Analysis of Doorway States in a Graphene Structure

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Doorway states (DWSs) are related to the strength function phenomenon and giant resonances; and arise when two systems interact: one with a high-density eigenvalue spectrum and the other with a comparatively lower density. They are important because they constitute a very efficient mechanism for energy absorption when a system has such a state. These concepts, studied first in nuclear physics in the 1940s, are analyzed here from a theoretical point of view in some particular graphene structures, obtained after applying appropriate voltages to a graphene sheet. The influence of the DWSs on the electronic transport in these systems is also studied. To analyze these effects, a graphene sheet is considered to which three electrodes are applied to produce two potential barriers separated by a well. It is shown that, for the thin barrier, the transmission coefficient as a function of the energy has well-localized maxima, each maximum occurring at the DWS energies. This transmission clearly shows the strength function phenomenon. This function is an envelope for the resonances of the composite system. The results suggest the possibility of building graphene electronic devices, such as filters matching the DWSs.

1. Introduction

Each new important discovery in physics has brought a new vision of the concepts and phenomena of nature. That happened in solid-state physics with the development of the first 2D material, graphene, which was obtained in 2004 by mechanical exfoliation of graphite.[1–3] Since then, researchers from different disciplines of science and technology[4–7] have turned their attention to this material due to the extraordinary properties it exhibits.

Graphene is a material made up of carbon atoms arranged in a honeycomb-shaped sheet, with the thickness of one carbon atom (0.1 nm). It has a very particular band structure, as it is a semimetal with a zero bandgap, and a linear dispersion relation with conical shape (the well-known Dirac cones) near the points $K$ and $K'$ (Dirac points) in the Brillouin zone.[8] It has been shown[1,9] that electrons behave then as relativistic particles even though they move at the speed of $v_F \approx c/300$, where $c$ is the speed of light, so $v_F \ll c$.

Therefore, in this work, the intersection of two important and different fields: the physics of 2D materials and that of DWSs, is studied. DWSs are present in nuclei, atoms, molecules; they also appear in classical systems, such as microwave resonators or sedimentary basins. In all these cases, a system with few eigenvalues called “distinct states” interacts with a second one with a spectrum, called the “sea of states,” which has a much higher eigenvalue density. The distinct states are called DWSs in the literature. Therefore, a composed system forms in which the DWSs somehow modulate the states of the sea. The strength function phenomenon then appears, which means that the excitation intensity of the eigenstates of the composite system is modulated by the DWSs, giving rise to an enveloping curve with a Lorentzian-like shape.[16]

To design the graphene system having DWSs, we must proceed differently than in nonrelativistic quantum mechanics as the electrons in graphene behave quasi-relativistically, and consequently, they will obey the Dirac equation instead of the Schrödinger equation. In the nonrelativistic case, the most simplistic system, having DWSs, consists of a narrow well coupled to a much broader well. However, we find that in graphene, the system that has DWSs consists of a thin electrostatic barrier linked to a wider one, separated by a well.

2. Methodology

The composite system we analyze in this work was generated by placing metallic contacts or gates kept at voltages $V_1$, $V_2$, and $V_3$. 

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respectively, on a graphene sheet deposited on a noninteracting substrate, such as SiO_2; see Figure 1a. The corresponding potential had two barriers and a well, as shown in Figure 1b. The first barrier, which will be called the thin barrier, has height \( V_1 \) and width \( d_1 \). In-between the two barriers, there was a well with depth \( V_2 = -V_1 \) and width \( d_2 \). The second barrier was wider than the first one so \( d_1 \ll d_2 \) but \( d_1 = d_2 \) and \( V_3 = V_1 \). The thin barrier generates the DWSs.

When the barriers were generated by gating, changes in the Dirac cones occurred only in the regions where the electrodes were localized (as shown in Figure 1 of ref. [2]). The particle moves on the XY plane and the transmission largely depends on the width of the barriers and the angle of incidence.

Our model considered perfect-rectangular barriers and without the presence of impurities that could come from the substrate. As it is well known, they can change the properties of graphene.\(^{[25]}\) However, in this work, these effects were neglected.

The transmission properties of the electrons traveling through the graphene sheet connected to the electrodes, as shown in Figure 1a, can be computed using the well-known transfer matrix method.\(^{[26,27]}\) To apply this methodology, we need the dispersion relations, the wave vectors, and the wave functions in the barriers, in the well and in the left and right semi-infinite regions. In the semi-infinite regions, the dispersion relations are

\[
E = \pm \hbar \nu_F k
\]

and the wave functions are

\[
\psi_k^\pm = \frac{1}{\sqrt{2 \left| u_\pm \right|}} e^{\pm i k_x x + i k_y y}
\]

where \( \nu_F \) is the Fermi velocity, \( k \) is the magnitude of the wave vector \( \mathbf{k} \) at the semi-infinite regions, \( k_x \) and \( k_y \) are the longitudinal and transversal components of \( \mathbf{k} \), and \( u_\pm = \pm \text{sgn}(E) e^{\pm i \theta} \) are the coefficients of the wave functions that depend on the angle of incidence of the electrons, \( \theta = \arctan(k_y/k_x) \).

