional to the reflectivity from the ribbon. We shall also analyse the circular dichroism, in terms of the dissymmetry factor (also known as the anisotropy factor),

$$
g(\omega, \mu, \mathcal{E}_y, B_z) = 2 \left| \frac{\Re \sigma_+ - \Re \sigma_-}{\Re \sigma_+ + \Re \sigma_-} \right|.
$$

(2.6)

If the above factor is larger than zero, this indicates that the originally circularly polarized light after the reflection becomes elliptically polarized. In other words, there is an angle between the original linear polarization and the reflected one.

Our numerical results for the energy bands, LDOS and conductance for semiconducting ANR ($N = 51$) in the presence/absence of electric and/or magnetic fields are presented in figure 2. Corresponding optical absorptions are shown in figure 3. The following material parameters have been used. Magnetic flux $\phi$ through a hexagon with C–C arm length $a_0 = 1.42 \ A$ is taken to be $\phi/\phi_0 = 1/150$ in units of the fundamental flux quantum $\phi_0 = \hbar c/e = 4.1356 \times 10^{-15} \ T m^2$. The flux is induced by the magnetic field $B_z = (2\phi_0/3\sqrt{3}a^2) = 526.28 \ T$. This is rather a large field, and well beyond experimental reach if one tries to achieve this value in a homogeneous and constant magnetic field. However, since such a large field has to be present only in a small region of space where the GNR is present, one can resort to a modulated magnetic field to reach locally such a value of the field. The electric field corresponds to the potential drop across the ribbon $U_0 = t_0/2$, where $t_0 = 2.7 \ eV$ of the jumping energy. This is much larger than the geometrical gap $t_0/W \approx t_0/75$. A corresponding electrical field yields $1.13 \times 10^8 \ V \ m^{-1}$.

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Figure 2. Column (i) represents the dispersion curves for the electrons (light curves) in the conduction band and holes (dark curves) in the valence band. The lowest conduction and highest valence sub-bands are given by the thick curves. Column (ii) shows local density of states. Column (iii) gives the corresponding ballistic conductance in units of $2e^2/h$. Row (a) corresponds to absence of the electromagnetic field. Row (b) corresponds to the sole magnetic field of the flux through a single hexagon placket $\phi/\phi_0 = 1/150$. Row (c) shows the effect of the sole electric field of the strength $U_0/t_0 = 1/2$. Row (d) demonstrates the combined effects owing to an electric and magnetic field with the same strength as that employed in rows (b,c). (Online version in colour.)

(a) No fields present

When either only an electric or magnetic field is applied, $E_y B_z = 0$, the electron/hole energy bands are symmetric with $E_{h,k} = -E_{e,k}$ and time-reversal symmetry is satisfied with $E_{n,k} = E_{n,-k}$ around the $k = 0$ Dirac point in

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Figure 3. (ai–di) Correspond to optical conductance induced by the linearly polarized light $\Re(\sigma^+ + \sigma^-)$ for the following cases: (ai) absence of the electromagnetic fields, (bi) magnetic field, (ci) electric field, (di) both electric and magnetic fields present. Subgraphs (aii–dii) indicate dependence of the optical conductance on both frequency of the light source and the chemical potential of the ribbon. Inset graph (diii) shows the dissymmetry factor. (Online version in colour.)

Figure 2bi. The latter means that if the time for the particle is reversed, the particle retraces its path along the same electron/hole branch. The LDOS also demonstrates the wave function symmetry with respect to the ribbon centre $\text{LDOS}(E, x) = \text{LDOS}(-E, x) = \text{LDOS}(E, -x)$. In accordance with the Landauer–Büttiker formalism, the conductivity demonstrates the familiar staggering pattern. Optical conductivity spectra are calculated assuming a constant relaxation rate $\hbar\delta = 0.01$. It exhibits sharp peaks at the resonances of JDOS; however, some of them are suppressed by the optical selection rules governed by the current matrix elements (2.5). The selection rules are simple for the ZNR type of ribbons saying that only transitions between the states of the same parity\(^3\) are allowed: $J^\pm_{\text{even, odd}; k} = J^\pm_{\text{odd, even}; k} = 0$. This selection rule (Hsu & Reichel 2007) is the consequence of the fact that the current matrix elements in equation (2.3) are given by the overlap of the wave functions at the $A$ and $B$ sub-lattices at the same site labelled as $y$, as follows from equation (A3). In the case of ANR ribbons, the selection rules are greatly relaxed by the fact that the current matrix elements are given by the wave functions overlap on $y$ as well as on $y \pm 1$ sites in accordance

\(^3\)This statement holds only for our labelling of the energy levels.

