Exclusive sub-lattices for extended and localized states in graphene ribbons: their role in Klein tunneling, disorder and magnetic field effects

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Abstract

We report the existence of two sub-lattices in metallic graphene nanoribbons that present a decoupled behavior. Each sub-lattice, one for extended states (ES) and another exclusively for localized states (LS), is formed by a combination of A and B graphene sites. In the sub-lattice ES all electronic transport phenomena occur, including the Klein tunneling through an external applied potential barrier. In contrast, the sub-lattice LS does not contribute to the transport of quasi-particles and strongly localized states are induced within the potential barrier region. The sub-lattices ES and LS are detected by analyzing Klein states and totally localized states that were systematically perturbed by the contributions of hyperboloid bands generated by the potential barrier. This is performed by gradually increasing the energy of the applied potential. The existence of both sub-lattices are tested by considering disorder and magnetic field effects in the system. The results indicate that both sub-lattices behave as if there are decoupled, even at the presence of an external applied barrier and that they can be coupled by applying an external magnetic field.

1. Introduction

Graphene, a two-dimensional material composed by a mono-layer of carbons distributed in a honeycomb lattice [1, 2], has shown interesting electronic properties in analogy with the ones observed in quantum electrodynamics. The pseudo-spin, the Dirac cone, the chirality and the absence of backscattering show the graphene’s relativistic behavior [3–5]. The study of these phenomena in condensed matter physics made possible the investigation of related effects that were not observed before, such as the Klein tunneling [6–8] for low energies. The graphene’s unique properties have attracted the interest of theoretical and experimental researches, mainly to develop applications in quantum computation, spintronics, valleytronics, gas sensors, fuel cells, field effect transistors, Fabry-Pérot interferometers, and pseudo-spin filters among other nano-electronic devices [9–14]. The properties of the graphene’s two-dimensional lattice represented by the sub-lattices A and B (known as pseudo-spins [2], mathematically very similar to spin and unique to graphene sub-lattice degeneracy) are the starting point to explain the analogies that the graphene has with the physics of relativistic particles. The pseudo-spin in graphene is the result of the superposition of the electron orbitals of two carbon atoms in the hexagonal lattice unit cell. The relativistic analogues can be elegantly studied in graphene using a tight-binding representation of the graphene’s hexagonal lattice, where the Dirac cone is very well reproduced by the tight-binding band at low energies [15, 16].

In the last years, quasi one-dimensional structures called nanoribbons were obtained from graphene. These structures are very similar to the carbon nanotubes [17], in which transverse confinement phenomena directly related to the nanoribbon border shape are expected [18, 19]. A special interest is given to the graphene nanoribbon with armchair edge (AGR), which presents a metallic or semiconductor behavior depending on its
width. The existence of metallic nanoribbons were reported for widths larger than 4 nm [20]. In this work we are mainly focus in their metallic behavior and for that reason we have considered nanoribbons with widths of 6 nm and above. In the metallic AGR a single K valley is observed in the band structure [21, 22], preventing a valleytronic in this ribbon. However, interesting properties related to the pseudo-spins can be used to generate a latticetronic of currents [9, 14].

The main objective of this work is to show that the metallic AGR behaves, at the presence of an applied potential barrier, as if there were two completely decoupled sub-lattices, each one formed by a combination of the graphene sites A and B. One of these sub-lattices is exclusively formed by extended states (ES) and the other exclusively by localized states (LS). In the sub-lattice ES all quasi-particle transport effects occur, including the Klein tunneling through the potential barrier. On the contrary, the sub-lattice formed by the localized states does not contribute to the transport of quasi-particles, i.e. the Klein tunneling is completely suppressed. The sub-lattices LS and ES reported here were obtained by analyzing Klein states gradually perturbed by hyperboloid band contributions due to an external applied barrier. This is performed by gradually increasing the energy of the applied barrier $V$. The existence of the sub-lattices LS and ES could lead to an asymmetry in the contributions of the impurities located on the lattice sites A and B. In general, this occurs if the impurities are randomly located in sites corresponding to the sub-lattice LS and therefore they do not contribute to the electronic transport. Thus, the recent reported phenomenon [23–26] in which doping occurs asymmetrically between the two sub-lattices (A and B) is a current interesting topic related to our work.