The kinetic energies in the region of the well and the barriers are

\[
E - V_j = \pm \hbar \nu_F q_j
\]

with \( j = 0, 1, 2, \) and \( 3, \) at \( j = 0 \rightarrow V_0 = 0 \rightarrow q_0 = k, \) and the eigenfunctions are

\[
\psi_q^\pm = \frac{1}{\sqrt{2 \left| v_\pm \right|}} e^{i q_x x + i q_y y}
\]

Here, \( q \) is the magnitude of the wave vector \( \mathbf{q} \) in these regions, \( q_x \) and \( q_y \) are the components of \( \mathbf{q} \), and \( v_\pm \) are the coefficients of the wave functions.

By imposing continuity of the wave function and conservation of the transverse momentum \( q_y = k_y \) at the boundaries, we can obtain the transfer matrix \( \mathbf{M} \) of the structure\(^{[26,27]}\)

\[
\mathbf{M} = \mathbf{M}_I \mathbf{M}_L \mathbf{M}_W \mathbf{M}_B \mathbf{M}_B \mathbf{M}_W \mathbf{M}_I
\]

with \( \mathbf{M}_I \) and \( \mathbf{M}_W \) the transfer matrices associated with the left and right semi-infinite regions, \( \mathbf{M}_W \) with the well and \( \mathbf{M}_B \) and \( \mathbf{M}_B \) with the thin and wide barrier, respectively. These matrices depend on the so-called dynamic and propagation matrices \( \mathbf{D}_j \) and \( \mathbf{P}_j \)\(^{[28,29]}\)

\[
\mathbf{M}_I = (\mathbf{D}_k)^{-1} \\
\mathbf{M}_L = (\mathbf{D}_k)^{-1} \mathbf{P}_B \mathbf{D}_B \\
\mathbf{M}_W = (\mathbf{D}_k)^{-1} \mathbf{P}_W \mathbf{D}_W \\
\mathbf{M}_B = (\mathbf{D}_k)^{-1} \mathbf{P}_B \mathbf{D}_B \\
\mathbf{M}_I = \mathbf{D}_k
\]

where

\[
\mathbf{D}_j = \begin{pmatrix} 1 & 1 \\ \frac{-q_y - i q_x}{q} & \frac{-q_y - i q_x}{q} \end{pmatrix} ; \quad \mathbf{P}_j = \begin{pmatrix} e^{-i q x_j - x_j} & 0 \\ 0 & e^{i q x_j + x_j} \end{pmatrix}
\]

\( j = 0, 1, 2, 3 \)

The transmission coefficient of the Dirac electrons is given by the (1,1) element of the transfer matrix \( \mathbf{M} \)\(^{[26,27]}\)

\[
|t(E, \theta)|^2 = \frac{1}{|\mathbf{M}_{11}|^2}
\]
3. Results and Discussion

3.1. Single Barrier

We first study a single barrier and calculate its transmission coefficient. We focus on a range of energies below the barrier potential. In Figure 2a, \( d_1 = 45a \) and in Figure 2b, \( d_1 = 200a \), where \( a \) is the carbon—carbon distance in graphene, which is equal to 0.142 nm. In Figure 2a, the transmission coefficient shows three maxima, whereas in Figure 2b, it shows fifteen. At these maxima, whose positions are indicated with dashed vertical lines, \(|t|^2 = 1\). Using Equation (1) and (3), and the necessary condition for a resonance \( q_d = n\pi \), we obtain an analytical expression for the number of maxima in these figures.

The energy must fulfill

\[
q_d = d_1 \sqrt{\left(\frac{E - V_1}{\hbar v_F} \right)^2 - k_F^2} = d_1 \frac{V_1}{\hbar v_F} \sqrt{\left(\frac{E}{V_1} - 1 \right)^2 - \left(\frac{E}{V_1} \sin \theta \right)^2}
\]

where \( \hbar v_F \approx 4a \text{ eV} \times 4 \times 0.142 \text{ eV} \cdot \text{nm} \). From this equation, we can see that there is a finite number of values of \( n \) for which \( 0 < E/V_1 < 1 \). For example, with \( \theta = \pi / 9 \) and \( d_1 = 45a \) one has \( n = 1, 2, 3 \), whereas changing \( d_1 \) to \( 200a \) one obtains \( n = 1, \ldots, 15 \). This matches the results shown in Figure 2a,b.