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with equation (A4) (Xin-Xiang et al. 2008). However, in the important region of far-infrared (FIR) and visible light, the optical conductivity is low for two fundamental reasons: the density of states vanishes near the Fermi energy and the interband transition amplitude is small. For instance, the transition between the lowest conduction \((n = N + 1)\) and highest valence \((n = N)\) bands is suppressed for all types of ribbons. The corresponding effect for ANR with \(N = 51\) is shown in figure 3a. To overcome this difficulty and make the GNRs good candidates for optoelectronic applications, such as sensors operating at low frequency, it was proposed to use strong magnetic fields (Liu et al. 2008b).

(b) Transverse magnetic field

The magnetic field by itself distorts the weak dispersion \((n \text{ close to } N)\) so that the partially formed Landau levels \(E_{n,0} \sim \sqrt{B_z n}\) show themselves up as the flat parts in the dispersion curves. The lowest Landau level provides the single conducting channel (along the ribbon edges), while the rest are doubly degenerate. When the wavevector evolves from the Dirac point, the degeneracy is lifted and the lowest sub-band acquires a local minimum. Of these two effects, the first one can be observed in the LDOS, while the second reveals itself as sharp spikes in the conductance as depicted in figure 2biii. For the high-energy sub-bands, when the radii of the Landau orbits (spread of the wave function in figure 2bii) become comparable with the ribbon width, the confinement effects dominate and the spectra become linear in magnetic field with \(E_{n,0} \sim B_z / n\). These sub-bands are not degenerate.

In the FIR and visible light regime, the GNRs\(^4\) demonstrate the optical absorption with resonances given by the transitions between the flat portions of the partially formed Landau levels. The selection rules are conventional for the magneto-optics and may be viewed as the overlap between the \(A\) and \(B\) wave functions given by the hermitian polynomials of the alternating order (see equation (2.7) with \(\beta = 0\)). As compared with the infinite graphene, the edges of the ribbon produce three significant effects on the magneto-optical absorption. First, the resonances strength is varied, while in the infinite graphene, all the resonances are of the same intensity. Second, and most important, the transition between the highest valence and lowest conduction bands become optically active owing to the acquired dispersion next to the boundaries (figure 3b). This effect is known as magnetic enhancement of the THz conductance (Liu et al. 2008b). However, it does not extend much into the visible range, keeping the nanoribbons mostly transparent. Third, for \(N\) odd types of the ribbons, one can observe circular dichroism owing to non-vanishing albeit small dissymmetry factor \((\max(g(\omega))\) has an order of magnitude approx. \(10^{-4}\)). In a stack of identical GNRs, this would lead to measurable Faraday rotation.

(c) Electric field across the ribbon

The main effect that the electric field has on the energy dispersion is to fracture the Fermi surface into small pockets for \(k \neq 0\), thereby closing the semiconducting energy gap. These zero energy points, where the group velocity abruptly changes sign, represent new Dirac points, which follow from the chirality of the wave

\(^4\)Both AGNR and ZNR.
function in their vicinity (Brey & Fertig 2009). The rapid changes in the group velocity cause the appearance of spikes in the conductance near $|\mu| \leq U_0/2$ and its step-like pattern is broken. Owing to the Dirac symmetry of the problem, the electron–hole band structure remains symmetric. The energy dispersion is not affected by the magnetic field at the original Dirac point $k = 0$. Time-reversal symmetry also persists. The LDOS shows that at high energies, the electric field confines the electrons and holes near opposite boundaries. However, at low energies, the LDOS does not change across the ribbon, which is a manifestation of the Zitterbewegung effect (attempts to confine Dirac fermions cause wave function delocalization (Neto et al. 2009)). With respect to the three cases considered above, we point out that the hallmark of Dirac fermions is the even symmetry of the dispersion with respect to the wavevector, and steams from time-reversal symmetry. Even though an attempt to confine them may lead to the broken electron/hole symmetry (Peres et al. 2006), the wavevector symmetry still persists.

Formation of the new $K$ points has an interesting effect on the optical conductance (Chang et al. 2008; Chen et al. 2010). Namely it makes the ribbons opaque in the visible range (figure 3c). The effect is easily traceable to the formation of large density of states in between the newly formed $K$ points. Although it is a common feature that the optical absorption grows with increasing chemical potential, this effect is largely amplified by the DC electric field across the ribbon (figure 3cii).