In previous works [27–29], destructive interference effects were reported at each three sites starting from the armchair graphene nanoribbon edge. This interference generate an armchair configuration for the available wavefunction of the system. Probability density and density of states (DOS) calculations had shown this destructive effects locally. The armchair configuration for the available wavefunction shown in those works arise as a result of a collective interference effect of all lattice sites. However, the individual role of each site in the total interference can not be inferred. For example, if we perturbed or change one (or several) lattice sites we will expect changes in the probability density as well as in the DOS. In this work we show that perturbations applied over the sites of the sub-lattices LS seem not to affect the extended states of the system. Also, we show in this work (using an external applied barrier $V$) that we can generate in the sub-lattice LS total localized states that apparently do not couple with the sites of the sub-lattice ES. This is performed via numerical simulations. Given a Hamiltonian of the form $H = H_{ES} + H_{LS} + V_{coupling}$, where $V_{coupling}$ couples the Hamiltonians $H_{ES}$ and $H_{LS}$ of the sub-lattices ES and LS, the transport properties of the system remain unaltered when changes in $H_{LS}$ are induced via artificial impurities, i.e. we do not have an effective coupling between $H_{LS} e H_{ES}$.

For the reasons above, the relevant states to consider in our work are not the pure Klein states. The hyperboloid band contributions, induced by high values of the applied barrier $V$, generate states with a mixture of Dirac and Schroedinger properties. It is possible to distinguish between extended and localized states. The extended states exhibit an opposite pseudo-spin polarization at both sides of the barrier while the localized states do not show any signs of polarization and are exclusively located inside the barrier region. These properties allow us to identify which sites of the nanoribbon are used by the extended and localized states and in this way to define the sub-lattices LS and ES studied in this work. The states in the sub-lattice LS are generated by applying a high potential values $V$ that strongly localize them inside the barrier region. These states are uniformly (and exclusively) distributed inside the barrier region. We will use the nomenclature $S_\alpha$ to refer us to the localized states in the sub-lattice LS.

On the other hand in the sub-lattice ES, when the chirality property that couples the hole-type wavefunction (inside the barrier) with the electron-type wavefunction (outside the barrier) is not longer robust, in comparison with the applied potential $V$, the Klein states are perturbed by the hyperboloid bands and the transport starts to decrease. While they still have the property of tunneling through the barrier, the states under this limit (since they are not pure Dirac states) were called in this work quasi-Klein states to avoid confusion with the pure Klein states. However, after a certain value of the applied potential $V$ the tunneling is totally destroyed and the transport ceases. Under this condition the quasi-Klein states are divided into two parts, a hole-type wavefunction inside the barrier region and an electron-type wavefunction at both sides of the barrier. The localized hole-type wavefunction that remains inside the barrier is similar to the one formed in the sub-lattice LS. We will refer to the localized hole-type wavefunction in the sub-lattice ES as $S_\beta$ state. Outside the barrier and around the Dirac point the wavefunctions in the sub-lattice ES continue to exhibit a topology similar to the pure Klein states, which is a sign of lack of scattering.

The detection of $S_\alpha$ states (and consequently the detection of the sub-lattice LS) can be hard, as we shall see in section 3.2, due to two important facts: (a) the quasi-Klein and $S_\alpha$ states have the same energy, i.e. they are degenerated, and (b) the $S_\alpha$ states are located in a sub-lattice that seems decoupled (or have small interactions) from the one that generates the electronic transport. As a consequence of this lack of coupling, the Fano resonances will not be observed in the conductance maps and therefore the detection of the sub-lattice LS related to the $S_\alpha$ states would remain hidden. So, in order to detect the $S_\alpha$ states in the conductance maps it is necessary a
mechanism that could couple the sub-lattices LS and ES. We will show that an applied magnetic field can be used for this purpose.

The paper is organized as follows, in the next section we briefly describe the method and the model considered. In section 3 we present and discuss our results. In section 4 some final considerations are made.

