Spin transport in a rippled graphene periodic chain

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Abstract. We discuss the solution of the scattering problem of ballistic electrons on the finite periodic chain. Each element of this chain is composed of a combination of a planar and rippled graphene elements. The analysis is carried out in the effective mass approximation when only the interaction between nearest neighbour atoms is taken into account. We find that, with the increase of number of elements, the chain becomes more transparent for electrons with spin up travelling in one direction and for electrons with spin down travelling in the opposite direction.

1. Introduction

In quantum mechanics the study of electron motion in an infinite or half-infinite one-dimensional periodic chain provides a valuable tool in understanding and prediction various physical properties of real materials. The most famous example is the Kronig-Penney model [1]. Nowadays, the problem of scattering with a finite number of scattering centres attracts a considerable interest in view of an ability of modern technology to create periodic rippled graphene structures. For example, the chemical vapor deposition provides quite promising way to create periodic nanoripples [2]. On the other hand, it is found that ripples or wrinkles act as potential barriers for charged carriers leading to their localization [3].

In this communication we discuss the electron scattering in the graphene based superlattice (figure 1). Each element of the periodic chain consists of the flat graphene piece continuously connected to the ripple that is connected again to the flat graphene piece. In our consideration a ripple consists of a curved graphene surface in the form of an arc of a circle. We analyze the transmission and reflection of an electron flow through a rippled system in the effective mass approximation. In this case only the interaction between nearest neighbour atoms is taken into account (see details in [4]).

Our study is based on the results discussed in Refs.[5, 6]. We suppose that the incident electrons move from the left planar part (L) to the right planar part (R) along the x axis (figure 1) and its energy is an integral of motion. Hereafter, we consider a wide enough graphene sheet $W \gg M$, where $W$ and $M$ being, respectively, as the width along the y axis and the length along x axis of the graphene sheet. It means that we keep the translational invariance along the y axis and neglect the edge effects.

In our system the scattering mechanism is due to the curvature-induced spin-orbit couplings characterized by the coefficients $\lambda_x$ and $\lambda_y$ in carbon nanotubes (see details in Refs.[4, 5, 6]). Considering the curved surface as part of the armchair nanotube, it was shown that the curvature-induced spin-orbit coupling [4] yields backscattering with spin inversion. This spin
2. Wave functions

The particular subsystems of the investigated structure can be characterized by the base wave function sets \([5]\). Each of these sets is composed of the four wave functions that depend on the momentum \(\mathbf{k} = (k_x, k_y)\) or angular momentum \(m\), respectively. In the calculations, we assume that \(k_y = 0\). In other words, we consider the one-dimensional problem.

For the planar parts, the eigen energy depends on the momentum as

\[ E = \pm \gamma k_x \]  

and the base wave functions have the form

\[ \psi_j^P = \frac{1}{2} \exp(\pm i k_x x) w_j, \quad j \in \{1, 2, 3, 4\} \]  

(signs “+” or “-”, correspond to the indices ”1,2” or ”3,4”, respectively), where \(\exp(\pm i k_x x)\) are the eigenfunctions of the momentum and \(w_1, w_2, w_3, w_4\) are the energy eigenvectors from the set

\[ S_P = \left\{ \begin{pmatrix} 1 \\ i \\ 1 \\ i \end{pmatrix}, \begin{pmatrix} 1 \\ -i \\ 1 \\ i \end{pmatrix}, \begin{pmatrix} -1 \\ i \\ -1 \\ -i \end{pmatrix}, \begin{pmatrix} -1 \\ -i \\ -1 \\ i \end{pmatrix} \right\}. \]  

For the planar piece, the wave function can be written in the form

\[ \psi = \frac{1}{2} \sum_{j=1}^{4} C_{P,j} \exp(\pm i k_x x) w_j, \]  

where \(C_{P,j}\) are the coefficients.
where \( C_{P,j} \) are the coefficients of the linear combination. The matrix form of this wave function has the following form

\[
M_0 \exp(iKx)C_P,
\]

where the columns of \( M_0 \) are created by the vectors from \( S_P \) and the components of \( C_P \) are created by the coefficients \( C_{P,j} \). The expression \( \exp(iKx) \) is a diagonal matrix

\[
\exp(iKx) = \text{diag}\{\exp(ikx), \exp(ikx), \exp(-ikx), \exp(-ikx)\}.
\]

