Tunable transmission due to defects in zigzag phosphorene nanoribbons

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Abstract – Transport of the edge-state electrons along zigzag phosphorene nanoribbons in the presence of two impurities/vacancies is analytically investigated. Considering the places of the defects, a number of different situations are examined. When both defects are placed on the edge zigzag chain, as is expected, by changing the energy of the traveling electrons the electrical conductance exhibits a resonance behavior. In this case, for two vacancies the observed resonant peaks become extremely sharp. An amazing behavior is seen when the second vacancy is located along an armchair chain while the first is placed at the intersection of the edge zigzag and this armchair chain. In this case, in a considerable range of energy, the conductance is strongly strengthened. In fact the presence of the second vacancy creates a shielded region around the first vacancy, consequently, the traveling wave bypasses this region and enhances the conductance. The analytical results are compared with numerical simulations showing very good agreement.

Introduction. – Graphene, as the most fundamental two-dimensional (2D) material in the world, has no electronic band gap in its electronic structure and this feature is an obstacle in practical application of this material in the design of semiconductor devices [1]. Therefore, it is natural to look for the applicable 2D materials with a gap in their band structures for such purposes. Phosphorene, as a new elemental quasi-2D material, has recently attracted great attention of the manufacturers of the electronic devices. This is due to the large direct band gap of phosphorene ranging from about 0.5 eV for the five-layer structures to 1.5 eV for the monolayer ones [2].

Bulk phosphorus is a layered crystal of the van der Waals type [3] which can be exfoliated into phosphorene as a separated single-layer material [4]. The peculiarity of phosphorene resides in the fact that each phosphorus atom is bonded covalently with three nearest neighbors via $sp^3$ hybridization to make a puckered 2D honeycomb structure which gives rise to various anisotropic properties [5–9]. Furthermore, a zigzag phosphorene nanoribbon (zPNR), which can be fabricated in experiment [10,11], supports an edge band in the middle of the main gap which is completely isolated from both the conduction and valence bands. Due to the presence of two edge boundaries in zPNRs, the quasi-flat band composed of edge modes is doubly degenerated [12] with interesting transport properties. Similarly, edge states in skewed-armchair phosphorene nanoribbons have been studied in ref. [13]. In the absence of defect, both zigzag and skewed-armchair phosphorene nanoribbons are metallic unless they undergo an edge reconstruction or passivation [14].

In addition to the above-mentioned properties, the negative differential resistance (NDR) behavior which is robust with respect to the edge reconstruction has been reported for a two-terminal zPNR device [15]. Also, using the first-principles calculations, it is shown that a transverse electric field can induce an insulator-metal transition in the zPNRs with hydrogen-saturated edges [16]. Finally, the effect of impurity defects on the quantum transport in zPNRs has been investigated recently [17–19]. The studies show that the presence of impurity defects, ranging from vacancies [17] to substitution of atoms via doping [18], changes the transport properties of pristine zPNRs. The presence of localized scattering centers near the edges of zPNR, has a significant effect on the electronic transmission through the edge states and reduces the transmittance of the sample depending on its distance from the edge [19]. On the other hand, it is important to explore new efficient ways to modulate the transport properties of zPNR such as tuning the band structure by mechanical...
As is schematically shown in fig. 1, phosphorene has a non-planar puckered honeycomb lattice which consists of two inequivalent sublattices denoted by A and B. In a tight-binding approach, the Hamiltonian of such a system including a number of lattices denoted by honeycomb lattice which consists of two inequivalent sublatetices shown in fig. 1, phosphorene has a non-planar puckered axes respectively. Also, two-defect structures along the x and y axes are shown schematically.

stress [20]. A possible subsequent step in these studies is to investigate the effect of the presence of multiple scattering centers, manipulated on the atomic scale in a nanoribbon, on the quantum transport properties of this material. For example, the influence of the edge states on the Ruderman-Kittel-Kasuya-Yosida (RKKY) exchange interaction between two doped on-site magnetic impurities in azpNR has been recently investigated [21].