2. The model and method

The system depicted in figure 1(a) was used to address and illustrate our discussions: a metallic AGR of width $W$ perturbed by the potential barrier of width $L$ and height $V/t$. The calculation of the electronic transport properties were performed using the Green function formalism in the tight-binding lattice $[30, 31]$, where the first neighbors free-electron Hamiltonian was written as

$$H = -\sum_{i,j} t(i|j) + \sum_j V(j)|j\rangle \langle j|,$$

(1)

with $i = (x, y)$. Here the hopping $t[32]$ is approximately 3 eV and $V(j)$ is the electrostatic potential applied on the AGR sites (along $L$) that acts as the scattering source for the calculated conductivity. The retarded Green propagators are calculated by

$$G(E) = (E - H - \Sigma^L - \Sigma^R + i\eta)^{-1},$$

(2)

where the self-energies $\Sigma^R$ and $\Sigma^L$ of the contact leads are numerically calculated using the recursive Green function method $[31, 33–36]$. With these propagators we computed the DOS and the local density of states (LDOS) as described in $[31, 35, 37]$. We used

$$\eta_k = -\frac{1}{\pi} \text{Im}\{\text{Tr}[G(E)]\},$$

(3)
for the DOS calculations and
\[
          \rho_E(i) = -\frac{1}{\pi} \text{Im}[G(i, E)],
\]
for the LDOS ones. For the calculation of the trace in equation (3) we considered all the diagonal elements of the matrix \( G(E) \).

The partial pseudo-spin polarization (PP) is defined, using the LDOS [14] at each side of the barrier (see figure 1(c)), as
\[
PP = \sum_i |\rho_{E,i}| - \sum_i |\rho_{E,\bar{a}}| \sum_i |\rho_{\bar{a}}|.
\]
Notice that the PP is defined for a specific energy \( E \), where the \( A \) (\( B \)) subscript corresponds to the use of solely \( A \) (\( B \)) sites in the calculations. In this work we do not show quantitative calculations of the PP. It is only used as a tool for the identification of the sub-lattices ES and LS.

Finally, the conductance (\( \sigma \)) is obtained by the Fisher-Lee relation [38],
\[
\sigma_E = \frac{2e^2}{h} \text{Tr}[\Gamma_L G_{1M}(E) \Gamma_R G(E)^\dagger].
\]
The trace in equation (6) is calculated using the diagonal elements of a sub-matrix in \( G(E) [G_{1M}(E)] \) that couples the entry (1) and exit (M) transversal chains. In this equation \( \Gamma_L (\Gamma_R) \) is the matrix that couples the central scattering region (the considered system) with the contact lead of the left (right).

The system considered in figure 1(a) is useful because it allows us to identify the PP in the LDOS (around the Dirac point) when the ribbon is perturbed by an applied barrier, see figure 1(c). This fact eases the detection of the sub-lattices LS and ES.

The main objective is to show that the metallic AGR behaves as if there were two decoupled sub-lattices, one for extended states and another for localized ones. In order to study the contribution of each sub-lattice to these physical quantities, we have calculated \( \eta_{\alpha}, \rho_E(i) \) and \( \sigma_E \) for each sub-lattice (LS and ES) separately. We performed this calculation by considering the contributions of the propagators \( G(E) \) for each sub-lattice.

In our simulations we have considered systems of metallic behavior, with widths between \( W = 6 \) nm (graphene nanoribbon) and \( W = 40 \) nm (graphene ribbon). All these systems have shown similar behaviors in the simulations performed. We have rescaled with \( t \) the energy, \( E/t \), and the potential barrier energy, \( V/t \), i.e. we will use dimensionless energies from now on.

### 3. Results and discussion

#### 3.1. Defining the sub-lattices ES and LS

In figure 1(b) a high potential barrier \( V/t \) applied over a region \( L \) of the graphene ribbon induces the participation of hyperboloid bands inside the barrier region. In this figure we show how the number of hyperboloid bands that pass through the Dirac point (\( E/t = 0 \)) increases as we vary \( V/t \). The LDOS of the system for \( V/t = 0 \) is presented in figure 1(a). We can see from this figure that the maxima and minima intensities of the LDOS are related to an upper and lower plane respectively. This is an important point since one of the goals of our work is to prove that the lattice sites related to the upper and lower planes are associated to extended and localized states respectively. We will use the nomenclature sub-lattice ES to refer us to the lattice sites that define the upper plane and sub-lattice LS for the ones of the lower plane.