For the arc pieces, there are four different values of the angular momentum \( m_1, m_2, m_3, m_4 \) since the angular momentum is not conserved in this case. They are connected with the eigenenergy as (see figure 2 and [5]):

\[
E = \mathcal{E}_1 = \lambda_x + \sqrt{\lambda_y^2 + t_{m_1}^2}, \quad E = \mathcal{E}_2 = \lambda_x - \sqrt{\lambda_y^2 + t_{m_2}^2},
\]

\[
E = \mathcal{E}_3 = -(\lambda_x - \sqrt{\lambda_y^2 + t_{m_3}^2}), \quad E = \mathcal{E}_4 = -(\lambda_x + \sqrt{\lambda_y^2 + t_{m_4}^2}),
\]

where \( t_{m_j} = \frac{\gamma}{\pi} m_j \). For the purpose of the simplification, we can write

\[
t_{m_{1,2}} = \pm t_{m_+}, \quad t_{m_{3,4}} = \pm t_{m_-}.
\]

Then,

\[
t_{m_+} = \sqrt{(E - \lambda_x)^2 - \lambda_y^2}, \quad t_{m_-} = \sqrt{(E + \lambda_x)^2 - \lambda_y^2}.
\]

The base eigenfunctions have the form

\[
\psi^A_j = \exp(\pm im \pm \theta) \exp(ik_y y)v,
\]

where \( v \) is an energy eigenvector from the list

\[
S_A = \begin{cases} 
\left( \begin{array}{c} \lambda_y - \frac{-it_m}{\sqrt{\lambda_y^2 + t_m^2}} \\ i(\lambda_y - \sqrt{\lambda_y^2 + t_m^2}) \end{array} \right), & \left( \begin{array}{c} \lambda_y + \frac{-it_m}{\sqrt{\lambda_y^2 + t_m^2}} \\ -i(\lambda_y + \sqrt{\lambda_y^2 + t_m^2}) \end{array} \right), & \left( \begin{array}{c} \lambda_y - \frac{-it_m}{\sqrt{\lambda_y^2 + t_m^2}} \\ -i(\lambda_y + \sqrt{\lambda_y^2 + t_m^2}) \end{array} \right), & \left( \begin{array}{c} \lambda_y + \frac{-it_m}{\sqrt{\lambda_y^2 + t_m^2}} \\ i(\lambda_y - \sqrt{\lambda_y^2 + t_m^2}) \end{array} \right) 
\end{cases}
\]

but here the choice of the appropriate vector in \( S_A \) is more complicated.

The electron eigenfunction, associated with the arc piece, can be (analogously to (5)) written as

\[
M_A(\theta) \exp(i\mathbf{\mathbf{m}} \theta)C_A,
\]

where \( M_A(\theta) = U(\theta)M_A(0) \). The structure of the matrix \( M_A(0) \) depends on the chosen interval of energy (figure 2). If we denote the particular vectors from \( S_A \) by \( v_1, v_2, v_3, v_4 \), it follows that:

- \( E > \lambda_x \Rightarrow E = \mathcal{E}_1 \vee E = \mathcal{E}_3 \); the base eigenfunctions are \( \exp(\pm im_+ \theta)v_1(\pm t_{m_+}) \) and \( \exp(\pm im_- \theta)v_3(\pm t_{m_-}) \). The columns of \( M_A(0) \) are created by \( v_1(t_{m_+}), v_3(t_{m_-}), v_1(-t_{m_-}), v_3(-t_{m_+}) \) adjusted by the normalization constants; the case \( E < \lambda_y + \lambda_x \) corresponds to the evanescent modes (\( m \) is imaginary);

- \( -\lambda_y < E < \lambda_x \Rightarrow E = \mathcal{E}_2 \vee E = \mathcal{E}_4 \); the base eigenfunctions are \( \exp(\pm im_+ \theta)v_2(\pm t_{m_+}) \) and \( \exp(\pm im_- \theta)v_4(\pm t_{m_-}) \). The columns of \( M_A(0) \) are created by \( v_2(t_{m_+}), v_4(t_{m_-}), v_2(-t_{m_-}), v_4(-t_{m_+}) \) adjusted by the normalization constants; the case when \( |E \pm \lambda_x| \leq \lambda_y \) corresponds to the evanescent modes;

