Controlled engineering of spin-polarized transport properties in a zigzag graphene nanojunction

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Abstract – We investigate a novel way to manipulate the spin-polarized transmission in a two-terminal zigzag graphene nanoribbon in the presence of the Rashba spin-orbit (SO) interaction with a circular-shaped cavity engraved into it. A usual technique to control the spin-polarized transport behaviour of a nanoribbon can be achieved by tuning the strength of the SO coupling, while we show that an efficient engineering of the spin-polarized transport properties can also be done via cavities of different radii engraved in the nanoribbon. Simplicity of the technique in creating such cavities in the experiments renders an additional handle to explore transport properties as a function of the location of the cavity in the nanoribbon. Further, a systematic assessment of the interplay of the Rashba interaction and the dimensions of the nanoribbon is presented. These results should provide useful input to the spintronic behaviour of such devices. In addition to the spin polarization, we have also included an interesting discussion on the charge transmission properties of the nanoribbon, where, in the absence of any SO interaction a metal-insulator transition induced by the presence of a cavity is observed.

Introduction. – Spin-based electronics or spintronics is one of the most promising field for future power-consuming high-operating speed, new forms of information storage and logic devices [1]. The key factor for the development of spin-based electronics [2] is the fine control of the spin-polarized current. For this purpose, a major challenge is developing a suitable spin transport channel with long spin diffusion length and spin lifetime. Graphene [3], believed to be a very promising candidate in the spintronic applications, owing to the achievement of room temperature spin transport with long spin diffusion lengths (up to ∼100 μm) [4–8]. Graphene has also several interesting electronic and transport properties [9], that make it very attractive for spintronic applications, such as quasirelativistic band structure [3,10], unconventional quantum Hall effect [3,10,11], half-metallicity [12,13] and high carrier mobility [14,15].

Recent experimental realization of free-standing graphene nanoribbons (GNRs) [16,17] has generated renewed interest in carbon-based materials with exotic properties. GNRs are basically single strips of graphene where electronic properties [18,19] depend on the geometry of the edges and the lateral width of the nanoribbons [20]. Depending upon the edge structures, GNRs can be of two types, namely armchair graphene nanoribbon (AGNR) and zigzag graphene nanoribbon (ZGNR). Irrespective of the width of the ZGNR, they are always metallic with zero bandgap, while the AGNRs are conditionally metallic, that is when the lateral width \(N_y = 3M - 1\) (\(M\) is an integer), else the AGNRs are semiconducting in nature [18] with a finite band gap. GNR is also known to have long spin diffusion length, spin relaxation time, and electron spin coherence time [21–23].

SO coupling (SOC) plays a crucial role in spintronic devices. Two kinds of SOC can be present in graphene, the intrinsic SOC and the Rashba SOC (RSOC) [24,25]. The strength of the intrinsic SOC is negligibly small in pristine graphene (up to ∼0.01–0.05 meV) [26,27]. On the other hand, the strength of the Rashba SOC can be modulated by an external electric field or by using substrates. Recent observations showed that the strength of the Rashba SOC can be enhanced up to 100 meV from...
gold (Au) intercalation at the graphene-Ni interface [28]. A Rashba splitting about 225 meV in epitaxial graphene layers grown on the surface of Ni [29] and a giant Rashba SOC (~600 meV) from Pb intercalation at the graphene-Ir surface [30] are noted in experiments. In view of the above discussion, GNRs can be used as spin-based devices. Consequently a variety of graphene-based spintronic devices have been proposed [31–39], for example, prediction of spin-valve devices based on graphene nanoribbons exhibit giant magnetoresistance (GMR) [33], spin-valve experiment on GNR [34], study of spin polarization and giant magnetoresistance in GNR [35], experiments of GNR as field-effect transistor [36] and p-n junctions [37] using the bottom-up fabrication technique and many more [38,39]. However, most of the studies have been dedicated to making GNR as information storage or attempted to get larger spin polarization. For a complete realization of spintronic applications, a fine control of the spin polarization is highly desirable.

Further, a few of the studies have been dedicated on the transport properties and band structures of graphene nanoribbons in the presence of antidots [40–43], which, in essence, is the same as our “cavity”. These studies were basically searching for possible ways to open up energy gaps at the Dirac points to propose an on-off switching mechanism using graphene nanoribbons. In this work, in addition to the charge transport properties being alluded briefly, our central focus is to deliberate on the spin-polarized transport in order to explore spintronic application elaborated in the subsequent discussion.

