Valley filtering by a line-defect in graphene: quantum interference and inversion of the filter effect

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Abstract
Valley filters are crucial to any device exploiting the valley degree of freedom. By using an atomistic model, we analyze the mechanism leading to the valley filtering produced by a line-defect in graphene and show how it can be inverted by external means. Thanks to a mode decomposition applied to a tight-binding model we can resolve the different transport channels in \( k \)-space while keeping a simple but accurate description of the band structure, both close and further away from the Dirac point. This allows the understanding of a destructive interference effect, specifically a Fano resonance or antiresonance located on the p-side of the Dirac point leading to a reduced conductance. We show that in the neighborhood of this feature the valley filtering can be reversed by changing the occupations with a gate voltage, the mechanism is explained in terms of a valley-dependent Fano resonance splitting. Our results open the door for enhanced control of valley transport in graphene-based devices.

Keywords: graphene, line defect, valley filter, valleytronics

(Some figures may appear in colour only in the online journal)
finds a conductance dip which we interpret as resulting from destructive interference (known in the literature as Fano resonance or antiresonance). Interestingly, we find that around this conductance dip the valley filtering effect can be reversed by applying a gate voltage. This is, if around the Dirac point electrons incident on the defect at a given angle are predominantly transmitted on the $K$ valley, close to the conductance dip one can tune the occupation so that they are transmitted mainly on the $K'$ valley. The mechanism is explained in terms of a valley-dependent Fano resonance splitting. This reversal of the filtering effect could be useful, for example, to produce the analog of a spin-valve effect.

In the following we introduce our model Hamiltonian and the scheme used to resolve the scattering in $k$-space produced by the defect. Later on we examine the operation of the valley filter both close and away from the Dirac point and present our main results.

2. Hamiltonian model and mode decomposition

Let us consider a simple $\pi$-orbitals Hamiltonian [2, 4] for graphene:

$$H_{\pi} = \sum_i E_i \hat{c}_i^\dagger \hat{c}_i - \sum_{\langle i,j \rangle} \gamma_{ij} \left( \hat{c}_i^\dagger \hat{c}_j + \text{h.c.} \right) \tag{1}$$

where $\hat{c}_i^\dagger$ and $\hat{c}_i$ are the electronic creation and anihilation operators at site $i$, $E_i$ is the site energy and $\langle i,j \rangle$ denote that the summation is restricted to nearest neighbors. The transfer integrals between nearest neighbors is chosen as $\gamma_{0} = 2.7$ eV [4]. Since we are interested in the two-dimensional limit, we impose periodic boundary conditions along the armchair edge. This makes the quasi-momentum along the vertical direction (see figure 1(a)) a good quantum number which we will exploit later on. The defect is modelled by taking into account the changes in the topology of the lattice according to a 8–5–5 linear structure (see figure 1(c)) as in [9].

A tight-binding model is, a priori, not well suited for obtaining transmission probabilities as a function of the incident angle of the electrons, i.e. $k_x$ and $k_y$. Since the Hamiltonian is written in a real space basis, the momentum resolved information is hidden when one follows the standard procedure to compute the transmission probabilities from left to right [22, 23].

To gain resolution in reciprocal space we exploit the periodic boundary conditions and switch to a basis where $k_y$ is well defined, a similar strategy was followed in [20, 21]. In this basis the Hamiltonian of a pristine armchair ribbon with periodic boundary conditions can be written in block-diagonal form [4], where each block can be represented as shown in figure 1(b). Since the line-defect doubles the periodicity of the lattice along $y$ it couples only those modes with $k_y$ differing in $|k_y - k'_y| = 2\pi/2a$, where $a$ is the lattice parameter, which leads to the ladder model represented in figure 1(d).

The eigenvectors defining the new basis can be worked out analytically. By choosing slices of the ribbon as shown in 1(a), so that the carbon atoms are along the same vertical line, the ribbon has a periodicity of four of such slices. Then, the problem can be decoupled by changing to the following basis [4]:

$$|k_q\rangle = \frac{1}{\sqrt{n}} \sum_{j=1}^{n} \exp(i k_q j a) |j\rangle, \tag{2}$$

where $k_q = 2\pi q / a, q = 1,2,\ldots,n$ ($n$ being an even integer number) and the sum on the right hand side is over the lattice sites on each slice of figure 1(a). Therefore, one can see that in this basis one gets independent modes as shown in figure 1(b).