- \( E < -\lambda_y \Rightarrow E = \mathcal{E}_2 \vee E = \mathcal{E}_4 \); the base eigenfunctions are \( \exp(\pm im_+ \theta)v_2(\pm t_{m_+}) \) and \( \exp(\pm im_- \theta)v_4(\pm t_{m_-}) \). The columns of \( M_A(0) \) are created by \( v_2(t_{m_+}), v_4(t_{m_-}), v_2(-t_{m_-}), v_4(-t_{m_+}) \) adjusted by the normalization constants; the case when \( E > -\lambda_x - \lambda_y \) corresponds to the evanescent modes.
Figure 2. Dependence of the energy on the quantum number $m$ for rippled graphene (purple line). There are two anticrossings (top and the bottom of the left panel) due to the presence of nonzero term $\lambda_y = 0.0043$ eV, which yields the energy gaps $2\lambda_y$. These gaps contain the evanescent modes. The shifts of these gaps with the respect to the zero energy are given by the term $\lambda_x = 0.32$ eV, so they are $\pm 0.32$ eV. The values of $\lambda_x, \lambda_y$ follow from the values of the parameters: $R = 10 \text{ Å}$, $\delta = 0.01$, $p = 0.1$, $\gamma = (4.5 \cdot 1.42) \text{ eV} \cdot \text{Å}$, $\gamma' = 8/3 \gamma$.

Next,

$$\exp(i m \theta) = \text{diag} \left( \exp(i m_+ \theta), \exp(i m_- \theta), \exp(-i m_+ \theta), \exp(-i m_- \theta) \right)$$

where the angular momenta

$$m_{\pm} = \frac{R}{\gamma} t_{m_{\pm}} = \frac{R}{\gamma} \sqrt{(E \mp \lambda_x)^2 - \lambda_y^2}$$

and $C_A$ is a vector of the coefficients of the linear combination.

3. Spin scattering

In the investigated system, we define the unit structure (figure 1) that is $(N-1)$—times repeated (plus the connection arc $A'$); and we denote $2N$ connection points. In these connection points, the eigenfunctions of the neighboring parts are equal. This fact leads to the system of $2N$ equations

$$M_0 \left( \Phi_{m r} \right) = M_A \left( -\frac{\varphi}{2} \right) \cdot \exp(-i m \frac{\varphi}{2}) C_{1A},$$

$$M_A \left( +\frac{\varphi}{2} \right) \cdot \exp(+i m \frac{\varphi}{2}) C_{1A} = M_0 \cdot \exp(-i K d/2) C_{1P},$$

$$M_0 \cdot \exp(+i K d/2) C_{1P} = M_A \left( -\frac{\varphi}{2} \right) \cdot \exp(-i m \frac{\varphi}{2}) C_{2A},$$

\vdots
\begin{equation}
M_0 \cdot \exp(+i \hat{K} d/2) C_{N-1,P} = M_A(-\frac{\varphi}{2}) \cdot \exp(-i \hat{m} \frac{\varphi}{2}) C_{N,A},
\end{equation}

\begin{equation}
M_A(+\frac{\varphi}{2}) \cdot \exp(+i \hat{m} \frac{\varphi}{2}) C_{N,A} = M_0 \begin{pmatrix} t \\ 0 \end{pmatrix}.
\end{equation}

\(-\varphi, \varphi\) are the edge angles of the arcs, \(d\) is the length of the planar part. The form of the eigenfunctions for the particular parts follows from (13) and (5), respectively. The symbols \(C_{1A}, C_{1P}, \ldots, C_{N-1,A}, C_{N-1,P}, C_{N,A}\) denote the vectors of the linear combination at planar part \((C_{1P})\) and rippled part \((C_{1A})\) of the graphene. Their forms for the left and the right planar part are \(\begin{pmatrix} \Phi_{in} \\ r \end{pmatrix}\) and \(\begin{pmatrix} t \\ 0 \end{pmatrix}\), respectively; where \(\Phi_{in}, r, t, 0\) represent two component vectors with \(\Phi_{in} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}\) and "0" represents two zeros. These forms follow from the idea that the electron flux moves from the left to the right, and the both components of the incoming state, corresponding to the positive momentum in \(\Phi_{in}\), are equal. The factor \(\frac{1}{\sqrt{2}}\) stands for the normalization.