In this letter, we have proposed a possible way of tuning the spin polarization in ZGNR modulated with a circular-shaped cavity in the presence of Rashba SOC. We have shown that the spin-polarized transmission of a two-terminal ZGNR can be tuned by varying the radius of the circular cavity. Recent experimental advancement in making nanoscale devices also indicates that our proposed theoretical model can be achieved experimentally. Fischbein et al. showed that it is possible to realize nanometer-scale pores in graphene by controlled exposure to the focused electron beam of a transmission electron microscope [44] and most importantly they do not evolve over time. Nanolithographic technique [45], template growth [46] technique can be used to achieve the desired shape and size of nanopores with great accuracy.

If graphene is grown on a corrugated target substrate, it acquires the morphology of the substrate, leading to ripples [44]. This, in turn, enhances local SO coupling [47]. For example a ~10 meV SO splitting has been reported in a flat Au monolayer [48], whereas graphene-Au hybridization enhances the Rashba splitting up to 100 meV [28]. Moreover, intercalation of a Pb monolayer between graphene and Ir(111) results into an almost negligible structural corrugation and reduces the overall SO coupling [49]. In this work, all the calculations are carried out by assuming a flat GNR (uncorrugated) and thus such corrugated scenario is not taken into consideration.

We organize our paper as follows. In the following section, we present the proposed model and the theoretical formalism for the total transmission and spin-polarized transmission using the Green’s function technique. Subsequently, we include an elaborate discussion of the results where we have demonstrated the cavity effect in ZGNR on the spin polarization, that is, how the spin polarized transmission behaves with the dimension of the system and with the position of the centre of the cavity. We end with a brief summary of our results.

**Model and theoretical formulation.** – We consider a zigzag graphene nanoribbon (ZGNR) inscribed with a circular-shaped cavity structure as shown in fig. 1 (top). The length and the width of the ZGNR are 2L and 2W, respectively. The radius of the circular-shaped cavity is r and the position of the centre of the cavity is (dx, dy). We consider a two-terminal setup as shown in fig. 1 (bottom) in order to calculate the charge and spintronic properties of the ZGNR, where two leads are attached to the central scattering region (ZGNR in this case). The leads are denoted by red color and are semi-infinite and free from any kind of SO interactions. The Rashba interaction is assumed to be present in the central scattering region only.

The length and the width of the system can be defined in the following way. Since along the length, the system has a zigzag shape and along the width an armchair one, we call the system mZ-nA as shown in fig. 1 (bottom). The system dimension can also be expressed in nm with the help of the following relations [50]: 

\[ L_x = \frac{\sqrt{3}}{2}(m - 1)a, \]

\[ L_y = \frac{3}{2}a(n - 1)a, \]

where a = 0.142 nm. Though the nm unit is useful to measure sample dimensions experimentally, the mZ-nA notation is also helpful in some cases to visualize...
the system. Thus, throughout this work, we shall use the nm unit as well as the mZnA notation. However, the radius of the cavity, \( r \), is measured in nm.

The tight-binding (TB) Hamiltonian modelled on a ZGNR in the presence of the Rashba SO interaction can be written as [24,25]

\[
H = -t\sum_{\langle ij \rangle} c_i^\dagger c_j + i\alpha\sum_{\langle ij \rangle} c_i^\dagger(\hat{\sigma} \times \hat{d}_{ij})_z c_j, \tag{1}
\]

where \( c_i^\dagger = (c_i^\uparrow, c_i^\downarrow) \). \( c_{i\sigma} \) \( (\sigma = \uparrow, \downarrow) \) is the creation operator of an electron at site \( i \) with spin \( \sigma \). The first term is the nearest-neighbor hopping term, with a hopping strength \( t = 2.7 \text{ eV} \). The second term is the nearest-neighbor Rashba term which explicitly violates the \( z \to -z \) symmetry. \( \hat{\sigma} \) denotes the Pauli spin matrices and \( \alpha \) is the strength of the Rashba SO interaction. \( \hat{d}_{ij} \) is the unit vector that connects the nearest-neighbor sites \( i \) and \( j \).

The total transmission coefficient \( T \) can be calculated via [51–53],

\[
T = \text{Tr}[\Gamma_L G_R \Gamma_R G_A]. \tag{2}
\]

\( \mathcal{G}_{R(A)} \) is the retarded (advanced) Green’s function. \( \Gamma_L (\Gamma_R) \) are the coupling matrices representing the coupling between the central region and the left (right) lead.

Finally, we calculate the spin-polarized transmission coefficient \( P_s \) from the relation as [54]

\[
P_s = \text{Tr}[\hat{\sigma}_s \Gamma_L G_R \Gamma_R G_A], \tag{3}
\]

where \( s = x, y, z \) and \( \sigma \) denotes the Pauli matrices.