These modes are indexed by $k_q$, the quasimomentum in the vertical direction, and are represented by dimers with hoppings $\gamma_{0}$ and $\gamma_q = 2\gamma_{0} \exp(-i\pi q/a) \cos(q\pi/n)$.

These modes will be mixed by the line defect. The corresponding matrix elements can be obtained by writing the matrix of the defect $H_d$ in the basis of equation (2). This gives:

$$\langle k_q'|H_d|k_q\rangle = \begin{cases} 
\gamma_0 \cos(k_q a) & \text{if } q = q' \in [1, \ldots, n/2]. \\
-\gamma_0 \cos(k_q a) & \text{if } q = q' \in [n/2 + 1, \ldots, n]. \\
\gamma_q \sin(k_q a) & \text{if } q' = q + n/2. \\
0 & \text{otherwise} 
\end{cases} \tag{3}$$

Therefore, as a result of placing the defect in the sample, the dimers are now connected in pairs as represented in figure 1(d). At low energies these two modes are not simultaneously metallic, which means that an electron cannot be scattered from one valley to the other.

Each leg of the ladder corresponds to a well defined $k_y$. Thus, we still need to resolve the information on $k_y$. This can be done by noticing that the asymptotic states also have a well defined $k_y$ which is fixed by the dispersion relation of bulk graphene and a boundary condition (direction of incidence). Therefore, an interesting aspect of this representation is that both the longitudinal and transversal quasi-momentum of the asymptotic states can be resolved within a tight-binding model.

3. Valley filtering and inversion of the filter effect

To motivate our discussion let us examine the transmission probability through a very wide ribbon containing a line defect perpendicular to the transport direction ($x$) as introduced in the previous section. The result of a tight-binding calculation is shown in figure 2 with a full line, as a reference the result for a pristine system is shown with a dashed line. Overall, we can see a reduction of the transmission probability consistent with a defect-induced enhanced backscattering. The most prominent difference is the dip observed in the p-doped region (i.e. for energies below the Dirac point). We will come back to the physical origin of this feature later on.

Figure 2(a) provides information on the scattering for different energies of the incident electrons but it does not discriminate between valleys. One might be tempted to infer that the transmission probabilities for electrons entering the sample at a given incident angle is independent on whether the quasimomentum lies close to $K$ or $K'$. Figure 2(b) shows that this is not the case. There, we observe the dependence of the transmission probability with the angle of incidence.
and valley calculated from our tight-binding model at a Fermi energy close to the Dirac point. At normal incidence (0°) the value of the transmission is equivalent for electrons from both valleys. In contrast, at high incident angle we see a larger difference of transmission probability between electrons from different valleys, which means a larger valley polarization for those angles. This behavior is stable at energies close to the Fermi level and is consistent with the results reported in [9].

Now, exploiting the capabilities of our atomistic description, we turn to the study of the valley polarization further

Figure 1. (a) Scheme showing a graphene ribbon lattice decomposed into successive interconnected layers. A mode decomposition of the lattice shown in (a) leads to the independent modes represented in (b). (c) Detail of the line defect considered in the text. The defect couples two of the modes represented in (b) as shown in panel (d).

Figure 2. (a) Transmission probability as a function of the incident electronic energy for a ribbon with a line-defect (solid line). The simulations are for a system 93.7 μm wide. The transmission for a pristine system of the same dimensions is shown for reference with a dotted line. Notice the dip around $E = -540$ meV. (b)–(d) Representative polar plots of the transmission probability as a function of the angle of incidence on the line defect (0° corresponds to normal incidence, see scheme). (b)–(d) differ in the energy of the incoming electrons which are marked on panel (a) with grey vertical lines (dash–dot): (b) is for $E = -23.3$ meV, (c) is for $E = -594$ meV and (d) is for $E = -729$ meV. The solid line is for scattering around the $K$ point while the dashed line is for the $K'$ point. (b) and (c) show that the valley polarization gets inverted close to the transmission dip in (a).
away from the Dirac point. We are interested, in particular,
in the behavior close to the dip observed for negative doping
in figure 2(a). Interestingly, we find that the valley polariza-
tion is reversed around the conductance dip. Figures 2(c) and
(d) illustrate the dramatic change in angular dependence of
the transmission probability when the Fermi energy is slightly
shifted.