The system (16)-(20) can be rewritten in the matrix form

\begin{equation}
\begin{pmatrix} \Phi_{in} \\ r \end{pmatrix} = M_0^{-1} A M_0 \begin{pmatrix} t \\ 0 \end{pmatrix} = M_C \begin{pmatrix} t \\ 0 \end{pmatrix},
\end{equation}

where

\begin{equation}
A = \left( \left[M_A(-\frac{\varphi}{2}) \exp(-i \hat{m} \varphi) M_A^{-1}(\frac{\varphi}{2}) \right] \cdot \left[M_0 \exp(-i \hat{K} d) M_0^{-1} \right] \right)^{N-1}.
\end{equation}

Introducing the notation

\begin{equation}
B = M_0^{-1} \left[M_A(-\frac{\varphi}{2}) \exp(-i \hat{m} \varphi) M_A^{-1}(\frac{\varphi}{2}) \right] M_0,
\end{equation}

we have

\begin{equation}
A = M_0(B \exp(-i \hat{K} d))^{N-1} B M_0^{-1}.
\end{equation}

As a result, it follows that

\begin{equation}
M_C = (B \exp(-i \hat{K} d))^{N-1} B.
\end{equation}

The schematic form of \(B\) is

\begin{equation}
\begin{pmatrix}
z_1 & 0 & 0 & z_1' \\
0 & z_2 & z_2' & 0 \\
0 & z_2'' & z_2'' & 0 \\
z_1'^* & 0 & 0 & z_1'^*
\end{pmatrix},
\end{equation}

where

\begin{equation}
\begin{aligned}
z_1 &= e^{i \frac{\varphi}{2}} \left[ \cos(m_- \varphi) - i \sgn(E + \lambda_x) \frac{\sqrt{\lambda_y^2 + t_{m-}^2}}{t_{m-}} \sin(m_- \varphi) \right], \\
z_2 &= e^{-i \frac{\varphi}{2}} \left[ \cos(m_+ \varphi) - i \sgn(E - \lambda_x) \frac{\sqrt{\lambda_y^2 + t_{m+}^2}}{t_{m+}} \sin(m_+ \varphi) \right], \\
z_1' &= -\frac{\lambda_y \sin(m_- \varphi)}{t_{m-}}, \\
z_2' &= -\frac{\lambda_y \sin(m_+ \varphi)}{t_{m+}}.
\end{aligned}
\end{equation}
Here, the application of the function "sgn" (signum) is a consequence of different forms of \( M_A(0) \) for different intervals of energies.

It can be easily proven that in the general case, if \( z_1, z_2, z_1', z_2' \) are complex numbers, an arbitrary product of the matrices of such a kind, including diagonal matrices, has the same structure. Because \( M_C \) is created by a product of the mentioned kind of matrices, (21) can be transformed to the following form

\[
\begin{pmatrix}
\alpha_1 & 0 & 0 & \beta_1 \\
0 & \alpha_2 & \beta_2 & 0 \\
0 & \beta_2' & \alpha_2' & 0 \\
\beta_1^* & 0 & 0 & \alpha_1^*
\end{pmatrix}
\begin{pmatrix}
t \\
0
\end{pmatrix},
\]

where \( \alpha_1, \alpha_2, \beta_1, \beta_2 \) are complex numbers. Because

\[
\begin{pmatrix}
\Phi_{in} \\
\Phi_{r}
\end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\
r_1 & r_2 \end{pmatrix}, \quad \begin{pmatrix}
t \\
0
\end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} t_1 \\
t_2 \\
0 \\
0 \end{pmatrix},
\]

we can immediately write

\[ t_1 = \frac{1}{\alpha_1}, \quad t_2 = \frac{1}{\alpha_2}. \] (32)

Note, that within our model, the transmission coefficient \( t_1 \) corresponds to spin up states, while the coefficient \( t_2 \) corresponds to spin down states; the both coefficients correspond to the positive pseudospin quantum number.