When \( V/t \) is non-zero, like in figure 1(c)(ii), we notice some changes only in the LDOS intensities of the sub-lattice ES. The pure Klein states (\( PP = 0 \) and \( V/t < 0.5 \)) have evolve to quasi–Klein states. The quasi–Klein states still have the property of tunneling through the barrier and they are characterized by a PP different from zero at both sides of the barrier region (pseudo-spin A in red and pseudo-spin B in blue). The PP increases a we increase \( V/t \). By further increasing \( V/t \), figures 1(c)(iii-iv), we observe that in the sub-lattice ES the connection between the polarized electron-type wavefunction (outside the barrier) and the hole-type wavefunction (inside the barrier) breaks. Under this situation the Klein tunneling is totally suppressed and the \( S_0 \) states are generated inside the barrier occupying the sites of the sub-lattice ES.

On the other hand, at low applied potentials values (\( V/t < 0.5 \)) the LDOS of the sub-lattice LS does not change. However, when we increase \( V/t \) we observe in this sub-lattice the appearance of high LDOS intensities only inside the barrier region. If we continue increasing \( V/t \), the LDOS intensities inside the barrier region continue to increase until the appearance of the \( S_0 \) states (figures 1(c)(iii–iv)). As far as we know, the appearance of these states due to the applied potential barrier has not been reported before.

The \( S_0 \) and \( S_3 \) states seem quite similar but they indeed have very different origins. The \( S_3 \) states were induced from extended states, in contraposition with the \( S_0 \) states that were always localized inside the barrier.
The $S_\beta$ are generated by the chirality loss induced by the high applied potential $V/t$ and so they can be directly associated to quasi-Klein states in a conductance $\sigma(V/t)$ profile. In those profiles the width of the conductance peaks (quasi-Klein states) decreases as we increase $V/t$\cite{39}. In general, in the tunneling regime (with hyperboloid band contributions) the extended states of the sub-lattice ES coexist with the $S_\alpha$ states without any coupling (as we will prove) between them.

The discussions about figure 1(c) suggest that the sub-lattice ES and LS could be decoupled from each other. To illustrate this point we identified from figure 1(c)(i) which graphene lattice sites are associated to each LDOS plane. We considered orange points for sites that are related to the sub-lattice ES and green ones for the sub-lattice LS. The results are displayed in figures 2(a) and (b). Note that figure 2(a) illustrate some important facts previously discussed in this work. The sub-lattices ES and LS are both form by A and B sites. Furthermore, the PP is an interference phenomenon that take place only in the sub-lattice ES (orange sites). Finally, the $S_\alpha$ states arise in the sub-lattice LS (green sites) and within the applied barrier region.

We can see from figure 2(b) that the sub-lattice ES and sub-lattice LS are related to periodic arrangements of combinations of graphene sites $A$ and $B$. It is important to mention that the graphene ribbon continues to exhibit this periodic arrangement if we modified the ribbon width $W$. These periodic arrangements are identical to the ones already reported in\cite{27–29} as probability density. Also, in those references were reported the absence of states at the sites that form the sub-lattice LS. However, we will prove in this work that we can induce in the sites $n = 3, 6, 9...$ (sub-lattice LS) localized states that do not (or slightly) interfered with the states located at the sites of the sub-lattice ES.

In order to prove that the sub-lattices ES and LS behave as if they were decoupled, and also that they are related to extended and localize states respectively, we computed the DOS and conductance contributions from

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**Figure 2.** (a) LDOS showing the relation between the pseudo-spins $A$ and $B$ with the sub-lattice ES (orange) and the sub-lattice LS (green). (b) Mapping of the graphene lattice sites identifying the sub-lattice ES (orange) and the sub-lattice LS (green). (c) Density of states (DOS) and conductance ($\sigma$) maps, as a function of $V/t$ and $E/t$, for each sub-lattice. The conductance maps show that the sub-lattices ES and LS are decoupled in the Dirac plateau. The dots on the DOS maps are related to $S_\alpha$ states (left panels) and the quasi-Klein states ($\sigma \approx 0$, right panels). We also observed $S_\beta$ states at $\sigma = 0$ for $V/t > 2$, right panels.
the sub-lattice LS (green sites, figure 2(c) left panels) and the sub-lattice ES (orange sites, figure 2(c) right panels) independently.