We have studied the charge and spin properties of ZGNR modulated with a circular-shaped cavity structure.

**Results and discussions.** – We set the hopping term \( t = 2.7 \text{ eV} \). All the energies are measured in units of \( t \). For most of our numerical calculations, we have used KWANT [55]. In order to visualize the critical roles of RSOI, and, for the sake of comprehensive analysis we have taken the RSOI strength over a wide range varying from a moderate value (0.05–0.135 eV) to a very large one (0.5–1.35 eV), which is referred to as a giant Rashba SO coupling.

Before going into the results, there is one important point about the spin-polarized transmission that should be mentioned. Since the ZGNR has longitudinal mirror symmetry along the \( x \) and \( z \) axes, the \( x \) and \( z \) components of the spin-polarized transmission are zero. Only the \( y \)-component has a non-zero value (due to the finite width of the ZGNR along the \( y \)-direction) [38,39]. Hence from now on, we shall call the \( y \)-component of the spin-polarized transmission coefficient by \( P \).

In fig. 2, the total transmission coefficient \( T \) is plotted as a function of the Fermi energy \( E \) in the absence of the Rashba SO interaction. We set the dimension of the ZGNR as 9.8 nm-8.4 nm (81Z-40A). The red color denotes the plot without a cavity, while the black one denotes the one with cavity with radius \( r \sim 2.5 \text{ nm} \). When the cavity is absent in the system, \( T \) shows the usual discrete step-like feature emphasizing the occurrence of quantum transport at discrete energy values. As the cavity is introduced, the transmission loses its step-like feature and also the magnitude of \( T \) gets suppressed. Another important observation is that, in the absence of the cavity, a \( 2e^2/h \) plateau is observed around the zero of the Fermi energy. This \( 2e^2/h \) plateau plays a vital role in determining the presence of edge states [18,56]. However, this \( 2e^2/h \) conductivity plateau vanishes as we introduce cavity in the system. For better clarity the behaviour of \( T \) is plotted, near the zero of the Fermi energy, in the inset in fig. 2(a).

In order to have more information about the vanishing nature of the \( 2e^2/h \) plateau near the zero of the Fermi energy, we have plotted the total transmission \( T \) as a function of the radius of the cavity as shown in fig. 2(b). Here, we set the Fermi energy at zero. From fig. 2(b), it is observed that \( T \) smoothly falls off as we increase the radius of the cavity and vanishes completely after a certain value of \( r \).

For \( r \lesssim 2.5 \text{ nm} \), the system shows metallic behavior, and, for \( r \gtrsim 2.5 \text{ nm} \) it acts as an insulator. Thus, a metal-to-insulator (MI) transition across the zero Fermi energy can be achieved in a ZGNR using an inscribed cavity. Most importantly, this feature is observed in the absence of any kind of SO interaction. Basically, as we increase the radius of the cavity, the transmission gap is enlarged due to the finite-size effect and, as a result, the MI transition occurs in the system. The same findings for larger system dimensions have also been obtained and we have found that though the behavior of \( T \) is not exactly the same as shown in fig. 2(b) but in all the cases, beyond a certain value of \( r \), the system looses the plateau and becomes an insulator.

Let us now include the effect of the Rashba SO interaction and explore the interplay between RSOI and cavity on the spin-polarized transport. The spin-polarized transmission behavior in the absence and presence of cavity are presented in fig. 3. All the plots for the spin-polarized transmission are antisymmetric in nature as a function of the Fermi energy \( E \) which is due to the electron-hole symmetry of the system. The radius of the cavity is taken as \( r \sim 2.5 \text{ nm} \) and the system size is kept fixed at
9.8 nm-8.4 nm (81Z-40A). For smaller values of RSOI, namely, \( \alpha = 0.05 \) and 0.1, the spin-polarized transmission shows reasonably large fluctuations for the cavity-free system as a function of \( E \), especially within the range \(-1 \leq E \leq 1\) (red lines of figs. 3(a) and (b)). Whereas the fluctuations get suppressed in the presence of the cavity (black lines of figs. 3(a) and (b)). Interestingly we see that for these smaller values of RSOI, much larger spin polarization is achieved in the presence of a cavity beyond the range \( E > 1 \) and \( E < 1 \), which may give an important hint of achieving a high degree of cavity-induced spin polarization, and, to the best of our knowledge, this phenomenon has not been discussed so far in the literature. Along with the cavity, the fluctuations get also suppressed with increasing the strength of RSOI, as clearly seen from fig. 3(c). Though a smooth curve is obtained, which is always favorable in the context of a physical measurement, the strength of RSOI in this case (fig. 3(c)) is too large and has not been achieved experimentally so far. For our theoretical study, we choose one such large value of \( \alpha \) along with other smaller ones, for the sake of a complete analysis. Comparing the spectra given in fig. 3, one can see that the overall magnitude of \( P \) enhances with the rise of \( \alpha \).