In this paper, motivated by recent experiments on creating and manipulating a single dopant atom on a black phosphorus surface [22] and similarly to what has been studied on the coherent electron transport along zigzag graphene nanoribbons [23], we study the effects of two impurities/vacancies on the electron transport along a zigzag chain in a zPNR. To this end, a Green’s function approach, which we have developed previously to study the influence of the impurity defects on the scattering of the traveling electrons in a zPNR [19,24], is employed. For different cases the conductance is evaluated as a function of the electron energy. This function displays a resonant structure when the defects are placed along the edge zigzag chain. A more interesting behavior is observed when the second vacancy is placed adjacent to the first one on an armchair chain. This combination maximizes the conductance in a certain range of energy.

**Theoretical preliminaries.** As is schematically shown in fig. 1, phosphorene has a non-planar puckered honeycomb lattice which consists of two inequivalent sublattices denoted by A and B. In a tight-binding approach, the Hamiltonian of such a system including a number of the on-site impurities is given as

$$H = \sum_{\langle i,j \rangle} t_{ij} c_i^\dagger c_j + \text{h.c.} + V,$$  \hspace{1cm} (1)

where $\langle i,j \rangle$ represents the index of summation that is taken over only the considered nearest neighbors, $t_{ij}$ is referred to as the hopping integral between atoms at sites $i$ and $j$, $c_i$ and $c_i^\dagger$ are the electron annihilation and creation operators in site $i$, h.c. stands for Hermitian conjugate and $V$ is the disorder potential energy. It is obvious that in absence of the defects, $V$ is zero.

The calculations based on the ab initio tight-binding method, show that taking only five nearest-neighbor interatomic interactions is a very good approximation to provide a reasonable description of the phosphorene band structure [25]. Referring to fig. 1, the hopping integrals corresponding to these interactions are denoted for simplicity by $t_1$ to $t_5$ and their corresponding values are assumed the same as reported in ref. [25]. These values are given as $t_1 = -1.220$ eV, $t_2 = 3.665$ eV, $t_3 = -0.205$ eV, $t_4 = -0.105$ eV, and $t_5 = -0.055$ eV.

Phosphorene can be cut into nanoribbons and the shape of their edges depends on the direction of the cut. Two typical crystal directions, namely the armchair and zigzag directions, were generally explored. The nanoribbons with zigzag edges exhibit some interesting behaviors representing important physical aspects. One of the interesting aspects of these nanoribbons is the existence of quantum edge states in the edge zigzag chains. In the following section, we are interested in studying the behavior of the edge-state electrons, traveling along a side zigzag chain, when they scatter off the impurities doped into the ribbon sites. In order to investigate this issue, the electronic properties of this type of nanoribbons are studied analytically. Also, a numerical simulation is made to study the tunable resonances due to the impurities and the validity of the analytical calculations is examined by comparing their obtained results with this numerical simulation.

The first step in the evaluation of the transport properties is to calculate the conductance which depends on the Hamiltonian of the specified system. Here, we use the Landauer formula,

$$g(E) = \frac{2e^2}{h} T(E),$$  \hspace{1cm} (2)

to evaluate the conductance of a zPNR. In this equation, $g(E)$ is conductance, e is the fundamental charge, $h$ is the Planck constant and $T(E)$ is the transmission coefficient. Both conductance $g(E)$ and the transmission coefficient $T(E)$ depend on the electron energy $E$. In order to calculate the transmission coefficient, we employ the Lippmann-Schwinger formalism in which we need the edge-states Green’s function. Hence, before proceeding any further, we will devote the following subsections to the calculation of edge-states wave functions and their corresponding lattice Green’s function.