We see from figure 2(c), for the considered $V/t$ interval and energies around the Dirac plateau, that the sub-lattice LS generates only localized states in the DOS. We can observed in this map high intensity points (red dots) over a background of zero intensity. This indicates a total localization of the states as we can infer from the conductance (zero values). On the other hand the sub-lattice ES contributes with extended states, which are used in the quasi-particle transport. In the last case the DOS maps show a background different from zero for $V/t < 2$, fact that is associated to extended states. Note the appearance over this background of discrete states coupled with extended ones. The conductance for this case emerges as Fabri-Perot resonances.

From these results and considering that: (i) conductance calculations using all lattice sites (sub-lattice ES + sub-lattice LS) exactly reproduce the conductance map obtained considering only the sites from the sub-lattice ES, and also that (ii) we did not observed in the conductance maps dips or asymmetric Fano resonances, which are signatures of couplings between extended and localized states, we can conclude that the sub-lattices LS and ES seems decoupled.

It is important to emphasize that the calculation of the conductances displayed in figure 2(c) for the sub-lattices ES and LS were performed following the procedure described in section 2 and by considering only the sites from the sub-lattice ES an LS respectively. Therefore, as the results show, the tunneling through the system is accomplished via the sub-lattice ES. Also, we could not find in the DOS map of the sub-lattice LS, as we found in the conductance $\sigma$ of the sub-lattice ES, interferences produced by the hyperboloid bands. In general, we could not observe fingerprints of the sub-lattice ES in the DOS of the sub-lattice LS, i.e. the similarities observed between the DOS and conductance maps of the sub-lattice ES are not observed in the DOS and conductance maps of the sub-lattice LS. This can also be interpreted as a sign of decoupling between the sub-lattices ES and LS.

In resume, our results confirm the interference effects previously published [27–29] around the $V/t = 0$ for metallic armchair nanoribbons, i.e. the absence of states in the sub-lattice LS and that the available states are distributed in the sub-lattice ES. However, we shown that we can induce totally localized states in the sub-lattice LS using potential barriers and more important, the above results confirm the existence of two sub-lattices for the scattering processes that behave as if there were decoupled. We will return to this point in section 3.3.

### 3.2. Characteristics of the $S_\alpha$ states: degeneracy between quasi-Klein and $S_\alpha$ states

A way to experimentally detect the existence of the sub-lattice LS is by the detection of the $S_\alpha$ states. In the regime of total localization of states (in our case for $V/t > 2$, figure 2(c)), the $S_\alpha$ states can not be detected in tunneling experiments of quasi-particles since there are no conductances to manipulate ($\sigma = 0$). However we can use the transport regime of $V/t < 2$ for that purpose. In the last case, it is necessary to have a mechanism to couple the $S_\alpha$ states with the quasi-Klein states. This mechanism will be presented in the next section. Meanwhile we will discuss the most important characteristics of the $S_\alpha$ states and by doing so explained how they can be detected.

The DOS results for the sub-lattice LS of figure 2(c) show the formation of $S_\alpha$ states (red dots) inside the barrier region as a function of $V/t$. Those states present a peculiar property, they are localized throughout the barrier region independently of the geometry of the barrier considered. We have verified that for each studied $S_\alpha$ state there is always another one in the sub-lattice ES with the same energy, i.e. they are degenerated. To show this we enlarge two regions of the DOS maps of figure 2(c) and display them in figure 3(a). With the help of the horizontal and vertical yellow lines within the maps, we can observe the existence of states that appear in both sub-lattices sharing the same $E/\hbar$ and $V/t$ values. This degeneracy of states occurs at both the tunneling ($V/t < 2$, upper panels) and the total localization regime ($V/t > 2$, lower panels).