It should be noted that in both figures, the maxima are equal to 1, the only difference being the density of resonances, which grows with the barrier width.

3.2. Composite System

We now study the composite system, which consists of two electrostatic barriers separated by a well. This case has been widely studied in the literature, but the phenomena of the strength function and the influence of the DWSs have not been discussed. Its transmission spectrum is compared in Figure 3 with that corresponding to the thin barrier. In Figure 3a, the parameters of the thin barrier are as in Figure 2a, whereas for the well and the wide barrier \( d_3 = 200a \). We can see that the 15 resonances of Figure 2b are now modified. Their intensities (purple line) are modulated by the transmission curve corresponding to that of the single barrier (green line). Furthermore, the vertical red dotted lines indicate that the position of the maxima along the energy axis changes slightly. In general, the maxima of the purple line are different from 1, so the composite system does not have a perfect transmission. However, the purple maxima whose energies are close to the energies of the green maxima are larger than the other purple maxima.

The shape of the transmission spectrum can be understood by the following argument: when the waves entering the system have a frequency close to or equal to any of the resonances, a quasi-standing wave is established along the whole system. To obtain a constructive interference pattern, the waves have to travel several times back and forth within the system. It is therefore clear that the waves will settle within the small body in a shorter period of time than it takes for the waves to settle in the composite system. So resonances with frequencies close to those of the small system will absorb energy faster than the other resonances and the peaks corresponding to these resonances are higher. For a more detailed discussion about the relation between the time that a resonance takes to be established and its strength, see the comments in the study by Morales et al.[17] related to its figures 3–5.

In Figure 3b, the well and the wide barrier widths were increased with respect to those of Figure 3a so the transmission spectrum shows many more resonances. The system in Figure 3b is much larger than in Figure 3a, but the behavior of the transmission coefficient is controlled in both cases by the thin barrier, so in the two figures the green curve is the envelope of the purple curve, showing the strength function phenomenon.

Up to now, the angle at which the electrons impinge has been \( \pi / 9 \). In what follows we shall present results for other values of \( \theta \). In Figure 4, the contour plots are shown. Again, the transmission spectrum of the thin barrier (Figure 4a) is compared with that of the composite system (Figure 4b). For the thin barrier, we see a spectrum with only three maxima. As the angle...
changes, these maxima shift slightly on the energy axis. On the other hand, for the composite system, the transmission coefficient shows many maxima. However, despite the change in the angle, the maxima are still modulated by the spectrum of the thin barrier.

If we overlap Figure 4a,b, the red zone of Figure 4a covers completely the red zone of Figure 4b. To guide the eye, the vertical white line has been inserted to indicate that the energy value $E/V_{1}$ of the third peak is $\approx 0.465$ in both figures; this is also true for the other two peaks in the graphs.

We now analyze the behavior of the transmission coefficient as a function of $\theta$. In Figure 5 the results for $\theta = 4\pi/9$ are presented. We see that there are still three maxima and that the green curve also modulates the behavior of the purple curve.

The minima of the transmission coefficient now approach zero and the width of each resonance in the transmission coefficient decreases as the angle increases, making the strength function phenomenon even more evident.

In the previous plots, the thin barrier has a width equal to 45 $\alpha$. In Figure 6, this width is 60 $\alpha$. This increases the number of maxima, so there are now four peaks instead of three, but the green curve still modulates the purple one.

4. Conclusions

In this work, we have studied a graphene structure that has DWSSs that allow a more efficient energy absorption. We analyze the electronic transmission as a function of the energy and of the angle of incidence. For the thin barrier, the transmission maxima will be equal to 1.0; this occurs at the DWSS energies. Here, the transmission coefficient of the thin barrier follows a smooth curve with well-localized maxima, and it turns out that this curve is an envelope for the resonances of the composite system.
In other fields of physics, when resonating systems with a DWS are dealt with, this envelope is obtained by interpolating the individual transmission, so it is a mathematical construction, whereas in the system, we have studied in this article, the green curve has a physical meaning as it corresponds to the transmission through a single barrier.

The DWSs, together with the angle of incidence variation can be useful to build optoelectronic devices, such as filters or sensors.

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Conflict of Interest

The authors declare no conflict of interest.

Data Availability Statement

Data sharing is not applicable to this article as no new data were created or analyzed in this study.

Keywords

doorway states, giant resonances, graphene, strength function phenomena

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