(d) Criss-crossed electric and magnetic fields

We now turn our attention to the most interesting case when both electric and magnetic fields are applied together. Concurrent action of the electric-field dragging force, the Lorentz force and confinement by the ribbon edges destroys the Dirac symmetry of the problem so that $E_{n,k} \neq E_{n,-k}$, as shown in figure 2di. The dispersion distortion is different for the electrons and holes, so the symmetry between the conduction and valence bands is also broken. On one hand, the partially formed Landau levels get distorted by the confinement owing to the electric field in conjunction with the edges. Their degeneracy is also lifted. On the other hand, the magnetic field does not allow the formation of additional Dirac points and wave function delocalization. At high energies, where the group velocity is decreased and the drag owing to the electric field prevails. The electrons and holes get gathered at the opposite ribbon edges (figure 2dii). For lower energies, in the region $|E_{n,k}| \leq U_0/2$, the electron/hole dispersions overlap. The electron bands have only local minima, whereas only the hole bands have local maxima. Regardless of the broken Dirac $k$ symmetry of the dispersion, our numerical simulation of the differential conductivity shows that the Landauer–Büttiker expression still applies. Therefore, in the overlapping region $|\mu| \leq U_0/2$, the conductivity oscillates since the minimum of the electron band is followed by the maximum on the hole band when the chemical potential grows. As for possible applications of the broken Dirac symmetry, the ribbon, subjected to mutually transverse electric and magnetic fields, may serve as a field-effect transistor with a tunable working point. An interesting feature of our results is that there is not only a breakdown in the even-$k$ symmetry of the energy-dispersion relation, but the energy bands are reversed with odd symmetry, satisfying $E_{e,k} = -E_{h,-k}$.
We explain this effect by adopting the method described in Novikov & Levitov (2006) and Brey & Fertig (2009). Let us focus on the energy region close to the original Dirac point \( k = 0 \), where the unperturbed wave functions are governed by the conventional Dirac equation. Both applied fields are treated perturbatively. The effect of magnetic field is included through the wavevector replacement \( k \rightarrow k - B_z e_y/c \). The electric field is treated by a chiral gauge transformation. This transformation shows that the spectrum at \( k = 0 \) is affected by the electric field in the presence of the magnetic field. An alternative approach based on Lorentz-boosted Landau levels was developed in Lukose et al. (2007). Both approaches yield the same spectrum and eigenvalues,

\[
E_{n', k} = sgn(n') \sqrt{2|n'|} \frac{\hbar v_F}{l_c} (1 - \beta^2)^{3/4} - \hbar v_F \beta k
\]  

(2.7)

and

\[
\psi_{n', k}(y) \sim \left( \frac{sgn(n')\phi_{|n'|-1}(\zeta)}{i\phi_{|n'|}(\zeta)} \right).
\]  

(2.8)

Here, \( \beta = \frac{E_y}{v_F B_z} \) is the field-dependent dimensionless parameter; \( v_F \) is the Fermi velocity; \( n' \) are the integer quantum numbers describing Landau levels for electrons \( n' \geq 0 \) and holes \( n' \leq 0 \); \( l_c = \sqrt{\hbar/eB_z} \) is the magnetic length; \( \phi_{n'}(\zeta) \) are the harmonic oscillator eigenfunctions; and

\[
\zeta = \left( \frac{1 - \beta^2}{l_c} \right)^{1/4} \left( y + l_c^2 k + sgn(n') \frac{\sqrt{2|n'|l_c \beta}}{(1 - \beta^2)^{1/4}} \right).
\]  

(2.9)

Owing to the \( 1 - \beta^2 \) factor, the Landau levels collapse under a large electric field. This feature is characteristic to graphene in crossed electromagnetic fields as compared with the standard two-dimensional electron gas. The last term in equation (2.9) indicates effective spatial separation between the electrons and holes, similar to the case shown in figure 2dii. As follows from the second term in equation (2.7), the boosted Landau levels are linearly dispersive with \( v_{n', k} = v_F \beta \). Figure 2dii shows that this feature holds true for nanoribbons. Regardless of the metallic or semiconducting ANR, the electron and hole dispersion become degenerate around \( k = 0 \) with \( E_{e, k} = -E_{h, -k} \sim -\hbar (E_y/B_z) k \).