Since the sub-lattices LS and ES are decoupled, it is difficult to detect the $S_\alpha$ states when the transport occurs in the sub-lattice ES because the $S_\alpha$ states do not leave traces in the conductance. Due to the degeneracy of the states, we would observe only an unique intense peak in the total DOS (a dot in the map) associated to both sub-lattices. This fact affects the experimental identification of the $S_\alpha$ states. The decoupling of the sub-lattices ES and LS means that the total DOS is calculated as the sum of the individual contributions of both sub-lattices. In the tunneling regime the intense peaks in the total DOS map can be related to contributions from $S_\alpha$ and quasi-Klein states. On the other hand, in the total localization regime the peaks can be associated to contributions from $S_\alpha$ and $S_\beta$ states. In the last case, as mentioned before, the detection of the $S_\alpha$ states is complicated since they are spatially entangled with the $S_\beta$ states. This entanglement can be seen in the LDOS of figure 3(b) where the green and orange LDOS coexist for several barrier widths $L$ (states labelled with stars). The intense peaks in the total DOS correspond to situations in which we have the contributions of both $S_\alpha$ and $S_\beta$ states inside the barrier region.

In figure 3(c) we show the coexistence of two states with the same energy, a $S_\alpha$ inside the barrier (green) and a quasi-Klein (orange), for the tunneling regime (upper figure, $V/t < 2$) and for the zero conductance regime.
In the last figure we show the coexistence inside the barrier region of $S_\alpha$ and $S_\beta$ states that are degenerated. In all cases the states from the sub-lattices $LS$ and $ES$ do not couple. In resume, the degeneracy shown in (a) and the entanglement in (b) and (c) prevent the experimental determination of the $S_\alpha$ states.

3.3. Detection of the sub-lattice $LS$: impurities and applied magnetic field effects in the system

In this section we will show an indirect way to detect the sub-lattice $LS$ via the detection of $S_\alpha$ states. We perform this by applying a magnetic field which couples the $S_\alpha$ states with the quasi-Klein states, leaving evidences of this coupling in the conductance map as Fano resonances. Also, we will further verify that the sub-lattices $LS$ and $ES$ behave as if there were decoupled. This is done by locally manipulating the lattice sites by the application of controllable impurities. The results will show the role of the sub-lattices $LS$ and $ES$ in the quasi-particles transport and will confirm the existence of these sub-lattices as an effect that goes beyond the global interference effect of all lattice sites, showing the local role of each sub-lattice in the transport properties.

In figure 4 an external magnetic field $B$ is perpendicularly applied to the system. The magnetic field was included via the Peierls substitution and as a result the longitudinal hopping parameter acquires a complex phase, which was developed in previous studies [31, 40]. Note that the applied magnetic field generates dips and asymmetric resonances (Fano resonances [41], dark dots in the conductance) in the conductance map of the sub-lattice $ES$. These resonances are not present in the conductance map of figure 2(c) that was obtained for the same sub-lattice and without magnetic field. Clearly the Fano resonances appear as the result of the coupling between a localized channel ($S_\alpha$ state of sub-lattice $LS$) and a continuous channel (quasi-Klein state of sub-lattice $ES$).

Figure 3. (a) DOS maps showing that for each $S_\alpha$ state another state exists in the sub-lattice $ES$ with the same energy. (b) Intense peaks (stars), seen as dots in (a), in the total DOS related to the contributions from both $S_\alpha$ and $S_\beta$ states ($V/t > 2$). In the continuous plateau, we identify the states (triangles) that are localized outside the barrier region. (c) LDOS mapping. The upper panel shows the coexistence between the quasi-Klein (orange) and the $S_\alpha$ states (green) for $V/t < 2$. The bottom panel shows the coexistence between the $S_\beta$ states (for the zero chirality limit, orange) and the $S_\alpha$ states (green) for $V/t > 2$. The mixture of the states from the sub-lattices $ES$ and $LS$ hinder the detection of the $S_\alpha$ states.
We already know that for low values of $V/t$ the $S_{\alpha}$ states are not present in the system. Also, for high values of $V/t$ the loss of chirality began to decouple the hole-type wavefunction inside the barrier from the electron-type wavefunction outside of it, destroying in this way the continuous channel of the sub-lattice ES. So, the $V/t$ range in which the quasi-Klein and $S_{\alpha}$ states can coexist is located in the central region of the conductance maps, and it is in this region where we found a high density of Fano resonances (figure 4, bottom right panel).