**Quantum edge states in a zPNR.** The presence of topological edge states at the zigzag edges of single-layer phosphorene has recently been investigated using the tight-binding model [12]. The existence of these edge states in zPNRs has created a great potential for this material to use it in science and technology. These states are also the essential ingredients in many of the fascinating properties...
of phosphorene. In this subsection we provide an overview on the wave function obtained in ref. [12] to describe the electronic edge states in a zPNR.

For two different cases, both conductance and band structure of a typical zPNR are shown in fig. 2. For the first case, we assumed that the hopping amplitude $t_4$ is zero. As is seen, in this case a flat edge band, which is completely separated form both conduction and valence bands, appears in the band structure. The second case is for a more real situation for which $t_4$ is zero. In this case the flat edge band tends to become a quasi-flat band.

Employing the tight-binding Hamiltonian given in eq. (1) and applying a first-order perturbation theory, a dispersion relation can be derived for the edge states of zPNRs and the properties represented in fig. 2 can be explained. To this end, at first we neglect the interaction terms including the hopping integrals of $t_3$ and $t_5$. Since $t_3$ and $t_5$ in comparison with $t_4$ and $t_2$ make a smaller contribution to the Hamiltonian, this assumption seems reasonable. Also, since $t_4$ is responsible for the dispersion of edge bands and breaks both particle-hole and lattice bipartition symmetries of the Hamiltonian [26,27], it is reasonable to consider its effect perturbatively. Taking $x$ and $y$ axes along the zigzag and armchair directions, each lattice site can be labeled by a pair of integers $(m, n)$ where $m$ and $n$ are armchair and zigzag chain numbers. Without loss of generality, we focus on an $A$-type edge chain in which the edge-state wave function has non-zero amplitudes only on the $A$ sublattice (top edge in fig. 1).

For this case, we notice that a typical unperturbed edge state is given as [12,19]

$$|\psi_k\rangle = \sum_{m,n} \gamma_k \alpha^m_k e^{i(k(m+n))} |m,n\rangle,$$

in which $k$ is the wave number which is normalized by the length of the primitive cell in the $x$-direction $(1/a)$, the constant value of $\delta_n$ is 0 (0.5) for even (odd) $n$, $\alpha_k$ is given by

$$\alpha_k = -2(t_1/t_2) \cos(k/2),$$

and $\gamma_k$, a normalization coefficient satisfying $(\psi_k|\psi_{k'}) = \delta(k-k')$, reads

$$\gamma_k^2 = \frac{1}{2\pi} (1 - \alpha_k^2).$$

Since $-2t_1 < t_2$, the partial wave amplitudes appearing in the edge wave states, $\alpha_k^m$, are always less than unit and they tend to vanish with increasing $n$. This means that the edge states are localized at the sites of the edge chain, and they decay to zero by penetrating from the edge into the inside sites. Furthermore, for the boundary values of $k$, $k = \pm \pi$, the wave states are zero unless $n = 0$. In other words, for $k = \pm \pi$ the edge states are strongly localized on the side zigzag chain.

Considering the $t_4$ term as a perturbation and applying a first-order approximation the wave state remains unperturbed, but the energy eigenvalue now depends on $k$ and reads

$$E_k = E_0 - 2\Delta \cos k,$$

where $E_0 = (-4t_1 t_2)/t_2$ and $\Delta = 2t_1 t_4/t_2$. This expression is very similar to the dispersion relation of a one-dimensional (1D) tight-binding atomic chain with hopping amplitude $\Delta$ to the nearest neighbors.

**Green’s function of the edge states in zPNRs.** With the above introduction, now we can apply a Green’s function technique to calculate the transmission coefficient of the doped lattice for the case in which the edge-state matter waves traveling along a zigzag chain are scattered by the on-site impurities.