Let us examine the changes in the valley filter effect as
we move away from the Dirac point. For energies above the
Dirac point we find that the lobes shift their dominant angle
from grazing angles to angles closer to normal incidence as
the energy increases. On the other hand, for negative ener-
gies we see a richer behavior: As the energy moves further
away from the Dirac point the transmission degrades, espe-
cially at normal incidence, the lobes become thinner and their
maxima do not reach unity, see figure 2(c). Furthermore, for
each valley one notices an incipient new lobe in the opposite
quadrant, which becomes dominant as the energy is lowered
even further, see figure 2(d). Therefore, the operation of the
valley filter can be inverted by introducing a small change in
the Fermi energy (e.g. through an applied gate voltage).

The mechanism behind the valley filter inversion turns out
to be closely related to that of the conductance suppression.
The conductance dip reported earlier is the manifestation of
a destructive interference effect, known as Fano resonance
[24–26] or antiresonance [27, 28]. This can be visualized by
analyzing the individual modes represented in figure 1(d), a set
of representative transmissions is shown in figures 3(a)–(d).
The Green’s function determining the transmission contains
two contributions that can compete with each other: One corre-
sponding to direct transmission from left to right on the same
leg of the ladder, and another one which where the mode on
the opposite leg (which has a larger energy gap) is explored.
This can be captured by a simple two-pole approximation for
the retarded Green’s function determining the transmission:
\[ G_{RL} \sim \frac{1}{(\epsilon - E_0) - i \gamma_0 + E_0 - E_d} + \frac{1}{(\epsilon - E_0) - i \gamma_0 + E_0 + E_d} \].
The pole in the first term is located at \( \Im(E_0) > 0.5 |\gamma_0| \) and dominates over the second one which is on the p-doped side. This is because the second pole comes from the non-conducting leg of the ladder and therefore can only provide for a virtual process. The competition between these two poles leads to a destructive interference located closer to the non-dominant pole, on the p-doped side of the spectrum. As shown in figure 3, the precise position of this antiresonance or Fano-resonance feature changes slightly from one mode to the other giving the overall behavior shown in figure 2(a).

Figure 3. Panels ((a)–(d)) show the transmission probabilities for individual channels corresponding to a well defined \( k_y \) (represented in the insets, the empty dot being the nearest Dirac point). \( k_y \) (as measured from the nearest Dirac points) are set to 0, 2\( \pi \Delta/a \), 4\( \pi \Delta/a \), and 6\( \pi \Delta/a \) respectively (\( \Delta = 1/130 \)). (e) Total transmission probability for electrons from the \( K \) and \( K' \) valleys in solid and dashed lines respectively, for the (0° – 90°) quadrant. Inversion of dominant polarization current occurs at \( E_6 = -620 \text{ meV} \) (marked with a vertical grey line).
Now, the question is how is this destructive interference linked to the inversion of the valley filter effect. To rationalize it let us examine more closely the panels in figure 3. One can see that while moving away from the Dirac point in a chosen direction (as in figures 3(b)–(d)) the poles in the two-pole approximation get closer together in one valley while they get further apart in the other. Therefore, as one moves away from the Dirac point, the destructive interferences on each valley, which are degenerate in figure 3(a), follow the movement of the pole on the p-doped side (3(b)–(d)), thereby suffering a valley-dependent splitting (the position of the Fano resonances is marked with arrows in figure 3). This splitting, in turn, produces the observed change in the valley polarization direction around the destructive interference. This behavior can also be verified analytically from the ladder model.

To better visualize the valley-dependent splitting of the Fano resonance let us consider the sum of all the transmission probabilities from electrons with incident angles in one valley, which means zero polarization for the whole quadrant (vertical line) and one has balanced transmission from both valleys, thereby suffering a valley-dependent splitting (the position of the Fano resonances is marked with arrows in figure 3). This splitting, in turn, produces the observed change in the valley polarization direction around the destructive interference. This behavior can also be verified analytically from the ladder model.

4. Conclusions

We have shown a new mechanism leading to an inversion of the valley filtering effect in graphene: the valley-dependent splitting of the Fano resonances. Our results for graphene with a line-defect show that this could be achieved on the p-doped side where a destructive interference is present. This would allow for better control of valley filtering in graphene and one could envisage, for example, the realization of the analog of a spin-valve [29] by using two valley filters in series with their easy valley axis inverted.

Indeed, previous works showed that line defects in series could provide for an enhanced control of the valley polarization [21]. Nonetheless, since the authors focused in the vicinity of the Dirac point, where the mechanism that we propose is not active, the use of creative configurations together with a gate voltage remains as an interesting problem for further study.

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