The above analysis raises an obvious question whether one can tune spin-polarized transmission by varying the radius of the cavity. To explore it, let us look into the spectra given in fig. 4 where the \( P-r \) characteristics are shown at three typical energies (\( E = -2.5, -1.5 \) and \(-0.5 \) (in units of \( t \))) considering a reasonably large system, compared to the previous one, having system size 15 nm-12.6 nm (121Z-60A). We choose arbitrarily these typical energies where the transmission probability \( T \) is sufficiently high (\( E = 0 \) is not a good choice, as in this case \( T \) goes to zero beyond a critical value of \( r \), as clearly seen from fig. 2). Several interesting features are noticed. For different values of \( E \), the signs of \( P \) are different depending on the dominating spin band (up or down). The most notable aspect is that, as we increase \( r \), up to \( r \sim 3 \) nm, the degree of polarization increases, beyond which it starts to decrease. For larger values of \( r \), i.e., when \( r \approx 6 \) nm, \( P \) almost drops to zero. This vanishing nature of \( P \) at large \( r \) is associated with the fact that the number of conducting channels gradually decreases with removing the lattice sites (that is, increasing cavity size), and beyond a critical radius, almost no paths are available for electronic conduction which yields vanishingly small polarization. But below this critical radius that is, where \( P \) is finite one may always expect that reduced spin polarization with increasing \( r \) as spin-dependent scattering mechanism, associated with the Rashba term, gets weaker with the removal of lattice sites. But the results of fig. 4 show a non-monotonic nature where \( P \) initially increases for smaller \( r \), and after reaching a maximum, it \( (P) \) decreases for large values of \( r \). There are several possible reasons for that as the polarization effectively depends on which spin channel (up or down) is dominating. One possible reason is the existence of large fluctuations at low cavity sizes, where for a particular energy \( E \), \( P \) differs by reasonably large values for two distinct cavity sizes. This difference gradually decreases with large values of \( r \), consistent with the suppression of fluctuations, and in that case, reduced values of \( P \) are observed with \( r \), as expected.

Fig. 3: (Color online) Spin-polarized transmission as a function of the Fermi energy \( E \) for three different strengths of RSOI (\( \alpha \)) considering the system dimension 9.8 nm-8.4 nm (81Z-40A), where the black and red colored curves correspond to the systems with and without cavity, respectively. The radius of the cavity is fixed at \( r \sim 2.5 \) nm.

Fig. 4: (Color online) \( P-r \) characteristics at three typical energies considering the system size \( \sim 15 \) nm-12.6 nm (121Z-60A).
From the spectra given in figs. 3 and 4 we get a clear hint that one can tune \( P \) by regulating the cavity size, which is our primary goal of the present analysis. Now, as the value of \( P \) depends on the specific choice of the energy \( E \), we need to scrutinize further by considering a wider range of energy in order to understand the precise role of cavity on spin polarization. In order to do that, in fig. 5 we show the variation of \( P_{\text{max}} \) (maximum value of \( P \)) with \( r \) for two different strengths of RSOI (namely \( \alpha = 0.05 \) and 0.1) considering the same system size as taken in fig. 4. \( P_{\text{max}} \) is computed by taking the maximum value of \( P \) over the complete energy window \([-3,3]\) (in units of \( t \)). It is seen that \( P_{\text{max}} \) decreases with \( r \) providing minor fluctuations, and eventually reduces nearly to zero. The decreasing nature can easily be understood, following the results of figs. 3 and 4, as the scanning is done over the full energy window. The reduction of \( P_{\text{max}} \) with \( r \) does not actually yield a negative response towards the tuning mechanism using a cavity, as in the calculation of \( P_{\text{max}} \) it takes the maximum value of \( P \). While in an experimental situation whenever we talk about possible tuning of \( P \) with a cavity, we need to fix the Fermi energy at a particular value and there is a high possibility to achieve favorable spin polarization and even much higher polarization than the cavity-free case, as reflected in figs. 3 and 4.