The Green’s function of a defect-free system with a discrete spectrum is defined as

$$\hat{G}_E = \sum_i \frac{|\psi_i\rangle\langle\psi_i|}{E - E_i + i0^+},$$

and the same for a system of a continuous spectrum reads

$$\hat{G}_E = \int \frac{|\psi_k\rangle\langle\psi_k|}{E - E_k + i0^+} dk.$$
these matrix elements which are listed as follows:

\[ G_E(0, 0; 0, 0) = G_E(m, 0; 0, m) = \frac{\gamma_k^2}{2i\Delta \sin k_0} - \frac{(2t_1/t_2)^2}{4\Delta}, \]  

(10)

and

\[ G_E(0, 0; m, 0) = \frac{\gamma_k^2 e^{ik_0m}}{2i\Delta \sin k_0}, \]  

(11)

where \( k_0 \) is the pole of the integrand in eq. (9) with \( \cos k_0 = (E_0 - E)/2\Delta \). Here, we should emphasize that the first term on the right-hand side of eq. (10) is identical to that in Green’s function of a 1D chain (up to the normalization factor \( \gamma_k \) \[28\]), while the second term is an additional term. This term originates from the dependence of edge-state wave functions in eq. (3) on the vertical index \( n \) in comparison to its corresponding wave functions for the 1D chain which are plane waves and depend only on the horizontal index \( m \).

Also, for certain cases in which \( |m - m'| \gg 1 \), it is easy to show

\[ G_E(m, n; m', n') = \frac{\gamma_k^2 \alpha_k^{n+n'} e^{i(m-m' + \delta_n - \delta_{n'})k_0}}{2i\Delta \sin k_0}. \]  

(12)

Furthermore, for two sites on an armchair chain with even \( n \) and \( n' \), since \( m = m' \) and \( \delta_n = \delta_{n'} = 0 \), the corresponding matrix element of \( \hat{G} \) reduces to

\[ G_E(m, n; m, n') = \int_0^\pi \frac{\gamma_k^2 \cos k + i\pi}{E - E_0 + 2\Delta \cos k + i\pi} dk. \]  

(13)

Inserting \( \alpha_k \) and \( \gamma_k \) from eqs. (4) and (5) into the above expression, it can be separated into two integrals. These integrals can be also evaluated analytically using the following identity integral;

\[ \int_{-\pi}^{+\pi} \frac{\cos^2(k/2)}{E - E_0 + 2\Delta \cos k + i\pi} dk = \frac{1}{2\pi} \sum_{j=0}^{\ell} \left( \frac{1}{2j+1} \right) \frac{1}{2^{2j}} \left\{ \cos[(j - 2j')k_0] + i \sin[(j - 2j')k_0] \right\}. \]  

(14)

where \( \ell \) is an integer.

Using the obtained analytical expressions for the matrix elements of the edge-state Green’s operator and applying the general theory of the potential scattering, we can calculate the transmission coefficient of the system in the presence of the on-site impurities and/or vacancies. This issue will be followed in the next section.

**Electrical conductance of the zPNR in the presence of two impurities.** – In this section, we present the results of the transport calculations in the pure and the defective zPNRs. Our aim of this study is the exploring of the influence of the defect type and its position on the transport properties of the considered system. To perform the calculations, we begin with the Lippmann-Schwinger equation in the potential scattering theory

\[ |\psi_{\text{out}}\rangle = |\psi_{\text{in}}\rangle + \hat{G}_E \hat{V} |\psi_{\text{out}}\rangle = |\psi_{\text{in}}\rangle + \hat{G}_E \hat{T} |\psi_{\text{in}}\rangle, \]  

(15)

where \( |\psi_{\text{in}}\rangle \) and \( |\psi_{\text{out}}\rangle \) are the quantum states of the incoming and outgoing charge carriers, \( \hat{G}_E \) is the Green operator for the unperturbed system, \( \hat{V} \) is the scattering potential and \( \hat{T} \) is the transition matrix corresponding to the scattering potential \( \hat{V} \) with \( \hat{V} |\psi_{\text{out}}\rangle = \hat{T} |\psi_{\text{in}}\rangle \). An attempt to solve the Lippmann-Schwinger equation by successive iterations leads to

\[ \hat{T} = \hat{V}(1 + \hat{G}_E \hat{V} + \hat{G}_E \hat{V} \hat{G}_E \hat{V} + \cdots). \]  