We have checked that the number of Fano resonances in the conductance maps increases as we increase the intensity of the applied magnetic field and always within the $V/t$ region analyzed before, where the conditions for the coexistence of the continuous and localized channels are optimized. Another important sign of the coupling between both sub-lattices can be seen in the DOS maps of the sub-lattice ES. The DOS maps (LS and ES) also exhibit the same Fano states.

Finally, we study impurity effects (disorder) in the system, figure 5. The effects of local impurities [42, 43] are included in our system by considering a randomly distributed potential $U$ in the diagonal elements of the Hamiltonian $H$ of equation (1). The disorder model used here consists in choosing randomly $N$ transverse chains with $n$ impurities in each chain. The position of the impurities are also randomly chosen. In this way we have $N \times n$ randomly chosen impurities at both sides of the barrier. To avoid imperfections over the barrier region, produced by the impurity’s potential, we have placed them far away from the central barrier. This allow us to exclusively and strictly study the impurity effects in the ribbon bulk. The barrier imperfections (not discussed in this work), beside destroying the Dirac plateau, generate tunneling peaks in regions where we once had a total localization of states with zero conductivity ($V/t > 2$). We normalized the impurity potential as $U/t$ in order to make it increase at the same rate as the central potential barrier $V/t$ does. Also, this normalization will allow us to compare these results with the maps obtained in figure 4 where no disorder was considered.

Physically, the model presented here can describe situations in which carbon atoms are substituted by other atoms due to the absorption of molecules present in the environment or by imperfections in the substrate [44–46].

In figure 5 we considered three different impurity distributions for the system. In cases (i) and (ii) we have randomly distributed the impurities over the graphene ribbon, i.e. the impurities are located in both sub-lattices. We can see in the conductance map of case (i) that some regions around the Dirac plateau are destroyed. For $V/t < 0.5$ the conductance remains roughly unchanged since the transport in this region is related mainly to pure Klein states. If we increase the number of impurities in the system, case (ii), the destruction of the Dirac plateau increases even more as we can see in the conductance map for this case. However, if we intentionally, and randomly, localize the impurities exclusively in the sub-lattice LS, case (iii), we recover the Dirac plateau. We can infer from this result that the impurities responsible for the destruction are the ones located in the sub-lattice ES since this is the sub-lattice that contributes with extended states. Also, the conductance behavior of case (iii) is similar to the one calculated considering only the contributions from the sub-lattice ES and without impurities.

Figure 4. DOS and conductance $\sigma$ maps, as a function of $V/t$ and $E/t$, for the sub-lattices LS and ES under a perpendicular applied magnetic field of 8 T. We have considered the same system of figure 3(c). The coupling between both sub-lattices can be identified as dark dots (i.e. Fano resonances) in the conductance maps of the sub-lattice ES. The DOS maps (LS and ES) also exhibit the same Fano states.
This fact corroborates the idea that the sub-lattice LS does not contribute to the transport of quasiparticles.

In figure 6 we test our results considering an intensionally built new system. We considered in the graphene ribbon an effective barrier that is exclusively located on the sites of the sub-lattice LS. Without magnetic field, the transport in the Dirac plateau behaves as if there were no applied potential barrier, i.e. the whole system, formed by the sub-lattices ES + LS, is not affected by the barrier. We can also infer from this result that the sub-lattice LS does not contribute to the transport.

To confirm that the sub-lattice ES is not affected by the barrier but the barrier indeed induce $S_{\alpha}$ states within the barrier region, we consider now an applied magnetic field, $B = 8 \, T$, (right panel). Under this condition Fano resonances began to appear in the conductance maps as a consequence of the coupling between states from both sub-lattices. Note that the pattern of the Fano resonances that we found inside the Dirac plateau for this case is different from the one observed in figure 4. The Fano resonances in figure 6 are uniformly distributed for high $V/t$ values, however the Fano resonances in figure 4 are found only at specific regions.