It is worth noticing that by substituting equations (2.7) and (2.8) into the current equation (2.3), we obtain an interesting result. Namely the first term in equation (2.3) vanishes since all boosted Landau levels provide right-moving carriers, both electrons and holes. Thus, there is a non-vanishing current in the absence of the bias between the source and the drain. This effect may be viewed as an inverse of the conventional Hall effect. Equation (2.7) indicates that by increasing the electric field one would pack in more and more boosted Landau levels to the energy region around \( k = 0 \), thus increasing this type of current. However, the boundary conditions for the nanoribbons restrain this current and result in an oscillating conductance, as shown in figure 2diii.

Now let us turn our attention to the optical properties of the GNR in criss-crossed electromagnetic fields. It is dominated by the optical transitions between the maximums for \( k < 0 \) and minimums for \( k > 0 \) (figure 2dii). The strong resonance in the FIR and visible regimes illustrated in figure 3di are obviously
attributed to formation of large density of states (figure 2di) in those regimes. Similar to the case of the electric field itself, the optical absorption may be greatly enhanced by increasing the chemical potential (figure 3dii).

The broken time-reversal symmetry has an effect on the absorption of the left- and right-circularly polarized light, resulting in relatively large circular dichroism, as shown in figure 3diii. The classical physical picture of the effect is the same as for any two-dimensional electron gas (2DEG) in criss-crossed fields: the DC electric field is either working along with the left- and against the right-polarized wave y-component or vice versa. At the same time, the action of the ‘drag force’ on the x-component of both left- and right-polarized waves is the same. This results in slightly different classical trajectories for the electrons subjected to the left- and right-polarized optical fields and ultimately in different optically induced currents. Although this effect is present in the infinite graphene, or a 2DEG for that matter, the underlying density of states is not just enough to make it well pronounced. In GNRs on the other hand, the edges do provide the required density of states. This effect can be alternatively described from the point of view of the asymmetry of the LDOS. When the magnetic field perpendicular to a GNR is non-zero, the Lorentz force acted on moving electrons will generate a transverse current in the presence of a longitudinal electric field. The existence of this induced transverse current contributes to a finite value to the off-diagonal dielectric matrix elements. This implies that no linearly polarized transverse electromagnetic field can exist in the electron plasma of a GNR. As a result of this, the phase velocities of a left- and right-circularly-polarized light must be different, leading to a Faraday rotation to linearly polarized incident light after it is either transmitted through or reflected from a GNR. The rotation angle is significant in a GNR in comparison to a 2DEG owing to higher carrier mobility and higher density of states of a GNR. Thus, one can, in principle, observe the electrically enhanced Faraday rotation of the transmitted (reflected) light originally linearly polarized along a single GNR.

3. Conclusion

We have demonstrated that when GNRs are placed in mutually perpendicular electric and magnetic fields, there are dramatic changes in their band structure and transport properties. The electric field across the ribbon induces multiple chiral Dirac points, whereas a perpendicular magnetic field induces partially formed Landau levels accompanied by dispersive surface-bound states. Each of the fields by itself preserves the original even parity of the sub-band dispersion, i.e. $E_{n,k} = E_{n,-k}$, maintaining the Dirac fermion symmetry. When applied together, their combined effect is to reverse the dispersion parity to being odd with $E_{e,k} = -E_{h,-k}$ and to mix electron and hole sub-bands within an energy range equal to the potential drop across the ribbon. Broken Dirac symmetry suppresses the wave function delocalization and the Zitterbewegung effect. The Büttiker formula for the conductance holds true for the odd $k$ symmetry. This, in turn, causes the ballistic conductance to oscillate within this region, which can be

5Compared to the magnetic field itself.

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used to design tunable field-effect transistors. The broken time-reversal symmetry
provides dichroism in the absorption of the circularly polarized light. As a
consequence, one can observe electrically enhanced Faraday rotation.