(16)

Now, we assume that two on-site defects are localized at positions \( (m_1, n_1) \) and \( (m_2, n_2) \), and consider the edge-state charge carriers traveling along the side zigzag chain. These traveling matter waves will be scattered by the defects. Consequently, the incoming wave in the Lippmann-Schwinger equation is the edge-state wave given in eq. (3). The scattering potential due to the presence of the defects is given in its explicit form as

\[ \hat{V} = \hat{V}_1 |m_1, n_1\rangle \langle m_1, n_1| + \hat{V}_2 |m_2, n_2\rangle \langle m_2, n_2|, \]  

(17)

where \( \hat{V}_1 \) and \( \hat{V}_2 \) are the on-site potentials due to the presence of the defects. With this form of the scattering potential the transition operator \( \hat{T} \) can be written in its matrix form as

\[ \hat{T} = [\hat{V}] + [\hat{G}_E][\hat{V}] + [\hat{G}_E][\hat{V}][\hat{G}_E][\hat{V}] + \cdots, \]  

(18)

where

\[ [\hat{V}] = \left( \begin{array}{cc} V_1 & 0 \\ 0 & V_2 \end{array} \right) \]  

and \( [\hat{G}_E] = \left( \begin{array}{cc} G_{11} & G_{12} \\ G_{21} & G_{22} \end{array} \right) \).  

(19)

It is obvious that the matrix elements of \([\hat{G}_E]\) are known as

\[ \begin{align*}
G_{11} &= G_E(m_1, n_1; m_1, n_1), \\
G_{12} &= G_E(m_1, n_1; m_2, n_2), \\
G_{21} &= G_E(m_2, n_2; m_1, n_1), \\
G_{22} &= G_E(m_2, n_2; m_2, n_2).
\end{align*} \]  

(20)

Since, the matrix forms of the scattering potential and the free-defect Green’s operator are exactly known, a closed-form expression can be evaluated for the transition matrix using the fact that

\[ \hat{T} = [\hat{V}][1 - [\hat{G}_E][\hat{V}])^{-1}. \]  

(21)

Substituting the edge-state wave function as the incoming wave, and the matrix forms of \( \hat{G}_E \) and \( \hat{T} \) into eq. (15), the outgoing wave function can be calculated. To this end, we introduce the quantum state \( |\chi\rangle \) as

\[ |\chi\rangle = \hat{T} |\psi_{\text{in}}\rangle = \alpha |n_1, m_1\rangle + \beta |n_2, m_2\rangle, \]  

(22)
where
\[ \alpha = T_{11}(n_1, m_1|\psi_{in}) + T_{12}(n_2, m_2|\psi_{in}), \]
\[ \beta = T_{21}(n_1, m_1|\psi_{in}) + T_{22}(n_2, m_2|\psi_{in}), \]

in which \( T_{11}, T_{12}, T_{21} \) and \( T_{22} \) are the calculated matrix elements of \( \hat{T} \) for the specified case. Having \( |\chi\rangle \), we find out
\[ |\psi_{\text{out}}\rangle = |\psi_{\text{in}}\rangle + \hat{G}_E|\chi\rangle. \]

Using the obtained result for the outgoing wave, both the transmitted and the reflected parts of the final state are derivable. Having these parts of the outgoing wave, the reflection and transmission coefficients can be evaluated. To evaluate these coefficients, for an arbitrary site of \((m', n')\) it is seen that
\[ \langle m', n'|\hat{G}_E|\chi\rangle = \alpha G_E(m', n'; m_1, n_1) + \beta G_E(m', n'; m_2, n_2), \]

Since the transmission coefficient is more of interest, we examine the transmitted part of the final wave state at an arbitrary position of \((m', n')\) with \( m' \gg m_2 \). In this case, using the form of the Green’s operator it is easy to show that the above expression is proportional to \( |m', n'|\psi_k\rangle \).