The pattern of the Fano resonances in figure 4 arises from the coupling between $S_{\alpha}$ and quasi-Klein states because it exhibits evidences of the chirality loss of the quasi-particles (behaving similar to the Schroedinger quasi-particle case). Also, this pattern is analogous to the one found in a conductance map (as a function of $B$ and $E$) of a 2DEG quantum box. In a 2DEG quantum box the magnetic field $B$ plays the same role of the quantity $V/t$ considered in this work [47]. The pattern observed in the Fano resonances of figure 6 for $B = 8 \, T$ arises from the

Figure 5. Conductance maps for the whole system (sub-lattices ES+LS), as a function of $V/t$ and $E/t$, for three different impurity situations: (i) with $N \times n = 40 \times 3$, (ii) and (iii) with $N \times n = 126 \times 9$. In cases (i) and (ii) we have randomly distributed the impurities over the graphene ribbon, i.e. the impurities are located in both sub-lattices. In case (iii) the impurities are exclusively located in the sub-lattice LS at both sides of the barrier. Notice from (i) to (ii) an increase in the destruction of the Dirac plateau. However in (ii) the Dirac plateau is recovered.

Figure 6. In the inset we show the system with a central barrier formed exclusively using sites from the sub-lattice LS. The conductance map for $B = 0 \, T$ is identical to the one obtained without a potential barrier, i.e. the considered barrier was invisible. With an applied magnetic field, $B = 8 \, T$, couplings between both sub-lattices (Fano resonances) appear.
coupling between $S_\alpha$ and pure Klein states. This confirms the idea that the continuous channel is not affected by the barrier. In resume, figures 5 and 6 corroborates the idea of having two decoupled sub-lattices, LS and ES.

4. Conclusion

We have reported the existence of two sub-lattices associated to extended and localized states in the scattering processes of metallic-AGRs. Both sub-lattices behave as if they were totally decoupled. The localized states related to the sub-lattice LS ($S_\alpha$ states) are only observed with high applied potential barriers for which the contributions of the hyperboloid bands are important. Moreover, the existence of the sub-lattice LS can largely decrease the disorder and impurities effects in the system. This is mainly due to the fact that the sub-lattice LS occupies an important portion of the ribbon and the imperfections that are localized in this particular sub-lattice do not participate in the transport process of quasi-particles. Furthermore, the sub-lattices reported here couple under the effect of a perpendicular applied magnetic field. The effects reported are strictly related to the metallic behavior of the AGR, for which the linear Dirac band exists. In semiconductor AGRs the effects discussed in this work were not observed, i.e. we cannot separate the ribbon into LS and ES sub-lattices. For future considerations, one can analyze spatially-resolved (ES and LS) states experimentally within local-in-space STM and laser pulse perturbations, with consequent local emission. Probably, a corresponding theoretical analysis as performed in this work would be also very useful.

Concerning the application of a strong magnetic field: in the limit of pure Landau levels the oscillations in the conductance plateaus will be completely suppressed. Also, the energy width of these plateaus should increase (well-separated Landau levels). In our work we still observe the oscillations in the conductance plateaus. This indicates that in our simulations we are still in the transition to a regime of pure Landau levels. Nevertheless, the increase of the magnetic field, besides eliminating the oscillations, will increase the localization of the extended states due to the increase of the couplings with the localized states. The final effect due to a strong magnetic field and to the existence of the sub-lattices LS and ES will be the generation of an energy gap.

Our main goal in this work is to study the free particle case without any further perturbation (as the Coulomb interaction). This is done in order to compare later our free electron results with the one-electron case or with the non-interacting electron flux case. The above two cases can be modeled by quantum wires without extra confinements or quantum dots. The system studied in the present work has perturbations typical of a Klein tunneling, and so the ballistic approximation is appropriate. Nevertheless, small Coulomb perturbations would only give rise to small variations in the confinement potential with little impact in the present results. This Coulomb perturbation can be included in our simulations as an increase in the effective mass of the quasi-particle, decreasing in this way the hooping energy $t$. However, at the presence of a strong Coulomb interaction our results will be certainly modified. So, a favorable condition to induce a free-particle case is when the Coulomb interaction is less stronger than the hooping energy $t$

Finally, the behaviors of the sub-lattices ES and LS reported and studied in this work contribute to a better understanding of the transport properties in AGRs that consider potential barriers, disorder and magnetic field. Moreover, the existence of the sub-lattices ES and LS and the effects reported here could also be observed in recent two-dimensional materials that are analogue to graphene, such as: Silicene, Germanene and Stanene [48–50]. This could generate a large area still open for research.

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