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Appendix A

Let us address the problem of finding eigenvalues/eigenfunctions of both types
of the nanoribbons when an electromagnetic field is applied as shown in figure 1.
We adopt the tight-binding model, where the magnetic field is taken in the form
of the Peierls phase added to the hopping coefficients between two sub-lattices.
GNRs are made of two equivalent sub-lattices $A$ and $B$ of carbon atoms with
sub-lattice constant $a$. The hybridization of $p_z$ valence electrons at each carbon
atom $|A(B); x, y\rangle$ provides the system electron wave function in the Bloch form
along the ribbon,

$$|\Psi_{n,k}\rangle = 2 \sum_{y=1}^{N} \Psi_{n,k}(y)(|A; y, k,\rangle, |B; y, k\rangle), \quad (A1)$$

where $k = k_x a$ is the particle wavevector along the ribbon; $|A(B); y, k,\rangle$ defines
the electron state in the $y$th unit cell on $A(B)$ carbon atom; and the spin index
is neglected. In the basis (A1), the wave functions $\Psi_{n,k}(y)$ satisfy the following
Schrodinger equations:

$$E_{n,k}\Psi_{n,k}(y) = [\mathcal{H}(\phi) + \mathcal{U}(U_0)]\Psi_{n,k}(y). \quad (A2)$$

Here, $E_{n,k}$ are hole $1 \leq n \leq N$ and electron $N + 1 \leq n \leq 2N$ energies given in the
unit of jumping energies between the sub-lattices $t_0 \approx 2.8$ eV. $\phi = 3\sqrt{3}B_z a^2/2$ is the
magnetic flux through the hexagon plaquette in units of quantum magnetic
flux $\phi_0 = \hbar c/e$. $U_0$ is the potential drop across the ribbon, also given in units of $t_0$. The first term in equation (A 2) is sensitive to the nanoribbon edge configuration
and can be written in the block-off-diagonal form using the corresponding $Q$ matrices,

$$\mathcal{H}_{ZNRR} = \begin{pmatrix} 0 & Q_{ZNRR} \\ Q_{ZNRR}^T & 0 \end{pmatrix}_{2N \times 2N} \quad \text{and} \quad \mathcal{H}_{ANR} = \begin{pmatrix} 0 & Q_{ANR} \\ Q_{ANR}^\dagger & 0 \end{pmatrix}_{2N \times 2N}. \quad (A3)$$

Here, the ZNR $Q$ matrix of $N \times N$ size is two diagonal, with its matrix elements
given by

$$(Q_{ZNRR})_{y,y'} = \delta_{y,y'} 2 \cos(\alpha_{y,k}) + \delta_{y,y'-1}, \quad (A3)$$

where the magnetic-field-dependent Peierls phase assumes the form $\alpha_{y,k} = \sqrt{3}k/2 + (y + 1/6)\pi \phi$ and the superscript ‘$\dagger$’ refers to the complex conjugate of the matrix and must not be confused with the Hermitian conjugate. The $Q$ matrix corresponding to the armchair configuration is three diagonal,

$$Q_{ANR}^{y,y'} = \delta_{y,y'} \exp(-i(2\alpha_{y,k} - \pi\phi/3)) + \delta_{y,y'-1} \exp(i\alpha_{y,k}) + \delta_{y,y'+1} \exp(i\alpha_{y-1,k}), \quad (A4)$$

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with the Peierls phase in the form of \( \alpha_{y,k} = \sqrt{3} k/\pi + (y + 1/2) \pi \phi/3 \).

The forms of \( Q \) matrices in equation (A3) and equation (A4) ascertain that
the hard-wall boundary conditions \( \psi_{y,k}(0) = \psi_{y,k}(N+1) = 0 \) are satisfied. For
the completeness of equation (A2), a fictional layer of carbon atoms has been
placed at both edges of the ribbon, so that the wave function vanishes on them.
For convenience we also change the coordinate origin to the centre of the ribbon,

\[
y \rightarrow \frac{N - 1}{2 - y_+} + 1. \tag{A 5}
\]

Alternatively, we may flip the nanoribbon with respect to its centre,

\[
y \rightarrow - \frac{N - 1}{2 - y_-} - 1. \tag{A 6}
\]

The above two transformations are used in the optical absorption of the left- and
right-polarized light. The DC electric field across the ribbon adds to the on-site
energies in the Hamiltonian (A2). Neglecting the potential drop within the unit
cell, the corresponding part of the Hamiltonian assumes block-diagonal form,

\[
U = \begin{pmatrix} U & 0 \\ 0 & U \end{pmatrix}_{2N \times 2N}, \tag{A 7}
\]

where \( N \times N \) sub-matrices have the diagonal form \( U_{y,y'} = U_0 \delta_{y,y'} (1/2 - y/N) \).

Note that in the absence of the electric field, the set of equation (A2) can be
split into the complimentary Harper equations for each of the sub-lattices.

References