Consequently, we obtain the transmission amplitude as
\[ \tau = 1 + \frac{\alpha G_E(m', n'; m_1, n_1) + \beta G_E(m', n'; m_2, n_2)}{\langle m', n'|\psi_k\rangle}, \]

in which it is obviously known that \( m' \gg m_2 \). Finally the transmission coefficient is obtained using \( T(E) = |\tau|^2 \).

In the following discussion, we consider two on-site impurities and/or vacancies in the nanoribbon. As is seen in fig. 1, one of the impurities/vacancies is located at one of the sites of the zigzag side of the nanoribbon. This site is labeled as \((m_1, n_1) = (0, 0)\). For the second impurity/vacancy, we consider two different positions. In the first case, the impurity/vacancy is also located at one of the sites of the side zigzag chain. So, this site is labeled as \((m_2, n_2) = (m, 0)\). For the second case, we consider the second defect located at the same armchair chain as the first one, but the related zigzag chain is labeled by an even integer. So, the detected site in this case is labeled as \((m_2, n_2) = (0, n)\) where \( n \) is even.

Also, for simplicity, we assume that the potential strengths \( V_1 \) and \( V_2 \) are equal, so we put \( V_1 = V_2 = U \), and we notice that for two vacancy defects, \( U \) tends to infinity (\( U \to \infty \)).

**Results and discussion.** – In all the following discussions, we assumed that the first impurity/vacancy is fixed at \((m_1, n_1) = (0, 0)\) on the edge zigzag chain.

Figure 3 shows the conductance as a function of the electron energy for the case in which the second impurity is located on the edge zigzag chain at \((m_2 = m, n_2 = 0)\). So, both defects are along the \( x \)-axis. The graphs are plotted for \( m = 4 \) and for two values of the potential strength, \( U = 0.1 \) and \( U = 0.5 \). As is seen the conductance presents a resonant behavior which is expected for successive reflection and transmissions of the matter waves from the impurities and the constructive or destructive interference of the transmitted parts. The number of the observed resonant peaks are equal to the number of the atomic sites between the impurities \((m - 1)\). This result follows from the expression for the transmission amplitude in eq. (26) which can be written explicitly in this case as
\[ \tau = 1 + \frac{U \gamma_0^2}{it' \sin k_0} \frac{(1 - U c_1) + U c_2 \cos (mk)}{(1 - U c_1)^2 - (U c_2)^2}, \]

where \( c_1 = G_E(0, 0; 0, 0) \) and \( c_2 = G_E(0, 0; m, 0) \). It is now obvious that the number of sites between two impurities, \( m - 1 \), which is the number of peaks in the transmission reality to the argument in \( \cos(mk) \) in the numerator of eq. (27) and the phase in \( c_2 \). This is due to the changes in the phase of the traveling electron when it travels the distance between impurities. Hence, we expect the number of resonant peaks to be related to \( m \). For the weaker interaction, \( U = 0.1 \), the peaks are not very sharp, but with increasing the interaction strength the peaks become sharper and shift toward the larger energies. The numerical simulations performed using the approach followed in ref. [19] are also depicted in this figure. As is seen, our present analytical results are in excellent agreement with the numerical simulations.

A similar situation for two vacancies on the edge zigzag chain is demonstrated in fig. 4. For this case, \( U \) tends to infinity. The resonant peaks which are also seen in this case are extremely sharp and the number of peaks are equal to \( m - 1 \). Figures 3 and 4 show that the behavior of the considered system is similar to what happens for a 1D tight-binding chain. For a 1D atomic chain the vacancy limit is meaningless, because this is equivalent to the chain being cut off. But for the present quasi 1D system this limit is completely meaningful.
Fig. 4: Same as fig. 3 but for two vacancies on the edge zigzag chain. The first vacancy is fixed at (0, 0), but for the second vacancy two positions are considered: (3, 0) and (4, 0).