### 4. Results

By using the mathematical induction, we can show that in the case of \( N \) samples in the ripple, \( \alpha_{1,2}^{(N)} = \frac{z_{1,2}((\lambda_{1,2}^{(+)})^N - (\lambda_{1,2}^{-})^N)}{\lambda_{1,2}^{(+) - \lambda_{1,2}^{-}}} \) (33)
and

\( \beta_{1,2}^{(N)} = \frac{z_{1,2}'((\lambda_{1,2}^{(+)})^N - (\lambda_{1,2}^{-})^N)}{\lambda_{1,2}^{(+) - \lambda_{1,2}^{-}}}, \) (34)

where

\[
\lambda_{1,2}^{(\pm)} = \Re(z_{1,2} \exp(-ikx_d)) \pm \sqrt{[\Re(z_{1,2} \exp(-ikx_d))]^2 - 1}.
\] (35)

Furthermore, \( |z_{1,2}|^2 = 1 + |z_{1,2}'|^2 \) (36) and at the same time, \( |\alpha_{1,2}^{(N)}|^2 = 1 + |\beta_{1,2}^{(N)}|^2 \) (37). Then, the final formula for the transmission probabilities is

\[
|t_{1,2}|^2 = \frac{1}{1 + |\beta_{1,2}^{(N)}|^2} = \frac{1}{1 + |z_{1,2}'|^2 \left( \frac{(\lambda_{1,2}^{(+)})^N - (\lambda_{1,2}^{-})^N}{\lambda_{1,2}^{(+) - \lambda_{1,2}^{-}}} \right)^2}. \] (38)
Taking into account (15), (1), (27) and (28), we obtain the following result

\[ |t_1(E)|^2 = |t_2(-E)|^2. \]  (39)

It follows from (38) and (29) that the perfect transmission (\(|t_{1,2}|^2 = 1\)) is ensured in the case when

\[ m_{\pm \varphi} = \pi j, \; j \in \mathbb{Z}. \]  (40)

We can show that the corresponding value of the angle equals

\[ \varphi = \frac{j \gamma}{R} \frac{\pi}{\sqrt{(E \pm \lambda_x)^2 - \lambda_y^2}}. \]  (41)

In [5], it is demonstrated that in the case of one sample, the transmission has a minimum close to point \( E = \mp \lambda_x \). So, it is reasonable to suppose that for a suitable value of the angle, the state corresponding to the opposite spin has a maximum in this range of values. Due to (39), we can conclude that the state with the minimum of the transmission in the point \( E = \mp \lambda_x \) has the appropriate maximum in the point \( E = \pm \lambda_x \). Then, in the case \( j = 1 \), the value of the corresponding angle is

\[ \varphi_c = \frac{j \gamma}{R} \frac{\pi}{\sqrt{4 \lambda_x^2 - \lambda_y^2}} \sim 0.996\pi. \]  (42)

So, let us do a choice \( \varphi_c = \pi \).

We show the plots of the transmission probabilities \(|t_1|^2\), \(|t_2|^2\) for the cases of \( N=2 \) and 200 samples in the investigated structure for \( d = 16 \) Å and 100 Å. The results are displayed in figure 3. The values of the parameters are specified in the description of figure 2 and \( \varphi = \pi \).

![Figure 3](image-url). Transmission probabilities \(|t_1|^2\) (red) and \(|t_2|^2\) (blue) for various lengths of the planar parts: \( d = 16 \) Å (up), \( d = 100 \) Å (bottom). The number \( N \) of elements in the superlattice: \( N = 2 \) (left), \( N = 200 \) (right).
In the case of $N=2$ elements in the system under consideration, the transmission change is almost negligible. With the increasing number of the elements in the superlattice, the effect strengthens but the interval of significance is getting narrower. If we increase the distance between the arcs in the structure, the number of the peaks in the corresponding plots increases but the interval of significance remains the same.

5. Conclusion
We have considered the electron scattering in the superlattice created by periodically repeated the semi-rippled and at graphene structures. One element of the superlattice acts as a semipermeable membrane in some energy range which is transparent for electrons with spin up travelling in one direction and for electrons with spin down travelling in the opposite direction. The results show that this effect is negligible for a few semi-ripples. However, it can acquire considerable values in the case of a few hundreds of the elements. Finally, we have derived the analytical formula for the transmission of electrons with different spin orientation through our one-dimensional superlattice. It would be useful to analyse further the curvature induced spin-orbit effects in various graphene based nanostructures for the purposes of spintronics.

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