For completeness, we have also studied the finite-size effects on the behavior of spin-polarized transmission, as shown in fig. 6 and fig. 7, respectively. In fig. 6(a), we have shown the effect of the length (in units nm) of the system on \( P \) without cavity and in fig. 6(b) with cavity of radius \( r \sim 3.7 \text{ nm} \). The width of the system is taken \( \sim 16.9 \text{ nm} \) (\( W = 80 \text{ A} \)). We set \( \alpha = 0.1 \). The spin-polarized transmission shows large fluctuations in fig. 6(a). However, in the presence of the cavity, the behavior of \( P \) is smooth and oscillating in nature as a function of the length of the system. Further, the effect of the width \( W \) (in units of nm) of the system on the spin-polarized transmission is shown in fig. 7. Here we have taken the system length as \( \sim 14.8 \text{ nm} \) (121Z) and fixed the Rashba SO interaction strength at \( \alpha = 0.1 \). In the absence of cavity, \( P \) shows more fluctuations (fig. 7(a)) than that with the cavity case (fig. 7(b)). In both the cases, \( P \) initially increases with \( W \) up to \( W \sim 15–16 \text{ nm} \), then it tends to saturate. However, the rate of change of \( P \) is more in the presence of cavity compared to the cavity-free case. Now, as we increase the width of the system the number of modes available for transport increases. As a result, initially \( P \) increases with \( W \). However, when \( W \) is large enough compared to the radius of the cavity, which is the case for \( r \sim 3.7 \text{ nm} \), the system tends to behave as that without cavity.

In all the results discussed so far the centre of the cavity was fixed at the origin or in other words, the position of the centre of the cavity was fixed at \((d_x, d_y) = (0, 0)\) (see fig. 1 (top)). It is also important to see how the position of the centre of the cavity affects the spin-polarized transport. In other words, in order to answer a rather important question, \( i.e., \) whether there is anything like the most suitable position for the cavity to exist in the system that would yield the maximum spin-polarized transmission. To do that, we have considered two different scenarios. First, we have varied the \( x \)-coordinate \((d_x)\) keeping the \( y \)-coordinate fixed at \( y = 0 \) \((d_y)\). In the second case, we have varied \( d_y \) along the \( x = 0 \) line. Thus, the translations of the cavity in both the \( x \) and \( y \) directions are considered.

The behavior of the spin-polarized transmission as a function of the \( x \)-coordinate of the centre of the cavity \( d_x \) (in units of nm) and symmetrically with respect to the origin is shown in fig. 8 for two different values of the Fermi energy, namely \( E = -2.5 \) and \(-1.5 \) in the presence of the Rashba SO interaction. We have taken three different values of \( \alpha \), which are \( \alpha = 0.05 \) (fig. 8(a)), \( \alpha = 0.1 \) (fig. 8(b)), and \( \alpha = 0.1 \) (fig. 8(c)).
The centre of the cavity is moving along the $y = 0$ line, and here we choose $r \sim 3.7$ nm.

The position of the centre of the cavity is also an important feature for larger dimensions of the system and for larger values of the width it tends to saturate. However, the main focus of this work, that is the tuning of the spin-polarized transmission, shows qualitatively similar behavior for larger dimensions of the system. The position of the centre of the cavity is also an important parameter for tuning the spin-polarized transmission. In order to achieve higher spin-polarized transmission, we issue a word of caution that one should not put the cavity at far left or far right edge of the system, since at these positions, $P$ has lower values compared to other intermediate locations.

**Conclusion.** – In summary, we have studied briefly the charge transmission and more elaborately spin-polarized transport properties in a two-terminal ZGNR modulated with a circular-shaped cavity in the presence of RSOI. The charge transmission shows interesting feature in the presence of the cavity. In particular, we notice a cavity-induced MI transition in the interacting free system. From the detailed analysis of spin-polarized transport we have shown that by varying the radius of the cavity, one can tune the spin-polarized transmission efficiently in a two-terminal ZGNR. All the results are obtained for fairly large dimensions of the system. Moreover, we have also studied the effect of the system dimension, such as the length and width of the system on the spin-polarized transmission. The spin-polarized transmission oscillates with the length of the system and for larger values of the width it tends to saturate. However, the main focus of this work, that is the tuning of the spin-polarized transmission, shows qualitatively similar behavior for larger dimensions of the system. The position of the centre of the cavity is also an important parameter for tuning the spin-polarized transmission.
at the extreme left or at the extreme right edge of the system.

Considering the success of fabricating “holey graphene” [57] seamlessly, our work may render a new direction to engineer tunable spin-polarized transport properties of GNRs via cavities of different shapes and sizes.

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