Fig. 5: Electrical conductance as a function of energy for a case in which two atomic impurities are located in the y-direction. The first impurity is on the edge zigzag chain and the second is inside the bulk. Two different positions for the second impurity are considered (0, 2) and (0, 8).

Figure 5 shows the conductance as a function of energy for two impurities located along the y-axis. The first impurity is on the edge zigzag chain and the second is inside the bulk. The defected sites are denoted as (0, 0) and (0, n), where n is an even integer. As is seen, in this case the conductance is in general weak. Whatever the second impurity which penetrates more into the bulk, its effect will be less. So that, for the large values of n the behavior of the system is closer to a system with a single impurity placed on the edge zigzag chain.

An interesting situation occurs when two vacancies are created along the y-axis. Figure 6 shows that if, instead of two atomic impurities, two vacancies are placed on an armchair chain along the y-axis the electrical conduction increases considerably with respect to the case in which there is only a single vacancy on (0, 0). As is seen, in a certain range of the electron energy, the conductance is maximized. Since the presence of the second vacancy not only does not reduce the conductance but increases it significantly, this situation is very interesting. However, the behavior of conductance by changing the energy in this case is non-resonant. This amazing behavior can be explained as follows. If we consider only the second vacancy which is located on (0, 2) and calculate the unperturbed Green’s operator, the result can be used to calculate $\rho_{(0,0)}(E)$ [19] which is the local density of states (LDoS) on the first vacancy site, (0, 0). As we can see in fig. 7 LDoS decreases strongly by the presence of a single vacancy on site (0, 2) with respect to the case in which there is no vacancy. If we use the Lippmann-Schwinger equation to study the scattering of the incoming matter waves from the first vacancy, it seems that, due to the presence of the second vacancy, these waves turn around this vacancy. In other words, the presence of the second vacancy reduces the penetration of the traveling waves into the spatial region around the first vacancy. So, the second vacancy creates a shielding around the first vacancy. In this case, for $n = 2$ the agreement between the present analytical results and their corresponding numerical simulations is excellent, but with increasing $n$, some discrepancies are observed between analytical and numerical calculations. The reason for this discrepancy is the formation of additional localized bound
states due to the presence of a vacancy defect. In the case of larger $n$ the corresponding binding energy of such impurity states lies inside the edge band. This will change the Green’s function and one needs to take into account the effect of such additional bound states which is discussed in detail in ref. [27].

Before ending this section, it is worth mentioning that although the presence of the $t_3$ and $t_5$ terms in the Hamiltonian of eq. (1) makes the edge band wider, it will not change quantitatively any of the conclusions drawn here. In order to show this fact, we have presented a comparison of the conductance as a function of energy in the presence of $t_3$ and $t_5$ and in the absence of these terms which is plotted by dotted lines in figs. 3 and 6.

**Summary and conclusion.** – Considering a tight-binding model and applying the general scattering theory, the electron transport in a zPNR in the presence of two impurities/vacancies was analytically investigated. For two impurities on the edge zigzag chain, the variations of the conductance with the electron energy exhibits a resonant behavior. For a similar situation with two vacancies, a similar resonant behavior with extremely sharp peaks has been observed. It was shown that the agreement between the analytical calculations and the numerical simulations in these cases is excellent. We found out that the presence of the impurities along the $y$-axis reduces the conductance considerably. If the distance between the impurities increases, the behavior of the system approaches the behavior of a system with a single impurity on the zigzag chain. Two adjacent vacancies induce considerable conduction in a certain range of the electron energy. This is due to creating a shielding by the second vacancy around the first one. For this final case, the agreement between the analytical and numerical calculations is excellent only for $n = 2$. For a larger value of $n$, although the overall behavior of analytical calculations and simulations is the same, they have considerable discrepancies in detail.

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